



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:37 AM UTC

PDB ID : 2QLR / pdb_00002qlr
Title : Crystal structure of human kynurenine aminotransferase II
Authors : Han, Q.; Robinson, R.; Li, J.
Deposited on : 2007-07-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

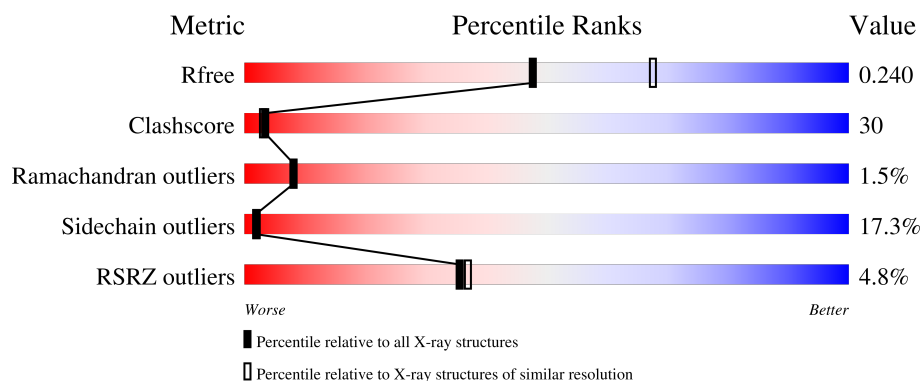
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	425	5% 48% 36% 10% 6%
1	B	425	4% 44% 39% 15% .
1	C	425	4% 45% 40% 12% .
1	D	425	5% 42% 40% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	D	427	-	-	X	-
2	GOL	D	428	-	-	X	-
2	GOL	D	429	-	X	X	-

2 Entry composition [i](#)

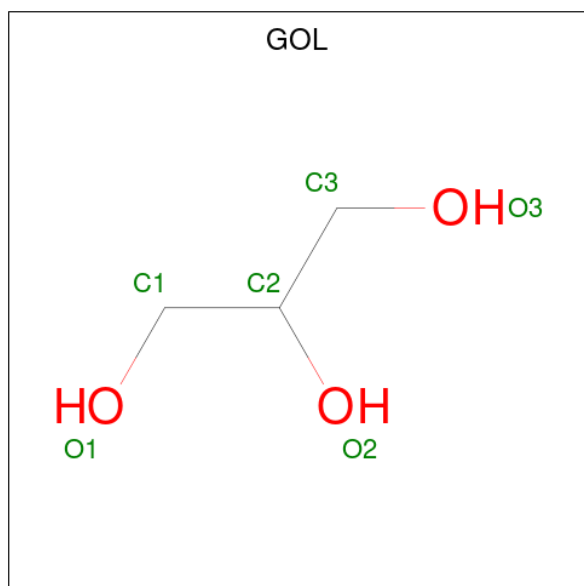
There are 3 unique types of molecules in this entry. The entry contains 14176 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Kynurenine/alpha-aminoadipate aminotransferase mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	P	S	0	0	0
			3347	2147	560	621	1	18			
1	B	425	Total	C	N	O	P	S	0	0	0
			3348	2147	560	622	1	18			
1	C	425	Total	C	N	O	P	S	0	0	0
			3347	2147	560	621	1	18			
1	D	425	Total	C	N	O	P	S	0	0	0
			3348	2147	560	622	1	18			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

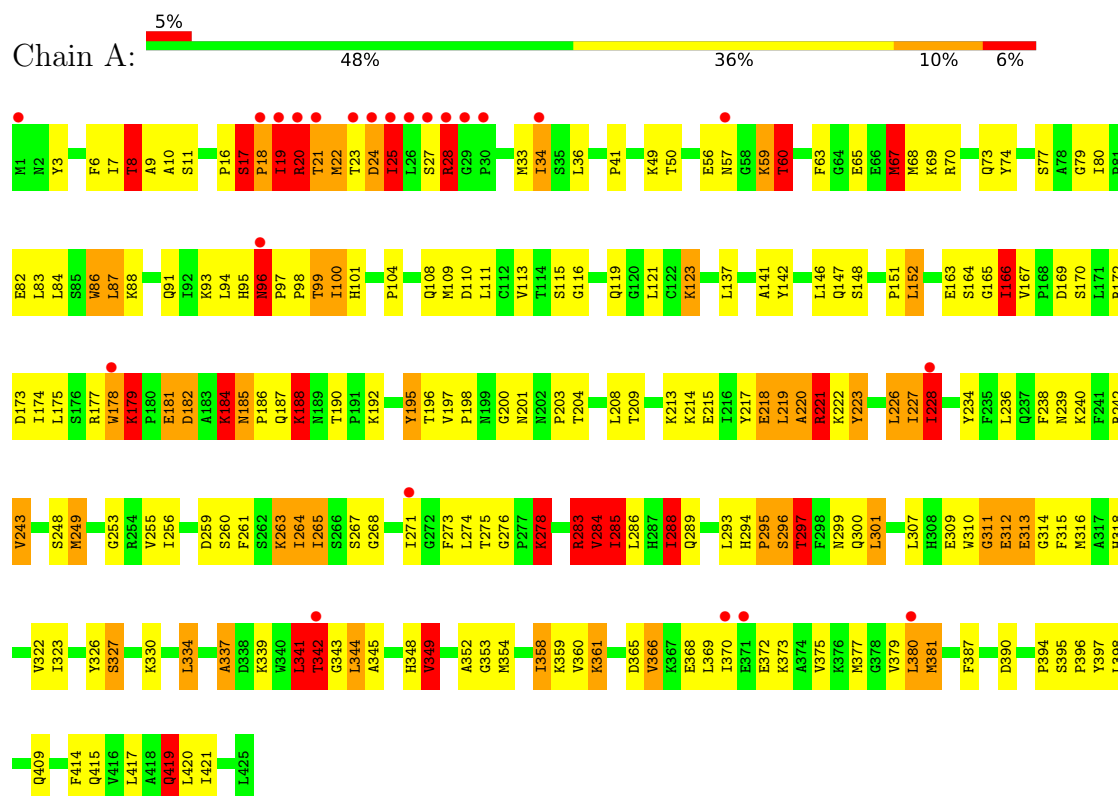
- Molecule 3 is water.

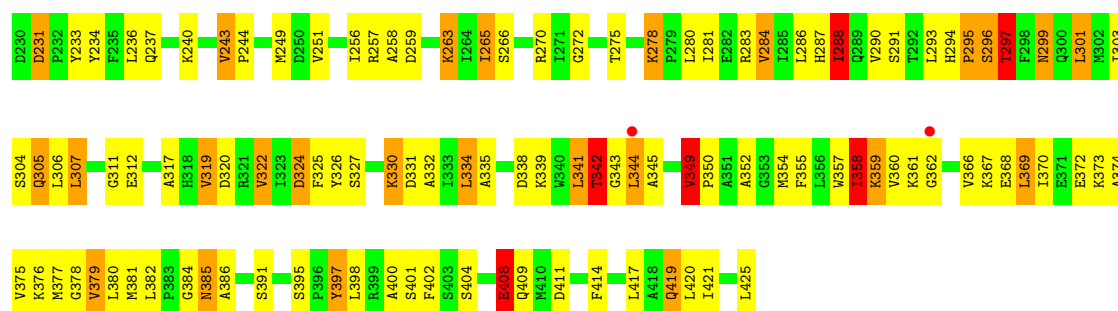
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	199	Total	O	0	0
			199	199		
3	C	166	Total	O	0	0
			166	166		
3	D	183	Total	O	0	0
			183	183		

3 Residue-property plots

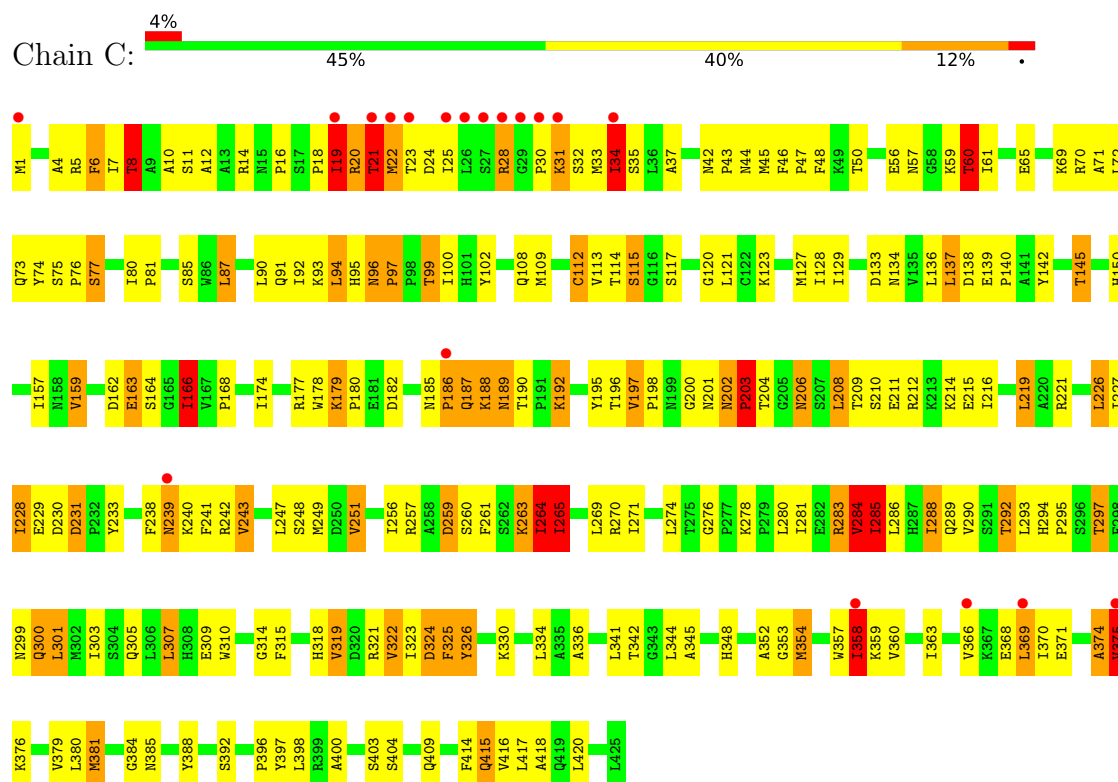
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial

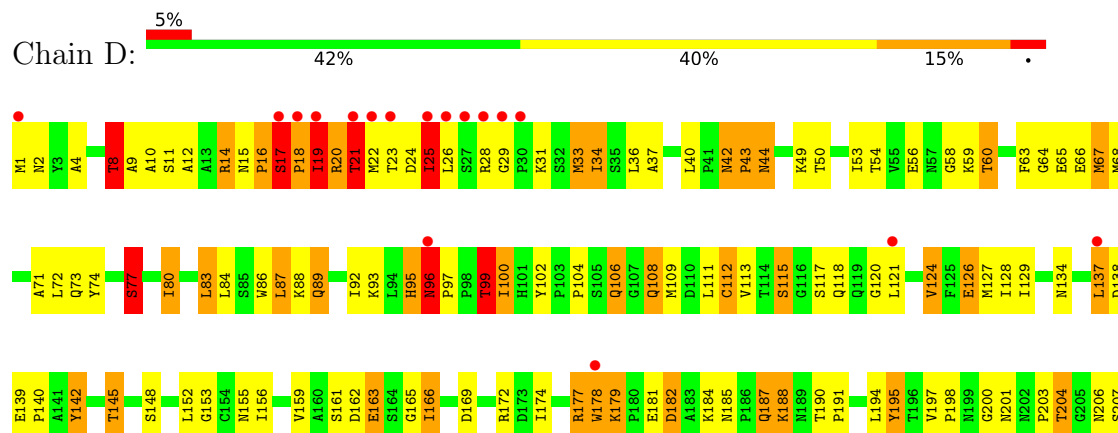


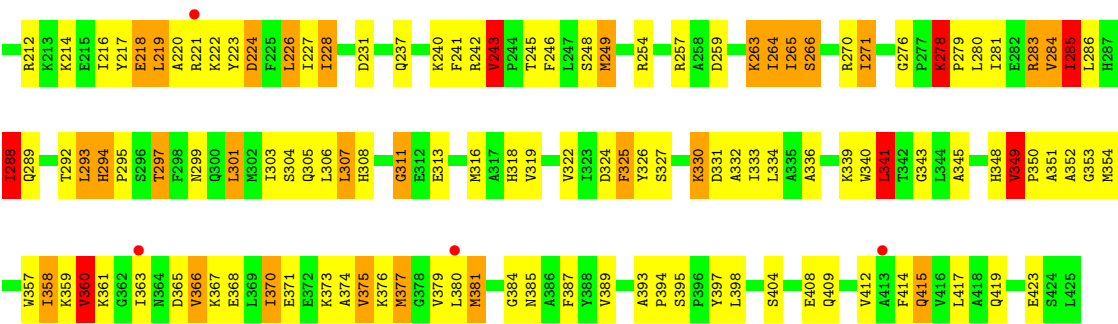


• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial



• Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.50Å 70.97Å 121.13Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	30.11 – 2.30 30.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.11-2.30) 96.3 (30.11-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.256 0.226 , 0.240	Depositor DCC
R_{free} test set	3883 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14176	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4387e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.59	29/3404 (0.9%)	1.62	66/4620 (1.4%)
1	B	1.65	36/3405 (1.1%)	1.60	68/4620 (1.5%)
1	C	1.63	30/3404 (0.9%)	1.62	51/4620 (1.1%)
1	D	1.67	42/3405 (1.2%)	1.63	70/4620 (1.5%)
All	All	1.63	137/13618 (1.0%)	1.62	255/18480 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	5
1	D	1	4
All	All	1	18

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ILE	CA-CB	9.93	1.66	1.54
1	D	12	ALA	CA-CB	9.89	1.69	1.53
1	D	288	ILE	CA-CB	9.69	1.66	1.54
1	D	96	ASN	CA-CB	9.29	1.60	1.52
1	C	34	ILE	CA-CB	8.73	1.64	1.54
1	A	342	THR	N-CA	8.36	1.54	1.46
1	A	349	VAL	CA-C	8.32	1.59	1.53
1	C	418	ALA	C-O	-8.15	1.14	1.24
1	D	9	ALA	C-O	-8.13	1.13	1.24
1	C	290	VAL	CA-CB	8.00	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	ARG	C-O	7.91	1.33	1.23
1	B	224	ASP	CA-C	7.85	1.63	1.53
1	B	385	ASN	N-CA	7.80	1.56	1.46
1	D	115	SER	CA-C	-7.73	1.44	1.53
1	A	227	ILE	CA-CB	7.70	1.63	1.53
1	C	322	VAL	CA-CB	7.66	1.64	1.54
1	D	351	ALA	CA-CB	-7.48	1.41	1.53
1	B	197	VAL	CA-CB	7.47	1.63	1.54
1	D	285	ILE	CA-C	7.46	1.62	1.52
1	D	271	ILE	CA-CB	7.36	1.64	1.54
1	B	349	VAL	CA-CB	7.25	1.64	1.53
1	C	4	ALA	CA-CB	7.16	1.65	1.53
1	C	60	THR	CA-CB	7.03	1.65	1.53
1	B	96	ASN	CA-CB	7.00	1.58	1.52
1	B	332	ALA	CA-CB	-7.00	1.42	1.53
1	C	325	PHE	CA-C	6.96	1.61	1.52
1	B	342	THR	CA-CB	6.96	1.64	1.53
1	C	248	SER	CA-C	6.88	1.62	1.52
1	A	349	VAL	CA-CB	6.86	1.63	1.53
1	A	166	ILE	CA-CB	6.80	1.61	1.54
1	B	296	SER	N-CA	6.74	1.54	1.46
1	B	322	VAL	CA-CB	6.74	1.63	1.54
1	B	196	THR	CA-C	-6.72	1.44	1.52
1	A	273	PHE	CA-C	-6.72	1.44	1.52
1	A	271	ILE	CA-CB	6.63	1.63	1.54
1	C	226	LEU	N-CA	-6.61	1.37	1.45
1	B	317	ALA	C-O	-6.59	1.16	1.24
1	A	96	ASN	C-O	-6.57	1.20	1.23
1	B	319	VAL	CA-CB	6.56	1.61	1.54
1	C	374	ALA	CA-CB	6.53	1.63	1.53
1	A	79	GLY	C-O	-6.49	1.18	1.23
1	D	67	MET	CA-C	6.47	1.61	1.52
1	D	142	TYR	CA-C	6.41	1.60	1.52
1	C	196	THR	CA-CB	6.25	1.65	1.53
1	C	360	VAL	CA-CB	6.25	1.62	1.54
1	A	119	GLN	N-CA	6.16	1.53	1.46
1	C	265	ILE	CA-CB	6.13	1.62	1.54
1	C	336	ALA	CA-CB	-6.11	1.43	1.53
1	C	10	ALA	CA-C	6.09	1.60	1.52
1	B	304	SER	N-CA	-6.04	1.39	1.46
1	D	294	HIS	CA-C	6.04	1.60	1.52
1	D	182	ASP	CB-CG	6.02	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	ILE	CA-CB	5.99	1.61	1.54
1	B	275	THR	CA-CB	5.96	1.64	1.53
1	A	195	TYR	N-CA	-5.96	1.38	1.46
1	C	166	ILE	CA-C	5.95	1.59	1.52
1	C	292	THR	CA-CB	5.93	1.63	1.53
1	A	190	THR	CA-C	5.91	1.60	1.52
1	D	283	ARG	C-O	5.91	1.31	1.24
1	A	223	TYR	N-CA	5.88	1.52	1.46
1	D	77	SER	N-CA	5.86	1.53	1.46
1	C	396	PRO	CA-C	5.82	1.58	1.52
1	C	197	VAL	CA-CB	5.81	1.61	1.54
1	D	19	ILE	CA-C	5.75	1.60	1.52
1	C	251	VAL	CA-CB	5.75	1.63	1.54
1	D	412	VAL	CA-CB	5.74	1.61	1.54
1	B	299	ASN	CA-C	5.71	1.60	1.52
1	D	156	ILE	C-O	-5.69	1.18	1.24
1	A	275	THR	N-CA	5.69	1.53	1.46
1	D	2	ASN	N-CA	5.67	1.54	1.46
1	B	352	ALA	CA-C	5.65	1.59	1.52
1	B	69	LYS	C-O	-5.59	1.17	1.24
1	B	305	GLN	C-O	-5.57	1.17	1.24
1	B	374	ALA	CA-CB	5.54	1.62	1.53
1	B	196	THR	CA-CB	5.52	1.63	1.53
1	D	195	TYR	CD1-CE1	5.51	1.55	1.38
1	D	278	LYS	CE-NZ	5.51	1.65	1.49
1	A	9	ALA	N-CA	5.50	1.53	1.46
1	C	150	HIS	N-CA	5.49	1.53	1.46
1	D	395	SER	CA-C	5.48	1.57	1.52
1	A	260	SER	CA-C	5.48	1.59	1.52
1	A	342	THR	CA-C	-5.48	1.45	1.53
1	B	297	THR	CA-CB	5.45	1.61	1.53
1	D	67	MET	C-O	5.43	1.30	1.24
1	B	402	PHE	N-CA	-5.42	1.39	1.46
1	A	349	VAL	C-N	5.40	1.39	1.33
1	B	295	PRO	C-O	5.39	1.29	1.23
1	B	404	SER	N-CA	5.38	1.52	1.46
1	D	374	ALA	CA-CB	5.37	1.61	1.53
1	A	182	ASP	CB-CG	5.36	1.65	1.52
1	D	325	PHE	CA-C	5.36	1.59	1.52
1	B	95	HIS	C-O	-5.35	1.17	1.23
1	C	409	GLN	C-O	-5.32	1.18	1.24
1	A	166	ILE	C-O	5.31	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	VAL	CA-CB	5.30	1.61	1.54
1	D	332	ALA	CA-CB	5.29	1.61	1.53
1	B	339	LYS	N-CA	-5.28	1.40	1.46
1	D	285	ILE	CA-CB	5.28	1.61	1.54
1	A	220	ALA	CA-CB	5.27	1.61	1.53
1	C	388	TYR	N-CA	5.27	1.52	1.46
1	B	141	ALA	CA-CB	5.26	1.64	1.53
1	D	129	ILE	CA-CB	5.26	1.60	1.54
1	C	259	ASP	N-CA	5.24	1.52	1.45
1	D	197	VAL	CA-C	5.24	1.58	1.52
1	D	278	LYS	CG-CD	5.24	1.68	1.52
1	D	43	PRO	CA-C	5.21	1.60	1.52
1	C	269	LEU	C-O	-5.20	1.17	1.24
1	D	108	GLN	C-O	5.19	1.30	1.23
1	A	339	LYS	CA-C	5.18	1.60	1.52
1	C	113	VAL	CA-CB	5.18	1.60	1.54
1	A	265	ILE	CA-CB	5.18	1.61	1.54
1	D	44	ASN	CA-C	-5.18	1.45	1.52
1	A	242	ARG	N-CA	5.17	1.52	1.46
1	C	6	PHE	CA-C	5.15	1.60	1.52
1	C	325	PHE	N-CA	5.15	1.52	1.46
1	A	243	VAL	CA-CB	5.13	1.60	1.54
1	A	278	LYS	CA-C	5.13	1.59	1.52
1	B	293	LEU	C-O	-5.13	1.17	1.24
1	C	385	ASN	CA-C	5.12	1.59	1.52
1	B	382	LEU	CA-C	5.12	1.59	1.52
1	A	337	ALA	CA-C	-5.11	1.46	1.52
1	D	72	LEU	CA-CB	5.11	1.62	1.53
1	D	153	GLY	N-CA	5.11	1.52	1.45
1	D	281	ILE	CA-CB	5.08	1.61	1.54
1	D	50	THR	CA-CB	5.08	1.62	1.53
1	C	231	ASP	N-CA	5.08	1.51	1.46
1	D	99	THR	C-O	5.07	1.30	1.23
1	B	44	ASN	N-CA	5.07	1.52	1.46
1	A	271	ILE	C-O	5.06	1.29	1.24
1	D	100	ILE	CG1-CD1	5.04	1.71	1.51
1	B	397	TYR	CA-C	-5.04	1.46	1.52
1	B	256	ILE	C-O	-5.03	1.18	1.24
1	B	362	GLY	N-CA	5.03	1.52	1.45
1	B	359	LYS	CE-NZ	5.03	1.64	1.49
1	D	285	ILE	CB-CG2	5.02	1.69	1.52
1	D	197	VAL	CA-CB	5.01	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	353	GLY	N-CA	5.00	1.50	1.45

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	ILE	N-CA-C	11.58	121.28	111.90
1	D	227	ILE	CA-C-N	-10.88	108.97	123.12
1	D	227	ILE	C-N-CA	-10.88	108.97	123.12
1	D	128	ILE	N-CA-C	10.76	120.61	111.90
1	C	22	MET	N-CA-C	-9.93	100.45	111.07
1	C	227	ILE	CA-C-N	-9.90	110.25	123.12
1	C	227	ILE	C-N-CA	-9.90	110.25	123.12
1	A	187	GLN	N-CA-C	9.13	121.31	111.36
1	A	285	ILE	N-CA-C	8.99	119.80	110.62
1	B	129	ILE	N-CA-C	8.98	120.88	107.51
1	B	243	VAL	CA-C-N	8.92	130.99	119.84
1	B	243	VAL	C-N-CA	8.92	130.99	119.84
1	A	285	ILE	N-CA-CB	8.85	122.58	110.54
1	A	278	LYS	CA-C-N	-8.80	111.06	120.47
1	A	278	LYS	C-N-CA	-8.80	111.06	120.47
1	B	124	VAL	N-CA-C	-8.72	101.50	111.00
1	D	188	LYS	N-CA-C	8.69	122.66	112.93
1	A	184	LYS	N-CA-C	-8.63	102.75	113.28
1	D	285	ILE	N-CA-CB	8.47	122.06	110.54
1	B	361	LYS	N-CA-C	8.44	121.69	111.40
1	D	17	SER	CA-C-N	8.43	130.37	119.84
1	D	17	SER	C-N-CA	8.43	130.37	119.84
1	B	189	ASN	CB-CA-C	-8.38	99.87	112.11
1	A	80	ILE	CA-C-N	8.20	127.77	119.24
1	A	80	ILE	C-N-CA	8.20	127.77	119.24
1	D	20	ARG	N-CA-C	8.20	121.11	110.53
1	B	107	GLY	N-CA-C	-8.17	101.65	115.62
1	B	228	ILE	N-CA-C	8.04	120.27	107.73
1	D	8	THR	CB-CA-C	7.93	120.73	109.71
1	D	29	GLY	CA-C-N	7.92	127.98	119.90
1	D	29	GLY	C-N-CA	7.92	127.98	119.90
1	A	227	ILE	CA-C-N	-7.80	112.62	122.37
1	A	227	ILE	C-N-CA	-7.80	112.62	122.37
1	A	152	LEU	N-CA-C	-7.66	103.91	113.18
1	B	96	ASN	CA-C-N	-7.64	112.51	120.38
1	B	96	ASN	C-N-CA	-7.64	112.51	120.38
1	B	15	ASN	CA-C-N	-7.53	111.87	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	ASN	C-N-CA	-7.53	111.87	119.93
1	A	228	ILE	CB-CA-C	7.51	120.05	110.96
1	D	324	ASP	N-CA-C	-7.46	103.23	111.36
1	B	228	ILE	N-CA-CB	7.42	120.44	111.31
1	D	77	SER	N-CA-C	7.41	120.29	111.33
1	D	126	GLU	N-CA-C	-7.35	102.24	112.45
1	B	211	GLU	N-CA-C	-7.34	102.67	111.69
1	D	187	GLN	CA-C-N	-7.23	110.65	122.65
1	D	187	GLN	C-N-CA	-7.23	110.65	122.65
1	D	349	VAL	CA-C-N	7.17	127.58	119.83
1	D	349	VAL	C-N-CA	7.17	127.58	119.83
1	A	25	ILE	N-CA-C	-7.12	103.32	113.07
1	A	100	ILE	N-CA-C	7.05	118.66	110.62
1	C	375	VAL	CB-CA-C	-7.01	99.79	111.29
1	C	188	LYS	N-CA-C	-6.92	104.91	113.15
1	D	66	GLU	N-CA-C	6.91	118.46	111.07
1	B	36	LEU	N-CA-C	-6.86	104.22	112.59
1	B	361	LYS	CA-C-N	-6.86	107.97	121.41
1	B	361	LYS	C-N-CA	-6.86	107.97	121.41
1	B	327	SER	N-CA-C	6.81	118.49	111.14
1	C	353	GLY	N-CA-C	6.79	123.15	111.47
1	C	264	ILE	CA-C-N	-6.78	116.08	122.66
1	C	264	ILE	C-N-CA	-6.78	116.08	122.66
1	C	128	ILE	N-CA-C	6.76	118.37	111.00
1	D	95	HIS	CA-C-N	-6.75	116.62	123.10
1	D	95	HIS	C-N-CA	-6.75	116.62	123.10
1	B	349	VAL	N-CA-C	-6.74	102.83	108.63
1	C	113	VAL	N-CA-C	-6.72	100.06	109.21
1	A	297	THR	CB-CA-C	6.71	121.92	110.79
1	D	106	GLN	CA-C-N	-6.67	108.35	121.41
1	D	106	GLN	C-N-CA	-6.67	108.35	121.41
1	A	349	VAL	CB-CA-C	6.65	117.13	110.94
1	C	14	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	A	285	ILE	CA-CB-CG2	6.61	121.73	110.50
1	D	190	THR	CA-C-N	-6.60	112.96	119.76
1	D	190	THR	C-N-CA	-6.60	112.96	119.76
1	D	124	VAL	N-CA-C	-6.57	103.84	111.00
1	B	284	VAL	N-CA-CB	6.56	120.42	110.58
1	A	283	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	D	384	GLY	N-CA-C	6.53	121.86	114.67
1	A	419	GLN	N-CA-C	6.53	120.35	112.38
1	C	342	THR	CA-C-N	-6.50	108.67	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	THR	C-N-CA	-6.50	108.67	121.41
1	C	129	ILE	N-CA-C	6.49	117.78	107.98
1	D	285	ILE	CA-CB-CG2	6.46	121.48	110.50
1	A	288	ILE	N-CA-CB	6.40	118.47	110.47
1	A	349	VAL	N-CA-CB	6.39	117.06	110.23
1	A	18	PRO	N-CA-C	6.37	122.38	111.03
1	A	366	VAL	N-CA-C	6.35	118.26	112.29
1	B	265	ILE	CB-CA-C	6.33	116.68	111.05
1	A	343	GLY	N-CA-C	-6.30	105.38	115.08
1	C	233	TYR	N-CA-C	-6.30	104.22	112.41
1	D	339	LYS	N-CA-C	6.29	117.94	111.14
1	D	226	LEU	CA-C-N	-6.25	115.04	123.10
1	D	226	LEU	C-N-CA	-6.25	115.04	123.10
1	D	33	MET	CA-C-N	-6.24	115.05	123.10
1	D	33	MET	C-N-CA	-6.24	115.05	123.10
1	D	393	ALA	CA-C-N	-6.22	113.54	120.14
1	D	393	ALA	C-N-CA	-6.22	113.54	120.14
1	D	8	THR	N-CA-CB	-6.22	99.83	109.34
1	D	128	ILE	CB-CA-C	-6.21	105.34	111.30
1	C	96	ASN	CA-C-N	6.18	126.75	120.38
1	C	96	ASN	C-N-CA	6.18	126.75	120.38
1	A	20	ARG	N-CA-C	6.14	123.87	110.80
1	B	312	GLU	CB-CA-C	6.13	122.44	110.67
1	C	219	LEU	N-CA-C	6.10	117.60	111.07
1	A	220	ALA	N-CA-C	6.06	117.55	111.07
1	B	325	PHE	N-CA-C	6.04	117.53	111.07
1	A	87	LEU	N-CA-C	5.98	117.47	111.07
1	C	60	THR	CB-CA-C	5.98	119.87	109.65
1	A	310	TRP	N-CA-C	5.97	118.58	111.71
1	A	179	LYS	N-CA-C	-5.97	102.55	110.07
1	B	288	ILE	N-CA-CB	5.95	120.83	110.65
1	C	239	ASN	CA-C-N	-5.93	111.03	122.06
1	C	239	ASN	C-N-CA	-5.93	111.03	122.06
1	C	360	VAL	N-CA-C	-5.93	100.04	108.58
1	A	228	ILE	N-CA-CB	5.92	117.75	111.00
1	A	238	PHE	N-CA-C	5.91	117.80	111.36
1	D	284	VAL	N-CA-CB	5.91	119.45	110.58
1	D	333	ILE	N-CA-C	5.91	117.44	111.00
1	A	373	LYS	N-CA-C	5.90	117.80	111.36
1	A	82	GLU	N-CA-C	5.90	118.50	111.71
1	A	204	THR	N-CA-C	5.87	119.63	112.23
1	C	77	SER	N-CA-C	5.87	121.05	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	THR	N-CA-C	5.86	117.75	111.36
1	B	227	ILE	CA-C-N	-5.82	115.09	122.43
1	B	227	ILE	C-N-CA	-5.82	115.09	122.43
1	C	115	SER	CB-CA-C	5.81	121.10	112.03
1	A	327	SER	N-CA-CB	5.81	118.66	110.12
1	C	228	ILE	CB-CA-C	5.80	119.42	110.96
1	D	243	VAL	CB-CA-C	5.75	116.64	111.00
1	B	113	VAL	N-CA-C	-5.74	101.32	108.89
1	A	249	MET	N-CA-C	5.73	119.26	112.72
1	B	75	SER	CA-C-N	-5.72	113.89	119.78
1	B	75	SER	C-N-CA	-5.72	113.89	119.78
1	A	7	ILE	CA-C-N	5.71	129.21	120.82
1	A	7	ILE	C-N-CA	5.71	129.21	120.82
1	B	53	ILE	N-CA-C	5.70	116.20	107.77
1	D	276	GLY	CA-C-N	5.69	126.58	119.98
1	D	276	GLY	C-N-CA	5.69	126.58	119.98
1	B	287	HIS	N-CA-C	-5.69	104.69	111.69
1	B	335	ALA	N-CA-C	5.68	117.47	111.28
1	D	188	LYS	N-CA-CB	5.66	118.37	110.56
1	A	342	THR	CA-C-N	-5.66	110.95	121.07
1	A	342	THR	C-N-CA	-5.66	110.95	121.07
1	C	285	ILE	N-CA-CB	5.65	118.23	110.54
1	B	312	GLU	CB-CG-CD	5.64	122.19	112.60
1	A	256	ILE	CB-CA-C	-5.64	102.43	110.83
1	C	206	ASN	N-CA-C	5.64	118.16	110.55
1	A	36	LEU	N-CA-C	-5.63	105.09	112.41
1	B	231	ASP	CA-C-N	5.63	125.72	119.87
1	B	231	ASP	C-N-CA	5.63	125.72	119.87
1	D	71	ALA	N-CA-C	5.63	118.18	111.71
1	A	349	VAL	CA-C-N	5.61	125.93	119.93
1	A	349	VAL	C-N-CA	5.61	125.93	119.93
1	D	311	GLY	N-CA-C	-5.61	105.70	112.48
1	A	276	GLY	CA-C-N	5.59	125.86	119.83
1	A	276	GLY	C-N-CA	5.59	125.86	119.83
1	A	283	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	4	ALA	N-CA-C	5.56	118.86	111.75
1	A	259	ASP	N-CA-C	5.56	119.11	110.17
1	C	284	VAL	N-CA-C	5.55	116.33	110.72
1	C	238	PHE	CA-C-N	5.54	129.23	121.02
1	C	238	PHE	C-N-CA	5.54	129.23	121.02
1	D	292	THR	N-CA-C	5.54	118.08	111.71
1	B	385	ASN	N-CA-C	5.54	118.84	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ALA	CA-C-N	5.52	125.94	120.31
1	C	37	ALA	C-N-CA	5.52	125.94	120.31
1	A	60	THR	N-CA-C	5.52	117.86	110.35
1	B	177	ARG	N-CA-C	-5.52	105.81	112.54
1	C	240	LYS	N-CA-C	5.50	119.99	113.28
1	B	173	ASP	N-CA-C	5.49	116.94	111.07
1	C	96	ASN	O-C-N	5.47	124.05	121.53
1	A	284	VAL	N-CA-CB	5.45	118.76	110.58
1	C	70	ARG	N-CA-C	-5.44	105.25	111.07
1	B	281	ILE	CB-CA-C	-5.44	104.79	112.14
1	D	318	HIS	N-CA-C	-5.44	105.25	111.07
1	D	99	THR	N-CA-CB	-5.43	102.45	110.49
1	D	100	ILE	N-CA-C	5.42	116.15	110.62
1	A	116	GLY	CA-C-O	-5.42	118.49	122.23
1	D	341	LEU	N-CA-C	5.41	120.75	113.72
1	A	295	PRO	N-CA-C	-5.41	102.65	111.68
1	D	288	ILE	CA-CB-CG2	5.40	119.67	110.50
1	B	408	GLU	CB-CG-CD	5.39	121.77	112.60
1	D	288	ILE	N-CA-CB	5.39	117.87	110.54
1	B	16	PRO	N-CA-C	5.38	120.03	111.26
1	D	373	LYS	N-CA-C	5.38	116.95	111.14
1	C	358	ILE	N-CA-C	5.36	115.62	108.11
1	A	86	TRP	N-CA-CB	5.35	117.77	110.01
1	B	404	SER	N-CA-C	5.35	119.56	112.72
1	B	58	GLY	CA-C-N	5.34	128.30	120.71
1	B	58	GLY	C-N-CA	5.34	128.30	120.71
1	A	315	PHE	N-CA-C	-5.33	105.11	111.03
1	B	324	ASP	N-CA-C	-5.32	105.48	111.28
1	C	8	THR	N-CA-CB	-5.32	102.76	110.36
1	D	370	ILE	N-CA-C	5.32	115.53	110.53
1	B	343	GLY	CA-C-N	-5.31	113.64	122.08
1	B	343	GLY	C-N-CA	-5.31	113.64	122.08
1	C	112	CYS	CB-CA-C	5.29	118.90	109.65
1	A	173	ASP	CB-CA-C	5.29	121.04	109.99
1	A	181	GLU	N-CA-C	5.29	119.73	113.28
1	C	283	ARG	N-CA-CB	5.28	117.97	110.16
1	D	243	VAL	N-CA-CB	5.28	115.43	109.99
1	B	297	THR	CA-C-N	5.25	127.57	120.65
1	B	297	THR	C-N-CA	5.25	127.57	120.65
1	C	322	VAL	N-CA-C	5.24	116.01	110.72
1	C	276	GLY	CA-C-N	5.24	125.49	119.83
1	C	276	GLY	C-N-CA	5.24	125.49	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	SER	CA-C-N	-5.23	114.64	120.45
1	D	395	SER	C-N-CA	-5.23	114.64	120.45
1	A	185	ASN	CA-C-N	5.23	125.54	119.47
1	A	185	ASN	C-N-CA	5.23	125.54	119.47
1	A	314	GLY	N-CA-C	-5.22	108.18	114.66
1	A	221	ARG	N-CA-CB	5.22	117.64	110.07
1	B	234	TYR	N-CA-C	-5.22	105.59	111.28
1	B	272	GLY	N-CA-C	-5.21	100.84	110.73
1	B	77	SER	N-CA-C	5.21	117.63	111.33
1	D	113	VAL	N-CA-C	-5.20	102.14	109.21
1	A	234	TYR	CA-C-N	-5.18	114.05	122.65
1	A	234	TYR	C-N-CA	-5.18	114.05	122.65
1	B	113	VAL	CB-CA-C	-5.18	104.42	111.15
1	C	4	ALA	N-CA-C	5.18	121.83	110.80
1	B	401	SER	N-CA-CB	5.17	118.14	110.29
1	D	254	ARG	CA-C-N	-5.16	116.45	123.10
1	D	254	ARG	C-N-CA	-5.16	116.45	123.10
1	D	360	VAL	N-CA-C	5.15	115.68	108.89
1	B	322	VAL	CB-CA-C	5.14	119.32	112.22
1	B	311	GLY	N-CA-C	-5.14	102.81	112.22
1	B	306	LEU	CA-C-N	5.14	128.12	120.31
1	B	306	LEU	C-N-CA	5.14	128.12	120.31
1	A	288	ILE	CA-CB-CG2	5.13	119.22	110.50
1	A	8	THR	N-CA-CB	-5.12	101.73	109.92
1	A	234	TYR	N-CA-C	-5.12	105.70	111.28
1	B	103	PRO	O-C-N	5.12	123.67	121.31
1	D	284	VAL	CA-C-N	-5.12	113.45	120.46
1	D	284	VAL	C-N-CA	-5.12	113.45	120.46
1	D	224	ASP	N-CA-C	5.11	118.38	111.17
1	D	16	PRO	CA-C-N	-5.11	109.33	121.80
1	D	16	PRO	C-N-CA	-5.11	109.33	121.80
1	C	128	ILE	CB-CA-C	-5.10	105.41	112.24
1	B	224	ASP	N-CA-C	5.09	118.23	111.30
1	C	242	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	B	355	PHE	N-CA-C	5.07	117.66	109.40
1	C	12	ALA	N-CA-C	5.07	117.54	111.71
1	D	265	ILE	N-CA-C	5.07	116.38	112.12
1	B	82	GLU	N-CA-C	5.06	116.80	111.28
1	B	189	ASN	N-CA-C	5.06	118.11	111.28
1	C	326	TYR	N-CA-C	-5.04	105.89	112.23
1	D	80	ILE	N-CA-C	5.04	114.50	108.96
1	C	248	SER	N-CA-C	5.03	118.19	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ILE	CB-CA-C	5.03	119.54	111.29
1	B	78	ALA	N-CA-C	-5.02	106.85	113.17
1	C	97	PRO	N-CA-C	-5.02	104.58	110.70
1	C	300	GLN	CB-CA-C	-5.02	102.32	110.85
1	B	154	CYS	CA-C-N	-5.01	115.53	122.30
1	B	154	CYS	C-N-CA	-5.01	115.53	122.30
1	B	382	LEU	CA-C-N	5.00	124.99	119.89
1	B	382	LEU	C-N-CA	5.00	124.99	119.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	188	LYS	CA

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	SER	Peptide
1	A	188	LYS	Peptide
1	A	19	ILE	Peptide
1	A	341	LEU	Peptide
1	A	342	THR	Peptide
1	B	106	GLN	Peptide
1	B	19	ILE	Peptide
1	B	202	ASN	Peptide
1	B	98	PRO	Peptide
1	C	187	GLN	Peptide
1	C	19	ILE	Peptide
1	C	202	ASN	Peptide
1	C	203	PRO	Peptide
1	C	21	THR	Peptide
1	D	17	SER	Peptide
1	D	19	ILE	Peptide
1	D	23	THR	Peptide
1	D	240	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3347	0	3357	214	0
1	B	3348	0	3356	213	0
1	C	3347	0	3357	212	0
1	D	3348	0	3357	212	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	30	0	40	7	0
2	D	24	0	32	24	0
3	A	166	0	0	24	0
3	B	199	0	0	27	0
3	C	166	0	0	17	0
3	D	183	0	0	34	0
All	All	14176	0	13523	809	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (809) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LEU:C	1:D:137:LEU:HD23	1.61	1.25
1:D:60:THR:HG22	3:D:555:HOH:O	1.38	1.22
1:D:182:ASP:HB2	3:D:568:HOH:O	1.40	1.22
1:C:166:ILE:HD11	1:C:216:ILE:CD1	1.71	1.18
1:C:166:ILE:HD11	1:C:216:ILE:HD11	1.24	1.16
1:B:344:LEU:HB2	3:B:571:HOH:O	1.43	1.16
1:A:182:ASP:HB2	3:A:537:HOH:O	1.43	1.15
1:D:22:MET:O	1:D:25:ILE:HB	1.46	1.15
1:C:214:LYS:HA	1:C:249:MET:HE1	1.29	1.13
1:A:41:PRO:HB3	1:B:354:MET:HE1	1.27	1.13
1:C:137:LEU:C	1:C:137:LEU:HD23	1.72	1.12
1:A:17:SER:HB2	1:A:18:PRO:HD3	1.25	1.11
1:A:41:PRO:CB	1:B:354:MET:HE1	1.80	1.10
1:A:342:THR:HB	1:A:344:LEU:HD22	1.33	1.10
1:D:201:ASN:HB2	2:D:428:GOL:H11	1.24	1.10
1:C:179:LYS:HG3	1:C:180:PRO:HD2	1.28	1.09
1:D:288:ILE:HD12	1:D:288:ILE:C	1.75	1.09
1:C:99:THR:HG21	3:C:531:HOH:O	1.52	1.07
1:B:67:MET:HG2	3:B:591:HOH:O	1.53	1.07
1:B:8:THR:HG22	1:B:11:SER:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:HG22	3:B:540:HOH:O	1.56	1.05
1:C:192:LYS:HE2	1:C:192:LYS:H	1.21	1.05
1:A:121:LEU:CD2	1:A:228:ILE:HD11	1.87	1.04
1:C:137:LEU:HD23	1:C:137:LEU:O	1.56	1.04
1:A:342:THR:O	1:A:342:THR:CG2	2.06	1.04
1:D:21:THR:HA	3:D:597:HOH:O	1.58	1.03
1:D:83:LEU:HD22	1:D:87:LEU:HD22	1.40	1.03
1:D:137:LEU:C	1:D:137:LEU:CD2	2.31	1.02
1:A:65:GLU:HG2	3:A:437:HOH:O	1.57	1.01
1:D:112:CYS:HB3	3:D:591:HOH:O	1.61	1.01
2:D:429:GOL:H31	3:D:480:HOH:O	1.62	1.00
1:C:370:ILE:HD11	1:C:398:LEU:HD21	1.43	0.99
1:B:121:LEU:CD1	1:B:228:ILE:HD11	1.94	0.98
1:B:96:ASN:HB3	3:B:572:HOH:O	1.62	0.98
1:A:22:MET:HG3	1:A:23:THR:H	1.27	0.97
1:C:261:PHE:HB3	1:C:265:ILE:CD1	1.95	0.96
1:A:121:LEU:HD21	1:A:228:ILE:HD11	1.47	0.96
1:A:59:LYS:CD	1:D:188:LYS:HD3	1.97	0.95
1:C:345:ALA:HB1	1:C:358:ILE:CD1	1.97	0.95
1:A:8:THR:HG22	1:A:11:SER:H	1.28	0.95
1:A:8:THR:HG21	3:A:561:HOH:O	1.65	0.94
1:B:56:GLU:O	1:B:57:ASN:HB2	1.66	0.94
1:A:214:LYS:HA	1:A:249:MET:HE1	1.50	0.94
1:B:243:VAL:HG13	3:B:534:HOH:O	1.68	0.94
1:B:30:PRO:HD2	1:B:33:MET:HE3	1.49	0.94
1:C:45:MET:HE2	1:D:322:VAL:HG22	1.47	0.94
1:D:126:GLU:HB3	2:D:429:GOL:O2	1.66	0.94
1:C:192:LYS:HE2	1:C:192:LYS:N	1.84	0.93
1:A:59:LYS:CB	1:A:59:LYS:NZ	2.30	0.93
1:D:137:LEU:HD23	1:D:137:LEU:O	1.68	0.93
1:D:16:PRO:O	1:D:17:SER:HB3	1.69	0.92
1:B:73:GLN:O	1:B:297:THR:HG21	1.70	0.91
1:B:121:LEU:HD12	1:B:228:ILE:HD11	1.52	0.90
1:C:137:LEU:C	1:C:137:LEU:CD2	2.44	0.90
1:A:342:THR:O	1:A:342:THR:HG22	1.69	0.89
1:C:415:GLN:HG3	1:C:416:VAL:N	1.77	0.89
1:B:301:LEU:O	1:B:305:GLN:HG3	1.70	0.89
1:D:201:ASN:HB2	2:D:428:GOL:C1	2.02	0.89
1:B:155:ASN:HB3	3:B:583:HOH:O	1.72	0.89
1:D:11:SER:HB2	2:D:429:GOL:H12	1.53	0.89
1:A:409:GLN:HB3	1:B:34:ILE:HD13	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:MET:HG3	1:B:420:LEU:HD11	1.54	0.88
1:C:257:ARG:HD3	1:C:259:ASP:OD2	1.74	0.87
1:B:341:LEU:HD22	1:B:414:PHE:CD2	2.09	0.87
1:A:170:SER:O	1:A:174:ILE:HG12	1.74	0.87
1:A:17:SER:HB2	1:A:18:PRO:CD	2.05	0.87
1:C:420:LEU:HG	3:C:499:HOH:O	1.73	0.87
1:C:8:THR:HG22	1:C:11:SER:H	1.38	0.86
1:B:28:ARG:HH11	1:B:28:ARG:HB3	1.39	0.86
1:D:325:PHE:HD1	3:D:546:HOH:O	1.57	0.86
1:D:20:ARG:C	1:D:22:MET:H	1.82	0.86
1:B:30:PRO:HD2	1:B:33:MET:CE	2.04	0.86
1:B:345:ALA:HB1	1:B:358:ILE:CD1	2.05	0.85
1:D:343:GLY:O	1:D:361:LYS:HE2	1.76	0.85
1:C:345:ALA:HB1	1:C:358:ILE:HD13	1.57	0.85
1:D:257:ARG:HD3	1:D:259:ASP:OD2	1.77	0.84
1:C:261:PHE:HB3	1:C:265:ILE:HD12	1.60	0.84
1:A:409:GLN:HB3	1:B:34:ILE:CD1	2.06	0.83
1:A:59:LYS:HD3	1:D:188:LYS:HD3	1.58	0.83
1:B:341:LEU:HD22	1:B:414:PHE:HD2	1.43	0.83
1:A:239:ASN:HB3	3:A:495:HOH:O	1.78	0.83
1:A:59:LYS:NZ	1:A:59:LYS:HB3	1.92	0.83
1:A:148:SER:HB2	1:B:290:VAL:HB	1.61	0.83
1:C:18:PRO:HG2	1:C:20:ARG:HB3	1.60	0.82
1:A:93:LYS:HG3	1:A:312:GLU:OE1	1.79	0.82
1:D:16:PRO:O	1:D:17:SER:CB	2.24	0.82
1:C:81:PRO:HG3	3:C:514:HOH:O	1.79	0.82
1:D:148:SER:O	1:D:152:LEU:HD13	1.80	0.81
1:D:179:LYS:HG3	3:D:559:HOH:O	1.79	0.80
1:A:17:SER:CB	1:A:18:PRO:HD3	2.08	0.80
1:D:42:ASN:HD22	1:D:44:ASN:H	1.30	0.80
1:A:59:LYS:CB	1:A:59:LYS:HZ1	1.93	0.80
1:C:8:THR:HB	1:C:127:MET:O	1.82	0.80
1:C:166:ILE:CD1	1:C:216:ILE:HD11	2.07	0.80
1:C:134:ASN:H	1:C:192:LYS:HZ1	1.30	0.80
1:C:179:LYS:HG3	1:C:180:PRO:CD	2.11	0.80
1:A:19:ILE:HA	1:A:22:MET:HE3	1.64	0.79
1:C:99:THR:HG22	1:C:109:MET:HB2	1.65	0.79
1:A:59:LYS:HD2	1:D:188:LYS:HD3	1.63	0.79
1:C:137:LEU:O	1:C:137:LEU:CD2	2.31	0.79
1:D:11:SER:HB2	2:D:429:GOL:C1	2.12	0.79
1:C:197:VAL:HB	1:C:201:ASN:HD22	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:TRP:NE1	2:C:427:GOL:H12	1.98	0.79
2:C:430:GOL:H32	1:D:56:GLU:OE2	1.81	0.79
1:D:8:THR:HG21	2:D:429:GOL:O1	1.83	0.78
1:A:342:THR:CB	1:A:344:LEU:HD22	2.12	0.78
1:D:8:THR:HG22	1:D:11:SER:H	1.47	0.78
1:A:56:GLU:O	1:A:57:ASN:HB2	1.82	0.78
1:A:220:ALA:CB	1:A:227:ILE:HD11	2.14	0.78
1:A:264:ILE:O	1:A:318:HIS:HE1	1.67	0.78
1:B:121:LEU:HD11	1:B:228:ILE:HD11	1.66	0.77
1:B:182:ASP:OD2	1:B:188:LYS:HB3	1.84	0.77
1:C:303:ILE:HG22	1:C:307:LEU:HD22	1.65	0.77
1:D:370:ILE:HG13	1:D:398:LEU:HD21	1.66	0.77
1:D:368:GLU:HB3	3:D:573:HOH:O	1.85	0.77
1:B:217:TYR:HB2	1:B:249:MET:CE	2.15	0.77
1:A:283:ARG:HD3	3:A:461:HOH:O	1.84	0.76
1:B:344:LEU:HB2	3:B:627:HOH:O	1.86	0.76
1:A:294:HIS:HD2	1:A:295:PRO:O	1.68	0.76
1:C:261:PHE:HB3	1:C:265:ILE:HD13	1.66	0.76
1:D:18:PRO:HB3	1:D:20:ARG:HG2	1.67	0.76
1:B:345:ALA:HB1	1:B:358:ILE:HD13	1.67	0.76
1:A:84:LEU:O	1:A:88:LYS:HG3	1.86	0.75
1:C:345:ALA:CB	1:C:358:ILE:HD13	2.16	0.75
1:C:134:ASN:H	1:C:192:LYS:NZ	1.84	0.75
1:B:212:ARG:O	1:B:216:ILE:HD12	1.86	0.75
1:B:217:TYR:HB2	1:B:249:MET:HE2	1.69	0.75
1:B:243:VAL:HG11	3:B:581:HOH:O	1.87	0.75
1:A:163:GLU:HG3	1:A:348:HIS:CE1	2.22	0.74
1:D:285:ILE:HD13	1:D:285:ILE:C	2.12	0.74
1:A:121:LEU:CD2	1:A:228:ILE:CD1	2.65	0.74
1:D:137:LEU:CD2	1:D:137:LEU:O	2.33	0.74
1:D:368:GLU:HB2	3:D:581:HOH:O	1.88	0.74
1:B:366:VAL:HG23	1:B:369:LEU:HD23	1.70	0.74
1:B:8:THR:HG22	1:B:11:SER:N	1.99	0.73
1:B:102:TYR:O	1:B:108:GLN:HG3	1.88	0.73
1:D:325:PHE:HB3	3:D:546:HOH:O	1.87	0.73
1:A:365:ASP:HB2	1:A:394:PRO:HB3	1.69	0.73
1:B:8:THR:CG2	1:B:11:SER:H	1.99	0.73
1:A:285:ILE:HG12	1:A:285:ILE:O	1.87	0.73
1:D:325:PHE:CD1	3:D:546:HOH:O	2.34	0.73
1:B:182:ASP:HB2	3:B:451:HOH:O	1.88	0.72
1:A:41:PRO:HB3	1:B:354:MET:CE	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:TYR:CD2	3:D:546:HOH:O	2.43	0.72
1:C:370:ILE:HD11	1:C:398:LEU:CD2	2.17	0.72
1:D:370:ILE:HG13	1:D:398:LEU:CD2	2.20	0.72
1:A:342:THR:H	1:A:344:LEU:H	1.38	0.72
1:A:41:PRO:CA	1:B:354:MET:HE1	2.18	0.72
1:C:185:ASN:O	1:C:186:PRO:C	2.33	0.72
1:A:172:ARG:NH2	1:A:215:GLU:OE2	2.22	0.71
1:A:60:THR:HG22	3:A:531:HOH:O	1.90	0.71
1:B:338:ASP:O	1:B:342:THR:HG23	1.91	0.71
1:A:17:SER:CB	1:A:18:PRO:CD	2.67	0.71
1:C:73:GLN:O	1:C:297:THR:HG21	1.89	0.71
1:C:179:LYS:HE3	1:C:180:PRO:HD3	1.72	0.71
1:C:221:ARG:HH21	1:C:251:VAL:CG1	2.03	0.71
1:A:97:PRO:C	1:A:99:THR:H	1.99	0.70
1:C:8:THR:CG2	1:C:11:SER:H	2.04	0.70
1:C:284:VAL:O	1:C:288:ILE:HG23	1.90	0.70
1:D:366:VAL:HG11	1:D:398:LEU:CD2	2.21	0.70
1:B:288:ILE:HD13	3:B:537:HOH:O	1.90	0.70
1:A:97:PRO:O	1:A:99:THR:N	2.23	0.70
1:D:303:ILE:HG22	1:D:307:LEU:HD22	1.71	0.70
1:A:19:ILE:HD12	3:A:549:HOH:O	1.93	0.69
1:C:45:MET:HE3	1:C:45:MET:HA	1.75	0.69
1:C:404:SER:O	2:C:428:GOL:H2	1.92	0.69
1:B:257:ARG:NH1	1:B:259:ASP:OD1	2.26	0.69
1:C:186:PRO:O	1:C:187:GLN:HG2	1.93	0.69
1:D:294:HIS:HD2	1:D:295:PRO:O	1.75	0.69
1:B:134:ASN:ND2	1:B:178:TRP:CH2	2.61	0.69
1:D:1:MET:N	3:D:431:HOH:O	2.22	0.69
1:D:169:ASP:HA	1:D:172:ARG:NH1	2.08	0.68
1:B:408:GLU:H	1:B:408:GLU:CD	2.00	0.68
1:B:283:ARG:HD3	3:B:553:HOH:O	1.93	0.68
1:C:140:PRO:HB2	1:C:203:PRO:HG3	1.76	0.68
1:A:59:LYS:NZ	1:A:59:LYS:HB2	2.08	0.67
1:B:231:ASP:OD2	1:B:257:ARG:NH2	2.26	0.67
1:C:345:ALA:CB	1:C:358:ILE:CD1	2.68	0.67
1:B:75:SER:HB2	1:B:76:PRO:CD	2.25	0.67
1:C:163:GLU:HG2	1:C:348:HIS:CE1	2.30	0.67
1:C:16:PRO:HA	1:C:286:LEU:HD22	1.77	0.67
1:D:73:GLN:O	1:D:297:THR:HG21	1.95	0.67
1:A:59:LYS:HB3	1:A:59:LYS:HZ1	1.54	0.67
1:D:89:GLN:HA	1:D:89:GLN:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASN:N	1:C:97:PRO:HD3	2.10	0.67
1:D:86:TRP:HZ2	3:D:583:HOH:O	1.76	0.67
1:D:358:ILE:O	1:D:358:ILE:HG13	1.95	0.67
1:D:366:VAL:CG1	1:D:398:LEU:HD21	2.25	0.67
1:A:59:LYS:HZ1	1:A:59:LYS:HB2	1.60	0.66
1:D:370:ILE:CG1	1:D:398:LEU:HD21	2.25	0.66
1:A:27:SER:O	1:A:28:ARG:HB3	1.95	0.66
1:C:185:ASN:O	1:C:187:GLN:N	2.28	0.66
1:A:361:LYS:HD3	3:A:560:HOH:O	1.95	0.66
1:D:24:ASP:CB	3:D:584:HOH:O	2.44	0.66
1:D:163:GLU:O	1:D:206:ASN:HB3	1.95	0.66
1:A:375:VAL:HG12	1:A:380:LEU:HD22	1.76	0.66
1:D:231:ASP:OD2	1:D:257:ARG:NH2	2.28	0.66
1:A:67:MET:O	1:A:70:ARG:N	2.27	0.66
1:A:59:LYS:HE2	1:D:178:TRP:CZ3	2.30	0.66
1:D:96:ASN:HB3	3:D:547:HOH:O	1.94	0.66
1:C:166:ILE:HD11	1:C:216:ILE:HD12	1.72	0.65
1:D:278:LYS:HB3	1:D:279:PRO:HD3	1.78	0.65
1:A:342:THR:O	1:A:342:THR:HG23	1.94	0.65
1:B:172:ARG:HG2	1:B:219:LEU:HD11	1.79	0.65
1:B:345:ALA:CB	1:B:358:ILE:CD1	2.75	0.65
1:C:34:ILE:HD12	1:D:409:GLN:HB3	1.78	0.65
1:B:143:SER:HB3	1:B:386:ALA:O	1.96	0.65
1:D:126:GLU:CB	2:D:429:GOL:O2	2.42	0.65
1:A:179:LYS:HB3	1:A:181:GLU:OE2	1.97	0.65
1:B:137:LEU:HD21	1:B:156:ILE:CG2	2.26	0.65
1:B:99:THR:HG23	1:B:109:MET:H	1.62	0.65
1:B:344:LEU:CB	3:B:627:HOH:O	2.43	0.65
1:D:163:GLU:HG2	1:D:348:HIS:CE1	2.32	0.65
1:A:86:TRP:HZ3	3:A:558:HOH:O	1.79	0.65
1:C:221:ARG:NH2	1:C:251:VAL:HG13	2.11	0.65
1:D:14:ARG:HH21	2:D:429:GOL:H2	1.61	0.65
1:D:120:GLY:O	1:D:124:VAL:HG23	1.97	0.65
1:B:345:ALA:CB	1:B:358:ILE:HD13	2.26	0.64
1:A:299:ASN:HD21	1:B:299:ASN:HD21	1.45	0.64
1:C:22:MET:HA	3:C:540:HOH:O	1.96	0.64
1:C:264:ILE:O	1:C:318:HIS:HE1	1.81	0.64
1:D:340:TRP:CE2	1:D:415:GLN:HB2	2.32	0.64
1:D:288:ILE:C	1:D:288:ILE:CD1	2.60	0.64
1:B:137:LEU:CD2	1:B:156:ILE:HG23	2.28	0.64
1:D:112:CYS:SG	3:D:591:HOH:O	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:HB2	1:A:227:ILE:HD11	1.78	0.63
1:B:344:LEU:HD12	1:B:421:ILE:CG2	2.27	0.63
1:C:303:ILE:CG2	1:C:307:LEU:HD22	2.28	0.63
1:C:415:GLN:CG	1:C:416:VAL:N	2.59	0.63
1:B:56:GLU:O	1:B:57:ASN:CB	2.43	0.63
1:A:288:ILE:HD11	1:A:293:LEU:O	1.99	0.63
1:C:239:ASN:ND2	1:C:241:PHE:O	2.32	0.63
1:D:99:THR:HG23	1:D:109:MET:HB2	1.78	0.63
1:C:133:ASP:OD2	1:C:192:LYS:HD2	1.98	0.63
1:C:310:TRP:CD1	2:C:427:GOL:H12	2.34	0.63
1:C:117:SER:HB3	1:C:260:SER:HB3	1.79	0.63
1:C:221:ARG:HH21	1:C:251:VAL:HG13	1.63	0.63
1:B:2:ASN:HD21	1:B:4:ALA:HB3	1.64	0.63
1:D:137:LEU:HD23	1:D:138:ASP:N	2.12	0.63
1:A:115:SER:O	1:A:115:SER:OG	2.16	0.62
1:C:294:HIS:HD2	1:C:295:PRO:O	1.82	0.62
1:D:42:ASN:ND2	1:D:44:ASN:HB2	2.14	0.62
1:A:300:GLN:NE2	3:A:478:HOH:O	2.25	0.62
1:C:192:LYS:CD	3:C:446:HOH:O	2.47	0.62
1:A:195:TYR:HD1	1:A:228:ILE:HG12	1.64	0.62
1:A:381:MET:HE2	1:A:398:LEU:HD13	1.82	0.62
1:A:196:THR:HG23	3:A:568:HOH:O	1.99	0.62
1:A:100:ILE:HD12	1:A:101:HIS:CE1	2.34	0.62
1:B:369:LEU:O	1:B:373:LYS:HB2	1.99	0.62
1:C:192:LYS:HD2	3:C:446:HOH:O	2.00	0.61
1:A:345:ALA:HB1	1:A:358:ILE:HD12	1.81	0.61
1:C:370:ILE:CD1	1:C:398:LEU:HD21	2.27	0.61
1:A:8:THR:CG2	1:A:10:ALA:HB3	2.31	0.61
1:B:99:THR:HG21	3:B:577:HOH:O	2.01	0.61
1:C:139:GLU:HA	1:C:140:PRO:C	2.26	0.61
1:B:222:LYS:HE2	1:B:223:TYR:CE2	2.34	0.61
1:A:73:GLN:O	1:A:297:THR:HG21	2.01	0.61
1:D:83:LEU:HD22	1:D:87:LEU:CD2	2.22	0.60
1:A:22:MET:HG3	1:A:23:THR:N	2.03	0.60
1:A:34:ILE:CD1	1:B:409:GLN:HB3	2.31	0.60
1:C:231:ASP:OD2	1:C:257:ARG:NH2	2.34	0.60
1:C:261:PHE:CB	1:C:265:ILE:HD12	2.29	0.60
1:C:30:PRO:HD2	1:C:33:MET:HE3	1.83	0.60
1:D:95:HIS:O	1:D:96:ASN:C	2.43	0.60
1:B:179:LYS:CG	1:B:180:PRO:HD2	2.32	0.60
1:C:73:GLN:O	1:C:297:THR:CG2	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ILE:HD11	1:C:293:LEU:O	2.02	0.60
1:B:84:LEU:HD13	1:B:113:VAL:HG23	1.85	0.59
1:A:197:VAL:C	3:A:568:HOH:O	2.45	0.59
1:B:190:THR:O	1:B:192:LYS:NZ	2.34	0.59
1:D:285:ILE:HD13	1:D:286:LEU:N	2.17	0.59
1:A:147:GLN:HG3	3:A:544:HOH:O	2.03	0.59
1:D:265:ILE:O	1:D:266:SER:HB2	2.03	0.59
1:A:142:TYR:CD1	1:A:263:LLP:H2'3	2.38	0.59
1:A:166:ILE:HD12	1:A:167:VAL:C	2.28	0.59
1:D:42:ASN:HD21	1:D:44:ASN:HB2	1.68	0.59
1:B:187:GLN:O	1:B:188:LYS:HB2	2.03	0.59
1:C:197:VAL:HB	1:C:201:ASN:ND2	2.18	0.59
1:C:34:ILE:HD13	1:D:409:GLN:O	2.03	0.58
1:C:384:GLY:N	1:C:397:TYR:O	2.32	0.58
1:C:178:TRP:HZ3	1:C:188:LYS:O	1.85	0.58
1:D:24:ASP:HB2	3:D:584:HOH:O	2.01	0.58
1:B:338:ASP:O	1:B:342:THR:CG2	2.51	0.58
1:D:10:ALA:HB2	3:D:469:HOH:O	2.02	0.58
1:B:42:ASN:HD22	1:B:44:ASN:H	1.51	0.58
1:D:99:THR:HG21	3:D:552:HOH:O	2.04	0.58
1:C:92:ILE:HG12	1:C:100:ILE:HG21	1.86	0.58
1:C:102:TYR:O	1:C:108:GLN:HB2	2.03	0.58
1:B:345:ALA:HB1	1:B:358:ILE:HD12	1.85	0.58
1:C:16:PRO:HA	1:C:286:LEU:CD2	2.32	0.58
1:C:261:PHE:CG	1:C:265:ILE:HD12	2.39	0.58
1:D:304:SER:O	1:D:308:HIS:HD2	1.87	0.58
1:C:99:THR:HG23	1:C:99:THR:O	2.04	0.57
1:C:163:GLU:CG	1:C:348:HIS:CE1	2.87	0.57
1:A:123:LYS:HB3	1:A:284:VAL:HB	1.85	0.57
1:B:134:ASN:ND2	1:B:178:TRP:HH2	2.02	0.57
1:A:59:LYS:HB3	1:A:59:LYS:HZ2	1.69	0.57
1:B:341:LEU:CD2	1:B:414:PHE:HD2	2.16	0.57
1:D:96:ASN:CB	3:D:547:HOH:O	2.50	0.57
1:D:237:GLN:HE22	1:D:243:VAL:H	1.53	0.57
1:C:1:MET:N	3:C:548:HOH:O	2.28	0.57
1:D:201:ASN:HB2	2:D:428:GOL:H2	1.87	0.56
1:D:365:ASP:HB2	1:D:394:PRO:HB2	1.86	0.56
1:A:34:ILE:HD13	1:B:409:GLN:HB3	1.87	0.56
1:D:86:TRP:CZ2	3:D:583:HOH:O	2.52	0.56
1:A:188:LYS:O	1:A:188:LYS:HD3	2.05	0.56
1:B:113:VAL:HG12	1:B:295:PRO:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:THR:HB	1:C:24:ASP:HB2	1.86	0.56
1:D:366:VAL:CG1	1:D:366:VAL:O	2.52	0.56
1:C:114:THR:HG21	1:C:120:GLY:HA3	1.87	0.56
1:B:20:ARG:HG3	1:B:22:MET:HE3	1.85	0.56
1:C:133:ASP:HB3	1:C:192:LYS:HE3	1.88	0.56
1:A:203:PRO:HG3	1:A:387:PHE:CG	2.40	0.56
1:D:16:PRO:O	1:D:289:GLN:OE1	2.24	0.56
1:A:370:ILE:HG21	1:A:381:MET:O	2.06	0.56
1:D:177:ARG:HB3	1:D:177:ARG:HH11	1.71	0.56
1:D:201:ASN:HB2	2:D:428:GOL:C2	2.35	0.56
1:A:163:GLU:HG2	3:A:550:HOH:O	2.06	0.55
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.71	0.55
1:C:221:ARG:NH2	1:C:251:VAL:CG1	2.69	0.55
1:D:102:TYR:O	1:D:108:GLN:HB2	2.07	0.55
1:D:231:ASP:HA	3:D:487:HOH:O	2.07	0.55
1:A:63:PHE:CB	1:A:68:MET:HE2	2.36	0.55
1:B:341:LEU:CD2	1:B:414:PHE:CD2	2.85	0.55
1:C:34:ILE:CD1	1:D:409:GLN:HB3	2.35	0.55
1:D:214:LYS:HA	1:D:249:MET:HE1	1.87	0.55
1:D:288:ILE:HD12	1:D:289:GLN:N	2.21	0.55
1:A:41:PRO:HA	1:B:354:MET:HE1	1.88	0.55
1:D:67:MET:H	2:D:427:GOL:H11	1.71	0.55
1:D:201:ASN:CB	2:D:428:GOL:H11	2.17	0.55
1:D:311:GLY:C	1:D:313:GLU:N	2.63	0.55
1:A:261:PHE:CD1	1:A:265:ILE:HD12	2.42	0.55
1:B:108:GLN:NE2	1:B:278:LYS:NZ	2.54	0.55
1:C:8:THR:HG22	1:C:11:SER:HB3	1.89	0.55
1:C:271:ILE:HD12	1:C:300:GLN:HG2	1.87	0.55
1:A:33:MET:HE2	1:B:378:GLY:HA2	1.89	0.55
1:A:169:ASP:OD1	1:A:172:ARG:NH1	2.40	0.55
1:D:366:VAL:CG1	1:D:398:LEU:CD2	2.85	0.55
1:A:179:LYS:HD2	1:A:179:LYS:N	2.22	0.55
1:B:217:TYR:CB	1:B:249:MET:CE	2.84	0.55
1:B:243:VAL:CG1	3:B:534:HOH:O	2.39	0.55
1:D:241:PHE:HD1	3:D:479:HOH:O	1.89	0.55
1:A:3:TYR:OH	1:A:253:GLY:O	2.22	0.54
1:B:330:LYS:HG2	1:B:334:LEU:HD22	1.89	0.54
1:C:99:THR:O	1:C:100:ILE:C	2.47	0.54
1:D:204:THR:OG1	2:D:428:GOL:H32	2.07	0.54
1:D:20:ARG:C	1:D:22:MET:N	2.58	0.54
1:D:316:MET:O	1:D:319:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:N	1:A:352:ALA:HB3	2.22	0.54
1:C:20:ARG:HD3	1:C:21:THR:N	2.22	0.54
1:A:163:GLU:CG	1:A:348:HIS:CE1	2.89	0.54
1:B:97:PRO:C	1:B:99:THR:H	2.16	0.54
1:B:137:LEU:HD21	1:B:156:ILE:HG23	1.87	0.54
1:B:237:GLN:HE22	1:B:243:VAL:H	1.55	0.54
1:B:30:PRO:HD2	1:B:33:MET:HE1	1.88	0.54
1:B:303:ILE:HG22	1:B:307:LEU:HD22	1.90	0.54
1:C:288:ILE:O	1:C:288:ILE:HD12	2.08	0.54
1:B:197:VAL:HB	1:B:201:ASN:HD22	1.73	0.54
1:C:22:MET:HG3	1:C:23:THR:HG23	1.90	0.53
1:B:368:GLU:O	1:B:372:GLU:HB2	2.08	0.53
1:C:99:THR:CG2	1:C:109:MET:HB2	2.37	0.53
1:C:261:PHE:CB	1:C:265:ILE:CD1	2.80	0.53
1:C:326:TYR:CE1	1:C:354:MET:HE2	2.43	0.53
1:C:363:ILE:HD13	3:C:564:HOH:O	2.08	0.53
1:D:341:LEU:HD22	1:D:414:PHE:CD2	2.44	0.53
1:A:377:MET:HG3	1:A:420:LEU:HD11	1.90	0.53
1:C:100:ILE:O	1:C:108:GLN:HG3	2.08	0.53
1:B:73:GLN:O	1:B:297:THR:CG2	2.52	0.53
1:B:108:GLN:NE2	1:B:278:LYS:HZ3	2.07	0.53
1:C:145:THR:HG21	1:C:195:TYR:OH	2.08	0.53
1:A:6:PHE:CE2	1:A:226:LEU:HD13	2.44	0.53
1:A:18:PRO:CD	1:A:289:GLN:HB3	2.38	0.53
1:B:179:LYS:HG3	1:B:180:PRO:HD2	1.91	0.53
1:D:359:LYS:HB2	1:D:397:TYR:CE1	2.43	0.53
1:C:45:MET:HE1	2:C:430:GOL:H12	1.90	0.53
1:C:99:THR:CG2	1:C:109:MET:N	2.72	0.53
1:D:288:ILE:HD12	1:D:288:ILE:O	2.06	0.53
1:A:59:LYS:NZ	1:D:177:ARG:HD3	2.24	0.52
2:D:428:GOL:H31	3:D:572:HOH:O	2.09	0.52
1:A:108:GLN:HE21	1:A:278:LYS:HD3	1.74	0.52
1:C:294:HIS:HB2	1:C:295:PRO:CD	2.40	0.52
1:D:203:PRO:HG3	1:D:387:PHE:CG	2.45	0.52
1:A:59:LYS:HZ3	1:D:177:ARG:HG2	1.73	0.52
1:A:264:ILE:O	1:A:318:HIS:CE1	2.56	0.52
1:A:334:LEU:HD21	1:A:349:VAL:HB	1.91	0.52
1:D:24:ASP:HB3	3:D:584:HOH:O	2.06	0.52
1:D:341:LEU:HD22	1:D:414:PHE:HD2	1.74	0.52
1:A:24:ASP:OD2	1:A:25:ILE:N	2.42	0.52
1:A:86:TRP:CD1	1:A:86:TRP:C	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TRP:CZ3	1:B:188:LYS:O	2.62	0.52
1:B:178:TRP:HZ3	1:B:188:LYS:O	1.92	0.52
1:B:303:ILE:O	1:B:307:LEU:HB2	2.09	0.52
1:D:366:VAL:O	1:D:366:VAL:HG13	2.08	0.52
1:B:295:PRO:O	1:B:296:SER:C	2.53	0.52
1:B:301:LEU:O	1:B:305:GLN:CG	2.51	0.52
1:C:74:TYR:HD1	1:C:294:HIS:HE1	1.58	0.52
1:D:198:PRO:O	1:D:207:SER:HA	2.09	0.52
1:A:86:TRP:CZ3	3:A:558:HOH:O	2.54	0.52
1:A:366:VAL:O	1:A:366:VAL:HG22	2.10	0.52
1:A:369:LEU:HD23	1:A:370:ILE:HD13	1.91	0.52
1:B:344:LEU:HD11	1:B:425:LEU:HD21	1.92	0.52
1:C:200:GLY:N	1:C:352:ALA:HB3	2.25	0.52
1:C:159:VAL:HG11	1:C:166:ILE:HD13	1.92	0.52
1:D:34:ILE:HD11	1:D:36:LEU:HD21	1.92	0.52
1:C:1:MET:HA	3:C:550:HOH:O	2.08	0.51
1:C:142:TYR:HD1	1:C:145:THR:CG2	2.23	0.51
1:D:159:VAL:HG11	1:D:166:ILE:HD13	1.91	0.51
1:A:74:TYR:HD1	1:A:294:HIS:HE1	1.57	0.51
1:A:97:PRO:HG2	1:A:109:MET:SD	2.51	0.51
1:A:217:TYR:O	1:A:220:ALA:HB3	2.10	0.51
1:A:366:VAL:O	1:A:370:ILE:HG12	2.11	0.51
1:B:142:TYR:CD2	1:B:145:THR:HG22	2.46	0.51
1:B:174:ILE:O	1:B:177:ARG:HD3	2.11	0.51
1:D:264:ILE:HG22	1:D:322:VAL:HG11	1.91	0.51
1:B:204:THR:HA	1:B:357:TRP:HB2	1.91	0.51
1:C:345:ALA:HB1	1:C:358:ILE:HD12	1.87	0.51
1:A:152:LEU:HD12	1:A:152:LEU:N	2.25	0.51
1:A:278:LYS:HD2	3:A:552:HOH:O	2.10	0.51
1:A:294:HIS:HB2	1:A:295:PRO:CD	2.40	0.51
1:A:345:ALA:HB1	1:A:358:ILE:CD1	2.40	0.51
1:B:22:MET:HE2	1:B:37:ALA:O	2.09	0.51
1:C:381:MET:HE2	1:C:398:LEU:HD13	1.91	0.51
1:C:138:ASP:HB3	1:C:166:ILE:HG22	1.92	0.51
1:D:8:THR:HG23	1:D:10:ALA:H	1.75	0.51
1:B:134:ASN:HD21	1:B:178:TRP:HH2	1.56	0.51
1:D:92:ILE:HG12	1:D:100:ILE:HG21	1.93	0.51
1:A:63:PHE:HB3	1:A:68:MET:HE2	1.92	0.51
1:C:61:ILE:HG23	1:C:305:GLN:HE21	1.76	0.51
1:C:345:ALA:HA	1:C:359:LYS:O	2.10	0.51
1:A:8:THR:HG22	1:A:11:SER:N	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:HG23	1:C:109:MET:N	2.25	0.51
1:C:285:ILE:O	1:C:289:GLN:HG3	2.10	0.51
1:D:126:GLU:CB	2:D:429:GOL:HO2	2.24	0.51
1:D:345:ALA:HB1	1:D:358:ILE:HD12	1.93	0.51
1:A:221:ARG:O	1:A:222:LYS:C	2.54	0.50
1:B:174:ILE:HD12	1:B:175:LEU:N	2.26	0.50
1:C:30:PRO:C	1:C:32:SER:H	2.20	0.50
1:A:227:ILE:HB	1:A:255:VAL:HG22	1.92	0.50
1:B:42:ASN:ND2	1:B:44:ASN:H	2.09	0.50
1:B:137:LEU:HD22	1:B:156:ILE:HG23	1.93	0.50
1:B:385:ASN:O	1:B:391:SER:HA	2.11	0.50
1:C:20:ARG:H	1:C:22:MET:HE3	1.77	0.50
1:C:142:TYR:HD1	1:C:145:THR:HG22	1.76	0.50
1:D:142:TYR:CD2	1:D:263:LLP:H2'3	2.46	0.50
1:B:96:ASN:CB	3:B:572:HOH:O	2.38	0.50
1:B:142:TYR:HD2	1:B:145:THR:HG22	1.76	0.50
1:B:283:ARG:CD	3:B:553:HOH:O	2.56	0.50
1:C:123:LYS:HD2	1:C:288:ILE:HG22	1.92	0.50
1:D:185:ASN:C	1:D:185:ASN:HD22	2.18	0.50
1:A:110:ASP:CG	1:A:278:LYS:HE2	2.36	0.50
1:A:209:THR:O	1:A:213:LYS:HG3	2.10	0.50
1:B:172:ARG:HG3	1:B:172:ARG:NH1	2.25	0.50
1:B:214:LYS:HA	1:B:249:MET:HE1	1.94	0.50
1:C:341:LEU:HD11	1:C:414:PHE:CE2	2.46	0.50
1:A:164:SER:O	1:A:208:LEU:HA	2.12	0.50
1:A:337:ALA:O	1:A:341:LEU:HB2	2.11	0.50
1:B:344:LEU:CB	3:B:571:HOH:O	2.24	0.50
1:B:344:LEU:HD12	1:B:421:ILE:HG23	1.93	0.50
1:C:24:ASP:O	1:C:28:ARG:HD2	2.11	0.50
1:C:99:THR:O	1:C:99:THR:CG2	2.58	0.50
1:B:233:TYR:CE1	1:B:263:LLP:HD3	2.47	0.50
1:C:71:ALA:HB2	1:C:301:LEU:HD23	1.94	0.50
1:A:18:PRO:HD3	1:A:289:GLN:HB3	1.92	0.50
1:B:366:VAL:HG12	1:B:395:SER:O	2.11	0.50
1:D:20:ARG:NH2	3:D:449:HOH:O	2.45	0.50
1:B:222:LYS:HE2	1:B:223:TYR:CZ	2.47	0.50
1:A:151:PRO:HG2	1:A:152:LEU:CD1	2.42	0.50
1:B:213:LYS:O	1:B:249:MET:HE1	2.11	0.50
1:B:408:GLU:OE1	1:B:408:GLU:N	2.27	0.50
1:C:256:ILE:HD11	1:C:280:LEU:HD13	1.94	0.49
1:D:80:ILE:HD13	1:D:301:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:O	1:A:68:MET:C	2.54	0.49
1:A:73:GLN:O	1:A:297:THR:CG2	2.59	0.49
1:D:270:ARG:O	1:D:271:ILE:HD13	2.12	0.49
1:D:366:VAL:HG11	1:D:398:LEU:HD21	1.89	0.49
1:A:299:ASN:HD21	1:B:299:ASN:ND2	2.09	0.49
1:C:60:THR:HG22	3:C:487:HOH:O	2.10	0.49
1:C:270:ARG:C	1:C:271:ILE:HG12	2.38	0.49
1:D:177:ARG:HG2	1:D:177:ARG:O	2.11	0.49
1:D:228:ILE:HG13	1:D:228:ILE:O	2.13	0.49
1:A:25:ILE:HG13	2:A:426:GOL:H12	1.92	0.49
1:A:342:THR:N	1:A:344:LEU:H	2.07	0.49
1:C:35:SER:HB2	1:D:380:LEU:HD12	1.93	0.49
1:A:104:PRO:HG3	1:A:108:GLN:NE2	2.28	0.49
1:B:240:LYS:HZ1	1:B:320:ASP:HB3	1.78	0.49
1:C:381:MET:HE2	1:C:398:LEU:CD1	2.43	0.49
1:B:381:MET:HE3	1:B:400:ALA:HB2	1.93	0.49
1:C:7:ILE:HD13	1:C:283:ARG:HD3	1.93	0.49
1:D:97:PRO:C	1:D:99:THR:H	2.21	0.49
1:B:89:GLN:NE2	1:B:89:GLN:HA	2.28	0.49
1:C:97:PRO:HG2	1:C:109:MET:SD	2.53	0.49
1:A:366:VAL:CG2	1:A:398:LEU:HD21	2.42	0.49
1:A:415:GLN:O	1:A:419:GLN:NE2	2.45	0.49
1:B:99:THR:HG23	1:B:109:MET:N	2.26	0.49
1:A:218:GLU:HG2	1:A:219:LEU:N	2.24	0.49
1:A:311:GLY:C	1:A:313:GLU:N	2.71	0.49
1:B:104:PRO:O	1:B:106:GLN:O	2.31	0.49
1:A:34:ILE:O	1:B:379:VAL:HA	2.13	0.48
1:A:174:ILE:O	1:A:177:ARG:HD3	2.13	0.48
1:A:236:LEU:HD23	1:A:353:GLY:HA2	1.94	0.48
1:C:288:ILE:HD11	1:C:293:LEU:C	2.37	0.48
1:D:145:THR:HG21	1:D:195:TYR:OH	2.12	0.48
1:A:195:TYR:CD1	1:A:228:ILE:HG12	2.47	0.48
1:C:95:HIS:HD2	3:C:458:HOH:O	1.95	0.48
1:C:133:ASP:CG	1:C:192:LYS:HD2	2.37	0.48
1:C:163:GLU:HG2	1:C:348:HIS:ND1	2.28	0.48
1:D:220:ALA:O	1:D:224:ASP:HA	2.13	0.48
1:A:68:MET:O	1:A:69:LYS:C	2.55	0.48
1:A:294:HIS:NE2	1:B:270:ARG:HD3	2.28	0.48
1:A:341:LEU:CD2	1:A:414:PHE:CE2	2.96	0.48
1:C:190:THR:O	1:C:192:LYS:NZ	2.42	0.48
1:B:2:ASN:ND2	1:B:4:ALA:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ILE:HG13	1:B:398:LEU:HD21	1.96	0.48
1:D:42:ASN:ND2	1:D:44:ASN:H	2.05	0.48
1:C:87:LEU:O	1:C:91:GLN:HG2	2.14	0.48
1:C:204:THR:HA	1:C:357:TRP:HB2	1.95	0.48
1:A:91:GLN:O	1:A:95:HIS:N	2.38	0.48
1:A:142:TYR:CG	1:A:263:LLP:H2'3	2.48	0.48
1:A:366:VAL:HG21	1:A:398:LEU:HD21	1.95	0.48
1:C:45:MET:HE3	1:C:45:MET:CA	2.39	0.48
1:D:99:THR:CG2	1:D:109:MET:HB2	2.44	0.48
1:D:200:GLY:N	1:D:352:ALA:HB3	2.29	0.48
1:A:95:HIS:O	1:A:248:SER:HA	2.14	0.48
1:D:127:MET:HA	2:D:429:GOL:H32	1.94	0.48
1:B:195:TYR:C	1:B:195:TYR:CD2	2.92	0.47
1:B:411:ASP:OD1	3:B:456:HOH:O	2.20	0.47
1:D:19:ILE:HG23	3:D:553:HOH:O	2.13	0.47
1:B:42:ASN:HD21	1:B:44:ASN:HD22	1.63	0.47
1:B:108:GLN:O	1:B:109:MET:C	2.56	0.47
1:D:245:THR:O	1:D:248:SER:OG	2.30	0.47
1:A:21:THR:HA	1:A:24:ASP:CG	2.38	0.47
1:A:196:THR:CB	3:A:568:HOH:O	2.62	0.47
1:D:42:ASN:HD21	1:D:44:ASN:HD22	1.62	0.47
1:D:117:SER:O	1:D:121:LEU:HD12	2.14	0.47
1:D:294:HIS:CD2	1:D:295:PRO:O	2.63	0.47
1:C:162:ASP:OD1	1:C:212:ARG:NH1	2.35	0.47
1:A:121:LEU:HD23	1:A:228:ILE:CD1	2.44	0.47
1:B:344:LEU:HG	3:B:571:HOH:O	2.14	0.47
1:C:21:THR:CB	1:C:24:ASP:HB2	2.43	0.47
1:D:349:VAL:HA	1:D:350:PRO:HD3	1.70	0.47
1:A:50:THR:C	1:A:68:MET:HE3	2.40	0.47
1:A:311:GLY:C	1:A:313:GLU:H	2.23	0.47
1:B:33:MET:HE3	1:B:33:MET:HB2	1.78	0.47
1:B:42:ASN:ND2	1:B:44:ASN:HB2	2.29	0.47
1:B:121:LEU:HD23	3:B:568:HOH:O	2.14	0.47
1:C:221:ARG:HH21	1:C:251:VAL:HG11	1.79	0.47
1:D:49:LYS:C	1:D:68:MET:HG2	2.39	0.47
1:A:198:PRO:N	3:A:568:HOH:O	2.48	0.47
1:A:359:LYS:HB2	1:A:397:TYR:CE2	2.49	0.47
1:A:390:ASP:C	1:A:390:ASP:OD2	2.58	0.47
1:B:16:PRO:HA	1:B:286:LEU:HD22	1.97	0.47
1:B:84:LEU:O	1:B:88:LYS:HG3	2.15	0.47
1:B:263:LLP:H5'2	1:B:263:LLP:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:CD1	1:C:301:LEU:HD13	2.45	0.47
1:C:97:PRO:C	1:C:99:THR:H	2.22	0.47
1:C:264:ILE:O	1:C:318:HIS:CE1	2.66	0.47
1:C:374:ALA:HA	1:C:420:LEU:CD1	2.44	0.47
1:A:152:LEU:N	1:A:152:LEU:CD1	2.78	0.47
1:A:341:LEU:HD22	1:A:414:PHE:CD2	2.49	0.47
1:C:243:VAL:HG13	3:C:544:HOH:O	2.15	0.47
1:A:192:LYS:HD3	3:A:492:HOH:O	2.14	0.47
1:C:186:PRO:C	1:C:187:GLN:HG2	2.39	0.47
1:A:341:LEU:CD2	1:A:414:PHE:CD2	2.98	0.47
1:B:163:GLU:HG2	3:B:561:HOH:O	2.15	0.47
1:A:342:THR:HB	1:A:344:LEU:CD2	2.24	0.46
1:B:185:ASN:O	1:B:187:GLN:O	2.33	0.46
1:D:162:ASP:CG	1:D:212:ARG:HH22	2.24	0.46
1:D:336:ALA:HA	3:D:519:HOH:O	2.13	0.46
1:B:377:MET:HE2	1:B:419:GLN:HE22	1.79	0.46
1:D:218:GLU:HG2	1:D:219:LEU:N	2.29	0.46
1:A:296:SER:O	1:A:300:GLN:HG3	2.15	0.46
1:B:136:LEU:CD2	1:B:174:ILE:HD13	2.44	0.46
1:B:334:LEU:HD21	1:B:349:VAL:HB	1.97	0.46
1:D:11:SER:HB2	2:D:429:GOL:H11	1.96	0.46
1:B:324:ASP:HB3	3:B:458:HOH:O	2.15	0.46
1:D:104:PRO:O	1:D:106:GLN:O	2.33	0.46
1:A:111:LEU:HA	1:A:274:LEU:O	2.14	0.46
1:B:190:THR:O	1:B:191:PRO:C	2.55	0.46
1:C:203:PRO:HB2	1:C:357:TRP:CE3	2.51	0.46
1:C:292:THR:HG22	1:D:115:SER:HB2	1.96	0.46
2:C:430:GOL:H32	1:D:56:GLU:CD	2.40	0.46
1:A:59:LYS:NZ	1:D:177:ARG:HG2	2.31	0.46
1:A:223:TYR:N	1:A:223:TYR:CD2	2.83	0.46
1:A:293:LEU:HD21	1:B:118:GLN:NE2	2.31	0.46
1:C:168:PRO:HG2	1:C:215:GLU:OE1	2.16	0.46
1:C:200:GLY:O	1:C:201:ASN:C	2.57	0.46
1:D:408:GLU:OE1	1:D:408:GLU:N	2.33	0.46
1:A:19:ILE:CA	1:A:22:MET:HE3	2.41	0.46
1:A:360:VAL:HG13	1:A:421:ILE:HD13	1.96	0.46
1:A:147:GLN:NE2	3:A:544:HOH:O	2.49	0.46
1:A:285:ILE:O	1:A:285:ILE:CG1	2.61	0.46
1:C:325:PHE:C	1:C:325:PHE:CD2	2.93	0.46
1:A:409:GLN:HB3	1:B:34:ILE:HD12	1.94	0.46
1:B:187:GLN:O	1:B:188:LYS:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:O	1:C:210:SER:C	2.59	0.46
1:C:299:ASN:HD21	1:D:299:ASN:HD21	1.63	0.46
1:C:288:ILE:CD1	1:C:293:LEU:C	2.89	0.45
1:D:360:VAL:HG23	1:D:363:ILE:HB	1.97	0.45
1:A:59:LYS:HD2	1:D:188:LYS:CD	2.40	0.45
1:B:220:ALA:O	1:B:224:ASP:HA	2.16	0.45
1:C:8:THR:HG22	1:C:11:SER:N	2.18	0.45
1:C:97:PRO:C	1:C:99:THR:N	2.74	0.45
1:D:330:LYS:O	1:D:331:ASP:C	2.59	0.45
1:C:303:ILE:O	1:C:307:LEU:HB2	2.16	0.45
1:A:263:LLP:NZ	1:A:263:LLP:C5'	2.77	0.45
1:B:166:ILE:HD11	1:B:216:ILE:HG12	1.97	0.45
1:C:134:ASN:N	1:C:192:LYS:HZ1	2.07	0.45
1:C:179:LYS:HE3	1:C:180:PRO:CD	2.45	0.45
1:D:16:PRO:HA	1:D:286:LEU:HD22	1.98	0.45
1:D:200:GLY:O	1:D:201:ASN:C	2.59	0.45
1:D:203:PRO:HB2	1:D:357:TRP:CE3	2.51	0.45
1:A:16:PRO:HA	1:A:286:LEU:HD22	1.98	0.45
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.47	0.45
1:A:196:THR:CG2	3:A:568:HOH:O	2.59	0.45
1:D:11:SER:O	1:D:283:ARG:NH2	2.24	0.45
1:D:242:ARG:NH2	1:D:316:MET:HE2	2.32	0.45
1:A:83:LEU:HD23	1:A:113:VAL:HG21	1.99	0.45
1:B:344:LEU:CG	3:B:571:HOH:O	2.63	0.45
1:C:371:GLU:O	1:C:375:VAL:CG2	2.65	0.45
1:A:268:GLY:O	1:B:296:SER:HA	2.17	0.45
1:C:203:PRO:HG2	1:C:204:THR:HG23	1.98	0.45
1:C:209:THR:HB	1:C:211:GLU:OE1	2.16	0.45
1:D:88:LYS:HE3	1:D:111:LEU:HB3	1.99	0.45
1:A:263:LLP:NZ	1:A:263:LLP:H5'2	2.31	0.45
1:B:119:GLN:O	1:B:123:LYS:HG3	2.17	0.45
1:C:164:SER:O	1:C:208:LEU:HA	2.17	0.45
1:C:381:MET:HA	1:D:37:ALA:HB2	1.99	0.45
1:A:175:LEU:O	1:A:178:TRP:HD1	2.00	0.45
1:D:15:ASN:HB3	1:D:16:PRO:HD2	1.99	0.45
1:D:58:GLY:HA2	3:D:571:HOH:O	2.16	0.45
1:D:311:GLY:C	1:D:313:GLU:H	2.24	0.45
1:D:325:PHE:CB	3:D:546:HOH:O	2.58	0.45
1:A:8:THR:HG23	1:A:10:ALA:H	1.81	0.44
1:A:184:LYS:HD2	1:A:184:LYS:N	2.32	0.44
1:B:162:ASP:C	1:B:162:ASP:OD1	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:HA	1:B:342:THR:HG22	1.99	0.44
1:C:75:SER:HB2	1:C:76:PRO:CD	2.47	0.44
1:C:270:ARG:HD3	1:D:294:HIS:CE1	2.52	0.44
1:C:310:TRP:HB3	1:C:314:GLY:HA3	1.99	0.44
1:A:330:LYS:HG2	1:A:334:LEU:HD22	1.99	0.44
1:B:115:SER:HA	1:B:270:ARG:O	2.18	0.44
1:C:197:VAL:HA	1:C:198:PRO:HD3	1.79	0.44
1:D:33:MET:HE3	1:D:33:MET:HB2	1.89	0.44
1:A:358:ILE:HG13	1:A:358:ILE:O	2.16	0.44
1:A:381:MET:HE2	1:A:398:LEU:CD1	2.47	0.44
1:B:22:MET:HG3	1:B:23:THR:HG23	1.98	0.44
1:B:42:ASN:HD21	1:B:44:ASN:HB2	1.83	0.44
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.66	0.44
1:D:204:THR:HG1	2:D:428:GOL:H32	1.81	0.44
1:D:305:GLN:NE2	3:D:596:HOH:O	2.46	0.44
1:B:42:ASN:HD22	1:B:44:ASN:N	2.16	0.44
1:C:257:ARG:CD	1:C:259:ASP:OD2	2.56	0.44
1:D:139:GLU:OE1	1:D:389:VAL:HG23	2.17	0.44
1:A:165:GLY:O	1:A:166:ILE:C	2.60	0.44
1:A:166:ILE:HD12	1:A:167:VAL:N	2.33	0.44
1:A:240:LYS:HE2	1:A:323:ILE:CG2	2.47	0.44
1:B:141:ALA:O	1:B:142:TYR:C	2.61	0.44
1:B:243:VAL:HA	1:B:244:PRO:HD2	1.47	0.44
1:C:42:ASN:OD1	1:C:44:ASN:HB2	2.17	0.44
1:D:139:GLU:HA	1:D:140:PRO:C	2.42	0.44
1:D:201:ASN:CB	2:D:428:GOL:H2	2.48	0.44
1:C:43:PRO:HA	1:C:46:PHE:CD2	2.53	0.44
1:B:345:ALA:HA	1:B:359:LYS:O	2.18	0.44
1:A:63:PHE:CZ	1:A:301:LEU:HB3	2.53	0.43
1:D:80:ILE:CD1	1:D:301:LEU:HD13	2.48	0.43
1:A:18:PRO:HD2	1:A:289:GLN:CD	2.43	0.43
1:A:95:HIS:O	1:A:96:ASN:C	2.61	0.43
1:A:285:ILE:O	1:A:289:GLN:HG3	2.19	0.43
1:B:237:GLN:NE2	1:B:243:VAL:HG12	2.33	0.43
1:B:366:VAL:HG11	1:B:397:TYR:O	2.18	0.43
1:C:45:MET:HE2	1:D:322:VAL:CG2	2.33	0.43
1:D:95:HIS:CE1	1:D:245:THR:HG21	2.52	0.43
1:D:134:ASN:ND2	1:D:178:TRP:HH2	2.16	0.43
1:D:365:ASP:HB2	1:D:394:PRO:CB	2.49	0.43
1:A:166:ILE:HD12	1:A:166:ILE:C	2.44	0.43
1:B:288:ILE:HA	1:B:291:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:THR:O	1:D:53:ILE:HA	2.19	0.43
1:D:67:MET:HB2	2:D:427:GOL:O1	2.17	0.43
1:D:285:ILE:O	1:D:289:GLN:HG3	2.17	0.43
1:B:109:MET:HE2	1:B:109:MET:HB3	1.89	0.43
1:B:167:VAL:HA	1:B:168:PRO:HD3	1.87	0.43
1:C:90:LEU:HG	1:C:94:LEU:HD22	2.00	0.43
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.78	0.43
1:B:121:LEU:HD12	1:B:228:ILE:CD1	2.37	0.43
1:B:172:ARG:HG3	1:B:172:ARG:HH11	1.82	0.43
1:C:59:LYS:HD3	1:C:309:GLU:HG2	2.00	0.43
1:D:64:GLY:HA3	2:D:427:GOL:H2	2.00	0.43
1:D:217:TYR:CG	1:D:249:MET:HE2	2.53	0.43
1:A:25:ILE:CG2	1:B:380:LEU:HD11	2.49	0.43
1:C:206:ASN:ND2	3:C:555:HOH:O	2.31	0.43
1:D:177:ARG:HD2	1:D:178:TRP:CE2	2.53	0.43
1:B:134:ASN:HB3	1:B:157:ILE:HD11	2.00	0.43
1:B:155:ASN:CB	3:B:583:HOH:O	2.43	0.43
1:C:99:THR:HG23	1:C:109:MET:H	1.83	0.43
1:C:133:ASP:CB	1:C:192:LYS:HE3	2.48	0.43
1:A:141:ALA:O	1:A:142:TYR:C	2.62	0.43
1:B:20:ARG:C	1:B:22:MET:H	2.27	0.43
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.82	0.43
1:A:6:PHE:CZ	1:A:226:LEU:HD13	2.53	0.42
1:A:163:GLU:HG3	1:A:348:HIS:NE2	2.33	0.42
1:C:179:LYS:O	1:C:182:ASP:HB2	2.18	0.42
1:C:323:ILE:O	1:C:324:ASP:C	2.62	0.42
1:A:299:ASN:ND2	1:B:299:ASN:HD21	2.12	0.42
1:C:56:GLU:HB2	1:D:49:LYS:HE3	2.01	0.42
1:A:278:LYS:CD	3:A:552:HOH:O	2.65	0.42
1:B:140:PRO:HB2	1:B:203:PRO:CG	2.49	0.42
1:A:41:PRO:HA	1:B:354:MET:CE	2.49	0.42
1:B:380:LEU:C	1:B:381:MET:HG3	2.43	0.42
1:C:48:PHE:HB2	1:C:72:LEU:HD11	2.00	0.42
1:D:377:MET:HE2	1:D:377:MET:HB3	1.77	0.42
1:A:366:VAL:HG22	1:A:370:ILE:HG12	2.01	0.42
1:B:240:LYS:NZ	1:B:320:ASP:HB3	2.34	0.42
1:D:17:SER:HA	1:D:18:PRO:HD3	1.79	0.42
1:D:134:ASN:O	1:D:191:PRO:HA	2.20	0.42
1:D:368:GLU:HA	3:D:592:HOH:O	2.20	0.42
1:A:197:VAL:N	3:A:568:HOH:O	2.52	0.42
1:B:117:SER:HB2	1:B:258:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLY:O	1:B:124:VAL:HG23	2.19	0.42
1:B:326:TYR:CE1	1:B:354:MET:HE2	2.55	0.42
1:C:46:PHE:HA	1:C:47:PRO:HD3	1.94	0.42
1:D:20:ARG:O	1:D:22:MET:N	2.51	0.42
1:D:419:GLN:N	1:D:419:GLN:CD	2.77	0.42
1:B:172:ARG:CG	1:B:219:LEU:HD11	2.49	0.42
1:C:69:LYS:HE2	3:C:560:HOH:O	2.20	0.42
1:C:315:PHE:O	1:C:319:VAL:HG13	2.19	0.42
1:A:59:LYS:HG2	1:A:309:GLU:HG2	2.02	0.42
1:B:100:ILE:CD1	1:B:101:HIS:CE1	3.02	0.42
1:A:396:PRO:HG3	3:A:497:HOH:O	2.20	0.42
1:B:99:THR:O	1:B:108:GLN:HA	2.20	0.42
1:B:178:TRP:CE2	1:B:191:PRO:HD3	2.54	0.42
1:B:229:GLU:OE2	3:B:500:HOH:O	2.22	0.42
1:A:185:ASN:HA	1:A:186:PRO:HD3	1.89	0.42
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.83	0.42
1:B:359:LYS:NZ	3:B:490:HOH:O	2.52	0.42
1:C:99:THR:CG2	1:C:109:MET:H	2.33	0.42
1:D:375:VAL:CG2	1:D:376:LYS:N	2.82	0.42
1:A:97:PRO:C	1:A:99:THR:N	2.65	0.41
1:A:263:LLP:H	1:A:263:LLP:HD3	1.85	0.41
1:B:172:ARG:HH11	1:B:172:ARG:CG	2.33	0.41
1:B:174:ILE:HD12	1:B:174:ILE:C	2.44	0.41
1:C:195:TYR:OH	1:C:230:ASP:OD2	2.29	0.41
1:D:161:SER:HA	1:D:165:GLY:O	2.19	0.41
1:D:367:LYS:HB3	1:D:367:LYS:HE3	1.89	0.41
1:D:370:ILE:HG21	1:D:381:MET:O	2.20	0.41
1:A:326:TYR:CE1	1:A:354:MET:HE2	2.54	0.41
1:B:243:VAL:CG1	3:B:581:HOH:O	2.56	0.41
1:C:140:PRO:HB2	1:C:203:PRO:CG	2.47	0.41
1:A:148:SER:O	1:A:152:LEU:HD13	2.20	0.41
1:B:71:ALA:HB2	1:B:301:LEU:HD23	2.02	0.41
1:C:381:MET:CE	1:C:400:ALA:HB2	2.51	0.41
1:C:50:THR:OG1	1:D:54:THR:OG1	2.19	0.41
1:C:341:LEU:HD11	1:C:414:PHE:HE2	1.86	0.41
1:B:179:LYS:HG2	1:B:180:PRO:HD2	2.02	0.41
1:B:384:GLY:N	1:B:397:TYR:O	2.49	0.41
1:C:57:ASN:HD22	1:C:321:ARG:NH1	2.18	0.41
1:D:222:LYS:HG2	1:D:223:TYR:CE2	2.56	0.41
1:A:220:ALA:HB1	1:A:227:ILE:HD11	2.00	0.41
1:A:415:GLN:O	1:A:419:GLN:CD	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:O	1:B:22:MET:HG2	2.21	0.41
1:B:95:HIS:O	1:B:96:ASN:C	2.63	0.41
1:C:314:GLY:CA	3:C:562:HOH:O	2.68	0.41
1:A:366:VAL:HG11	1:A:398:LEU:CD2	2.51	0.41
1:B:107:GLY:O	1:B:108:GLN:C	2.64	0.41
1:B:204:THR:HA	1:B:357:TRP:CG	2.56	0.41
1:B:294:HIS:HD2	1:B:295:PRO:O	2.03	0.41
1:D:288:ILE:HD11	1:D:293:LEU:O	2.20	0.41
1:C:7:ILE:HD13	1:C:7:ILE:HG21	1.91	0.41
1:C:283:ARG:HD2	3:C:486:HOH:O	2.21	0.41
1:C:403:SER:O	1:D:42:ASN:HB2	2.20	0.41
1:A:288:ILE:HG13	1:A:289:GLN:N	2.34	0.41
1:B:6:PHE:CD2	1:B:226:LEU:HD22	2.56	0.41
1:B:74:TYR:HD1	1:B:294:HIS:HE1	1.69	0.41
1:B:141:ALA:HB3	1:B:146:LEU:HD11	2.03	0.41
1:B:265:ILE:O	1:B:266:SER:HB2	2.20	0.41
1:C:19:ILE:HG22	1:C:22:MET:SD	2.60	0.41
1:C:65:GLU:HB3	3:C:557:HOH:O	2.20	0.41
1:C:80:ILE:HD13	1:C:80:ILE:HG21	1.82	0.41
1:C:114:THR:HG21	1:C:120:GLY:CA	2.49	0.41
1:C:204:THR:HA	1:C:357:TRP:CB	2.51	0.41
1:C:404:SER:O	2:C:428:GOL:C2	2.65	0.41
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.41
1:D:381:MET:HB3	1:D:381:MET:HE3	1.54	0.41
1:B:204:THR:HA	1:B:357:TRP:CB	2.51	0.41
1:B:257:ARG:HH11	1:B:259:ASP:CG	2.28	0.41
1:C:142:TYR:CD1	1:C:263:LLP:H2'3	2.55	0.41
1:D:20:ARG:HD2	1:D:21:THR:H	1.85	0.41
1:D:142:TYR:HD2	1:D:145:THR:HG22	1.84	0.41
1:D:166:ILE:HG13	1:D:216:ILE:HD11	2.02	0.41
2:D:429:GOL:C3	3:D:480:HOH:O	2.41	0.41
1:C:157:ILE:HG21	1:C:174:ILE:HG21	2.02	0.40
1:C:293:LEU:HD21	1:D:118:GLN:HG2	2.03	0.40
1:D:217:TYR:CB	1:D:249:MET:HE2	2.51	0.40
1:A:49:LYS:HE3	1:B:56:GLU:OE1	2.20	0.40
1:B:164:SER:HB3	1:B:209:THR:HG23	2.03	0.40
1:D:246:PHE:HA	1:D:249:MET:HG3	2.02	0.40
1:B:28:ARG:HB3	1:B:28:ARG:NH1	2.19	0.40
1:B:103:PRO:HD2	1:B:106:GLN:NE2	2.35	0.40
1:C:257:ARG:O	1:C:274:LEU:HA	2.22	0.40
1:D:288:ILE:HD11	1:D:293:LEU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:MET:HE2	1:A:354:MET:HB3	1.83	0.40
1:B:22:MET:H	1:B:22:MET:HG2	1.67	0.40
1:C:204:THR:HG22	1:C:357:TRP:CD1	2.57	0.40
1:C:212:ARG:O	1:C:216:ILE:HG12	2.21	0.40
1:C:281:ILE:O	1:C:285:ILE:HG23	2.22	0.40
1:C:369:LEU:O	1:C:374:ALA:N	2.48	0.40
1:D:65:GLU:N	2:D:427:GOL:H2	2.37	0.40
1:D:77:SER:HA	1:D:294:HIS:HB3	2.04	0.40
1:D:83:LEU:HG	1:D:304:SER:HB2	2.04	0.40
1:D:117:SER:C	1:D:121:LEU:HD12	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	6	5
1	B	422/425 (99%)	391 (93%)	26 (6%)	5 (1%)	10	12
1	C	422/425 (99%)	393 (93%)	24 (6%)	5 (1%)	10	12
1	D	422/425 (99%)	381 (90%)	33 (8%)	8 (2%)	6	5
All	All	1688/1700 (99%)	1546 (92%)	116 (7%)	26 (2%)	8	8

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	28	ARG
1	B	203	PRO
1	C	203	PRO
1	D	19	ILE

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Mol	Chain	Res	Type
1	A	21	THR
1	B	331	ASP
1	D	21	THR
1	D	25	ILE
1	D	293	LEU
1	B	57	ASN
1	C	186	PRO
1	C	189	ASN
1	D	18	PRO
1	A	20	ARG
1	A	67	MET
1	A	98	PRO
1	B	21	THR
1	B	202	ASN
1	C	31	LYS
1	D	17	SER
1	D	74	TYR
1	D	266	SER
1	A	19	ILE
1	C	202	ASN
1	A	311	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/369 (100%)	310 (84%)	59 (16%)	2	2
1	B	369/369 (100%)	308 (84%)	61 (16%)	2	2
1	C	369/369 (100%)	304 (82%)	65 (18%)	2	2
1	D	369/369 (100%)	299 (81%)	70 (19%)	1	1
All	All	1476/1476 (100%)	1221 (83%)	255 (17%)	2	2

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	20	ARG
1	A	22	MET
1	A	24	ASP
1	A	25	ILE
1	A	28	ARG
1	A	34	ILE
1	A	59	LYS
1	A	60	THR
1	A	67	MET
1	A	77	SER
1	A	87	LEU
1	A	94	LEU
1	A	96	ASN
1	A	99	THR
1	A	123	LYS
1	A	137	LEU
1	A	166	ILE
1	A	178	TRP
1	A	179	LYS
1	A	184	LYS
1	A	188	LYS
1	A	218	GLU
1	A	219	LEU
1	A	221	ARG
1	A	226	LEU
1	A	228	ILE
1	A	243	VAL
1	A	264	ILE
1	A	267	SER
1	A	278	LYS
1	A	283	ARG
1	A	284	VAL
1	A	285	ILE
1	A	288	ILE
1	A	296	SER
1	A	297	THR
1	A	301	LEU
1	A	307	LEU
1	A	312	GLU
1	A	313	GLU
1	A	316	MET
1	A	322	VAL

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Mol	Chain	Res	Type
1	A	327	SER
1	A	334	LEU
1	A	341	LEU
1	A	342	THR
1	A	344	LEU
1	A	349	VAL
1	A	358	ILE
1	A	361	LYS
1	A	368	GLU
1	A	372	GLU
1	A	379	VAL
1	A	380	LEU
1	A	381	MET
1	A	395	SER
1	A	417	LEU
1	A	419	GLN
1	B	8	THR
1	B	19	ILE
1	B	20	ARG
1	B	25	ILE
1	B	28	ARG
1	B	33	MET
1	B	34	ILE
1	B	42	ASN
1	B	59	LYS
1	B	60	THR
1	B	65	GLU
1	B	77	SER
1	B	83	LEU
1	B	84	LEU
1	B	87	LEU
1	B	96	ASN
1	B	99	THR
1	B	109	MET
1	B	137	LEU
1	B	145	THR
1	B	152	LEU
1	B	163	GLU
1	B	164	SER
1	B	166	ILE
1	B	172	ARG
1	B	179	LYS

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Mol	Chain	Res	Type
1	B	182	ASP
1	B	184	LYS
1	B	188	LYS
1	B	192	LYS
1	B	218	GLU
1	B	219	LEU
1	B	226	LEU
1	B	228	ILE
1	B	236	LEU
1	B	251	VAL
1	B	278	LYS
1	B	280	LEU
1	B	284	VAL
1	B	288	ILE
1	B	297	THR
1	B	301	LEU
1	B	307	LEU
1	B	319	VAL
1	B	322	VAL
1	B	330	LYS
1	B	334	LEU
1	B	341	LEU
1	B	342	THR
1	B	344	LEU
1	B	349	VAL
1	B	358	ILE
1	B	360	VAL
1	B	367	LYS
1	B	369	LEU
1	B	375	VAL
1	B	376	LYS
1	B	379	VAL
1	B	408	GLU
1	B	417	LEU
1	B	419	GLN
1	C	5	ARG
1	C	6	PHE
1	C	8	THR
1	C	19	ILE
1	C	20	ARG
1	C	21	THR
1	C	25	ILE

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Mol	Chain	Res	Type
1	C	28	ARG
1	C	31	LYS
1	C	34	ILE
1	C	60	THR
1	C	77	SER
1	C	85	SER
1	C	87	LEU
1	C	93	LYS
1	C	94	LEU
1	C	99	THR
1	C	112	CYS
1	C	115	SER
1	C	121	LEU
1	C	136	LEU
1	C	137	LEU
1	C	145	THR
1	C	159	VAL
1	C	163	GLU
1	C	166	ILE
1	C	177	ARG
1	C	179	LYS
1	C	189	ASN
1	C	192	LYS
1	C	208	LEU
1	C	219	LEU
1	C	226	LEU
1	C	228	ILE
1	C	229	GLU
1	C	243	VAL
1	C	247	LEU
1	C	264	ILE
1	C	265	ILE
1	C	278	LYS
1	C	284	VAL
1	C	285	ILE
1	C	288	ILE
1	C	297	THR
1	C	301	LEU
1	C	307	LEU
1	C	319	VAL
1	C	322	VAL
1	C	324	ASP

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Mol	Chain	Res	Type
1	C	330	LYS
1	C	334	LEU
1	C	344	LEU
1	C	354	MET
1	C	358	ILE
1	C	366	VAL
1	C	368	GLU
1	C	369	LEU
1	C	375	VAL
1	C	376	LYS
1	C	379	VAL
1	C	380	LEU
1	C	381	MET
1	C	392	SER
1	C	415	GLN
1	C	417	LEU
1	D	8	THR
1	D	21	THR
1	D	25	ILE
1	D	26	LEU
1	D	28	ARG
1	D	31	LYS
1	D	34	ILE
1	D	40	LEU
1	D	42	ASN
1	D	43	PRO
1	D	59	LYS
1	D	60	THR
1	D	77	SER
1	D	83	LEU
1	D	84	LEU
1	D	87	LEU
1	D	89	GLN
1	D	93	LYS
1	D	96	ASN
1	D	99	THR
1	D	112	CYS
1	D	137	LEU
1	D	145	THR
1	D	155	ASN
1	D	163	GLU
1	D	166	ILE

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Mol	Chain	Res	Type
1	D	174	ILE
1	D	177	ARG
1	D	178	TRP
1	D	179	LYS
1	D	181	GLU
1	D	184	LYS
1	D	187	GLN
1	D	194	LEU
1	D	218	GLU
1	D	219	LEU
1	D	221	ARG
1	D	226	LEU
1	D	228	ILE
1	D	243	VAL
1	D	249	MET
1	D	264	ILE
1	D	278	LYS
1	D	280	LEU
1	D	284	VAL
1	D	285	ILE
1	D	288	ILE
1	D	297	THR
1	D	301	LEU
1	D	306	LEU
1	D	307	LEU
1	D	327	SER
1	D	330	LYS
1	D	334	LEU
1	D	341	LEU
1	D	349	VAL
1	D	354	MET
1	D	358	ILE
1	D	360	VAL
1	D	366	VAL
1	D	371	GLU
1	D	375	VAL
1	D	377	MET
1	D	379	VAL
1	D	381	MET
1	D	385	ASN
1	D	404	SER
1	D	415	GLN

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Mol	Chain	Res	Type
1	D	417	LEU
1	D	423	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	89	GLN
1	A	91	GLN
1	A	96	ASN
1	A	101	HIS
1	A	108	GLN
1	A	187	GLN
1	A	189	ASN
1	A	199	ASN
1	A	201	ASN
1	A	206	ASN
1	A	239	ASN
1	A	289	GLN
1	A	294	HIS
1	A	299	ASN
1	A	305	GLN
1	A	318	HIS
1	A	419	GLN
1	B	2	ASN
1	B	42	ASN
1	B	89	GLN
1	B	101	HIS
1	B	106	GLN
1	B	108	GLN
1	B	118	GLN
1	B	134	ASN
1	B	185	ASN
1	B	189	ASN
1	B	201	ASN
1	B	237	GLN
1	B	239	ASN
1	B	294	HIS
1	B	299	ASN
1	B	305	GLN
1	B	308	HIS
1	B	348	HIS

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Mol	Chain	Res	Type
1	B	419	GLN
1	C	15	ASN
1	C	57	ASN
1	C	89	GLN
1	C	91	GLN
1	C	96	ASN
1	C	101	HIS
1	C	106	GLN
1	C	108	GLN
1	C	118	GLN
1	C	155	ASN
1	C	187	GLN
1	C	201	ASN
1	C	294	HIS
1	C	299	ASN
1	C	305	GLN
1	C	318	HIS
1	C	328	ASN
1	D	2	ASN
1	D	42	ASN
1	D	44	ASN
1	D	57	ASN
1	D	89	GLN
1	D	106	GLN
1	D	150	HIS
1	D	185	ASN
1	D	187	GLN
1	D	201	ASN
1	D	237	GLN
1	D	239	ASN
1	D	294	HIS
1	D	299	ASN
1	D	305	GLN
1	D	308	HIS
1	D	328	ASN
1	D	385	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	263	1	23,24,25	1.70	5 (21%)	25,32,34	1.85	7 (28%)
1	LLP	C	263	1	23,24,25	2.04	7 (30%)	25,32,34	1.96	7 (28%)
1	LLP	D	263	1	23,24,25	1.84	5 (21%)	25,32,34	2.04	9 (36%)
1	LLP	B	263	1	23,24,25	2.26	7 (30%)	25,32,34	1.81	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	263	1	-	3/16/17/19	0/1/1/1
1	LLP	C	263	1	-	5/16/17/19	0/1/1/1
1	LLP	D	263	1	-	5/16/17/19	0/1/1/1
1	LLP	B	263	1	-	6/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	LLP	O3-C3	-6.25	1.22	1.36
1	B	263	LLP	CE-NZ	5.28	1.58	1.46
1	D	263	LLP	O3-C3	-4.73	1.26	1.36
1	A	263	LLP	O3-C3	-4.73	1.26	1.36
1	B	263	LLP	C4-C4'	4.33	1.55	1.46
1	B	263	LLP	O3-C3	-4.25	1.27	1.36
1	D	263	LLP	CE-NZ	3.75	1.55	1.46
1	C	263	LLP	C2-N1	3.64	1.40	1.33
1	B	263	LLP	C3-C2	-3.44	1.37	1.41
1	D	263	LLP	C2-N1	3.35	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	LLP	C4'-NZ	2.97	1.37	1.27
1	A	263	LLP	C2-N1	2.96	1.39	1.33
1	A	263	LLP	C6-N1	2.93	1.40	1.34
1	D	263	LLP	C6-C5	2.67	1.43	1.37
1	C	263	LLP	P-OP3	-2.60	1.45	1.54
1	B	263	LLP	C4-C5	-2.57	1.38	1.42
1	C	263	LLP	C6-N1	2.48	1.39	1.34
1	D	263	LLP	C4-C4'	2.45	1.51	1.46
1	B	263	LLP	C6-N1	2.40	1.39	1.34
1	C	263	LLP	CE-NZ	2.26	1.51	1.46
1	C	263	LLP	CB-CA	2.12	1.56	1.53
1	A	263	LLP	CE-NZ	2.08	1.51	1.46
1	A	263	LLP	C4-C4'	2.07	1.51	1.46
1	C	263	LLP	CD-CE	2.07	1.58	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	LLP	OP2-P-OP4	-4.55	94.80	106.67
1	C	263	LLP	CE-NZ-C4'	-4.49	104.33	118.72
1	D	263	LLP	C5'-C5-C6	-4.34	112.29	119.36
1	D	263	LLP	CD-CE-NZ	4.12	121.74	110.83
1	D	263	LLP	C4-C4'-NZ	-4.02	105.48	124.04
1	A	263	LLP	C3-C4-C5	3.85	121.37	118.28
1	A	263	LLP	CE-NZ-C4'	-3.41	107.79	118.72
1	B	263	LLP	C5'-C5-C6	-3.38	113.84	119.36
1	C	263	LLP	C3-C4-C5	3.38	120.99	118.28
1	A	263	LLP	OP4-P-OP1	-3.32	97.48	106.44
1	D	263	LLP	OP2-P-OP4	-3.29	98.08	106.67
1	A	263	LLP	C4-C4'-NZ	-3.24	109.10	124.04
1	D	263	LLP	C5-C6-N1	-3.03	118.90	123.83
1	B	263	LLP	OP2-P-OP4	-2.82	99.32	106.67
1	C	263	LLP	C5-C6-N1	-2.78	119.30	123.83
1	B	263	LLP	C4-C3-C2	2.76	121.70	120.14
1	C	263	LLP	C5-C4-C4'	-2.76	117.21	121.47
1	C	263	LLP	C2'-C2-N1	2.68	122.69	117.64
1	B	263	LLP	O3-C3-C2	-2.63	112.13	117.58
1	B	263	LLP	OP3-P-OP2	2.52	117.24	107.80
1	A	263	LLP	C5-C6-N1	-2.51	119.74	123.83
1	A	263	LLP	C4-C3-C2	-2.50	118.73	120.14
1	B	263	LLP	O3-C3-C4	2.49	126.14	119.44
1	D	263	LLP	OP3-P-OP2	2.42	116.86	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	LLP	OP3-P-OP4	-2.37	100.50	106.67
1	B	263	LLP	C5-C6-N1	-2.27	120.14	123.83
1	B	263	LLP	OP4-P-OP1	2.26	112.54	106.44
1	C	263	LLP	C2'-C2-C3	-2.25	118.17	120.80
1	D	263	LLP	C6-C5-C4	2.18	121.96	118.21
1	A	263	LLP	OP2-P-OP4	-2.14	101.09	106.67
1	D	263	LLP	OP4-C5'-C5	2.13	113.34	109.36
1	B	263	LLP	CD-CE-NZ	2.02	116.18	110.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	263	LLP	N-CA-CB-CG
1	B	263	LLP	C-CA-CB-CG
1	C	263	LLP	C5-C4-C4'-NZ
1	C	263	LLP	CG-CD-CE-NZ
1	C	263	LLP	C4-C4'-NZ-CE
1	C	263	LLP	C3-C4-C4'-NZ
1	D	263	LLP	CE-CD-CG-CB
1	B	263	LLP	CA-CB-CG-CD
1	B	263	LLP	CE-CD-CG-CB
1	B	263	LLP	CG-CD-CE-NZ
1	A	263	LLP	CD-CE-NZ-C4'
1	D	263	LLP	N-CA-CB-CG
1	C	263	LLP	CE-CD-CG-CB
1	A	263	LLP	C3-C4-C4'-NZ
1	D	263	LLP	C3-C4-C4'-NZ
1	D	263	LLP	C5-C4-C4'-NZ
1	D	263	LLP	CG-CD-CE-NZ
1	A	263	LLP	C4-C4'-NZ-CE
1	B	263	LLP	C3-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	263	LLP	5	0
1	C	263	LLP	1	0
1	D	263	LLP	1	0
1	B	263	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	D	426	-	5,5,5	0.75	0	5,5,5	1.05	0
2	GOL	C	429	-	5,5,5	0.54	0	5,5,5	0.54	0
2	GOL	D	427	-	5,5,5	0.40	0	5,5,5	0.58	0
2	GOL	C	427	-	5,5,5	0.58	0	5,5,5	1.13	0
2	GOL	C	426	-	5,5,5	0.54	0	5,5,5	0.67	0
2	GOL	C	428	-	5,5,5	0.57	0	5,5,5	1.32	0
2	GOL	C	430	-	5,5,5	0.65	0	5,5,5	0.85	0
2	GOL	D	429	-	5,5,5	1.15	0	5,5,5	2.32	3 (60%)
2	GOL	A	426	-	5,5,5	0.32	0	5,5,5	0.95	0
2	GOL	D	428	-	5,5,5	0.96	0	5,5,5	1.72	1 (20%)
2	GOL	A	427	-	5,5,5	0.39	0	5,5,5	0.60	0
2	GOL	B	426	-	5,5,5	0.53	0	5,5,5	1.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	426	-	-	4/4/4/4	-
2	GOL	C	429	-	-	2/4/4/4	-
2	GOL	D	427	-	-	2/4/4/4	-
2	GOL	C	427	-	-	2/4/4/4	-
2	GOL	C	426	-	-	2/4/4/4	-
2	GOL	C	428	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	430	-	-	4/4/4/4	-
2	GOL	D	429	-	-	3/4/4/4	-
2	GOL	A	426	-	-	2/4/4/4	-
2	GOL	D	428	-	-	3/4/4/4	-
2	GOL	A	427	-	-	4/4/4/4	-
2	GOL	B	426	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	429	GOL	O1-C1-C2	3.49	126.09	110.38
2	D	429	GOL	O2-C2-C3	-3.00	96.75	109.18
2	D	428	GOL	O3-C3-C2	2.57	121.97	110.38
2	D	429	GOL	O3-C3-C2	2.38	121.10	110.38

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	426	GOL	O2-C2-C3-O3
2	C	426	GOL	C1-C2-C3-O3
2	C	426	GOL	O2-C2-C3-O3
2	C	427	GOL	C1-C2-C3-O3
2	C	428	GOL	O1-C1-C2-C3
2	C	428	GOL	C1-C2-C3-O3
2	C	429	GOL	C1-C2-C3-O3
2	C	430	GOL	O1-C1-C2-O2
2	C	430	GOL	C1-C2-C3-O3
2	D	426	GOL	O1-C1-C2-C3
2	D	428	GOL	O1-C1-C2-C3
2	D	429	GOL	O1-C1-C2-C3
2	D	426	GOL	O1-C1-C2-O2
2	A	426	GOL	C1-C2-C3-O3
2	A	427	GOL	O1-C1-C2-C3
2	A	427	GOL	C1-C2-C3-O3
2	B	426	GOL	C1-C2-C3-O3
2	C	430	GOL	O1-C1-C2-C3
2	D	426	GOL	C1-C2-C3-O3
2	D	428	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	427	GOL	O2-C2-C3-O3
2	C	428	GOL	O2-C2-C3-O3
2	D	426	GOL	O2-C2-C3-O3
2	D	428	GOL	O1-C1-C2-O2
2	A	427	GOL	O1-C1-C2-O2
2	A	427	GOL	O2-C2-C3-O3
2	C	428	GOL	O1-C1-C2-O2
2	C	429	GOL	O2-C2-C3-O3
2	C	430	GOL	O2-C2-C3-O3
2	A	426	GOL	O2-C2-C3-O3
2	D	429	GOL	O1-C1-C2-O2
2	D	427	GOL	O1-C1-C2-O2
2	D	429	GOL	O2-C2-C3-O3
2	D	427	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	427	GOL	4	0
2	C	427	GOL	2	0
2	C	428	GOL	2	0
2	C	430	GOL	3	0
2	D	429	GOL	11	0
2	A	426	GOL	1	0
2	D	428	GOL	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/425 (99%)	0.38	23 (5%) 31 33	24, 36, 54, 78	0
1	B	424/425 (99%)	0.33	19 (4%) 38 40	23, 34, 51, 92	0
1	C	424/425 (99%)	0.32	19 (4%) 38 40	23, 35, 52, 77	0
1	D	424/425 (99%)	0.36	21 (4%) 34 35	23, 35, 52, 84	0
All	All	1696/1700 (99%)	0.35	82 (4%) 35 37	23, 35, 53, 92	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	ILE	6.4
1	C	29	GLY	6.3
1	A	25	ILE	5.4
1	B	25	ILE	5.1
1	B	26	LEU	4.7
1	B	27	SER	4.6
1	A	21	THR	4.5
1	D	26	LEU	4.4
1	C	19	ILE	4.4
1	A	18	PRO	4.2
1	B	28	ARG	4.2
1	A	28	ARG	4.2
1	D	18	PRO	4.2
1	A	380	LEU	4.0
1	A	29	GLY	4.0
1	B	107	GLY	4.0
1	A	19	ILE	4.0
1	D	28	ARG	3.7
1	B	21	THR	3.6
1	C	25	ILE	3.6
1	A	27	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	21	THR	3.4
1	B	19	ILE	3.4
1	D	17	SER	3.4
1	B	344	LEU	3.3
1	C	28	ARG	3.2
1	D	30	PRO	3.1
1	C	375	VAL	3.1
1	C	23	THR	3.0
1	A	57	ASN	3.0
1	C	30	PRO	3.0
1	A	96	ASN	3.0
1	C	366	VAL	2.9
1	D	25	ILE	2.9
1	D	23	THR	2.9
1	C	34	ILE	2.9
1	A	23	THR	2.9
1	C	1	MET	2.9
1	D	1	MET	2.9
1	B	30	PRO	2.9
1	C	21	THR	2.8
1	C	22	MET	2.8
1	B	24	ASP	2.7
1	D	22	MET	2.7
1	A	34	ILE	2.7
1	A	24	ASP	2.7
1	C	27	SER	2.7
1	A	1	MET	2.6
1	D	413	ALA	2.6
1	B	23	THR	2.6
1	B	218	GLU	2.6
1	B	22	MET	2.5
1	B	362	GLY	2.5
1	D	27	SER	2.5
1	D	29	GLY	2.5
1	D	96	ASN	2.4
1	A	30	PRO	2.4
1	A	371	GLU	2.4
1	A	342	THR	2.4
1	D	380	LEU	2.3
1	B	178	TRP	2.3
1	C	186	PRO	2.3
1	A	228	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	34	ILE	2.3
1	A	26	LEU	2.3
1	A	178	TRP	2.2
1	D	137	LEU	2.2
1	A	271	ILE	2.2
1	C	26	LEU	2.2
1	D	363	ILE	2.2
1	C	358	ILE	2.1
1	C	239	ASN	2.1
1	B	187	GLN	2.1
1	D	221	ARG	2.1
1	A	370	ILE	2.1
1	D	178	TRP	2.1
1	B	29	GLY	2.1
1	C	369	LEU	2.1
1	D	121	LEU	2.1
1	C	31	LYS	2.0
1	B	36	LEU	2.0
1	A	20	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	C	263	24/25	0.95	0.07	27,30,34,37	0
1	LLP	D	263	24/25	0.95	0.09	23,32,35,35	0
1	LLP	A	263	24/25	0.96	0.07	23,33,36,36	0
1	LLP	B	263	24/25	0.96	0.07	23,30,33,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	C	430	6/6	0.64	0.18	48,53,56,57	0
2	GOL	C	429	6/6	0.66	0.16	63,66,68,69	0
2	GOL	D	427	6/6	0.68	0.17	55,56,59,62	0
2	GOL	A	426	6/6	0.69	0.19	68,70,71,72	0
2	GOL	C	426	6/6	0.76	0.16	59,64,65,65	0
2	GOL	D	429	6/6	0.76	0.33	23,30,40,43	0
2	GOL	D	428	6/6	0.77	0.22	46,51,52,53	0
2	GOL	B	426	6/6	0.79	0.15	63,64,66,66	0
2	GOL	C	428	6/6	0.80	0.17	54,56,58,60	0
2	GOL	D	426	6/6	0.81	0.14	44,52,55,59	0
2	GOL	C	427	6/6	0.85	0.13	34,47,53,54	0
2	GOL	A	427	6/6	0.88	0.10	58,61,62,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.