



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:56 AM UTC

PDB ID : 3AK5 / pdb_00003ak5
Title : Hemoglobin protease (Hbp) passenger missing domain-2
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Deposited on : 2010-07-07
Resolution : 2.20 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
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

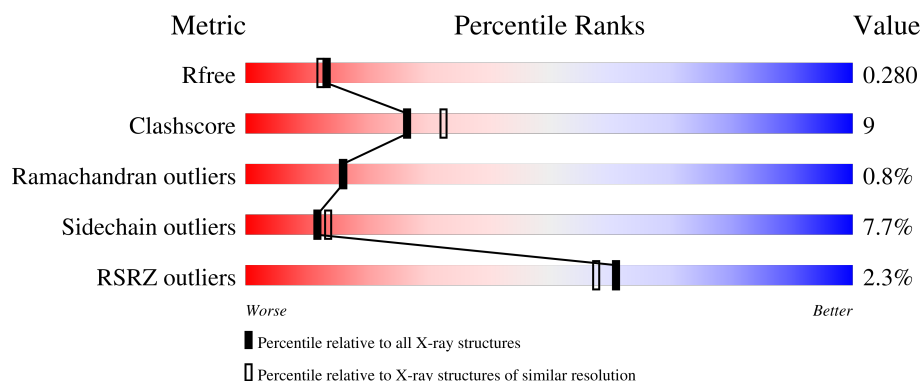
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	975	2% 74% 22% ..
1	B	975	2% 75% 20% ..
1	C	975	2% 73% 22% ..
1	D	975	3% 73% 20% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30307 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 Hemoglobin-binding protease hbp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	970	Total	C	N	O	S	7	0	0
			7278	4511	1268	1485	14			
1	B	970	Total	C	N	O	S	4	0	0
			7278	4511	1268	1485	14			
1	C	952	Total	C	N	O	S	4	1	0
			7149	4435	1241	1459	14			
1	D	948	Total	C	N	O	S	9	0	0
			7113	4411	1236	1452	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLY	-	SEE REMARK 999	UNP O88093
B	607	GLY	-	SEE REMARK 999	UNP O88093
C	607	GLY	-	SEE REMARK 999	UNP O88093
D	607	GLY	-	SEE REMARK 999	UNP O88093

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

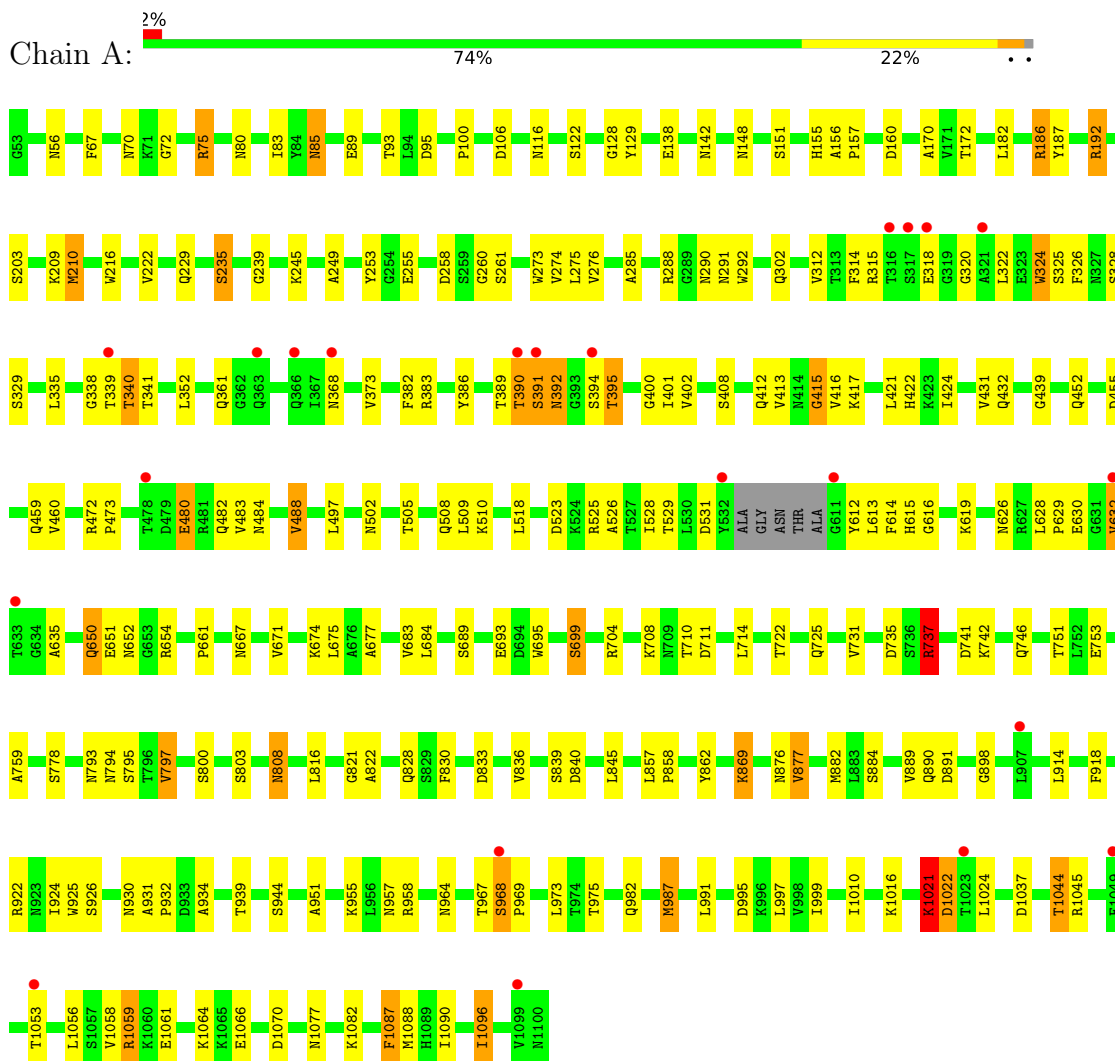
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	426	Total 426	O 426	0	0
3	B	430	Total 430	O 430	0	0
3	C	321	Total 321	O 321	0	0
3	D	308	Total 308	O 308	0	0

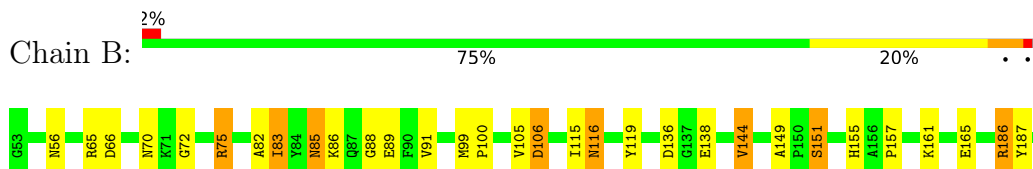
3 Residue-property plots [i](#)

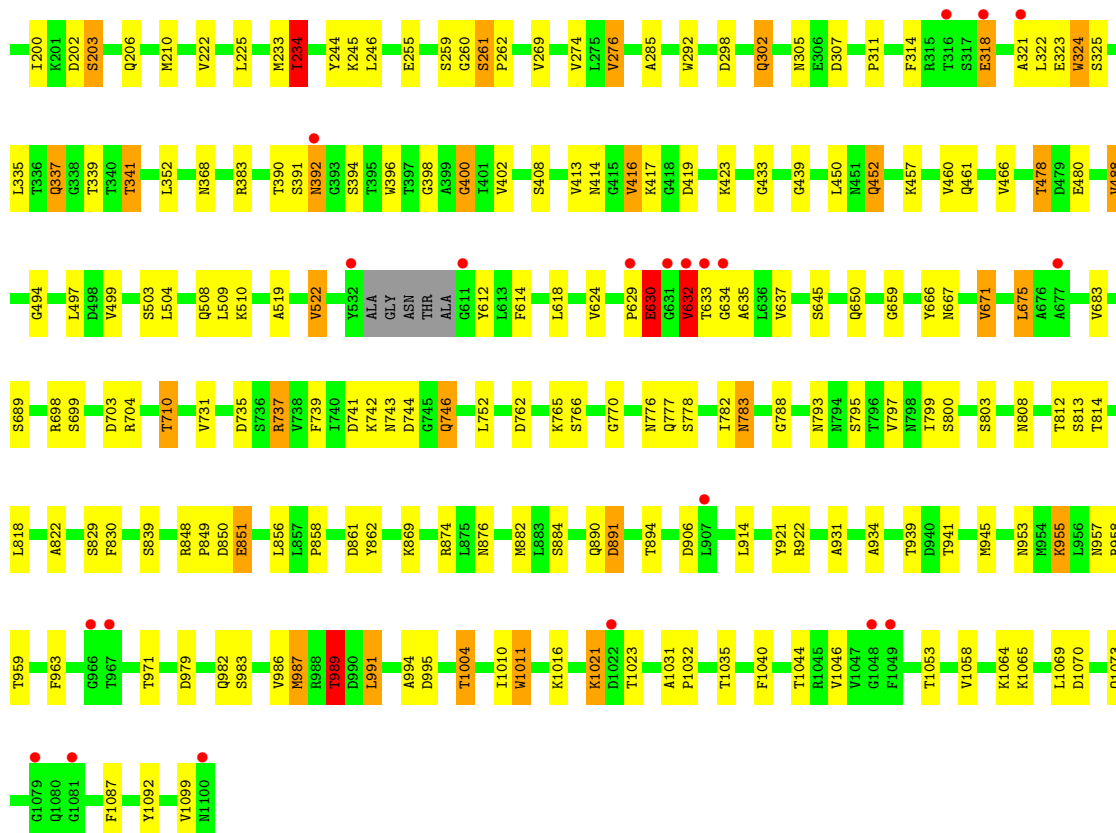
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemoglobin-binding protease hbp

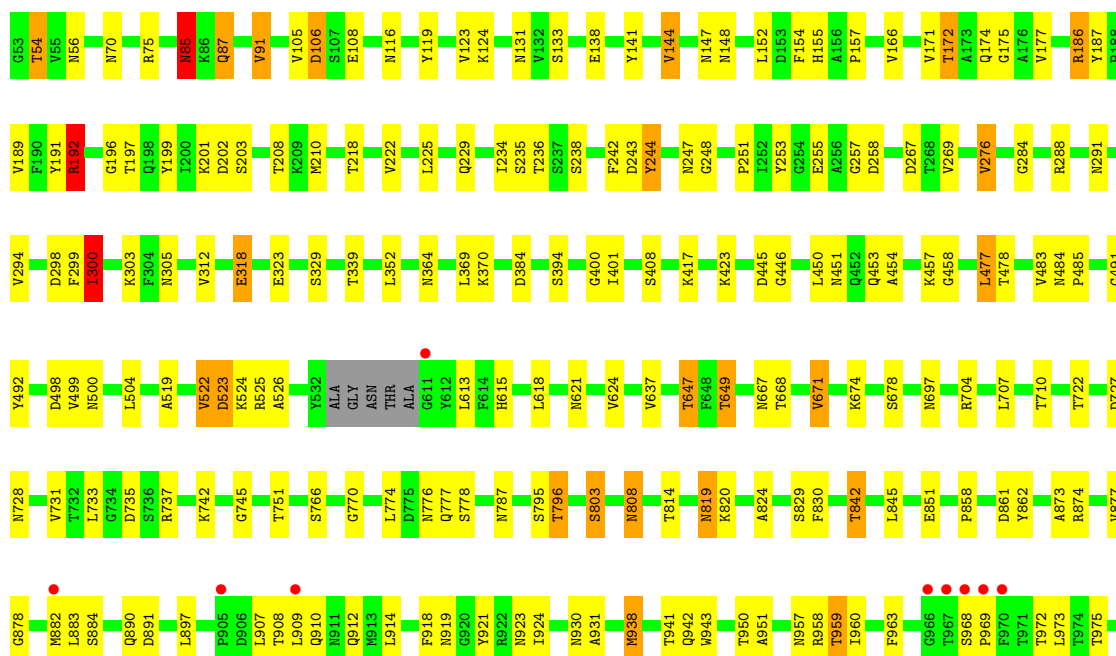
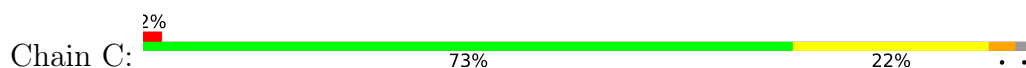


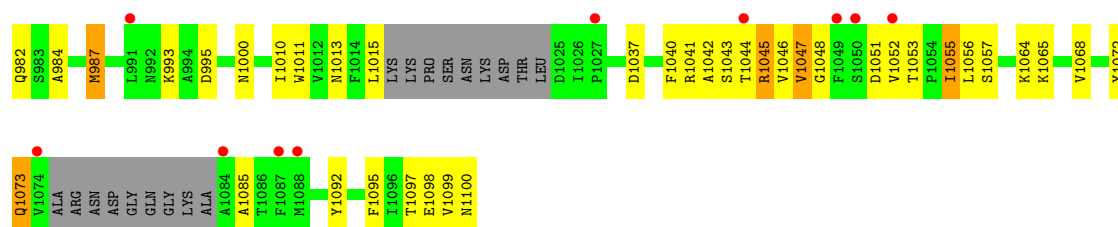
• Molecule 1: Hemoglobin-binding protease hbp



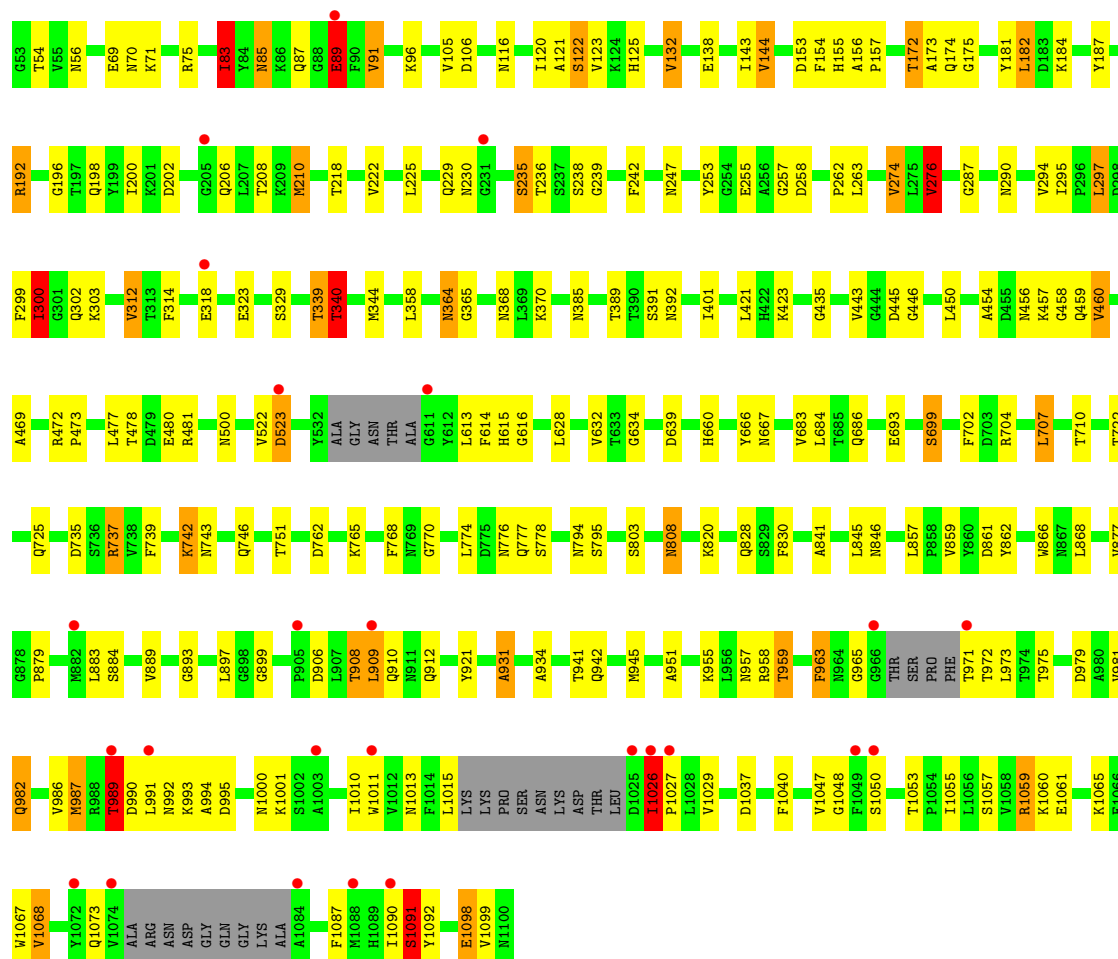
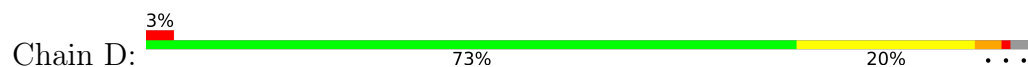


• Molecule 1: Hemoglobin-binding protease hbp





● Molecule 1: Hemoglobin-binding protease hbp



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	292.80Å 53.94Å 335.95Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	48.56 – 2.20 48.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.20) 93.1 (48.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.280 0.226 , 0.280	Depositor DCC
R_{free} test set	11985 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30307	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 94.28 % 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 3.1752e-09. 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:
CA

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	1.33	28/7407 (0.4%)	1.25	31/10069 (0.3%)
1	B	1.35	18/7407 (0.2%)	1.32	32/10069 (0.3%)
1	C	1.28	17/7278 (0.2%)	1.25	25/9895 (0.3%)
1	D	1.36	16/7236 (0.2%)	1.29	37/9835 (0.4%)
All	All	1.33	79/29328 (0.3%)	1.28	125/39868 (0.3%)

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	1
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	7

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	GLU	CD-OE2	-29.59	0.69	1.25
1	B	955	LYS	CE-NZ	24.49	2.22	1.49
1	C	523	ASP	CG-OD1	22.15	1.67	1.25
1	D	523	ASP	CG-OD2	21.63	1.66	1.25
1	D	523	ASP	CG-OD1	-21.44	0.84	1.25
1	A	619	LYS	CE-NZ	-19.93	0.89	1.49
1	B	851	GLU	CG-CD	-19.05	1.04	1.52
1	A	417	LYS	CE-NZ	-16.14	1.00	1.49
1	C	523	ASP	CG-OD2	-15.74	0.95	1.25
1	D	89	GLU	CD-OE1	14.79	1.53	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1021	LYS	CA-CB	-13.87	1.35	1.52
1	C	138	GLU	CD-OE2	13.44	1.50	1.25
1	C	138	GLU	CD-OE1	-13.32	1.00	1.25
1	B	633	THR	CA-CB	10.13	1.67	1.53
1	D	138	GLU	CD-OE2	9.30	1.43	1.25
1	A	632	VAL	CA-CB	8.44	1.63	1.54
1	D	138	GLU	CD-OE1	-8.37	1.09	1.25
1	D	276	VAL	CA-CB	7.90	1.64	1.54
1	A	276	VAL	CA-C	-7.66	1.44	1.52
1	B	416	VAL	CA-CB	7.16	1.64	1.54
1	D	300	ILE	CA-CB	7.05	1.62	1.54
1	D	443	VAL	CA-CB	6.76	1.62	1.54
1	A	964	ASN	N-CA	-6.65	1.41	1.47
1	B	115	ILE	N-CA	6.64	1.53	1.46
1	D	122	SER	CA-CB	-6.59	1.48	1.54
1	C	819	ASN	CA-C	-6.54	1.44	1.52
1	B	614	PHE	CA-C	6.48	1.60	1.52
1	B	83	ILE	CA-CB	6.45	1.63	1.54
1	A	416	VAL	CA-CB	6.44	1.62	1.55
1	B	144	VAL	CA-C	6.29	1.60	1.53
1	A	390	THR	CA-C	6.29	1.61	1.52
1	A	390	THR	CA-CB	-6.19	1.43	1.53
1	A	312	VAL	CA-C	6.13	1.59	1.53
1	C	300	ILE	CA-CB	5.98	1.61	1.54
1	A	80	ASN	CA-C	-5.87	1.45	1.53
1	A	759	ALA	C-O	-5.85	1.17	1.24
1	A	151	SER	N-CA	5.79	1.53	1.45
1	A	431	VAL	C-O	5.78	1.30	1.23
1	C	803	SER	CA-C	-5.77	1.46	1.53
1	C	697	ASN	CA-C	-5.75	1.45	1.52
1	B	151	SER	N-CA	5.72	1.53	1.45
1	B	324	TRP	N-CA	-5.70	1.39	1.46
1	B	452	GLN	CA-C	5.70	1.60	1.52
1	B	307	ASP	CA-C	5.70	1.60	1.52
1	C	873	ALA	CA-CB	-5.63	1.44	1.53
1	C	824	ALA	CA-CB	-5.60	1.43	1.53
1	A	389	THR	N-CA	5.58	1.52	1.45
1	D	121	ALA	CA-C	-5.57	1.45	1.52
1	A	699	SER	N-CA	-5.49	1.39	1.46
1	B	149	ALA	CA-CB	-5.47	1.43	1.53
1	D	329	SER	C-O	-5.45	1.16	1.24
1	D	457	LYS	N-CA	5.43	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	VAL	CA-CB	-5.39	1.47	1.54
1	C	166	VAL	CA-CB	5.37	1.62	1.54
1	A	502	ASN	CA-C	-5.35	1.45	1.52
1	A	395	THR	C-O	5.34	1.30	1.23
1	D	931	ALA	CA-CB	-5.33	1.47	1.53
1	A	275	LEU	C-O	5.30	1.30	1.24
1	C	1055	ILE	CA-CB	5.22	1.60	1.54
1	B	115	ILE	CA-CB	5.21	1.60	1.54
1	C	973	LEU	N-CA	-5.20	1.40	1.46
1	A	632	VAL	CA-C	5.18	1.58	1.52
1	A	390	THR	N-CA	5.16	1.52	1.46
1	A	382	PHE	CA-C	-5.16	1.46	1.52
1	A	488	VAL	C-O	-5.14	1.18	1.24
1	B	413	VAL	C-O	-5.14	1.18	1.24
1	C	276	VAL	CA-CB	5.10	1.61	1.54
1	D	456	ASN	CA-C	5.07	1.59	1.52
1	A	422	HIS	C-O	5.06	1.30	1.24
1	A	508	GLN	C-O	5.06	1.30	1.23
1	C	454	ALA	C-O	5.05	1.29	1.23
1	A	324	TRP	CA-C	-5.04	1.46	1.53
1	C	647	THR	CA-CB	5.04	1.60	1.53
1	B	276	VAL	CA-CB	5.04	1.61	1.54
1	A	368	ASN	N-CA	5.03	1.52	1.46
1	A	326	PHE	N-CA	-5.03	1.40	1.46
1	C	457	LYS	N-CA	5.02	1.51	1.46
1	D	739	PHE	C-O	5.01	1.29	1.23
1	B	311	PRO	CA-C	5.00	1.58	1.52

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	851	GLU	CB-CG-CD	29.67	163.03	112.60
1	D	89	GLU	CG-CD-OE1	-17.50	78.14	118.40
1	D	523	ASP	CB-CG-OD2	-17.00	79.29	118.40
1	B	851	GLU	CG-CD-OE1	16.83	157.10	118.40
1	D	89	GLU	OE1-CD-OE2	16.03	161.37	122.90
1	B	851	GLU	CG-CD-OE2	-15.89	81.85	118.40
1	C	238	SER	N-CA-C	-10.45	101.29	114.56
1	C	523	ASP	CB-CG-OD1	-10.35	94.59	118.40
1	D	172	THR	CB-CA-C	-9.55	94.52	109.61
1	D	116	ASN	N-CA-C	-9.17	97.62	108.25
1	D	318	GLU	CB-CG-CD	-8.23	98.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	686	GLN	CA-C-N	-7.93	111.55	119.56
1	D	686	GLN	C-N-CA	-7.93	111.55	119.56
1	A	415	GLY	N-CA-C	-7.91	101.53	112.13
1	D	1026	ILE	N-CA-C	7.75	116.83	107.61
1	C	116	ASN	N-CA-C	-7.74	101.25	108.22
1	D	238	SER	N-CA-C	-7.66	104.43	114.31
1	A	967	THR	N-CA-C	-7.02	105.25	114.31
1	B	321	ALA	N-CA-C	6.99	119.32	110.24
1	B	116	ASN	CA-C-N	-6.92	112.68	119.87
1	B	116	ASN	C-N-CA	-6.92	112.68	119.87
1	B	400	GLY	N-CA-C	-6.88	100.62	110.46
1	D	144	VAL	N-CA-CB	-6.85	102.89	112.35
1	B	65	ARG	N-CA-C	-6.77	103.52	111.03
1	A	312	VAL	N-CA-C	6.76	116.97	107.37
1	B	244	TYR	N-CA-C	6.68	119.57	111.82
1	B	488	VAL	N-CA-CB	6.65	117.97	110.72
1	A	192	ARG	NE-CZ-NH2	6.52	125.06	119.20
1	A	192	ARG	NE-CZ-NH1	-6.49	115.02	121.50
1	B	192	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	D	274	VAL	N-CA-C	-6.42	99.84	108.06
1	B	414	ASN	N-CA-C	6.40	118.29	110.41
1	C	244	TYR	N-CA-C	6.37	119.04	111.33
1	B	261	SER	N-CA-C	6.33	116.88	109.60
1	C	288	ARG	N-CA-C	6.32	121.17	112.90
1	D	683	VAL	N-CA-C	6.28	117.18	108.89
1	D	132	VAL	CB-CA-C	6.28	121.78	110.48
1	B	192	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	D	469	ALA	N-CA-C	6.18	118.17	108.96
1	C	1000	ASN	N-CA-C	6.15	118.95	111.82
1	C	192	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	C	305	ASN	N-CA-C	6.12	118.75	111.71
1	A	116	ASN	CA-C-N	-6.10	113.84	119.82
1	A	116	ASN	C-N-CA	-6.10	113.84	119.82
1	B	989	THR	CB-CA-C	-6.10	96.64	109.38
1	A	1021	LYS	CB-CA-C	-6.08	103.00	112.12
1	C	144	VAL	N-CA-CB	-6.04	103.96	112.12
1	D	972	THR	N-CA-C	6.01	119.28	109.24
1	C	878	GLY	CA-C-N	5.97	126.31	119.92
1	C	878	GLY	C-N-CA	5.97	126.31	119.92
1	A	390	THR	N-CA-C	5.93	123.44	110.80
1	C	243	ASP	N-CA-C	5.89	118.81	108.56
1	D	743	ASN	CB-CA-C	-5.82	101.59	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASN	N-CA-C	5.81	118.78	110.24
1	A	67	PHE	N-CA-C	-5.81	104.87	111.14
1	B	368	ASN	N-CA-C	5.79	118.16	108.02
1	D	187	TYR	CA-C-N	5.77	125.14	118.85
1	D	187	TYR	C-N-CA	5.77	125.14	118.85
1	A	714	LEU	N-CA-C	-5.76	97.94	108.02
1	C	1052	VAL	N-CA-C	5.72	116.11	107.75
1	A	1082	LYS	N-CA-C	5.69	117.64	110.24
1	D	247	ASN	N-CA-C	5.68	120.20	113.16
1	D	230	ASN	CB-CA-C	-5.67	102.12	111.36
1	D	364	ASN	CA-C-N	5.66	125.35	119.92
1	D	364	ASN	C-N-CA	5.66	125.35	119.92
1	D	628	LEU	CA-C-N	-5.65	113.89	119.99
1	D	628	LEU	C-N-CA	-5.65	113.89	119.99
1	C	787	ASN	CB-CA-C	-5.61	103.26	111.23
1	C	247	ASN	N-CA-C	5.60	120.10	113.16
1	A	737	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	B	234	ILE	CA-CB-CG2	5.60	120.02	110.50
1	C	147	ASN	N-CA-C	5.59	119.14	111.54
1	A	170	ALA	CA-C-N	-5.58	116.18	122.48
1	A	170	ALA	C-N-CA	-5.58	116.18	122.48
1	D	340	THR	CB-CA-C	5.56	119.19	110.19
1	B	635	ALA	N-CA-C	5.55	118.24	109.96
1	C	119	TYR	N-CA-C	5.55	118.51	109.24
1	B	392	ASN	N-CA-C	-5.53	105.89	113.30
1	A	402	VAL	CB-CA-C	-5.53	102.60	110.83
1	B	494	GLY	N-CA-C	5.52	121.28	111.02
1	D	83	ILE	N-CA-C	5.51	116.67	108.46
1	C	257	GLY	N-CA-C	-5.49	107.36	113.79
1	A	615	HIS	N-CA-C	-5.49	106.63	113.38
1	C	192	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	A	390	THR	CB-CA-C	-5.46	99.55	110.42
1	B	66	ASP	N-CA-C	5.46	117.99	111.71
1	C	300	ILE	CB-CA-C	5.46	118.96	111.97
1	D	392	ASN	N-CA-CB	-5.45	102.39	111.06
1	B	856	LEU	N-CA-C	5.43	117.96	110.35
1	C	187	TYR	CA-C-N	5.43	125.25	119.28
1	C	187	TYR	C-N-CA	5.43	125.25	119.28
1	D	257	GLY	N-CA-C	-5.42	107.05	114.64
1	A	821	GLY	N-CA-C	-5.42	107.88	114.92
1	B	305	ASN	N-CA-C	5.40	117.86	111.33
1	D	312	VAL	CB-CA-C	5.38	117.58	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1070	ASP	N-CA-CB	-5.38	103.88	110.98
1	A	836	VAL	N-CA-C	-5.35	98.26	107.24
1	B	260	GLY	N-CA-C	-5.33	107.32	114.25
1	D	794	ASN	N-CA-C	5.32	118.77	111.54
1	B	82	ALA	CA-C-N	-5.29	115.75	123.06
1	B	82	ALA	C-N-CA	-5.29	115.75	123.06
1	D	699	SER	CB-CA-C	5.29	119.27	109.70
1	B	402	VAL	CB-CA-C	-5.26	103.28	110.96
1	B	1011	TRP	N-CA-C	-5.25	101.72	110.17
1	D	667	ASN	N-CA-C	5.24	115.21	108.34
1	D	803	SER	CB-CA-C	-5.21	103.46	111.74
1	A	876	ASN	CA-C-N	-5.21	116.03	123.11
1	A	876	ASN	C-N-CA	-5.21	116.03	123.11
1	C	483	VAL	N-CA-C	5.19	114.71	108.06
1	A	249	ALA	N-CA-C	5.18	118.70	112.38
1	B	632	VAL	CB-CA-C	-5.17	102.95	110.81
1	D	1000	ASN	N-CA-C	5.15	118.82	112.54
1	D	989	THR	N-CA-C	5.15	118.46	110.17
1	A	898	GLY	N-CA-C	5.12	118.68	112.48
1	C	972	THR	N-CA-C	5.12	117.91	109.72
1	A	869	LYS	N-CA-C	5.11	116.95	109.24
1	B	83	ILE	CB-CA-C	5.11	118.23	110.62
1	A	260	GLY	N-CA-C	-5.10	109.01	115.08
1	B	165	GLU	N-CA-C	5.09	117.72	111.82
1	A	619	LYS	CD-CE-NZ	5.07	128.12	111.90
1	A	392	ASN	N-CA-C	-5.06	107.11	113.28
1	D	297	LEU	N-CA-C	5.05	116.48	111.07
1	C	318	GLU	N-CA-C	-5.05	105.87	112.23
1	A	999	ILE	N-CA-C	5.04	114.84	107.37
1	A	340	THR	N-CA-C	5.02	116.77	110.24

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	968	SER	Peptide
1	B	1069	LEU	Peptide
1	B	963	PHE	Peptide
1	C	523	ASP	Sidechain
1	C	968	SER	Peptide
1	D	391	SER	Peptide
1	D	523	ASP	Sidechain

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	7278	0	6993	120	0
1	B	7278	0	6993	114	0
1	C	7149	0	6858	152	0
1	D	7113	0	6823	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	426	0	0	15	0
3	B	430	0	0	15	0
3	C	321	0	0	9	0
3	D	308	0	0	7	0
All	All	30307	0	27667	523	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 9.

All (523) 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:C:364[B]:ASN:OD1	1:D:364:ASN:ND2	1.76	1.16
1:B:632:VAL:HG12	1:B:634:GLY:H	1.27	0.99
1:A:401:ILE:HD12	1:A:421:LEU:HD11	1.40	0.99
1:C:210:MET:HE3	1:C:210:MET:HA	1.43	0.99
1:C:842:THR:HG22	3:C:1285:HOH:O	1.62	0.97
1:D:172:THR:HG22	1:D:174:GLN:H	1.31	0.94
1:C:1013:ASN:ND2	1:C:1048:GLY:HA3	1.84	0.92
1:C:525:ARG:HE	1:C:621:ASN:HD21	1.18	0.92
1:C:938:MET:HE2	1:C:943:TRP:HB2	1.52	0.92
1:B:979:ASP:OD1	1:B:1004:THR:HG22	1.69	0.92
1:C:921:TYR:CE2	1:C:942:GLN:NE2	2.37	0.92
1:A:75:ARG:HH21	1:A:75:ARG:HG3	1.32	0.90
1:C:248:GLY:O	1:C:251:PRO:HD3	1.72	0.89
1:A:138:GLU:HG2	3:A:1239:HOH:O	1.71	0.89
1:A:383:ARG:HD3	3:A:1413:HOH:O	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1011:TRP:HE3	1:D:1047:VAL:HG23	1.40	0.86
1:D:987:MET:HB3	1:D:995:ASP:HB2	1.58	0.86
1:D:85:ASN:ND2	1:D:89:GLU:HG2	1.90	0.86
1:C:921:TYR:HE2	1:C:942:GLN:NE2	1.75	0.84
1:C:450:LEU:O	1:C:478:THR:HG23	1.76	0.84
1:D:1011:TRP:HE3	1:D:1047:VAL:CG2	1.91	0.83
1:A:667:ASN:HB3	1:A:671:VAL:CG2	2.08	0.83
1:C:957:ASN:O	1:C:959:THR:HG22	1.77	0.83
1:D:210:MET:HE2	1:D:210:MET:HA	1.61	0.82
1:B:302:GLN:NE2	3:B:1262:HOH:O	2.14	0.80
1:C:1011:TRP:HE3	1:C:1047:VAL:CG2	1.95	0.80
1:D:1013:ASN:OD1	1:D:1048:GLY:HA3	1.82	0.79
1:C:735:ASP:OD1	1:C:737:ARG:HD3	1.83	0.79
1:D:987:MET:CB	1:D:995:ASP:HB2	2.13	0.78
1:C:647:THR:HG22	1:C:649:THR:HG22	1.65	0.76
1:D:1011:TRP:CE3	1:D:1047:VAL:CG2	2.69	0.76
1:A:401:ILE:CD1	1:A:421:LEU:HD11	2.14	0.76
1:A:735:ASP:OD1	1:A:737:ARG:HD3	1.85	0.76
1:D:192:ARG:NH1	3:D:539:HOH:O	2.19	0.76
1:C:649:THR:HG23	3:C:1160:HOH:O	1.86	0.75
1:C:1013:ASN:HD21	1:C:1048:GLY:HA3	1.48	0.75
1:D:957:ASN:O	1:D:959:THR:HG22	1.86	0.75
1:C:525:ARG:HE	1:C:621:ASN:ND2	1.83	0.75
1:D:172:THR:HG21	1:D:181:TYR:OH	1.87	0.75
1:C:1011:TRP:CE3	1:C:1047:VAL:HG22	2.22	0.74
1:B:225:LEU:HD22	1:B:234:ILE:HG23	1.69	0.74
1:C:192:ARG:NH1	3:C:1153:HOH:O	2.04	0.74
1:D:908:THR:HG22	1:D:909:LEU:H	1.53	0.74
1:B:383:ARG:HD3	3:B:1489:HOH:O	1.87	0.74
1:B:735:ASP:OD1	1:B:737:ARG:HD3	1.88	0.73
1:D:908:THR:HG22	1:D:909:LEU:N	2.04	0.73
1:C:298:ASP:HB2	3:C:1366:HOH:O	1.89	0.72
1:C:186:ARG:HD3	1:C:267:ASP:OD1	1.89	0.72
1:A:987:MET:HB3	1:A:995:ASP:HB2	1.72	0.72
1:C:364[B]:ASN:ND2	1:D:385:ASN:HD22	1.87	0.71
1:C:210:MET:CE	1:C:674:LYS:HB3	2.20	0.71
1:A:987:MET:CB	1:A:995:ASP:HB2	2.21	0.71
1:D:989:THR:HG23	1:D:994:ALA:HB2	1.72	0.71
1:C:938:MET:CE	1:C:943:TRP:HB2	2.21	0.70
1:A:778:SER:O	1:A:795:SER:HB3	1.90	0.70
1:D:196:GLY:HA3	1:D:258:ASP:OD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLY:O	1:A:75:ARG:NH2	2.26	0.69
1:A:650:GLN:NE2	1:A:652:ASN:O	2.26	0.69
1:C:1011:TRP:HE3	1:C:1047:VAL:HG22	1.54	0.68
1:D:965:GLY:HA3	1:D:971:THR:HG21	1.75	0.68
1:B:503:SER:O	1:B:504:LEU:HD23	1.93	0.68
1:C:154:PHE:HE1	1:C:300:ILE:CD1	2.07	0.67
1:A:918:PHE:HA	1:A:924:ILE:HD12	1.76	0.67
1:D:154:PHE:CE1	1:D:300:ILE:HD11	2.29	0.67
1:B:793:ASN:HD22	1:B:812:THR:HB	1.58	0.67
1:C:186:ARG:HG2	1:C:269:VAL:HG23	1.76	0.67
1:D:154:PHE:CZ	1:D:300:ILE:HD11	2.29	0.67
1:C:85:ASN:HB3	1:C:87:GLN:H	1.59	0.67
1:C:210:MET:HA	1:C:210:MET:CE	2.23	0.67
1:A:1059:ARG:NH1	1:A:1066:GLU:OE1	2.27	0.67
1:C:451:ASN:HD21	1:C:453:GLN:HE21	1.42	0.66
1:C:154:PHE:CE1	1:C:300:ILE:HD11	2.29	0.66
1:C:364[A]:ASN:OD1	1:D:364:ASN:ND2	2.28	0.66
1:B:971:THR:HG22	3:B:1401:HOH:O	1.95	0.66
1:B:675:LEU:HD13	1:B:683:VAL:HG21	1.77	0.65
1:B:75:ARG:HH21	1:B:75:ARG:HG3	1.61	0.65
1:B:858:PRO:HB2	1:B:914:LEU:HD23	1.78	0.65
1:A:509:LEU:N	1:A:612:TYR:OH	2.21	0.65
1:B:341:THR:O	3:B:579:HOH:O	2.15	0.65
1:D:198:GLN:NE2	1:D:218:THR:HG23	2.11	0.65
1:D:1011:TRP:CZ2	1:D:1098:GLU:HG2	2.32	0.64
1:A:339:THR:HG23	1:A:340:THR:H	1.61	0.64
1:B:234:ILE:HG22	1:B:292:TRP:HB2	1.79	0.64
1:C:253:TYR:HE2	1:C:255:GLU:OE2	1.81	0.64
1:D:210:MET:HA	1:D:210:MET:CE	2.27	0.64
1:C:731:VAL:HG12	1:C:733:LEU:CD1	2.27	0.64
1:D:323:GLU:HB3	1:D:370:LYS:HD2	1.80	0.64
1:D:229:GLN:HG3	3:D:1326:HOH:O	1.98	0.63
1:D:1013:ASN:ND2	1:D:1015:LEU:HD23	2.13	0.63
1:A:858:PRO:HB2	1:A:914:LEU:HD23	1.81	0.63
1:C:987:MET:HB3	1:C:995:ASP:HB2	1.79	0.63
1:C:1046:VAL:HG23	3:C:1463:HOH:O	1.97	0.63
1:B:667:ASN:HB3	1:B:671:VAL:HG22	1.80	0.62
1:A:973:LEU:HD23	1:A:997:LEU:HD13	1.82	0.62
1:C:91:VAL:HG11	1:C:244:TYR:CE1	2.34	0.62
1:D:1026:ILE:HG22	1:D:1027:PRO:HD2	1.81	0.62
1:B:1058:VAL:CG1	1:B:1065:LYS:HD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLY:HA3	3:B:1130:HOH:O	2.00	0.62
1:D:450:LEU:O	1:D:478:THR:HG23	2.00	0.62
1:C:154:PHE:HE1	1:C:300:ILE:HD11	1.65	0.61
1:A:400:GLY:HA2	3:A:1115:HOH:O	1.99	0.61
1:A:667:ASN:HB3	1:A:671:VAL:HG22	1.82	0.61
1:C:1072:TYR:O	1:C:1073:GLN:HB3	2.00	0.61
1:D:85:ASN:HB2	1:D:89:GLU:H	1.66	0.61
1:C:845:LEU:HD12	1:C:877:VAL:HG22	1.82	0.61
1:B:522:VAL:HG13	3:B:1375:HOH:O	2.00	0.60
1:B:667:ASN:HB3	1:B:671:VAL:CG2	2.32	0.60
1:C:882:MET:HG2	1:C:918:PHE:CZ	2.36	0.60
1:A:186:ARG:HD2	1:A:187:TYR:CZ	2.37	0.60
1:C:154:PHE:CE1	1:C:300:ILE:CD1	2.85	0.59
1:A:918:PHE:HA	1:A:924:ILE:CD1	2.32	0.59
1:D:368:ASN:ND2	3:D:1334:HOH:O	2.35	0.59
1:C:225:LEU:HG	1:C:236:THR:HB	1.84	0.59
1:B:931:ALA:HB1	1:B:934:ALA:HB3	1.85	0.58
1:B:245:LYS:HG3	1:B:246:LEU:N	2.17	0.58
1:D:735:ASP:OD1	1:D:737:ARG:HD3	2.02	0.58
1:A:210:MET:HE2	1:A:210:MET:HA	1.84	0.58
1:B:233:MET:O	1:B:234:ILE:HD12	2.02	0.58
1:C:253:TYR:CE2	1:C:255:GLU:OE2	2.56	0.58
1:C:1011:TRP:CE3	1:C:1047:VAL:CG2	2.81	0.58
1:D:1011:TRP:CE3	1:D:1047:VAL:HG23	2.30	0.58
1:C:1045:ARG:NH1	1:C:1097:THR:OG1	2.34	0.58
1:A:452:GLN:N	1:A:482:GLN:OE1	2.27	0.58
1:B:298:ASP:O	1:B:302:GLN:HG3	2.04	0.58
1:C:451:ASN:ND2	1:C:453:GLN:HE21	2.01	0.57
1:C:1013:ASN:OD1	1:C:1015:LEU:HD23	2.03	0.57
1:D:454:ALA:HA	1:D:460:VAL:HB	1.86	0.57
1:D:85:ASN:HB2	1:D:89:GLU:N	2.19	0.57
1:C:987:MET:CB	1:C:995:ASP:HB2	2.35	0.57
1:A:210:MET:HA	1:A:210:MET:CE	2.35	0.57
1:B:987:MET:HB3	1:B:995:ASP:HB2	1.86	0.57
1:D:778:SER:O	1:D:795:SER:HB3	2.03	0.56
1:D:879:PRO:HG3	1:D:899:GLY:O	2.05	0.56
1:C:707:LEU:HB3	1:C:710:THR:CG2	2.35	0.56
1:A:797:VAL:HG22	1:A:816:LEU:CD1	2.35	0.56
1:A:845:LEU:HD12	1:A:877:VAL:HB	1.87	0.56
1:D:253:TYR:CE2	1:D:255:GLU:OE2	2.58	0.56
1:B:770:GLY:O	1:B:788:GLY:HA3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:MET:CB	1:B:995:ASP:HB2	2.35	0.56
1:C:451:ASN:HD21	1:C:453:GLN:NE2	2.04	0.56
1:A:235:SER:HB2	1:A:291:ASN:HD22	1.70	0.56
1:B:396:TRP:CH2	1:B:398:GLY:HA3	2.41	0.56
1:A:395:THR:CG2	1:A:415:GLY:O	2.54	0.55
1:A:951:ALA:HB3	1:A:975:THR:HG22	1.89	0.55
1:B:743:ASN:OD1	1:B:746:GLN:HG3	2.05	0.55
1:B:1010:ILE:CD1	1:B:1040:PHE:HB3	2.36	0.55
1:C:1037:ASP:OD1	1:C:1065:LYS:NZ	2.28	0.55
1:A:930:ASN:C	1:A:930:ASN:HD22	2.13	0.55
1:D:990:ASP:HB3	1:D:992:ASN:H	1.72	0.55
1:C:210:MET:HE1	1:C:674:LYS:HB3	1.88	0.55
1:D:423:LYS:HD3	1:D:423:LYS:C	2.32	0.55
1:A:704:ARG:HD3	1:A:725:GLN:OE1	2.07	0.54
1:C:795:SER:C	1:C:814:THR:HG23	2.33	0.54
1:C:618:LEU:HD13	1:C:624:VAL:HG21	1.89	0.54
1:B:1058:VAL:HG13	1:B:1065:LYS:HD2	1.88	0.54
1:D:253:TYR:HE2	1:D:255:GLU:OE2	1.91	0.54
1:B:298:ASP:HB2	3:B:1181:HOH:O	2.08	0.54
1:D:154:PHE:CE1	1:D:300:ILE:CD1	2.91	0.54
1:A:186:ARG:HD2	1:A:187:TYR:CE1	2.43	0.54
1:A:958:ARG:HA	1:A:982:GLN:O	2.08	0.54
1:C:862:TYR:CD1	1:C:884:SER:HB3	2.43	0.54
1:D:704:ARG:HD3	1:D:725:GLN:OE1	2.08	0.53
1:C:499:VAL:HG22	1:C:519:ALA:O	2.07	0.53
1:B:56:ASN:C	1:B:56:ASN:OD1	2.51	0.53
1:D:845:LEU:HD12	1:D:877:VAL:HG22	1.91	0.53
1:D:155:HIS:CD2	1:D:157:PRO:HD3	2.43	0.53
1:D:908:THR:CG2	1:D:909:LEU:H	2.18	0.53
1:D:1026:ILE:CG2	1:D:1027:PRO:HD2	2.39	0.53
1:B:452:GLN:HG2	1:B:461:GLN:C	2.34	0.53
1:D:951:ALA:HB3	1:D:975:THR:HG22	1.89	0.53
1:D:921:TYR:CD2	1:D:942:GLN:HB2	2.44	0.53
1:B:776:ASN:O	1:B:777:GLN:HB2	2.09	0.53
1:C:423:LYS:HD3	1:C:423:LYS:C	2.33	0.53
1:C:649:THR:CG2	3:C:1160:HOH:O	2.48	0.53
1:D:861:ASP:O	1:D:883:LEU:HD12	2.08	0.53
1:B:323:GLU:O	1:B:335:LEU:HA	2.09	0.52
1:B:200:ILE:HG12	1:B:210:MET:HE2	1.91	0.52
1:B:991:LEU:HD22	1:B:1016:LYS:HG3	1.91	0.52
1:A:75:ARG:HH21	1:A:75:ARG:CG	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1010:ILE:CD1	1:D:1040:PHE:HB3	2.39	0.52
1:A:314:PHE:HD2	1:A:322:LEU:HD12	1.74	0.52
1:A:890:GLN:O	1:A:891:ASP:HB2	2.09	0.52
1:B:782:ILE:HD12	1:B:799:ILE:HG12	1.91	0.52
1:D:941:THR:H	1:D:959:THR:HB	1.73	0.52
1:C:842:THR:HB	1:C:874:ARG:HB2	1.91	0.52
1:D:1098:GLU:C	1:D:1098:GLU:CD	2.78	0.52
1:A:626:ASN:HB3	1:A:650:GLN:HG2	1.91	0.52
1:A:987:MET:HB2	1:A:995:ASP:HB2	1.90	0.52
1:D:987:MET:HB2	1:D:995:ASP:HB2	1.91	0.52
1:A:930:ASN:C	1:A:930:ASN:ND2	2.68	0.52
1:B:419:ASP:OD2	3:B:1136:HOH:O	2.19	0.51
1:C:745:GLY:HA2	3:C:1300:HOH:O	2.10	0.51
1:A:674:LYS:O	1:A:677:ALA:HB3	2.10	0.51
1:B:186:ARG:HD2	1:B:187:TYR:CZ	2.46	0.51
1:B:423:LYS:C	1:B:423:LYS:HD3	2.36	0.51
1:A:800:SER:HA	1:A:822:ALA:HB2	1.93	0.51
1:A:930:ASN:ND2	1:A:932:PRO:HD3	2.25	0.51
1:C:941:THR:H	1:C:959:THR:HB	1.75	0.51
1:A:395:THR:HG22	1:A:415:GLY:O	2.10	0.51
1:B:632:VAL:HG12	1:B:634:GLY:N	2.11	0.51
1:C:707:LEU:HB3	1:C:710:THR:HG22	1.91	0.51
1:C:1013:ASN:ND2	1:C:1048:GLY:CA	2.67	0.51
1:D:1059:ARG:HG2	1:D:1060:LYS:N	2.25	0.51
1:A:83:ILE:HA	3:A:1490:HOH:O	2.11	0.50
1:B:186:ARG:HG3	1:B:269:VAL:HG23	1.94	0.50
1:D:294:VAL:O	1:D:295:ILE:C	2.55	0.50
1:D:1090:ILE:HG22	1:D:1091:SER:O	2.11	0.50
1:A:488:VAL:HG11	1:A:497:LEU:HD22	1.92	0.50
1:A:1010:ILE:N	1:A:1010:ILE:HD12	2.26	0.50
1:B:302:GLN:HG2	3:B:1376:HOH:O	2.10	0.50
1:C:229:GLN:O	1:C:229:GLN:HG2	2.11	0.50
1:A:235:SER:CB	1:A:291:ASN:HD22	2.24	0.50
1:B:958:ARG:HA	1:B:982:GLN:O	2.11	0.50
1:A:797:VAL:HG22	1:A:816:LEU:HD12	1.93	0.50
1:C:722:THR:O	1:C:770:GLY:HA3	2.11	0.50
1:C:613:LEU:HD21	1:C:615:HIS:CE1	2.45	0.50
1:B:255:GLU:OE1	1:B:285:ALA:HA	2.12	0.50
1:B:800:SER:HA	1:B:822:ALA:HB2	1.93	0.50
1:C:795:SER:C	1:C:796:THR:OG1	2.55	0.50
1:D:931:ALA:HB1	1:D:934:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LEU:O	1:B:478:THR:HG23	2.12	0.49
1:C:408:SER:OG	3:C:1224:HOH:O	2.19	0.49
1:D:632:VAL:HG12	1:D:634:GLY:H	1.77	0.49
1:A:210:MET:HE1	1:A:674:LYS:HG2	1.93	0.49
1:C:776:ASN:O	1:C:777:GLN:HB2	2.12	0.49
1:C:1013:ASN:HD22	1:C:1047:VAL:C	2.20	0.49
1:B:314:PHE:O	3:B:1458:HOH:O	2.20	0.49
1:A:693:GLU:HG2	3:A:1455:HOH:O	2.12	0.49
1:D:990:ASP:O	1:D:991:LEU:HB2	2.13	0.49
1:C:323:GLU:HB3	1:C:370:LYS:HD2	1.93	0.49
1:C:861:ASP:O	1:C:883:LEU:HD12	2.12	0.49
1:C:1098:GLU:C	1:C:1100:ASN:H	2.21	0.49
1:D:921:TYR:CD1	1:D:1092:TYR:HD2	2.30	0.49
1:D:1013:ASN:ND2	1:D:1015:LEU:CD2	2.76	0.49
1:C:91:VAL:CG1	1:C:244:TYR:CD1	2.96	0.49
1:D:722:THR:O	1:D:770:GLY:HA3	2.12	0.49
1:C:921:TYR:CD1	1:C:1092:TYR:HD2	2.31	0.49
1:A:324:TRP:CE2	1:A:373:VAL:HG21	2.48	0.48
1:A:613:LEU:HD21	1:A:741:ASP:HB2	1.95	0.48
1:A:742:LYS:HE3	1:A:753:GLU:OE2	2.13	0.48
1:C:667:ASN:HB3	1:C:671:VAL:HG22	1.94	0.48
1:C:918:PHE:HA	1:C:924:ILE:CD1	2.42	0.48
1:C:774:LEU:HB3	1:C:778:SER:HB2	1.94	0.48
1:D:122:SER:OG	1:D:123:VAL:N	2.46	0.48
1:A:472:ARG:N	1:A:473:PRO:CD	2.77	0.48
1:C:192:ARG:HH22	1:C:258:ASP:CG	2.21	0.48
1:D:992:ASN:O	1:D:1026:ILE:HD13	2.13	0.48
1:B:72:GLY:O	1:B:75:ARG:NH2	2.47	0.48
1:C:303:LYS:HE2	1:C:303:LYS:HA	1.94	0.48
1:C:830:PHE:C	1:C:830:PHE:CD2	2.91	0.48
1:C:522:VAL:HG13	1:C:524:LYS:H	1.78	0.48
1:C:951:ALA:HB3	1:C:975:THR:HG22	1.96	0.48
1:D:472:ARG:N	1:D:473:PRO:CD	2.76	0.48
1:D:868:LEU:HB3	3:D:1306:HOH:O	2.13	0.48
1:A:412:GLN:O	3:A:1274:HOH:O	2.20	0.48
1:C:731:VAL:HG12	1:C:733:LEU:HD13	1.95	0.48
1:A:156:ALA:N	1:A:157:PRO:HD3	2.29	0.48
1:B:186:ARG:HD2	1:B:187:TYR:CE1	2.49	0.48
1:B:882:MET:HE3	1:B:882:MET:HB3	1.82	0.48
1:C:1013:ASN:HD22	1:C:1048:GLY:HA3	1.71	0.48
1:D:1010:ILE:HD11	1:D:1040:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HD21	1:A:528:ILE:HD12	1.96	0.48
1:D:445:ASP:OD1	1:D:446:GLY:N	2.44	0.48
1:D:762:ASP:OD2	1:D:765:LYS:HE3	2.14	0.48
1:D:1053:THR:HB	1:D:1073:GLN:HB2	1.95	0.48
1:A:1021:LYS:O	1:A:1022:ASP:HB2	2.12	0.47
1:B:989:THR:HG23	1:B:994:ALA:HB2	1.96	0.47
1:A:629:PRO:O	1:A:632:VAL:HG13	2.13	0.47
1:B:650:GLN:HG2	1:B:710:THR:HG21	1.95	0.47
1:C:1010:ILE:CD1	1:C:1040:PHE:HB3	2.44	0.47
1:C:1046:VAL:HG12	1:C:1047:VAL:N	2.28	0.47
1:A:290:ASN:HB2	1:A:292:TRP:CH2	2.48	0.47
1:A:742:LYS:HB2	1:A:751:THR:HB	1.97	0.47
1:B:659:GLY:HA2	1:B:698:ARG:HG2	1.96	0.47
1:B:1021:LYS:HE3	1:B:1021:LYS:HA	1.96	0.47
1:A:505:THR:HA	1:A:529:THR:O	2.14	0.47
1:A:862:TYR:CD1	1:A:884:SER:HB3	2.49	0.47
1:A:1087:PHE:HA	1:A:1090:ILE:HG13	1.96	0.47
1:D:299:PHE:O	1:D:302:GLN:HB2	2.14	0.47
1:D:458:GLY:O	1:D:481:ARG:NH1	2.45	0.47
1:B:105:VAL:O	1:B:106:ASP:C	2.54	0.47
1:C:105:VAL:O	1:C:106:ASP:C	2.53	0.47
1:C:498:ASP:OD1	1:C:498:ASP:C	2.56	0.47
1:D:154:PHE:HE1	1:D:300:ILE:CD1	2.27	0.47
1:A:939:THR:HA	1:A:957:ASN:O	2.15	0.47
3:A:1409:HOH:O	1:B:138:GLU:HG2	2.15	0.47
1:B:196:GLY:O	1:B:197:THR:C	2.58	0.47
1:B:849:PRO:HG3	1:B:876:ASN:ND2	2.30	0.47
1:C:171:VAL:O	1:C:172:THR:C	2.56	0.47
1:C:229:GLN:O	1:C:229:GLN:CG	2.62	0.47
1:D:614:PHE:CZ	1:D:616:GLY:HA3	2.50	0.47
1:A:793:ASN:OD1	1:A:794:ASN:ND2	2.48	0.47
1:C:897:LEU:HD22	1:C:938:MET:HE3	1.97	0.47
1:D:239:GLY:HA3	1:D:287:GLY:O	2.15	0.47
1:D:908:THR:CG2	1:D:909:LEU:N	2.71	0.47
1:A:56:ASN:OD1	1:A:56:ASN:C	2.58	0.46
1:A:931:ALA:HB1	1:A:934:ALA:HB3	1.97	0.46
1:B:637:VAL:HG11	1:B:739:PHE:HB2	1.97	0.46
1:D:172:THR:HG22	1:D:173:ALA:N	2.30	0.46
1:D:846:ASN:ND2	1:D:859:VAL:HG22	2.29	0.46
1:D:989:THR:HG22	1:D:993:LYS:O	2.14	0.46
1:D:989:THR:CG2	1:D:994:ALA:HB2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:ARG:HB2	3:A:1452:HOH:O	2.15	0.46
1:B:400:GLY:HA2	3:B:1104:HOH:O	2.14	0.46
1:C:1011:TRP:CZ2	1:C:1098:GLU:HG3	2.50	0.46
1:D:368:ASN:HA	1:D:389:THR:O	2.15	0.46
1:B:416:VAL:O	1:B:417:LYS:C	2.57	0.46
1:D:841:ALA:C	3:D:1213:HOH:O	2.58	0.46
1:B:630:GLU:H	1:B:630:GLU:HG2	1.40	0.46
1:A:889:VAL:HG11	1:A:934:ALA:HB2	1.98	0.46
1:B:848:ARG:C	1:B:850:ASP:H	2.23	0.46
1:B:1031:ALA:O	1:B:1032:PRO:C	2.56	0.46
1:A:1077:ASN:HB2	3:A:1172:HOH:O	2.15	0.46
1:D:963:PHE:CD1	1:D:963:PHE:N	2.84	0.46
1:D:963:PHE:HB2	1:D:995:ASP:OD2	2.15	0.46
1:A:455:ASP:OD1	1:A:455:ASP:C	2.58	0.46
1:C:54:THR:OG1	1:C:199:TYR:HB2	2.16	0.46
1:A:75:ARG:HG3	1:A:75:ARG:NH2	2.15	0.46
1:A:85:ASN:HB3	1:A:89:GLU:H	1.81	0.46
1:A:830:PHE:C	1:A:830:PHE:CD2	2.93	0.46
1:C:731:VAL:HG12	1:C:733:LEU:HD11	1.98	0.46
1:A:412:GLN:HG2	1:A:432:GLN:HB3	1.97	0.45
1:A:628:LEU:HD13	1:A:632:VAL:HG21	1.98	0.45
1:C:958:ARG:HA	1:C:982:GLN:O	2.16	0.45
1:D:339:THR:HG22	1:D:340:THR:HG22	1.98	0.45
1:B:433:GLY:N	1:B:452:GLN:OE1	2.50	0.45
1:B:202:ASP:OD1	1:B:206:GLN:HB3	2.17	0.45
1:D:830:PHE:C	1:D:830:PHE:CD2	2.95	0.45
1:A:651:GLU:HG3	1:A:708:LYS:HB3	1.97	0.45
1:A:833:ASP:OD2	1:A:833:ASP:C	2.60	0.45
1:A:944:SER:HB2	1:A:1088:MET:HE3	1.97	0.45
1:B:390:THR:OG1	1:B:394:SER:HB2	2.16	0.45
1:B:1035:THR:O	1:B:1065:LYS:HE2	2.16	0.45
1:D:85:ASN:CB	1:D:89:GLU:H	2.29	0.45
1:D:1057:SER:O	1:D:1068:VAL:HG12	2.17	0.45
1:C:525:ARG:HG3	1:C:526:ALA:N	2.31	0.45
1:C:858:PRO:HB2	1:C:914:LEU:HD23	1.98	0.45
1:C:56:ASN:OD1	1:C:56:ASN:C	2.60	0.45
1:C:85:ASN:HB3	1:C:87:GLN:N	2.29	0.45
1:C:445:ASP:OD1	1:C:446:GLY:N	2.47	0.45
1:D:435:GLY:HA3	3:D:1295:HOH:O	2.16	0.45
1:D:666:TYR:HA	3:D:1300:HOH:O	2.17	0.45
1:C:707:LEU:HD22	1:C:710:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:957:ASN:O	1:C:958:ARG:C	2.58	0.45
1:A:383:ARG:NH1	3:A:1105:HOH:O	2.50	0.44
1:C:796:THR:N	1:C:814:THR:HG23	2.31	0.44
1:D:477:LEU:O	1:D:500:ASN:HB3	2.17	0.44
1:B:509:LEU:H	1:B:612:TYR:HH	1.60	0.44
1:C:484:ASN:C	1:C:484:ASN:OD1	2.60	0.44
1:D:862:TYR:CD1	1:D:884:SER:HB3	2.53	0.44
1:D:989:THR:O	1:D:1015:LEU:HB2	2.18	0.44
1:B:75:ARG:HG3	1:B:75:ARG:NH2	2.31	0.44
1:C:877:VAL:HG21	1:C:883:LEU:HD22	1.99	0.44
1:B:939:THR:HA	1:B:957:ASN:O	2.17	0.44
1:C:175:GLY:C	1:C:294:VAL:HG11	2.42	0.44
1:D:96:LYS:HD3	1:D:96:LYS:HA	1.70	0.44
1:A:1024:LEU:O	1:A:1070:ASP:HA	2.18	0.44
1:D:941:THR:HB	1:D:959:THR:HB	2.00	0.44
1:A:711:ASP:C	1:A:711:ASP:OD2	2.59	0.44
1:A:1044:THR:HG22	1:A:1045:ARG:HG3	1.99	0.44
1:A:1096:ILE:HA	1:A:1096:ILE:HD12	1.75	0.44
1:C:201:LYS:O	1:C:242:PHE:CZ	2.70	0.44
1:C:963:PHE:HB2	1:C:995:ASP:OD2	2.18	0.44
1:D:172:THR:CG2	1:D:175:GLY:H	2.29	0.44
1:D:235:SER:HB2	1:D:290:ASN:O	2.17	0.44
1:D:1059:ARG:HD3	1:D:1061:GLU:HB2	2.00	0.44
1:B:499:VAL:HG22	1:B:519:ALA:O	2.17	0.44
1:B:783:ASN:ND2	3:B:1389:HOH:O	2.45	0.44
1:C:154:PHE:CZ	1:C:300:ILE:HD11	2.52	0.44
1:C:196:GLY:O	1:C:197:THR:C	2.61	0.44
1:D:196:GLY:O	1:D:198:GLN:HG2	2.18	0.44
1:C:477:LEU:O	1:C:500:ASN:HB3	2.18	0.44
1:C:819:ASN:O	1:C:820:LYS:C	2.61	0.44
1:D:120:ILE:O	1:D:156:ALA:HA	2.17	0.44
1:D:989:THR:HB	1:D:991:LEU:H	1.82	0.44
1:A:951:ALA:O	1:A:975:THR:HA	2.18	0.43
1:B:795:SER:O	1:B:814:THR:HA	2.18	0.43
1:C:174:GLN:O	1:C:177:VAL:HG23	2.18	0.43
1:C:931:ALA:H	1:C:950:THR:HG23	1.83	0.43
1:C:960:ILE:HG13	1:C:984:ALA:HB3	1.98	0.43
1:D:120:ILE:HG13	1:D:157:PRO:HD2	1.99	0.43
1:D:1087:PHE:HA	1:D:1090:ILE:HG13	1.99	0.43
1:B:741:ASP:HB3	1:B:744:ASP:HB2	2.00	0.43
1:C:727:ASP:O	1:C:728:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:LEU:HD22	1:D:778:SER:HB3	2.00	0.43
1:A:1037:ASP:OD1	1:A:1058:VAL:HG11	2.19	0.43
1:D:299:PHE:CE2	1:D:303:LYS:HE3	2.54	0.43
1:A:142:ASN:ND2	1:A:160:ASP:OD1	2.41	0.43
1:C:491:GLY:O	1:C:492:TYR:C	2.61	0.43
1:C:668:THR:OG1	1:C:671:VAL:HG13	2.19	0.43
1:D:1037:ASP:OD1	1:D:1065:LYS:NZ	2.43	0.43
1:A:122:SER:HB3	1:A:155:HIS:NE2	2.33	0.43
1:B:1010:ILE:HD11	1:B:1040:PHE:CD2	2.54	0.43
1:C:1010:ILE:HD12	1:C:1010:ILE:N	2.34	0.43
1:C:1041:ARG:HD2	1:C:1042:ALA:O	2.18	0.43
1:D:69:GLU:HB3	1:D:71:LYS:HD2	1.99	0.43
1:D:56:ASN:HB2	1:D:242:PHE:CE1	2.54	0.43
1:D:125:HIS:ND1	1:D:153:ASP:OD2	2.44	0.43
1:C:1043:SER:O	1:C:1053:THR:HG23	2.19	0.43
1:D:263:LEU:HD23	1:D:276:VAL:HG22	2.01	0.43
1:A:100:PRO:HB3	1:A:273:TRP:CD1	2.54	0.43
1:B:192:ARG:HD2	3:B:1101:HOH:O	2.19	0.43
1:B:762:ASP:HA	1:B:765:LYS:HD2	2.01	0.43
1:B:830:PHE:O	1:B:861:ASP:HA	2.19	0.43
1:B:931:ALA:HB1	1:B:934:ALA:CB	2.47	0.43
1:C:1056:LEU:HA	1:C:1068:VAL:O	2.19	0.43
1:A:229:GLN:O	1:A:229:GLN:HG2	2.19	0.43
1:D:955:LYS:HG3	1:D:979:ASP:HB3	2.01	0.43
1:D:1026:ILE:O	1:D:1068:VAL:HA	2.18	0.43
1:D:1029:VAL:HB	1:D:1067:TRP:HB2	2.01	0.43
1:A:704:ARG:HE	1:A:704:ARG:HB2	1.75	0.42
1:B:155:HIS:C	1:B:157:PRO:HD3	2.44	0.42
1:B:629:PRO:O	1:B:632:VAL:CG2	2.67	0.42
1:B:778:SER:O	1:B:795:SER:HB3	2.19	0.42
1:A:614:PHE:CZ	1:A:616:GLY:HA3	2.54	0.42
1:B:324:TRP:CE2	1:B:335:LEU:HD11	2.52	0.42
1:C:484:ASN:HA	1:C:485:PRO:HD3	1.90	0.42
1:D:105:VAL:HG22	1:D:262:PRO:HG3	2.01	0.42
1:D:808:ASN:HD22	1:D:828:GLN:HB3	1.83	0.42
1:D:986:VAL:HG22	1:D:1011:TRP:HB2	2.00	0.42
1:A:302:GLN:NE2	3:A:1262:HOH:O	2.49	0.42
1:B:862:TYR:CD1	1:B:884:SER:HB3	2.55	0.42
1:B:957:ASN:ND2	1:B:958:ARG:HG3	2.34	0.42
1:C:923:ASN:O	1:C:924:ILE:HG13	2.19	0.42
1:C:1057:SER:O	1:C:1068:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:SER:HA	3:A:1233:HOH:O	2.18	0.42
1:B:618:LEU:HD13	1:B:624:VAL:HG21	2.01	0.42
1:B:783:ASN:ND2	1:B:800:SER:OG	2.53	0.42
1:C:364[B]:ASN:CG	1:D:385:ASN:HD22	2.27	0.42
1:D:314:PHE:CD1	1:D:365:GLY:HA2	2.55	0.42
1:D:344:MET:HG3	1:D:358:LEU:HD11	2.01	0.42
1:D:889:VAL:HG11	1:D:934:ALA:HB2	2.01	0.42
1:A:155:HIS:CD2	1:A:157:PRO:HD3	2.55	0.42
1:A:258:ASP:O	1:A:261:SER:HB3	2.19	0.42
1:A:689:SER:HB2	3:A:1218:HOH:O	2.19	0.42
1:A:925:TRP:CD1	1:A:926:SER:N	2.88	0.42
1:B:890:GLN:O	1:B:891:ASP:HB2	2.19	0.42
1:C:155:HIS:CD2	1:C:157:PRO:HD3	2.54	0.42
1:C:253:TYR:OH	1:C:284:GLY:O	2.36	0.42
1:C:960:ILE:HD12	1:C:1095:PHE:CD2	2.55	0.42
1:A:216:TRP:CZ3	1:A:671:VAL:HG11	2.54	0.42
1:A:480:GLU:HG2	3:A:1426:HOH:O	2.20	0.42
1:C:369:LEU:HD23	1:C:394:SER:HB3	2.02	0.42
1:D:613:LEU:HD21	1:D:615:HIS:CE1	2.54	0.42
1:A:484:ASN:OD1	1:A:484:ASN:C	2.62	0.42
1:A:635:ALA:HA	1:A:654:ARG:HB2	2.01	0.42
1:A:661:PRO:HA	1:A:695:TRP:HA	2.02	0.42
1:B:261:SER:HB2	1:B:262:PRO:HD2	2.02	0.42
1:D:182:LEU:CD1	1:D:225:LEU:O	2.68	0.42
1:A:128:GLY:O	1:A:129:TYR:C	2.60	0.42
1:B:86:LYS:C	1:B:88:GLY:H	2.27	0.42
1:B:116:ASN:HB3	1:B:119:TYR:HB2	2.02	0.42
1:B:396:TRP:CZ2	1:B:398:GLY:HA3	2.55	0.42
1:C:210:MET:HE2	1:C:674:LYS:HB3	2.00	0.42
1:D:196:GLY:HA3	1:D:258:ASP:CG	2.45	0.42
1:D:83:ILE:HG13	1:D:91:VAL:HG22	2.02	0.41
1:D:198:GLN:HE22	1:D:218:THR:HG23	1.82	0.41
1:D:945:MET:HE1	1:D:973:LEU:HB2	2.02	0.41
1:C:401:ILE:HD13	1:C:401:ILE:HG21	1.86	0.41
1:C:613:LEU:HD12	1:C:637:VAL:O	2.19	0.41
1:C:930:ASN:HA	1:C:950:THR:HG22	2.02	0.41
1:C:931:ALA:H	1:C:950:THR:CG2	2.32	0.41
1:D:776:ASN:O	1:D:777:GLN:HB2	2.20	0.41
1:A:288:ARG:HD2	3:A:1459:HOH:O	2.20	0.41
1:B:743:ASN:O	1:B:746:GLN:HG2	2.19	0.41
1:C:918:PHE:HA	1:C:924:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:ILE:HD12	1:D:421:LEU:HD11	2.02	0.41
1:D:957:ASN:O	1:D:958:ARG:C	2.61	0.41
1:A:675:LEU:HD13	1:A:683:VAL:HG21	2.03	0.41
1:B:136:ASP:OD2	1:B:136:ASP:C	2.62	0.41
1:C:108:GLU:HG2	1:C:133:SER:HB2	2.03	0.41
1:C:890:GLN:O	1:C:891:ASP:HB2	2.21	0.41
1:C:1013:ASN:OD1	1:C:1015:LEU:CD2	2.67	0.41
1:D:202:ASP:OD1	1:D:206:GLN:HB3	2.21	0.41
1:A:361:GLN:O	1:A:386:TYR:OH	2.27	0.41
1:A:390:THR:CG2	1:A:394:SER:H	2.34	0.41
1:B:986:VAL:HG22	1:B:1011:TRP:HB2	2.02	0.41
1:C:131:ASN:HA	1:C:141:TYR:O	2.21	0.41
1:C:907:LEU:C	1:C:908:THR:O	2.63	0.41
1:D:981:VAL:O	1:D:982:GLN:C	2.64	0.41
1:C:1098:GLU:C	1:C:1098:GLU:CD	2.88	0.41
1:D:742:LYS:HB2	1:D:751:THR:HB	2.02	0.41
1:A:340:THR:CG2	1:A:341:THR:N	2.84	0.41
1:A:390:THR:OG1	1:A:413:VAL:HG22	2.21	0.41
1:C:1010:ILE:HD11	1:C:1040:PHE:HB3	2.02	0.41
1:A:391:SER:HB2	1:B:508:GLN:HE22	1.86	0.41
1:B:457:LYS:HG2	3:B:1408:HOH:O	2.21	0.41
1:A:93:THR:HG23	1:A:95:ASP:OD2	2.20	0.41
1:A:390:THR:HG21	1:A:394:SER:N	2.35	0.41
1:A:808:ASN:HD22	1:A:828:GLN:HB3	1.85	0.41
1:B:85:ASN:HB3	1:B:89:GLU:H	1.86	0.41
1:B:645:SER:O	1:B:703:ASP:HB2	2.21	0.41
1:B:666:TYR:OH	1:B:746:GLN:NE2	2.54	0.41
1:A:255:GLU:OE1	1:A:285:ALA:HA	2.20	0.41
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.93	0.41
1:B:1035:THR:O	1:B:1065:LYS:CE	2.69	0.41
1:D:639:ASP:O	1:D:660:HIS:HB2	2.20	0.41
1:D:877:VAL:HG21	1:D:883:LEU:HD22	2.03	0.41
1:D:1013:ASN:HD21	1:D:1015:LEU:HD23	1.85	0.41
1:A:930:ASN:HD22	1:A:932:PRO:HD3	1.85	0.40
1:B:874:ARG:HD3	1:B:894:THR:HB	2.02	0.40
1:B:921:TYR:CD1	1:B:1092:TYR:HD2	2.40	0.40
1:D:707:LEU:HD22	1:D:710:THR:HG21	2.02	0.40
1:A:525:ARG:CG	1:A:526:ALA:N	2.84	0.40
1:B:161:LYS:NZ	1:B:398:GLY:O	2.40	0.40
1:B:322:LEU:HD23	1:B:337:GLN:HB3	2.03	0.40
1:B:457:LYS:HE3	1:B:457:LYS:HB2	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PHE:O	1:C:303:LYS:HG2	2.22	0.40
1:C:808:ASN:ND2	1:C:829:SER:H	2.19	0.40
1:A:239:GLY:HA2	1:A:253:TYR:HB2	2.03	0.40
1:B:99:MET:SD	1:B:100:PRO:HD2	2.60	0.40
1:B:941:THR:O	1:B:959:THR:HG23	2.21	0.40
1:C:148:ASN:HA	1:C:155:HIS:HB3	2.03	0.40
1:D:143:ILE:HG23	1:D:157:PRO:HB3	2.04	0.40
1:D:768:PHE:CD1	1:D:768:PHE:C	3.00	0.40
1:D:866:TRP:CE2	1:D:883:LEU:HD11	2.55	0.40
1:B:922:ARG:HB2	3:B:1475:HOH:O	2.22	0.40
1:C:124:LYS:HE2	1:C:152:LEU:O	2.22	0.40
1:C:189:VAL:CG2	1:C:191:TYR:CE1	3.05	0.40
1:C:742:LYS:HB2	1:C:751:THR:HB	2.03	0.40
1:B:959:THR:O	1:B:983:SER:HB3	2.21	0.40
1:C:400:GLY:HA2	3:C:1:HOH:O	2.20	0.40
1:D:56:ASN:OD1	1:D:56:ASN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	966/975 (99%)	898 (93%)	55 (6%)	13 (1%)	9	8
1	B	966/975 (99%)	900 (93%)	61 (6%)	5 (0%)	24	27
1	C	945/975 (97%)	876 (93%)	63 (7%)	6 (1%)	21	23
1	D	938/975 (96%)	870 (93%)	60 (6%)	8 (1%)	14	14
All	All	3815/3900 (98%)	3544 (93%)	239 (6%)	32 (1%)	16	16

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	GLY
1	A	1022	ASP
1	C	85	ASN
1	D	85	ASN
1	A	85	ASN
1	A	320	GLY
1	A	531	ASP
1	B	203	SER
1	B	318	GLU
1	C	1073	GLN
1	C	1085	ALA
1	A	318	GLU
1	A	510	LYS
1	A	840	ASP
1	A	969	PRO
1	A	1061	GLU
1	B	630	GLU
1	B	891	ASP
1	D	908	THR
1	B	85	ASN
1	D	982	GLN
1	D	1050	SER
1	D	1091	SER
1	D	460	VAL
1	A	328	SER
1	C	1099	VAL
1	A	439	GLY
1	D	1099	VAL
1	A	424	ILE
1	C	969	PRO
1	D	893	GLY
1	C	458	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	785/787 (100%)	729 (93%)	56 (7%)	13	16
1	B	785/787 (100%)	713 (91%)	72 (9%)	8	9
1	C	772/787 (98%)	716 (93%)	56 (7%)	13	15
1	D	767/787 (98%)	711 (93%)	56 (7%)	13	15
All	All	3109/3148 (99%)	2869 (92%)	240 (8%)	12	13

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	75	ARG
1	A	106	ASP
1	A	172	THR
1	A	182	LEU
1	A	186	ARG
1	A	192	ARG
1	A	203	SER
1	A	209	LYS
1	A	210	MET
1	A	222	VAL
1	A	235	SER
1	A	245	LYS
1	A	274	VAL
1	A	315	ARG
1	A	325	SER
1	A	335	LEU
1	A	352	LEU
1	A	391	SER
1	A	392	ASN
1	A	408	SER
1	A	459	GLN
1	A	460	VAL
1	A	480	GLU
1	A	483	VAL
1	A	523	ASP
1	A	630	GLU
1	A	650	GLN
1	A	684	LEU
1	A	699	SER
1	A	710	THR
1	A	722	THR
1	A	731	VAL

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Mol	Chain	Res	Type
1	A	737	ARG
1	A	746	GLN
1	A	797	VAL
1	A	803	SER
1	A	808	ASN
1	A	839	SER
1	A	857	LEU
1	A	869	LYS
1	A	877	VAL
1	A	882	MET
1	A	955	LYS
1	A	968	SER
1	A	987	MET
1	A	991	LEU
1	A	1016	LYS
1	A	1021	LYS
1	A	1044	THR
1	A	1053	THR
1	A	1056	LEU
1	A	1059	ARG
1	A	1064	LYS
1	A	1087	PHE
1	A	1096	ILE
1	B	70	ASN
1	B	75	ARG
1	B	83	ILE
1	B	91	VAL
1	B	106	ASP
1	B	144	VAL
1	B	151	SER
1	B	186	ARG
1	B	192	ARG
1	B	203	SER
1	B	222	VAL
1	B	234	ILE
1	B	259	SER
1	B	274	VAL
1	B	276	VAL
1	B	302	GLN
1	B	318	GLU
1	B	325	SER
1	B	337	GLN

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Mol	Chain	Res	Type
1	B	339	THR
1	B	341	THR
1	B	352	LEU
1	B	391	SER
1	B	392	ASN
1	B	408	SER
1	B	460	VAL
1	B	478	THR
1	B	480	GLU
1	B	488	VAL
1	B	497	LEU
1	B	510	LYS
1	B	522	VAL
1	B	630	GLU
1	B	632	VAL
1	B	671	VAL
1	B	675	LEU
1	B	689	SER
1	B	699	SER
1	B	704	ARG
1	B	710	THR
1	B	731	VAL
1	B	737	ARG
1	B	742	LYS
1	B	746	GLN
1	B	766	SER
1	B	783	ASN
1	B	797	VAL
1	B	803	SER
1	B	808	ASN
1	B	813	SER
1	B	818	LEU
1	B	829	SER
1	B	839	SER
1	B	851	GLU
1	B	869	LYS
1	B	906	ASP
1	B	945	MET
1	B	953	ASN
1	B	955	LYS
1	B	987	MET
1	B	989	THR

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Mol	Chain	Res	Type
1	B	991	LEU
1	B	1004	THR
1	B	1021	LYS
1	B	1023	THR
1	B	1044	THR
1	B	1046	VAL
1	B	1053	THR
1	B	1064	LYS
1	B	1073	GLN
1	B	1087	PHE
1	B	1099	VAL
1	C	54	THR
1	C	70	ASN
1	C	75	ARG
1	C	85	ASN
1	C	87	GLN
1	C	91	VAL
1	C	106	ASP
1	C	123	VAL
1	C	144	VAL
1	C	172	THR
1	C	186	ARG
1	C	192	ARG
1	C	202	ASP
1	C	203	SER
1	C	208	THR
1	C	218	THR
1	C	222	VAL
1	C	234	ILE
1	C	235	SER
1	C	276	VAL
1	C	291	ASN
1	C	300	ILE
1	C	312	VAL
1	C	318	GLU
1	C	329	SER
1	C	339	THR
1	C	352	LEU
1	C	384	ASP
1	C	417	LYS
1	C	477	LEU
1	C	504	LEU

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Mol	Chain	Res	Type
1	C	522	VAL
1	C	649	THR
1	C	671	VAL
1	C	678	SER
1	C	704	ARG
1	C	766	SER
1	C	796	THR
1	C	803	SER
1	C	808	ASN
1	C	842	THR
1	C	851	GLU
1	C	909	LEU
1	C	910	GLN
1	C	912	GLN
1	C	919	ASN
1	C	938	MET
1	C	959	THR
1	C	987	MET
1	C	993	LYS
1	C	1044	THR
1	C	1045	ARG
1	C	1047	VAL
1	C	1051	ASP
1	C	1055	ILE
1	C	1064	LYS
1	D	54	THR
1	D	70	ASN
1	D	75	ARG
1	D	83	ILE
1	D	87	GLN
1	D	89	GLU
1	D	91	VAL
1	D	106	ASP
1	D	132	VAL
1	D	144	VAL
1	D	182	LEU
1	D	184	LYS
1	D	192	ARG
1	D	200	ILE
1	D	208	THR
1	D	210	MET
1	D	222	VAL

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Mol	Chain	Res	Type
1	D	235	SER
1	D	236	THR
1	D	274	VAL
1	D	276	VAL
1	D	297	LEU
1	D	300	ILE
1	D	312	VAL
1	D	339	THR
1	D	340	THR
1	D	459	GLN
1	D	480	GLU
1	D	522	VAL
1	D	684	LEU
1	D	693	GLU
1	D	699	SER
1	D	702	PHE
1	D	707	LEU
1	D	737	ARG
1	D	742	LYS
1	D	746	GLN
1	D	808	ASN
1	D	820	LYS
1	D	857	LEU
1	D	897	LEU
1	D	906	ASP
1	D	909	LEU
1	D	910	GLN
1	D	912	GLN
1	D	959	THR
1	D	963	PHE
1	D	987	MET
1	D	989	THR
1	D	1001	LYS
1	D	1026	ILE
1	D	1055	ILE
1	D	1059	ARG
1	D	1068	VAL
1	D	1091	SER
1	D	1098	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	148	ASN
1	A	198	GLN
1	A	206	GLN
1	A	271	ASN
1	A	291	ASN
1	A	302	GLN
1	A	350	ASN
1	A	385	ASN
1	A	432	GLN
1	A	451	ASN
1	A	709	ASN
1	A	728	ASN
1	A	746	GLN
1	A	794	ASN
1	A	808	ASN
1	A	912	GLN
1	A	930	ASN
1	A	1089	HIS
1	A	1100	ASN
1	B	80	ASN
1	B	87	GLN
1	B	131	ASN
1	B	348	GLN
1	B	368	ASN
1	B	410	ASN
1	B	432	GLN
1	B	451	ASN
1	B	467	ASN
1	B	686	GLN
1	B	721	ASN
1	B	769	ASN
1	B	781	ASN
1	B	783	ASN
1	B	793	ASN
1	B	808	ASN
1	B	876	ASN
1	B	957	ASN
1	B	1006	HIS
1	B	1008	ASN
1	B	1020	ASN
1	B	1100	ASN
1	C	57	ASN

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Mol	Chain	Res	Type
1	C	80	ASN
1	C	85	ASN
1	C	148	ASN
1	C	174	GLN
1	C	350	ASN
1	C	368	ASN
1	C	410	ASN
1	C	412	GLN
1	C	451	ASN
1	C	621	ASN
1	C	725	GLN
1	C	781	ASN
1	C	794	ASN
1	C	808	ASN
1	C	912	GLN
1	C	919	ASN
1	C	946	ASN
1	C	957	ASN
1	C	964	ASN
1	C	992	ASN
1	C	1000	ASN
1	C	1013	ASN
1	D	85	ASN
1	D	131	ASN
1	D	350	ASN
1	D	385	ASN
1	D	410	ASN
1	D	412	GLN
1	D	432	GLN
1	D	453	GLN
1	D	743	ASN
1	D	794	ASN
1	D	808	ASN
1	D	957	ASN
1	D	992	ASN
1	D	1073	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	970/975 (99%)	0.02	22 (2%) 61 58	13, 31, 53, 66	4 (0%)
1	B	970/975 (99%)	0.01	21 (2%) 62 59	13, 30, 53, 70	2 (0%)
1	C	952/975 (97%)	0.03	19 (1%) 65 62	14, 32, 54, 69	3 (0%)
1	D	948/975 (97%)	0.02	25 (2%) 57 54	15, 32, 54, 65	4 (0%)
All	All	3840/3900 (98%)	0.02	87 (2%) 61 58	13, 31, 54, 70	13 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	633	THR	10.5
1	D	966	GLY	7.2
1	B	633	THR	6.0
1	D	1049	PHE	5.8
1	C	967	THR	5.0
1	A	632	VAL	5.0
1	C	1049	PHE	4.7
1	C	966	GLY	4.3
1	C	968	SER	4.3
1	B	967	THR	3.8
1	A	318	GLU	3.7
1	B	321	ALA	3.7
1	A	390	THR	3.6
1	B	1049	PHE	3.5
1	C	991	LEU	3.4
1	B	632	VAL	3.4
1	D	971	THR	3.3
1	A	316	THR	3.2
1	A	968	SER	3.1
1	C	1074	VAL	3.1
1	D	1088	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	970	PHE	3.0
1	D	905	PRO	3.0
1	B	634	GLY	2.9
1	A	532	TYR	2.8
1	D	89	GLU	2.8
1	C	909	LEU	2.7
1	C	969	PRO	2.7
1	D	1084	ALA	2.7
1	D	611	GLY	2.7
1	C	1084	ALA	2.7
1	A	1049	PHE	2.7
1	A	1023	THR	2.7
1	A	478	THR	2.6
1	B	677	ALA	2.6
1	C	1087	PHE	2.6
1	C	1050	SER	2.6
1	C	1088	MET	2.5
1	C	905	PRO	2.5
1	C	611	GLY	2.5
1	A	363	GLN	2.5
1	D	1074	VAL	2.5
1	D	1025	ASP	2.5
1	B	611	GLY	2.5
1	B	1022	ASP	2.4
1	A	907	LEU	2.4
1	A	1053	THR	2.4
1	C	1044	THR	2.4
1	A	366	GLN	2.4
1	D	1011	TRP	2.4
1	D	523	ASP	2.3
1	B	1079	GLY	2.3
1	A	317	SER	2.3
1	B	318	GLU	2.3
1	D	231	GLY	2.3
1	A	391	SER	2.3
1	D	991	LEU	2.2
1	B	1100	ASN	2.2
1	B	631	GLY	2.2
1	A	611	GLY	2.2
1	A	321	ALA	2.2
1	D	909	LEU	2.2
1	C	1052	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	205	GLY	2.2
1	A	339	THR	2.2
1	D	1003	ALA	2.2
1	B	629	PRO	2.1
1	D	318	GLU	2.1
1	A	394	SER	2.1
1	D	989	THR	2.1
1	D	882	MET	2.1
1	A	368	ASN	2.1
1	B	1081	GLY	2.1
1	B	532	TYR	2.1
1	D	1027	PRO	2.1
1	B	1048	GLY	2.1
1	D	1050	SER	2.1
1	B	966	GLY	2.1
1	B	316	THR	2.0
1	C	882	MET	2.0
1	B	392	ASN	2.0
1	B	907	LEU	2.0
1	D	1026	ILE	2.0
1	C	1027	PRO	2.0
1	D	1072	TYR	2.0
1	A	1099	VAL	2.0
1	D	1090	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	CA	A	1200	1/1	0.99	0.03	22,22,22,22	0
2	CA	B	1200	1/1	0.99	0.02	19,19,19,19	0
2	CA	C	1200	1/1	0.99	0.02	19,19,19,19	0
2	CA	D	1200	1/1	0.99	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.