



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:15 PM UTC

PDB ID : 1ECQ / pdb_00001ecq
Title : E. COLI GLUCARATE DEHYDRATASE BOUND TO 4-DEOXYGLUCARATE
Authors : Gulick, A.M.; Hubbard, B.K.; Gerlt, J.A.; Rayment, I.
Deposited on : 2000-01-25
Resolution : 2.00 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

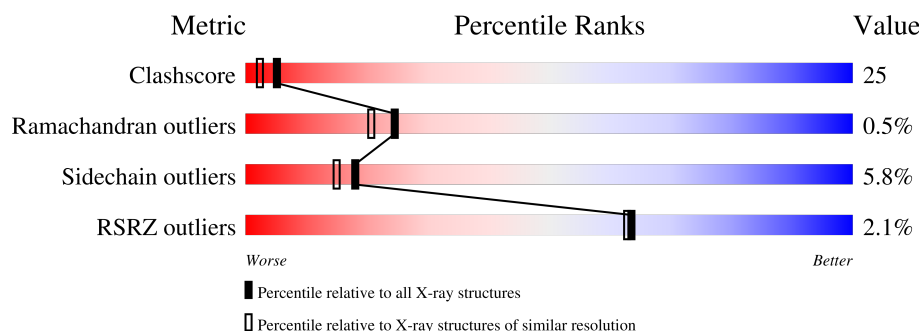
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	446	3% 60% 34% 5%
1	B	446	% 52% 41% 6%
1	C	446	2% 63% 33%
1	D	446	3% 56% 37% 6%

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	DXG	D	502	-	-	X	-
4	IPA	C	604	-	-	X	-

2 Entry composition [i](#)

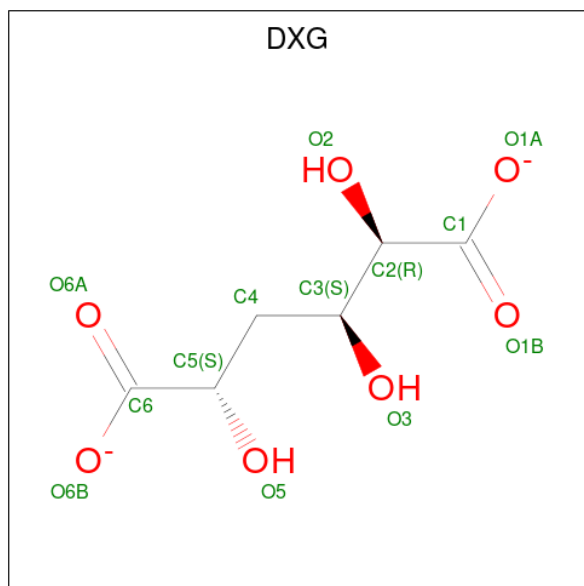
There are 5 unique types of molecules in this entry. The entry contains 14643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCARATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3436	2171	602	642	21			
1	B	442	Total	C	N	O	S	0	0	0
			3408	2153	598	636	21			
1	C	443	Total	C	N	O	S	0	1	0
			3421	2161	599	640	21			
1	D	442	Total	C	N	O	S	0	0	0
			3405	2153	595	636	21			

- Molecule 2 is 4-DEOXYGLUCARATE (CCD ID: DXG) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

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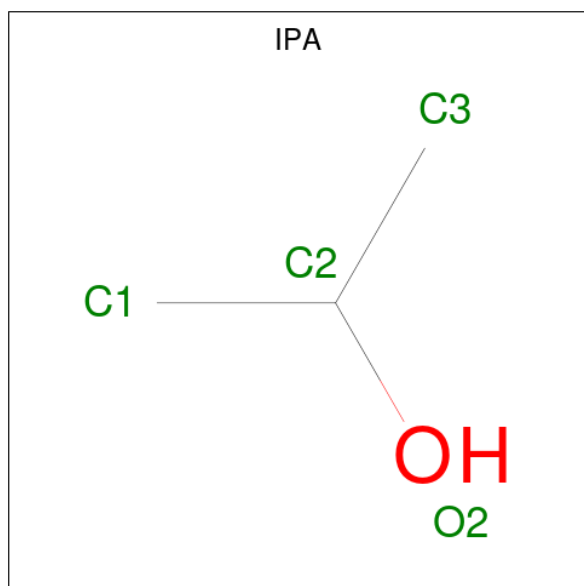
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	C	1	Total	C	O	0	0
			4	3	1		

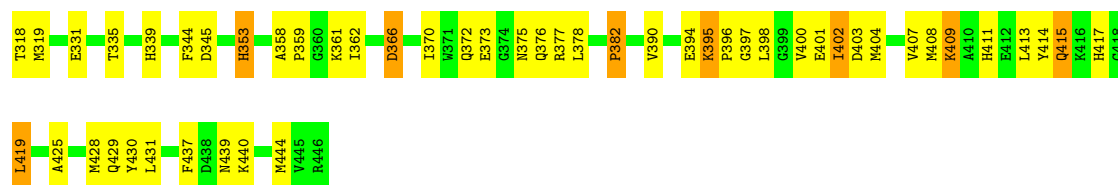
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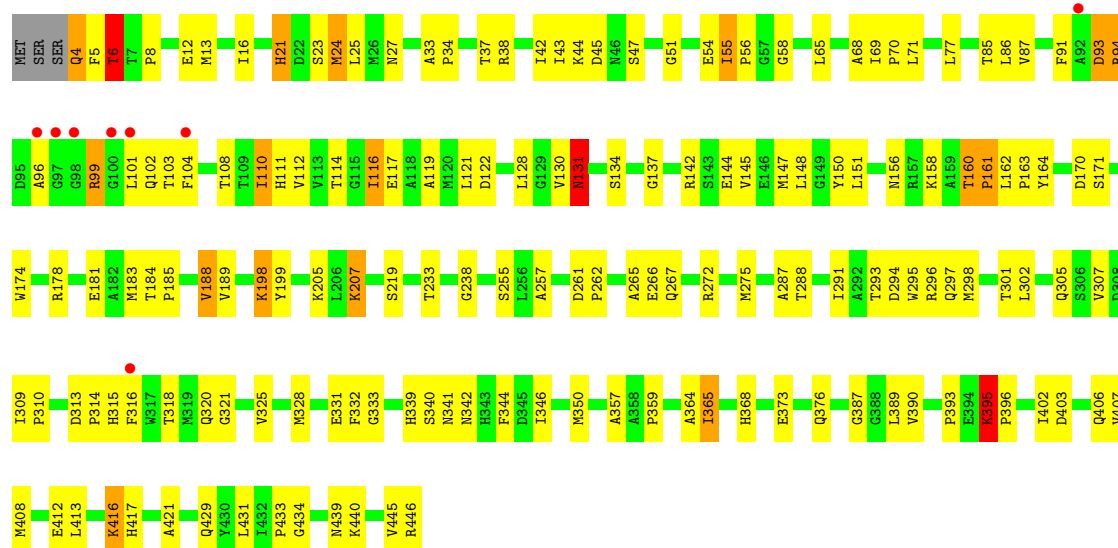
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is water.

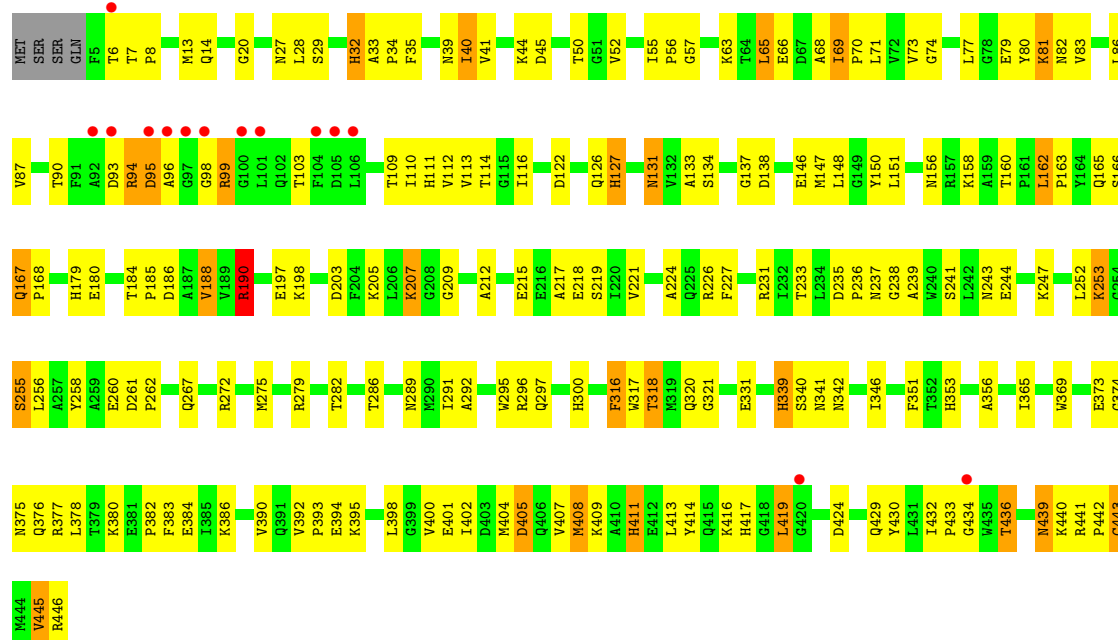
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	229	Total	O		0	0
			229	229			
5	B	168	Total	O		0	0
			168	168			
5	C	276	Total	O		0	0
			276	276			
5	D	228	Total	O		0	0
			228	228			



• Molecule 1: GLUCARATE DEHYDRATASE



• Molecule 1: GLUCARATE DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.11Å 84.60Å 98.78Å 103.46° 93.97° 113.03°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 93.8 (30.00-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.01Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.209 , 0.305 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 99.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, MG, DXG

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	1.29	4/3515 (0.1%)	1.49	22/4763 (0.5%)
1	B	1.18	2/3486 (0.1%)	1.46	18/4725 (0.4%)
1	C	1.29	2/3500 (0.1%)	1.48	23/4746 (0.5%)
1	D	1.28	2/3484 (0.1%)	1.53	33/4724 (0.7%)
All	All	1.26	10/13985 (0.1%)	1.49	96/18958 (0.5%)

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	D	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	190	ARG	NE-CZ	14.20	1.48	1.33
1	D	190	ARG	CD-NE	6.19	1.54	1.46
1	A	184	THR	C-O	6.03	1.29	1.24
1	B	21	HIS	CA-C	-5.78	1.45	1.52
1	C	389	LEU	CA-C	-5.37	1.46	1.52
1	A	146	GLU	N-CA	-5.29	1.39	1.46
1	B	189	VAL	CA-CB	-5.23	1.48	1.54
1	A	319	MET	N-CA	-5.23	1.40	1.46
1	C	183	MET	CA-C	-5.12	1.46	1.53
1	A	13	MET	C-N	-5.11	1.27	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	VAL	CB-CA-C	9.53	123.35	111.25
1	B	202	ASN	N-CA-C	-8.51	103.03	113.41
1	C	94	ARG	N-CA-C	8.41	123.27	112.34
1	D	227	PHE	CA-C-N	8.20	127.92	119.56
1	D	227	PHE	C-N-CA	8.20	127.92	119.56
1	A	163	PRO	CB-CA-C	-8.03	102.37	112.89
1	D	80	TYR	N-CA-C	8.02	120.73	111.11
1	C	365	ILE	N-CA-CB	-7.96	101.86	110.53
1	C	163	PRO	N-CA-CB	7.83	107.96	102.79
1	D	98	GLY	CA-C-N	7.77	130.55	120.44
1	D	98	GLY	C-N-CA	7.77	130.55	120.44
1	B	366	ASP	CA-CB-CG	7.77	120.37	112.60
1	D	351	PHE	N-CA-C	7.36	120.17	111.71
1	D	395	LYS	CA-C-N	7.24	127.29	119.90
1	D	395	LYS	C-N-CA	7.24	127.29	119.90
1	D	190	ARG	CD-NE-CZ	-7.07	114.51	124.40
1	C	393	PRO	N-CA-CB	7.05	109.48	103.35
1	D	127	HIS	CA-CB-CG	-6.95	106.85	113.80
1	A	167	GLN	CA-C-N	6.74	127.29	119.47
1	A	167	GLN	C-N-CA	6.74	127.29	119.47
1	D	167	GLN	CA-C-N	6.70	128.21	119.84
1	D	167	GLN	C-N-CA	6.70	128.21	119.84
1	D	411	HIS	CA-CB-CG	-6.53	107.28	113.80
1	B	92	ALA	N-CA-C	6.49	118.36	111.28
1	A	300	HIS	CA-CB-CG	-6.48	107.32	113.80
1	D	318	THR	N-CA-CB	6.45	121.39	110.49
1	D	351	PHE	N-CA-CB	6.45	120.15	110.22
1	A	424	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	395	LYS	CA-C-N	6.31	126.28	119.78
1	B	395	LYS	C-N-CA	6.31	126.28	119.78
1	C	395	LYS	CA-C-N	6.29	126.30	119.89
1	C	395	LYS	C-N-CA	6.29	126.30	119.89
1	A	95	ASP	CA-CB-CG	6.26	118.86	112.60
1	D	7	THR	N-CA-C	-6.19	101.77	110.31
1	C	6	THR	N-CA-C	6.13	119.63	109.46
1	C	257	ALA	N-CA-C	-5.96	104.86	111.36
1	A	368	HIS	N-CA-C	-5.94	106.07	113.38
1	B	411	HIS	CA-CB-CG	-5.94	107.86	113.80
1	B	289	ASN	N-CA-C	-5.94	103.57	112.54
1	C	387	GLY	N-CA-C	-5.92	105.17	114.10
1	C	364	ALA	CA-C-N	5.88	129.78	121.66
1	C	364	ALA	C-N-CA	5.88	129.78	121.66
1	C	350	MET	CA-C-N	-5.84	110.91	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	MET	C-N-CA	-5.84	110.91	121.14
1	D	316	PHE	N-CA-CB	5.84	119.43	110.61
1	B	167	GLN	CA-C-N	5.74	125.59	119.28
1	B	167	GLN	C-N-CA	5.74	125.59	119.28
1	D	93	ASP	N-CA-C	5.71	118.24	111.33
1	A	395	LYS	CA-C-N	5.70	125.65	119.78
1	A	395	LYS	C-N-CA	5.70	125.65	119.78
1	A	444	MET	CA-C-N	-5.70	115.25	122.43
1	A	444	MET	C-N-CA	-5.70	115.25	122.43
1	B	153	PHE	N-CA-C	-5.70	100.00	109.46
1	C	93	ASP	CA-C-N	5.63	129.70	120.63
1	C	93	ASP	C-N-CA	5.63	129.70	120.63
1	C	96	ALA	N-CA-C	5.61	117.26	111.03
1	B	353	HIS	CA-CB-CG	-5.59	108.21	113.80
1	B	211	LEU	CB-CA-C	-5.54	101.84	112.43
1	B	201	PHE	N-CA-C	5.50	118.32	110.24
1	A	422	ARG	N-CA-C	5.49	117.98	110.24
1	A	153	PHE	N-CA-C	-5.49	102.36	110.48
1	A	232	ILE	N-CA-C	5.49	116.64	108.46
1	C	145	VAL	N-CA-C	5.46	115.75	108.11
1	D	365	ILE	CB-CA-C	-5.42	103.02	111.26
1	D	316	PHE	CB-CA-C	5.40	119.29	110.17
1	B	184	THR	O-C-N	5.39	125.16	121.71
1	C	21	HIS	CA-CB-CG	-5.38	108.42	113.80
1	D	289	ASN	N-CA-C	-5.35	104.74	113.19
1	D	94	ARG	N-CA-C	5.34	119.28	112.34
1	A	163	PRO	N-CA-CB	5.33	105.98	102.25
1	B	382	PRO	N-CA-CB	5.33	107.99	103.19
1	C	56	PRO	N-CA-CB	5.32	107.79	103.32
1	A	127	HIS	CA-CB-CG	-5.31	108.49	113.80
1	D	383	PHE	CA-C-N	-5.28	114.52	122.81
1	D	383	PHE	C-N-CA	-5.28	114.52	122.81
1	A	340	SER	N-CA-C	5.26	117.19	109.24
1	D	45	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	202	ASN	N-CA-C	-5.22	107.03	113.41
1	D	395	LYS	N-CA-C	5.22	117.28	110.08
1	B	253	LYS	N-CA-C	5.21	117.38	111.02
1	B	72	VAL	N-CA-C	5.20	116.29	111.45
1	D	32	HIS	CA-CB-CG	-5.19	108.61	113.80
1	D	445	VAL	N-CA-C	5.19	115.09	107.15
1	D	300	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	351	PHE	N-CA-C	5.16	117.81	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ALA	N-CA-C	5.16	116.71	111.14
1	C	170	ASP	N-CA-C	5.13	117.53	110.35
1	D	393	PRO	N-CA-CB	5.12	107.80	103.35
1	C	131	ASN	CA-CB-CG	5.12	117.72	112.60
1	C	433	PRO	N-CA-CB	5.09	107.77	103.19
1	D	419	LEU	N-CA-C	5.08	116.88	110.33
1	A	8	PRO	N-CA-C	5.07	119.02	111.41
1	B	240	TRP	N-CA-C	5.07	117.65	110.50
1	D	433	PRO	O-C-N	5.07	128.78	123.10
1	C	421	ALA	N-CA-CB	5.03	118.09	110.45
1	A	307	VAL	N-CA-CB	-5.00	103.24	111.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	351	PHE	CA

There are no planarity outliers.

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	3436	0	3368	169	0
1	B	3408	0	3332	201	0
1	C	3421	0	3333	150	0
1	D	3405	0	3318	172	0
2	A	13	0	8	5	0
2	B	13	0	8	3	0
2	C	13	0	8	4	0
2	D	13	0	8	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	8	0	0
4	B	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	8	5	0
4	D	4	0	8	1	0
5	A	229	0	0	9	0
5	B	168	0	0	11	0
5	C	276	0	0	12	0
5	D	228	0	0	10	0
All	All	14643	0	13415	667	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 25.

All (667) 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:339:HIS:NE2	2:C:501:DXG:H51	1.66	1.11
1:B:287:ALA:HB1	1:B:311:LEU:HD21	1.29	1.10
1:B:24:MET:HG2	1:B:26:MET:HE3	1.35	1.07
1:A:339:HIS:NE2	2:A:499:DXG:H51	1.70	1.07
1:A:26:MET:HE2	1:A:444:MET:HE2	1.32	1.06
1:B:339:HIS:NE2	2:B:500:DXG:H51	1.76	0.99
1:B:55:ILE:HB	1:B:56:PRO:HD2	1.45	0.98
1:A:414:TYR:HA	1:A:419:LEU:HD12	1.45	0.97
1:B:293:THR:H	1:B:297:GLN:NE2	1.66	0.94
1:B:293:THR:H	1:B:297:GLN:HE21	1.01	0.93
1:A:240:TRP:HB3	1:A:244:GLU:HG3	1.51	0.91
1:D:122:ASP:O	1:D:126:GLN:HG3	1.70	0.90
1:A:60:LYS:HZ2	1:A:94:ARG:HD3	1.38	0.89
1:A:293:THR:H	1:A:297:GLN:HE21	1.21	0.87
1:B:156:ASN:HB2	1:B:181:GLU:OE2	1.74	0.86
1:D:66:GLU:O	1:D:69:ILE:HG13	1.76	0.86
1:B:24:MET:HG2	1:B:26:MET:CE	2.05	0.86
1:A:417:HIS:HB2	1:A:419:LEU:HD11	1.59	0.85
1:A:60:LYS:NZ	1:A:94:ARG:HD3	1.91	0.85
1:C:150:TYR:CZ	1:C:205:LYS:HE2	2.11	0.84
1:C:16:ILE:HD13	1:C:408:MET:HE1	1.58	0.84
1:A:293:THR:H	1:A:297:GLN:NE2	1.75	0.83
1:B:151:LEU:CD1	1:B:223:LEU:HD21	2.08	0.83
1:B:339:HIS:CD2	2:B:500:DXG:H51	2.14	0.81
1:D:253:LYS:HE2	1:D:282:THR:O	1.80	0.81
1:A:267:GLN:NE2	5:A:1498:HOH:O	2.12	0.81
1:C:293:THR:H	1:C:297:GLN:NE2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:HD23	1:D:116:ILE:HD11	1.63	0.81
1:B:294:ASP:OD1	1:B:297:GLN:HG3	1.81	0.81
1:D:339:HIS:HE2	2:D:502:DXG:H51	1.46	0.80
1:A:55:ILE:HB	1:A:56:PRO:HD2	1.64	0.80
1:B:188:VAL:O	1:B:191:LEU:HB2	1.81	0.80
5:A:1815:HOH:O	1:C:85:THR:HG22	1.80	0.80
1:A:8:PRO:HG3	1:A:47:SER:HB3	1.63	0.79
1:A:147:MET:HG2	1:A:365:ILE:HG13	1.65	0.79
1:D:339:HIS:NE2	2:D:502:DXG:H51	1.97	0.79
1:D:185:PRO:HA	1:D:188:VAL:CG2	2.12	0.79
1:B:415:GLN:NE2	1:B:415:GLN:HA	1.99	0.77
1:A:346:ILE:HD11	1:A:402:ILE:HD13	1.66	0.77
1:C:205:LYS:HG3	1:C:233:THR:HG23	1.67	0.77
1:B:313:ASP:HB3	1:B:316:PHE:CE1	2.20	0.76
1:C:205:LYS:HG3	1:C:233:THR:CG2	2.16	0.76
1:B:14:GLN:OE1	1:B:16:ILE:HD11	1.87	0.75
1:B:221:VAL:O	1:B:225:GLN:HG3	1.87	0.75
1:C:407:VAL:HG12	1:C:408:MET:HE2	1.69	0.75
1:B:33:ALA:HB1	1:B:34:PRO:HD2	1.69	0.75
1:B:218:GLU:HB3	5:B:1454:HOH:O	1.85	0.75
1:B:24:MET:HE2	1:B:431:LEU:HD11	1.67	0.74
1:B:409:LYS:HD3	1:B:409:LYS:N	2.00	0.74
1:C:313:ASP:HB3	1:C:316:PHE:CE1	2.22	0.74
1:C:339:HIS:CD2	2:C:501:DXG:H51	2.22	0.74
1:A:21:HIS:H	1:A:376:GLN:HE22	1.35	0.74
1:B:401:GLU:HG2	5:B:1750:HOH:O	1.86	0.74
1:D:186:ASP:O	1:D:190:ARG:HD3	1.87	0.74
1:A:67:ASP:O	1:A:70:PRO:HD2	1.88	0.73
1:A:147:MET:HE2	1:A:365:ILE:HD11	1.70	0.73
1:A:26:MET:HE2	1:A:444:MET:CE	2.16	0.73
1:A:147:MET:HG2	1:A:365:ILE:CG1	2.17	0.73
1:C:4:GLN:HB2	5:C:1892:HOH:O	1.87	0.73
1:B:68:ALA:C	1:B:70:PRO:HD2	2.14	0.73
1:B:404:MET:HA	1:B:407:VAL:CG2	2.19	0.73
1:C:313:ASP:HB3	1:C:316:PHE:CD1	2.24	0.72
1:D:417:HIS:HB2	1:D:419:LEU:CD1	2.19	0.72
1:C:293:THR:H	1:C:297:GLN:HE21	1.35	0.72
1:A:99:ARG:HG3	1:A:105:ASP:OD2	1.89	0.71
1:A:4:GLN:HA	1:C:4:GLN:N	2.05	0.71
1:A:416:LYS:HD3	1:A:417:HIS:CE1	2.25	0.71
1:D:405:ASP:O	1:D:409:LYS:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD11	1:A:430:TYR:CE1	2.25	0.71
1:B:262:PRO:HD2	1:B:275:MET:SD	2.31	0.71
1:C:267:GLN:NE2	5:C:1401:HOH:O	2.24	0.71
1:A:142:ARG:NH1	1:A:362:ILE:HG12	2.06	0.70
1:A:142:ARG:HH12	1:A:362:ILE:HG12	1.56	0.70
1:D:95:ASP:N	1:D:95:ASP:OD2	2.24	0.70
1:C:185:PRO:HA	1:C:188:VAL:CG1	2.20	0.69
1:B:55:ILE:HB	1:B:56:PRO:CD	2.21	0.69
1:B:226:ARG:HD2	1:B:226:ARG:O	1.92	0.69
1:A:313:ASP:HB3	1:A:316:PHE:CE1	2.27	0.69
1:A:380:LYS:HD2	1:A:401:GLU:HB3	1.74	0.69
1:B:26:MET:HE1	1:B:31:ALA:CB	2.23	0.69
1:A:7:THR:HG21	1:C:128:LEU:HD23	1.74	0.69
1:A:168:PRO:HD2	5:A:1356:HOH:O	1.93	0.69
1:A:348:LEU:CD2	1:A:383:PHE:HB2	2.23	0.69
1:B:39:ASN:ND2	1:B:57:GLY:HA2	2.08	0.68
1:B:59:GLU:OE2	1:B:62:ARG:NE	2.25	0.68
1:A:7:THR:HG21	1:C:128:LEU:HA	1.75	0.68
1:A:71:LEU:HD22	1:A:86:LEU:HD21	1.75	0.68
1:A:205:LYS:NZ	1:A:366:ASP:OD2	2.22	0.68
1:D:203:ASP:OD1	1:D:231:ARG:HB2	1.94	0.68
1:D:384:GLU:HB2	1:D:386:LYS:HE2	1.76	0.68
1:A:103:THR:O	2:A:499:DXG:H42	1.93	0.68
1:C:294:ASP:OD1	1:C:297:GLN:HG3	1.94	0.68
1:D:55:ILE:HB	1:D:56:PRO:CD	2.24	0.68
1:D:417:HIS:CB	1:D:419:LEU:HG	2.24	0.68
1:B:311:LEU:N	1:B:311:LEU:HD22	2.08	0.68
1:B:265:ALA:O	1:B:266:GLU:HB3	1.94	0.68
1:C:185:PRO:HA	1:C:188:VAL:HG12	1.76	0.67
1:D:346:ILE:HD11	1:D:402:ILE:HD13	1.75	0.67
1:B:147:MET:HE3	1:B:390:VAL:HG21	1.76	0.67
1:A:262:PRO:HD2	1:A:275:MET:SD	2.34	0.67
1:A:415:GLN:O	1:A:418:GLY:N	2.22	0.67
1:A:241:SER:H	1:A:244:GLU:CG	2.07	0.67
1:C:21:HIS:H	1:C:376:GLN:HE22	1.40	0.67
1:A:207:LYS:HE2	1:A:237:ASN:OD1	1.94	0.67
1:B:24:MET:CE	1:B:431:LEU:HD11	2.24	0.67
1:B:71:LEU:HD13	1:B:86:LEU:HG	1.75	0.67
1:A:55:ILE:HD11	1:A:65:LEU:HD11	1.75	0.66
1:A:310:PRO:HG2	1:A:329:CYS:SG	2.36	0.66
1:D:407:VAL:HG12	1:D:408:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:PHE:CG	1:B:378:LEU:HD11	2.30	0.66
1:D:133:ALA:H	1:D:353:HIS:HD2	1.40	0.66
1:B:415:GLN:HA	1:B:415:GLN:HE21	1.60	0.66
1:B:404:MET:HA	1:B:407:VAL:HG22	1.77	0.66
1:A:378:LEU:O	1:A:402:ILE:HD12	1.96	0.66
1:D:68:ALA:C	1:D:70:PRO:HD2	2.21	0.66
1:C:188:VAL:HG11	1:C:219:SER:OG	1.95	0.66
1:A:241:SER:H	1:A:244:GLU:HG2	1.60	0.65
1:A:105:ASP:OD1	1:A:107:ARG:HB2	1.97	0.65
1:B:99:ARG:HG3	1:B:105:ASP:OD2	1.97	0.65
1:D:339:HIS:CD2	2:D:502:DXG:H51	2.31	0.65
1:B:28:LEU:HG	1:B:437:PHE:HE2	1.60	0.65
1:B:26:MET:HE1	1:B:31:ALA:HB1	1.79	0.65
1:B:122:ASP:OD2	1:B:398:LEU:HD12	1.96	0.65
1:D:243:ASN:ND2	5:D:1883:HOH:O	2.29	0.65
1:B:167:GLN:O	1:B:176:ARG:HB2	1.97	0.65
1:B:107:ARG:NH2	5:B:1085:HOH:O	2.15	0.64
1:A:205:LYS:HD2	5:A:1727:HOH:O	1.96	0.64
1:A:209:GLY:O	1:A:442:PRO:HA	1.97	0.64
1:B:293:THR:N	1:B:297:GLN:HE21	1.85	0.64
1:A:26:MET:CE	1:A:444:MET:HE2	2.18	0.64
1:A:414:TYR:CA	1:A:419:LEU:HD12	2.25	0.64
1:D:378:LEU:O	1:D:402:ILE:HD12	1.97	0.64
1:D:33:ALA:HB1	1:D:34:PRO:HD2	1.78	0.64
1:B:226:ARG:HG3	1:B:227:PHE:CD1	2.32	0.64
1:B:108:THR:O	1:B:112:VAL:HG23	1.98	0.64
1:B:344:PHE:CD1	1:B:378:LEU:HD11	2.31	0.64
1:C:68:ALA:C	1:C:70:PRO:HD2	2.23	0.63
1:D:27:ASN:OD1	1:D:29:SER:N	2.30	0.63
1:C:340:SER:HB2	5:C:1573:HOH:O	1.97	0.63
1:B:157:ARG:NH2	1:B:180:GLU:OE1	2.25	0.63
1:D:185:PRO:HA	1:D:188:VAL:HG22	1.80	0.63
1:A:21:HIS:H	1:A:376:GLN:NE2	1.97	0.63
1:A:429:GLN:OE1	1:A:429:GLN:HA	1.97	0.63
1:B:59:GLU:OE1	1:B:62:ARG:NH2	2.27	0.62
1:D:404:MET:HE3	1:D:408:MET:HE3	1.80	0.62
1:C:12:GLU:HG3	1:C:44:LYS:HB2	1.81	0.62
1:D:205:LYS:HE3	1:D:260:GLU:OE1	1.99	0.62
1:B:172:CYS:HB3	1:B:175:TYR:HB2	1.81	0.62
1:A:34:PRO:HD3	1:A:164:TYR:CZ	2.34	0.62
1:B:417:HIS:HB2	1:B:419:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ASP:CG	1:B:398:LEU:HD12	2.25	0.62
1:B:417:HIS:HB2	1:B:419:LEU:CD1	2.30	0.62
1:A:109:THR:O	1:A:113:VAL:HG23	2.00	0.62
1:A:338:SER:HB3	5:A:1372:HOH:O	2.00	0.62
1:A:405:ASP:O	1:A:409:LYS:HD3	2.00	0.62
1:A:219:SER:O	1:A:223:LEU:HD12	2.00	0.61
1:A:104:PHE:CE1	1:A:106:LEU:HD21	2.36	0.61
1:B:210:VAL:O	1:B:444:MET:HB2	2.00	0.61
1:C:416:LYS:HG2	1:C:417:HIS:CD2	2.34	0.61
1:D:156:ASN:OD1	1:D:158:LYS:HE3	1.99	0.61
1:D:55:ILE:HB	1:D:56:PRO:HD2	1.83	0.61
1:B:151:LEU:HD12	1:B:223:LEU:HD21	1.83	0.61
1:D:316:PHE:HD2	5:D:1377:HOH:O	1.84	0.61
1:B:425:ALA:O	1:B:428:MET:HB2	2.01	0.61
1:B:8:PRO:HB3	1:B:47:SER:HB3	1.82	0.60
1:D:69:ILE:N	1:D:70:PRO:HD2	2.16	0.60
1:C:293:THR:OG1	1:C:297:GLN:NE2	2.34	0.60
1:D:39:ASN:ND2	1:D:57:GLY:HA2	2.16	0.60
1:D:241:SER:N	1:D:244:GLU:OE1	2.27	0.60
1:D:404:MET:CE	1:D:408:MET:HE3	2.32	0.60
1:B:168:PRO:HD2	5:B:1451:HOH:O	2.01	0.60
1:C:8:PRO:HB3	1:C:47:SER:HB3	1.82	0.60
1:C:156:ASN:HB2	1:C:181:GLU:OE1	2.02	0.60
1:C:58:GLY:HA3	5:C:1097:HOH:O	2.00	0.60
1:B:287:ALA:HB1	1:B:311:LEU:CD2	2.19	0.60
1:A:14:GLN:HB3	5:A:1609:HOH:O	2.01	0.60
1:A:150:TYR:OH	1:A:205:LYS:HE2	2.02	0.60
1:B:161:PRO:HG2	1:B:430:TYR:CE2	2.37	0.60
1:B:288:THR:H	1:B:311:LEU:HD23	1.67	0.60
1:B:233:THR:HA	1:B:256:LEU:HD22	1.82	0.59
1:C:160:THR:HB	1:C:161:PRO:HD2	1.83	0.59
1:A:440:LYS:HE3	5:A:1628:HOH:O	2.01	0.59
1:B:226:ARG:HG3	1:B:227:PHE:CE1	2.38	0.59
1:D:8:PRO:HD3	1:D:127:HIS:CE1	2.38	0.59
1:D:408:MET:O	1:D:411:HIS:HB3	2.03	0.59
1:C:205:LYS:HD2	5:C:1001:HOH:O	2.02	0.59
1:B:55:ILE:CB	1:B:56:PRO:HD2	2.28	0.58
1:C:117:GLU:OE1	1:C:320:GLN:HG3	2.02	0.58
1:A:168:PRO:HD2	1:A:169:ASP:H	1.67	0.58
1:B:267:GLN:OE1	5:B:1833:HOH:O	2.17	0.58
1:A:348:LEU:HD23	1:A:383:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:MET:O	1:C:412:GLU:HG3	2.04	0.58
1:A:184:THR:O	1:A:187:ALA:HB3	2.03	0.58
1:C:287:ALA:HA	1:C:309:ILE:O	2.04	0.58
1:A:13:MET:HA	1:A:42:ILE:O	2.04	0.58
1:B:33:ALA:HB1	1:B:34:PRO:CD	2.33	0.58
1:A:184:THR:O	1:A:188:VAL:N	2.29	0.58
1:A:365:ILE:HA	5:A:1503:HOH:O	2.03	0.58
1:C:34:PRO:HG3	1:C:162:LEU:HB3	1.85	0.58
1:D:411:HIS:O	1:D:414:TYR:HB3	2.03	0.58
1:D:436:THR:HG22	5:D:1708:HOH:O	2.03	0.58
1:B:13:MET:HE3	1:B:116:ILE:HD11	1.85	0.58
1:A:241:SER:N	1:A:244:GLU:HG2	2.19	0.57
1:D:162:LEU:HD11	1:D:430:TYR:CE2	2.39	0.57
1:D:217:ALA:O	1:D:221:VAL:HG23	2.04	0.57
1:B:205:LYS:HG3	1:B:233:THR:CG2	2.35	0.57
1:A:55:ILE:HB	1:A:56:PRO:CD	2.32	0.57
1:B:27:ASN:HD22	1:B:27:ASN:N	2.03	0.57
1:B:288:THR:N	1:B:311:LEU:HD23	2.20	0.57
1:C:65:LEU:HG	1:C:112:VAL:HG13	1.87	0.57
1:C:150:TYR:OH	1:C:205:LYS:HE2	2.03	0.57
1:D:247:LYS:NZ	5:D:1782:HOH:O	2.37	0.57
1:A:41:VAL:C	1:A:42:ILE:HG13	2.29	0.57
1:A:238:GLY:N	1:A:261:ASP:O	2.35	0.57
1:C:445:VAL:O	1:C:446:ARG:HD3	2.04	0.57
1:C:332:PHE:CD2	4:C:604:IPA:H12	2.40	0.57
1:D:339:HIS:HD2	2:D:502:DXG:O6B	1.87	0.57
1:D:417:HIS:HB2	1:D:419:LEU:HD11	1.85	0.57
1:A:339:HIS:NE2	2:A:499:DXG:C5	2.57	0.56
1:C:373:GLU:OE2	5:C:1868:HOH:O	2.18	0.56
1:A:442:PRO:HG2	1:A:445:VAL:HG11	1.86	0.56
1:C:267:GLN:NE2	1:D:296:ARG:HH12	2.03	0.56
1:C:429:GLN:OE1	1:C:434:GLY:N	2.37	0.56
1:B:65:LEU:CD2	1:B:116:ILE:HD11	2.35	0.56
1:B:288:THR:H	1:B:311:LEU:CD2	2.17	0.56
1:C:151:LEU:N	1:C:205:LYS:O	2.35	0.56
1:B:344:PHE:CB	1:B:378:LEU:HD12	2.36	0.56
1:A:101:LEU:HD13	1:A:439:ASN:ND2	2.20	0.56
1:A:267:GLN:NE2	1:B:296:ARG:HH12	2.02	0.55
1:D:218:GLU:OE2	1:D:218:GLU:HA	2.06	0.55
1:D:394:GLU:OE2	1:D:394:GLU:HA	2.05	0.55
1:B:273:GLU:O	1:B:277:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:O	5:C:1663:HOH:O	2.17	0.55
1:A:21:HIS:N	1:A:376:GLN:HE22	2.04	0.55
1:A:99:ARG:CG	1:A:105:ASP:OD2	2.55	0.55
1:A:162:LEU:HD11	1:A:430:TYR:HE1	1.72	0.55
1:D:207:LYS:HE2	1:D:237:ASN:ND2	2.22	0.55
1:A:409:LYS:HD2	1:A:409:LYS:N	2.22	0.55
1:D:185:PRO:O	1:D:188:VAL:HG23	2.06	0.55
1:A:150:TYR:CZ	1:A:205:LYS:HE2	2.41	0.55
1:B:81:LYS:NZ	1:D:137:GLY:O	2.38	0.55
1:B:85:THR:CG2	1:D:138:ASP:HB3	2.36	0.55
1:A:348:LEU:HD21	1:A:383:PHE:HB2	1.88	0.55
1:B:185:PRO:O	1:B:188:VAL:N	2.40	0.55
1:A:365:ILE:HG13	1:A:365:ILE:O	2.06	0.55
1:C:238:GLY:N	1:C:261:ASP:O	2.37	0.55
1:C:294:ASP:HB2	5:C:1434:HOH:O	2.06	0.55
1:B:184:THR:O	1:B:188:VAL:HG23	2.07	0.54
1:B:331:GLU:HB3	1:D:295:TRP:HB3	1.89	0.54
1:C:307:VAL:HG12	1:C:310:PRO:HD3	1.88	0.54
1:D:69:ILE:N	1:D:70:PRO:CD	2.70	0.54
1:D:203:ASP:CG	1:D:231:ARG:HB2	2.32	0.54
1:C:403:ASP:HB3	1:C:406:GLN:HB2	1.88	0.54
1:D:166:SER:HA	1:D:179:HIS:CG	2.42	0.54
1:A:103:THR:HG22	1:A:237:ASN:CG	2.32	0.54
1:A:253:LYS:HE2	1:A:282:THR:O	2.07	0.54
1:D:86:LEU:C	1:D:86:LEU:HD23	2.33	0.54
1:C:24:MET:HE1	1:C:431:LEU:HD21	1.89	0.54
4:C:604:IPA:H11	5:C:1572:HOH:O	2.06	0.54
1:A:205:LYS:HG3	1:A:233:THR:HG23	1.90	0.54
1:D:162:LEU:HB3	1:D:163:PRO:HD2	1.89	0.54
1:A:200:GLY:HA3	1:A:387:GLY:HA2	1.90	0.54
1:D:384:GLU:HB2	1:D:386:LYS:CE	2.37	0.54
1:D:207:LYS:HE2	1:D:237:ASN:HD21	1.73	0.53
1:B:178:ARG:NH1	1:B:370:ILE:O	2.41	0.53
1:B:344:PHE:HB3	1:B:378:LEU:HD12	1.90	0.53
1:C:91:PHE:HD1	1:C:94:ARG:CZ	2.21	0.53
1:D:272:ARG:HA	1:D:291:ILE:HD12	1.89	0.53
1:B:122:ASP:O	1:B:126:GLN:HG3	2.09	0.53
1:B:344:PHE:CG	1:B:378:LEU:CD1	2.91	0.53
1:C:13:MET:HE1	1:C:116:ILE:HD11	1.90	0.53
1:D:79:GLU:O	1:D:83:VAL:HG23	2.08	0.53
1:B:192:ALA:HB2	1:B:223:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HG21	1:C:315:HIS:HA	1.90	0.53
1:A:411:HIS:O	1:A:414:TYR:HB3	2.08	0.53
1:D:41:VAL:O	1:D:52:VAL:HA	2.09	0.53
1:C:346:ILE:HD11	1:C:402:ILE:CD1	2.39	0.53
1:D:65:LEU:HD23	1:D:116:ILE:CD1	2.36	0.53
1:B:377:ARG:HB2	1:B:382:PRO:HG3	1.90	0.53
1:D:148:LEU:HD12	1:D:148:LEU:C	2.34	0.53
1:A:414:TYR:HA	1:A:419:LEU:CD1	2.30	0.52
1:A:202:ASN:O	1:A:230:ALA:HB1	2.10	0.52
1:B:86:LEU:O	1:B:86:LEU:HD12	2.09	0.52
1:B:95:ASP:OD2	1:B:107:ARG:HB3	2.09	0.52
1:C:131:ASN:ND2	1:C:134:SER:OG	2.42	0.52
1:D:233:THR:HA	1:D:256:LEU:HD22	1.91	0.52
1:D:238:GLY:N	1:D:261:ASP:O	2.40	0.52
1:A:437:PHE:CE2	1:A:439:ASN:HB3	2.44	0.52
1:D:63:LYS:O	1:D:66:GLU:HB3	2.10	0.52
1:D:162:LEU:HD11	1:D:430:TYR:HE2	1.75	0.52
1:D:417:HIS:HB2	1:D:419:LEU:HG	1.91	0.52
1:D:445:VAL:C	1:D:446:ARG:HG2	2.34	0.52
1:A:261:ASP:N	1:A:262:PRO:HD3	2.25	0.52
1:C:267:GLN:HE22	1:D:296:ARG:HH12	1.56	0.52
1:D:111:HIS:CE1	1:D:316:PHE:HB3	2.45	0.52
1:D:35:PHE:CD1	1:D:413:LEU:HD21	2.45	0.52
1:A:403:ASP:HB3	1:A:406:GLN:HB2	1.91	0.52
1:C:207:LYS:HE3	1:C:207:LYS:HA	1.91	0.52
1:D:236:PRO:HG2	1:D:262:PRO:HA	1.91	0.52
1:B:12:GLU:HB2	1:B:44:LYS:HG3	1.92	0.52
1:A:24:MET:HG3	1:A:164:TYR:CZ	2.45	0.51
1:D:375:ASN:OD1	1:D:376:GLN:HG3	2.11	0.51
1:B:43:ILE:HD12	1:B:119:ALA:HB3	1.92	0.51
1:B:147:MET:CE	1:B:390:VAL:HG21	2.38	0.51
1:B:398:LEU:HB2	1:B:400:VAL:HG22	1.93	0.51
1:D:39:ASN:C	1:D:40:ILE:HD13	2.34	0.51
1:D:110:ILE:CG2	1:D:111:HIS:N	2.73	0.51
1:D:131:ASN:C	1:D:131:ASN:HD22	2.18	0.51
1:B:293:THR:OG1	1:B:297:GLN:NE2	2.43	0.51
1:B:376:GLN:OE1	5:B:1443:HOH:O	2.19	0.51
1:C:429:GLN:OE1	1:C:429:GLN:HA	2.11	0.51
1:D:133:ALA:H	1:D:353:HIS:CD2	2.26	0.51
1:A:17:PRO:HG3	1:A:62:ARG:HD3	1.93	0.51
1:B:402:ILE:HG13	1:B:403:ASP:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:PRO:HD2	1:D:260:GLU:O	2.10	0.51
1:A:105:ASP:OD2	1:A:107:ARG:NH2	2.44	0.51
1:B:148:LEU:C	1:B:148:LEU:HD12	2.35	0.51
1:C:162:LEU:HB2	1:C:164:TYR:CE1	2.45	0.51
1:D:429:GLN:OE1	1:D:434:GLY:N	2.40	0.51
1:A:29:SER:OG	1:A:102:GLN:NE2	2.43	0.51
1:A:83:VAL:O	1:A:87:VAL:HG23	2.11	0.51
1:A:105:ASP:OD1	1:A:107:ARG:N	2.43	0.51
1:A:27:ASN:OD1	1:A:29:SER:HB2	2.11	0.51
1:A:292:ALA:HA	1:A:297:GLN:HB3	1.92	0.50
1:B:35:PHE:CD1	1:B:413:LEU:HD21	2.46	0.50
1:B:242:LEU:HD11	1:B:246:ILE:HD11	1.91	0.50
1:B:287:ALA:HA	1:B:309:ILE:O	2.10	0.50
1:C:147:MET:HE3	1:C:390:VAL:HG21	1.93	0.50
1:B:17:PRO:HB2	1:B:414:TYR:CD1	2.47	0.50
1:D:184:THR:O	1:D:188:VAL:HG22	2.11	0.50
1:A:4:GLN:CA	1:C:4:GLN:N	2.72	0.50
1:A:417:HIS:HB2	1:A:419:LEU:CD1	2.38	0.50
1:B:26:MET:HE1	1:B:31:ALA:HB2	1.92	0.50
1:C:110:ILE:CG2	1:C:111:HIS:N	2.74	0.50
1:D:86:LEU:C	1:D:86:LEU:CD2	2.84	0.50
1:B:91:PHE:O	1:B:94:ARG:HG3	2.12	0.50
1:C:21:HIS:H	1:C:376:GLN:NE2	2.07	0.50
1:A:309:ILE:HA	1:A:335:THR:O	2.12	0.50
1:B:24:MET:CG	1:B:26:MET:CE	2.86	0.50
1:C:111:HIS:HD2	1:C:315:HIS:O	1.94	0.50
1:A:273:GLU:O	1:A:277:GLU:HG3	2.11	0.50
1:A:8:PRO:HD3	1:C:5:PHE:HD2	1.77	0.49
1:B:17:PRO:HB2	1:B:414:TYR:CE1	2.47	0.49
1:B:73:VAL:HG12	1:B:74:GLY:N	2.27	0.49
1:C:321:GLY:O	1:C:325:VAL:HG23	2.12	0.49
1:C:346:ILE:HD11	1:C:402:ILE:HD13	1.95	0.49
1:D:73:VAL:HG12	1:D:74:GLY:N	2.26	0.49
1:D:417:HIS:HB2	1:D:419:LEU:CG	2.41	0.49
1:A:184:THR:O	1:A:188:VAL:HG12	2.13	0.49
1:A:415:GLN:O	1:A:416:LYS:C	2.55	0.49
1:B:117:GLU:CD	1:B:319:MET:HB2	2.38	0.49
1:B:261:ASP:N	1:B:262:PRO:HD3	2.26	0.49
1:A:7:THR:CG2	1:C:128:LEU:HD23	2.41	0.49
1:B:103:THR:HG22	1:B:237:ASN:CG	2.37	0.49
1:B:214:GLU:O	1:B:217:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HB3	4:C:604:IPA:H32	1.93	0.49
1:C:13:MET:HE1	1:C:116:ILE:CD1	2.42	0.49
1:C:341:ASN:O	1:C:342:ASN:C	2.56	0.49
1:B:407:VAL:HG23	1:B:408:MET:N	2.27	0.49
1:C:69:ILE:N	1:C:70:PRO:CD	2.75	0.49
1:A:437:PHE:CZ	1:A:439:ASN:HB3	2.48	0.49
1:B:26:MET:CE	1:B:31:ALA:CB	2.91	0.49
1:B:309:ILE:HA	1:B:335:THR:O	2.12	0.49
1:D:73:VAL:CG1	1:D:74:GLY:N	2.75	0.49
1:D:150:TYR:CZ	1:D:205:LYS:NZ	2.78	0.49
1:A:43:ILE:HD12	1:A:119:ALA:HB3	1.95	0.49
1:B:69:ILE:N	1:B:70:PRO:CD	2.76	0.49
1:D:71:LEU:HD13	1:D:86:LEU:HD22	1.94	0.49
1:A:185:PRO:HA	1:A:188:VAL:CG1	2.42	0.49
1:C:68:ALA:O	1:C:71:LEU:HB2	2.13	0.49
1:A:261:ASP:N	1:A:262:PRO:CD	2.76	0.48
1:D:8:PRO:CD	1:D:127:HIS:ND1	2.76	0.48
1:C:198:LYS:O	1:C:198:LYS:HG3	2.11	0.48
1:D:262:PRO:HD2	1:D:275:MET:SD	2.54	0.48
1:D:292:ALA:HA	1:D:297:GLN:HB3	1.95	0.48
1:A:260:GLU:C	1:A:262:PRO:HD3	2.39	0.48
1:B:80:TYR:O	1:B:84:LEU:HG	2.13	0.48
1:C:275:MET:HG3	1:C:291:ILE:HD13	1.95	0.48
1:D:445:VAL:O	1:D:446:ARG:HD3	2.14	0.48
1:C:99:ARG:HD2	1:C:293:THR:HG21	1.95	0.48
1:C:93:ASP:OD1	1:C:94:ARG:HG3	2.14	0.48
1:D:110:ILE:HG23	1:D:111:HIS:N	2.28	0.48
1:D:205:LYS:HD2	5:D:1012:HOH:O	2.14	0.48
1:C:23:SER:O	1:C:25:LEU:HG	2.14	0.48
1:C:332:PHE:CD2	4:C:604:IPA:C1	2.96	0.48
1:D:65:LEU:HG	1:D:112:VAL:HG13	1.94	0.48
1:D:109:THR:O	1:D:113:VAL:HG23	2.13	0.48
1:A:110:ILE:HD12	1:A:110:ILE:HA	1.75	0.48
1:A:168:PRO:CD	1:A:169:ASP:H	2.26	0.48
1:D:20:GLY:O	1:D:35:PHE:HA	2.14	0.48
1:D:218:GLU:HB3	5:D:1783:HOH:O	2.13	0.48
1:C:174:TRP:O	1:C:178:ARG:HG2	2.14	0.48
1:D:417:HIS:CB	1:D:419:LEU:CG	2.90	0.48
1:A:260:GLU:O	1:A:261:ASP:C	2.57	0.48
1:B:185:PRO:HB3	1:B:219:SER:HA	1.96	0.48
1:B:13:MET:CE	1:B:116:ILE:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:OG1	1:B:318:THR:HA	2.14	0.47
1:C:185:PRO:O	1:C:189:VAL:HG23	2.14	0.47
1:A:39:ASN:C	1:A:40:ILE:HD13	2.39	0.47
1:C:198:LYS:HG2	1:C:199:TYR:CE1	2.50	0.47
1:D:190:ARG:HD3	1:D:190:ARG:N	2.29	0.47
1:B:311:LEU:N	1:B:311:LEU:CD2	2.76	0.47
1:C:357:ALA:O	1:C:359:PRO:HD3	2.14	0.47
1:D:377:ARG:HB2	1:D:382:PRO:HG3	1.95	0.47
1:A:60:LYS:NZ	1:A:94:ARG:CD	2.72	0.47
1:A:317:TRP:O	1:A:318:THR:OG1	2.29	0.47
1:C:440:LYS:HE3	5:C:1428:HOH:O	2.15	0.47
1:D:167:GLN:N	1:D:168:PRO:HD3	2.29	0.47
1:D:212:ALA:O	1:D:215:GLU:HB3	2.15	0.47
1:B:295:TRP:HB3	1:D:331:GLU:HB3	1.95	0.47
1:C:160:THR:CB	1:C:161:PRO:CD	2.92	0.47
1:D:28:LEU:CD1	1:D:442:PRO:HA	2.44	0.47
1:D:111:HIS:HE1	1:D:316:PHE:HB3	1.78	0.47
1:A:313:ASP:CB	1:A:316:PHE:CE1	2.96	0.47
1:A:438:ASP:OD2	1:A:438:ASP:C	2.58	0.47
1:B:19:ALA:HA	1:B:36:PHE:O	2.13	0.47
1:B:85:THR:HG21	1:D:138:ASP:HB3	1.95	0.47
1:B:190:ARG:HA	1:B:190:ARG:HD3	1.61	0.47
1:C:160:THR:HB	1:C:161:PRO:CD	2.45	0.47
1:C:265:ALA:O	1:C:266:GLU:HB3	2.15	0.47
1:D:147:MET:HE3	1:D:390:VAL:HG21	1.96	0.47
1:B:37:THR:HG22	1:B:414:TYR:HD2	1.79	0.47
1:B:170:ASP:OD1	1:B:172:CYS:N	2.35	0.47
1:B:298:MET:O	1:B:302:LEU:HG	2.14	0.47
1:D:353:HIS:HE1	1:D:398:LEU:O	1.97	0.47
1:A:320:GLN:HG2	5:A:1013:HOH:O	2.13	0.46
1:B:86:LEU:HD12	1:B:86:LEU:C	2.40	0.46
1:B:211:LEU:HD13	1:B:215:GLU:OE1	2.15	0.46
1:C:102:GLN:HG3	1:C:104:PHE:CZ	2.50	0.46
1:C:148:LEU:C	1:C:148:LEU:HD12	2.40	0.46
1:D:275:MET:HG3	1:D:291:ILE:HD13	1.97	0.46
1:A:73:VAL:HG12	1:A:74:GLY:N	2.31	0.46
1:B:207:LYS:HE3	1:B:207:LYS:HA	1.97	0.46
1:B:404:MET:CA	1:B:407:VAL:HG22	2.43	0.46
1:C:339:HIS:CD2	2:C:501:DXG:C5	2.96	0.46
1:A:138:ASP:O	1:C:85:THR:HG21	2.15	0.46
1:D:320:GLN:HG2	5:D:1054:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HA	1:A:163:PRO:HD3	1.84	0.46
1:B:404:MET:C	1:B:407:VAL:HG22	2.41	0.46
1:D:8:PRO:CD	1:D:127:HIS:CE1	2.98	0.46
1:D:99:ARG:HD3	5:D:1897:HOH:O	2.15	0.46
1:D:198:LYS:HD2	1:D:198:LYS:O	2.16	0.46
1:A:104:PHE:CE1	1:A:106:LEU:CD2	2.98	0.46
1:B:361:LYS:HE2	1:B:362:ILE:O	2.16	0.46
1:B:21:HIS:N	1:B:21:HIS:CD2	2.84	0.46
1:B:288:THR:O	1:B:311:LEU:HD23	2.14	0.46
1:C:110:ILE:HD12	1:C:110:ILE:HA	1.68	0.46
1:C:184:THR:O	1:C:188:VAL:HG12	2.15	0.46
1:D:148:LEU:HD12	1:D:148:LEU:O	2.16	0.46
1:D:224:ALA:HB2	1:D:255:SER:HB3	1.97	0.46
1:B:24:MET:HE1	1:B:431:LEU:HD21	1.97	0.46
1:B:331:GLU:HG2	5:B:1599:HOH:O	2.16	0.46
1:C:130:VAL:O	1:C:396:PRO:HA	2.16	0.46
1:D:339:HIS:HD2	2:D:502:DXG:C6	2.29	0.46
1:D:86:LEU:HD23	1:D:86:LEU:O	2.15	0.46
1:B:137:GLY:HA2	5:B:1330:HOH:O	2.16	0.46
1:B:232:ILE:CG2	1:B:233:THR:N	2.79	0.46
1:D:339:HIS:CD2	2:D:502:DXG:C6	2.99	0.46
1:D:353:HIS:O	1:D:356:ALA:HB3	2.16	0.46
1:A:313:ASP:HB3	1:A:316:PHE:CD1	2.51	0.45
1:A:34:PRO:HG3	1:A:162:LEU:HB3	1.98	0.45
1:A:293:THR:N	1:A:297:GLN:HE21	2.02	0.45
1:C:37:THR:C	1:C:38:ARG:HG2	2.41	0.45
1:C:43:ILE:HD12	1:C:119:ALA:HB3	1.99	0.45
1:C:101:LEU:HD23	1:C:101:LEU:HA	1.77	0.45
1:C:261:ASP:N	1:C:262:PRO:CD	2.79	0.45
1:C:262:PRO:HD2	1:C:275:MET:SD	2.56	0.45
1:B:375:ASN:OD1	1:B:376:GLN:HG3	2.16	0.45
1:B:404:MET:HA	1:B:407:VAL:HG21	1.97	0.45
1:D:83:VAL:O	1:D:87:VAL:HG23	2.16	0.45
1:D:252:LEU:O	1:D:253:LYS:C	2.55	0.45
1:B:66:GLU:O	1:B:69:ILE:HG13	2.15	0.45
1:B:183:MET:HE3	1:B:183:MET:HB3	1.62	0.45
1:C:131:ASN:ND2	1:C:134:SER:H	2.13	0.45
1:C:147:MET:CE	1:C:390:VAL:HG21	2.46	0.45
1:A:110:ILE:CG2	1:A:111:HIS:N	2.79	0.45
1:B:39:ASN:C	1:B:40:ILE:HD13	2.42	0.45
1:B:395:LYS:HB2	1:B:396:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLN:C	1:B:431:LEU:N	2.74	0.45
1:A:188:VAL:HG11	1:A:219:SER:HB3	1.98	0.45
1:B:132:VAL:HG23	1:B:397:GLY:C	2.42	0.45
1:B:205:LYS:HG3	1:B:233:THR:HG22	1.99	0.45
1:C:288:THR:HG22	1:C:307:VAL:HG21	1.99	0.45
1:D:185:PRO:HB3	1:D:219:SER:HA	1.99	0.45
1:B:24:MET:O	1:B:26:MET:HE3	2.16	0.45
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.75	0.45
1:C:332:PHE:CG	4:C:604:IPA:H12	2.52	0.45
1:A:147:MET:HG2	1:A:365:ILE:HG12	1.99	0.45
1:A:295:TRP:HB3	1:C:331:GLU:HB3	1.99	0.45
1:B:199:TYR:OH	1:B:373:GLU:OE1	2.34	0.45
1:D:29:SER:O	1:D:424:ASP:HB2	2.17	0.45
1:D:190:ARG:N	1:D:190:ARG:CD	2.80	0.45
1:D:439:ASN:C	1:D:440:LYS:HG2	2.42	0.45
1:D:392:VAL:O	5:D:1147:HOH:O	2.21	0.44
1:C:365:ILE:HD12	1:C:365:ILE:HG23	1.78	0.44
1:D:86:LEU:HD23	1:D:90:THR:OG1	2.18	0.44
1:C:185:PRO:CA	1:C:188:VAL:HG12	2.46	0.44
1:D:13:MET:HE1	1:D:116:ILE:CD1	2.48	0.44
1:D:86:LEU:CD2	1:D:90:THR:OG1	2.65	0.44
1:A:68:ALA:O	1:A:69:ILE:C	2.60	0.44
1:A:442:PRO:HG2	1:A:445:VAL:CG1	2.46	0.44
1:C:108:THR:O	1:C:112:VAL:HG23	2.17	0.44
1:D:185:PRO:CA	1:D:188:VAL:HG22	2.48	0.44
1:D:341:ASN:O	1:D:342:ASN:C	2.60	0.44
1:A:231:ARG:C	1:A:232:ILE:HG13	2.41	0.44
1:B:185:PRO:O	1:B:186:ASP:C	2.61	0.44
1:C:296:ARG:HH12	1:D:267:GLN:NE2	2.16	0.44
1:D:131:ASN:ND2	1:D:134:SER:H	2.16	0.44
1:D:165:GLN:HG3	1:D:179:HIS:CE1	2.53	0.44
1:A:142:ARG:NH1	1:A:362:ILE:CG1	2.80	0.44
1:A:426:MET:O	1:A:429:GLN:HB2	2.17	0.44
1:B:211:LEU:HB2	1:B:216:GLU:CG	2.47	0.44
1:B:345:ASP:OD2	1:B:345:ASP:N	2.48	0.44
1:C:33:ALA:HB1	1:C:34:PRO:HD2	1.99	0.44
1:C:54:GLU:OE1	1:C:344:PHE:HB2	2.18	0.44
1:A:39:ASN:ND2	1:A:57:GLY:HA2	2.33	0.44
1:A:77:LEU:O	1:A:80:TYR:HB3	2.16	0.44
1:A:361:LYS:HE2	1:A:362:ILE:O	2.18	0.44
1:A:202:ASN:O	1:A:230:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:THR:O	2:C:501:DXG:H42	2.18	0.44
1:D:114:THR:OG1	1:D:318:THR:HA	2.18	0.44
1:A:339:HIS:CG	1:A:340:SER:N	2.86	0.43
1:C:261:ASP:OD1	1:C:288:THR:OG1	2.34	0.43
1:D:197:GLU:OE1	1:D:197:GLU:HA	2.16	0.43
1:D:233:THR:HG21	1:D:258:TYR:CE2	2.53	0.43
1:D:416:LYS:O	1:D:416:LYS:CG	2.66	0.43
1:C:413:LEU:O	1:C:417:HIS:HD2	2.01	0.43
1:D:103:THR:HG22	1:D:237:ASN:CG	2.43	0.43
1:A:331:GLU:HB3	1:C:295:TRP:HB3	2.00	0.43
1:B:110:ILE:HA	1:B:110:ILE:HD12	1.69	0.43
1:B:114:THR:O	1:B:117:GLU:HB3	2.18	0.43
1:B:233:THR:HA	1:B:256:LEU:CD2	2.47	0.43
1:B:366:ASP:OD2	5:B:1335:HOH:O	2.21	0.43
1:C:86:LEU:O	1:C:87:VAL:C	2.61	0.43
1:A:185:PRO:O	1:A:189:VAL:HG23	2.19	0.43
1:B:68:ALA:C	1:B:70:PRO:CD	2.88	0.43
1:B:398:LEU:CB	1:B:400:VAL:HG22	2.48	0.43
1:C:298:MET:O	1:C:301:THR:HB	2.18	0.43
1:D:417:HIS:C	1:D:419:LEU:N	2.74	0.43
1:A:18:VAL:HB	1:A:410:ALA:HB1	1.99	0.43
1:B:27:ASN:N	1:B:27:ASN:ND2	2.65	0.43
1:A:81:LYS:HD3	1:C:137:GLY:O	2.18	0.43
1:C:288:THR:CG2	1:C:307:VAL:HG21	2.49	0.43
1:D:373:GLU:CD	1:D:374:GLY:N	2.77	0.43
1:A:244:GLU:O	1:A:248:ILE:HG13	2.18	0.43
1:B:232:ILE:HG22	1:B:233:THR:N	2.33	0.43
1:C:131:ASN:C	1:C:131:ASN:HD22	2.27	0.43
1:C:272:ARG:HA	1:C:291:ILE:HD12	2.01	0.43
1:D:27:ASN:OD1	1:D:29:SER:HB2	2.19	0.43
1:B:134:SER:OG	1:D:82:ASN:ND2	2.48	0.43
1:B:8:PRO:HA	1:B:46:ASN:OD1	2.18	0.43
1:B:280:ARG:NH2	1:C:305:GLN:OE1	2.52	0.43
1:B:404:MET:SD	1:B:407:VAL:HG21	2.59	0.43
1:C:130:VAL:C	1:C:396:PRO:HA	2.43	0.43
1:A:346:ILE:HD11	1:A:402:ILE:CD1	2.43	0.42
1:C:51:GLY:HA2	1:C:122:ASP:OD2	2.19	0.42
1:D:13:MET:HB3	1:D:69:ILE:HG23	2.00	0.42
1:A:28:LEU:HD12	1:A:442:PRO:HA	2.01	0.42
1:A:339:HIS:HD2	2:A:499:DXG:O6B	2.02	0.42
1:B:103:THR:O	2:B:500:DXG:H42	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:O	1:D:226:ARG:HG3	2.19	0.42
1:B:156:ASN:OD1	1:B:158:LYS:HB2	2.19	0.42
1:B:375:ASN:OD1	1:B:375:ASN:N	2.52	0.42
1:C:114:THR:O	1:C:117:GLU:HB3	2.19	0.42
1:C:307:VAL:CG1	1:C:310:PRO:HD3	2.49	0.42
1:C:313:ASP:HA	1:C:314:PRO:HD2	1.89	0.42
1:D:50:THR:O	1:D:126:GLN:NE2	2.52	0.42
1:B:13:MET:HA	1:B:42:ILE:O	2.19	0.42
1:B:203:ASP:OD1	1:B:231:ARG:HB2	2.18	0.42
1:D:6:THR:O	1:D:127:HIS:HE1	2.02	0.42
1:D:151:LEU:N	1:D:205:LYS:O	2.48	0.42
1:D:429:GLN:OE1	1:D:429:GLN:HA	2.17	0.42
1:C:102:GLN:NE2	1:C:102:GLN:HA	2.34	0.42
1:D:28:LEU:HD22	1:D:239:ALA:HB2	2.02	0.42
1:A:80:TYR:OH	1:A:81:LYS:HE2	2.19	0.42
1:B:59:GLU:CD	1:B:62:ARG:HE	2.21	0.42
1:B:403:ASP:O	1:B:407:VAL:HG22	2.20	0.42
1:C:23:SER:O	1:C:25:LEU:N	2.46	0.42
1:D:373:GLU:HG2	1:D:374:GLY:H	1.84	0.42
1:D:373:GLU:CG	1:D:374:GLY:N	2.83	0.42
1:A:110:ILE:HG23	1:A:111:HIS:N	2.35	0.42
1:B:69:ILE:N	1:B:70:PRO:HD2	2.34	0.42
1:D:158:LYS:HD2	5:D:1517:HOH:O	2.19	0.42
1:A:138:ASP:HB3	1:C:85:THR:CG2	2.49	0.42
1:B:148:LEU:HD12	1:B:148:LEU:O	2.19	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.82	0.42
1:C:156:ASN:OD1	1:C:158:LYS:HB2	2.20	0.42
1:D:417:HIS:CB	1:D:419:LEU:HD11	2.50	0.42
1:A:105:ASP:CG	1:A:107:ARG:HE	2.28	0.42
1:A:395:LYS:HA	1:A:396:PRO:HD3	1.80	0.42
1:B:206:LEU:O	1:B:234:LEU:HD12	2.20	0.42
1:C:142:ARG:HH11	1:C:142:ARG:HD3	1.72	0.42
1:A:310:PRO:HD2	1:A:335:THR:O	2.20	0.42
1:A:411:HIS:O	1:A:414:TYR:N	2.52	0.42
1:A:442:PRO:HB2	1:A:445:VAL:HG12	2.02	0.42
1:B:278:PHE:CD1	1:B:278:PHE:C	2.98	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.87	0.42
1:B:287:ALA:HB2	1:B:309:ILE:HB	2.02	0.42
1:D:235:ASP:OD2	1:D:235:ASP:C	2.63	0.42
1:B:128:LEU:HA	1:B:128:LEU:HD23	1.64	0.41
1:B:440:LYS:HE3	5:B:1074:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLY:HA2	5:C:1686:HOH:O	2.19	0.41
1:B:317:TRP:O	1:B:318:THR:OG1	2.26	0.41
1:C:13:MET:HA	1:C:42:ILE:O	2.20	0.41
1:A:142:ARG:NH1	1:A:362:ILE:CD1	2.83	0.41
1:B:5:PHE:HA	1:D:6:THR:O	2.20	0.41
1:B:7:THR:HA	1:B:8:PRO:HD3	1.96	0.41
1:B:358:ALA:HA	1:B:359:PRO:HD3	1.80	0.41
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.79	0.41
1:D:162:LEU:HA	1:D:163:PRO:HD3	1.92	0.41
1:B:192:ALA:CB	1:B:223:LEU:HD11	2.48	0.41
1:C:68:ALA:O	1:C:69:ILE:C	2.62	0.41
1:C:77:LEU:N	1:C:77:LEU:HD23	2.34	0.41
1:D:407:VAL:HG12	1:D:408:MET:CE	2.48	0.41
1:B:202:ASN:O	1:B:230:ALA:CB	2.68	0.41
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.68	0.41
1:C:45:ASP:OD2	1:C:45:ASP:C	2.64	0.41
1:C:328:MET:HE2	1:C:328:MET:HB3	1.99	0.41
1:A:86:LEU:O	1:A:87:VAL:C	2.64	0.41
1:C:24:MET:HG3	1:C:164:TYR:CZ	2.55	0.41
1:C:395:LYS:HA	1:C:396:PRO:HD3	1.80	0.41
1:B:25:LEU:HB3	1:B:152:PHE:CD1	2.56	0.41
1:B:26:MET:CE	1:B:31:ALA:HB1	2.48	0.41
1:B:372:GLN:HA	1:B:376:GLN:NE2	2.36	0.41
1:C:114:THR:OG1	1:C:318:THR:HA	2.20	0.41
1:D:32:HIS:CE1	1:D:342:ASN:OD1	2.73	0.41
1:D:40:ILE:HD13	1:D:40:ILE:N	2.36	0.41
1:A:158:LYS:C	1:A:160:THR:H	2.27	0.41
1:B:10:VAL:CG1	1:B:73:VAL:HA	2.50	0.41
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.89	0.41
1:A:4:GLN:O	1:C:6:THR:OG1	2.29	0.41
1:A:282:THR:OG1	1:A:284:LEU:HB2	2.21	0.41
1:A:331:GLU:HB3	1:C:295:TRP:CB	2.50	0.41
1:B:117:GLU:OE1	1:B:319:MET:HB2	2.21	0.41
1:B:137:GLY:O	1:D:81:LYS:NZ	2.40	0.41
1:C:342:ASN:HA	1:C:368:HIS:CB	2.51	0.41
1:C:395:LYS:CB	1:C:396:PRO:HD2	2.50	0.41
1:D:27:ASN:O	1:D:443:CYS:HB3	2.21	0.41
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.86	0.41
1:D:279:ARG:HG3	1:D:286:THR:HG23	2.03	0.41
1:B:33:ALA:CB	1:B:34:PRO:CD	2.98	0.41
1:C:440:LYS:NZ	5:C:1565:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:ARG:HG3	1:D:442:PRO:HD2	2.03	0.41
1:A:261:ASP:OD1	1:A:288:THR:OG1	2.35	0.40
1:A:301:THR:HG23	1:A:306:SER:HB2	2.02	0.40
1:A:341:ASN:O	1:A:342:ASN:C	2.63	0.40
1:B:43:ILE:HG22	1:B:123:LEU:HD11	2.01	0.40
1:B:99:ARG:HG3	1:B:105:ASP:CG	2.46	0.40
1:B:302:LEU:HB3	4:D:601:IPA:H33	2.03	0.40
1:A:162:LEU:HD11	1:A:430:TYR:CD1	2.56	0.40
1:B:353:HIS:CE1	5:B:1119:HOH:O	2.73	0.40
1:D:28:LEU:HD12	1:D:442:PRO:HA	2.03	0.40
1:D:209:GLY:O	1:D:442:PRO:HA	2.21	0.40
1:D:380:LYS:HG3	1:D:401:GLU:HB3	2.02	0.40
1:B:13:MET:HE3	1:B:116:ILE:CD1	2.51	0.40
1:C:21:HIS:N	1:C:376:GLN:HE22	2.14	0.40
1:D:110:ILE:HD12	1:D:110:ILE:HA	1.78	0.40
1:D:317:TRP:O	1:D:321:GLY:HA3	2.21	0.40
1:B:288:THR:C	1:B:311:LEU:HD23	2.47	0.40
1:C:16:ILE:CD1	1:C:408:MET:HE1	2.41	0.40
1:D:369:TRP:NE1	1:D:373:GLU:HG3	2.36	0.40
1:A:16:ILE:HD13	1:A:16:ILE:HG21	1.83	0.40
1:A:180:GLU:O	1:A:181:GLU:C	2.64	0.40
1:A:339:HIS:CD2	2:A:499:DXG:O6B	2.75	0.40
1:B:13:MET:HE2	1:B:69:ILE:HG12	2.04	0.40
1:C:55:ILE:HD11	1:C:65:LEU:HD11	2.03	0.40
1:C:407:VAL:CG1	1:C:408:MET:HE2	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	442/446 (99%)	414 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/446 (99%)	405 (92%)	30 (7%)	5 (1%)	11	7
1	C	442/446 (99%)	412 (93%)	28 (6%)	2 (0%)	24	21
1	D	440/446 (99%)	409 (93%)	30 (7%)	1 (0%)	43	42
All	All	1764/1784 (99%)	1640 (93%)	116 (7%)	8 (0%)	24	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	ARG
1	B	102	GLN
1	B	80	TYR
1	C	24	MET
1	D	443	CYS
1	B	181	GLU
1	B	266	GLU
1	C	161	PRO

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	359/362 (99%)	342 (95%)	17 (5%)	23	22
1	B	354/362 (98%)	333 (94%)	21 (6%)	18	14
1	C	355/362 (98%)	338 (95%)	17 (5%)	23	21
1	D	353/362 (98%)	326 (92%)	27 (8%)	12	9
All	All	1421/1448 (98%)	1339 (94%)	82 (6%)	18	15

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	THR
1	A	12	GLU

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Mol	Chain	Res	Type
1	A	24	MET
1	A	95	ASP
1	A	99	ARG
1	A	107	ARG
1	A	130	VAL
1	A	131	ASN
1	A	160	THR
1	A	188	VAL
1	A	207	LYS
1	A	338	SER
1	A	361	LYS
1	A	409	LYS
1	A	419	LEU
1	A	429	GLN
1	B	15	VAL
1	B	16	ILE
1	B	27	ASN
1	B	40	ILE
1	B	44	LYS
1	B	55	ILE
1	B	160	THR
1	B	171	SER
1	B	190	ARG
1	B	207	LYS
1	B	233	THR
1	B	253	LYS
1	B	255	SER
1	B	275	MET
1	B	311	LEU
1	B	394	GLU
1	B	402	ILE
1	B	409	LYS
1	B	415	GLN
1	B	419	LEU
1	B	439	ASN
1	C	4	GLN
1	C	6	THR
1	C	27	ASN
1	C	55	ILE
1	C	99	ARG
1	C	110	ILE
1	C	116	ILE

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Mol	Chain	Res	Type
1	C	131	ASN
1	C	160	THR
1	C	171	SER
1	C	188	VAL
1	C	198	LYS
1	C	207	LYS
1	C	255	SER
1	C	395	LYS
1	C	416	LYS
1	C	439	ASN
1	D	14	GLN
1	D	40	ILE
1	D	44	LYS
1	D	65	LEU
1	D	69	ILE
1	D	81	LYS
1	D	94	ARG
1	D	95	ASP
1	D	99	ARG
1	D	131	ASN
1	D	146	GLU
1	D	160	THR
1	D	162	LEU
1	D	180	GLU
1	D	188	VAL
1	D	190	ARG
1	D	207	LYS
1	D	253	LYS
1	D	255	SER
1	D	339	HIS
1	D	340	SER
1	D	400	VAL
1	D	405	ASP
1	D	408	MET
1	D	432	ILE
1	D	436	THR
1	D	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	102	GLN
1	A	111	HIS
1	A	131	ASN
1	A	243	ASN
1	A	267	GLN
1	A	297	GLN
1	A	341	ASN
1	A	376	GLN
1	A	415	GLN
1	A	439	ASN
1	B	21	HIS
1	B	27	ASN
1	B	39	ASN
1	B	49	HIS
1	B	111	HIS
1	B	297	GLN
1	B	341	ASN
1	B	353	HIS
1	B	372	GLN
1	B	415	GLN
1	C	4	GLN
1	C	39	ASN
1	C	102	GLN
1	C	111	HIS
1	C	131	ASN
1	C	140	GLN
1	C	141	GLN
1	C	225	GLN
1	C	243	ASN
1	C	267	GLN
1	C	297	GLN
1	C	341	ASN
1	C	376	GLN
1	C	406	GLN
1	C	415	GLN
1	C	417	HIS
1	C	439	ASN
1	D	102	GLN
1	D	131	ASN
1	D	140	GLN
1	D	229	GLN
1	D	237	ASN

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Mol	Chain	Res	Type
1	D	243	ASN
1	D	267	GLN
1	D	339	HIS
1	D	353	HIS
1	D	415	GLN

5.3.3 RNA [i](#)

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	DXG	C	501	3	12,12,12	1.48	2 (16%)	12,16,16	2.09	5 (41%)
4	IPA	D	601	-	3,3,3	0.70	0	3,3,3	0.31	0
2	DXG	B	500	3	12,12,12	1.52	2 (16%)	12,16,16	1.74	3 (25%)
4	IPA	C	604	-	3,3,3	0.54	0	3,3,3	0.26	0
4	IPA	B	603	-	3,3,3	0.21	0	3,3,3	0.57	0
2	DXG	D	502	3	12,12,12	1.23	0	12,16,16	1.99	6 (50%)
2	DXG	A	499	3	12,12,12	1.51	3 (25%)	12,16,16	1.82	3 (25%)
4	IPA	A	602	-	3,3,3	0.67	0	3,3,3	0.24	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	DXG	A	499	3	-	4/16/16/16	-
2	DXG	B	500	3	-	6/16/16/16	-
2	DXG	C	501	3	-	5/16/16/16	-
2	DXG	D	502	3	-	6/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	DXG	C5-C6	-3.43	1.47	1.52
2	A	499	DXG	O1B-C1	2.57	1.29	1.22
2	C	501	DXG	C5-C6	-2.53	1.48	1.52
2	C	501	DXG	C2-C1	-2.53	1.49	1.52
2	B	500	DXG	C2-C1	-2.43	1.49	1.52
2	A	499	DXG	C2-C1	-2.36	1.49	1.52
2	A	499	DXG	C3-C2	-2.18	1.50	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	499	DXG	O5-C5-C4	4.01	118.20	108.31
2	C	501	DXG	O6B-C6-C5	3.74	120.65	112.74
2	D	502	DXG	O6B-C6-C5	3.62	120.39	112.74
2	C	501	DXG	O5-C5-C4	3.17	116.14	108.31
2	D	502	DXG	O1A-C1-C2	3.06	121.82	113.31
2	A	499	DXG	O6B-C6-C5	2.95	118.97	112.74
2	B	500	DXG	O6B-C6-C5	2.88	118.82	112.74
2	A	499	DXG	O5-C5-C6	2.62	117.02	110.36
2	B	500	DXG	O5-C5-C4	2.55	114.60	108.31
2	C	501	DXG	O5-C5-C6	2.54	116.82	110.36
2	B	500	DXG	O3-C3-C4	2.45	114.05	109.15
2	C	501	DXG	O3-C3-C2	2.42	113.19	109.67
2	D	502	DXG	O5-C5-C4	2.25	113.87	108.31
2	D	502	DXG	O3-C3-C4	2.24	113.64	109.15
2	D	502	DXG	O1B-C1-C2	-2.19	115.79	121.62
2	C	501	DXG	O6A-C6-C5	-2.17	118.26	122.60
2	D	502	DXG	O6A-C6-C5	-2.16	118.29	122.60

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	499	DXG	C3-C4-C5-O5
2	B	500	DXG	C3-C4-C5-O5
2	B	500	DXG	C3-C4-C5-C6
2	C	501	DXG	C3-C4-C5-O5
2	D	502	DXG	C3-C4-C5-O5
2	D	502	DXG	O5-C5-C6-O6A
2	D	502	DXG	O5-C5-C6-O6B
2	A	499	DXG	C4-C5-C6-O6A
2	A	499	DXG	C4-C5-C6-O6B
2	B	500	DXG	C4-C5-C6-O6A
2	B	500	DXG	C4-C5-C6-O6B
2	D	502	DXG	C4-C5-C6-O6A
2	D	502	DXG	C4-C5-C6-O6B
2	B	500	DXG	O5-C5-C6-O6B
2	C	501	DXG	C4-C5-C6-O6A
2	C	501	DXG	C4-C5-C6-O6B
2	B	500	DXG	O5-C5-C6-O6A
2	C	501	DXG	O5-C5-C6-O6B
2	A	499	DXG	C3-C4-C5-C6
2	C	501	DXG	C3-C4-C5-C6
2	D	502	DXG	C3-C4-C5-C6

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	DXG	4	0
4	D	601	IPA	1	0
2	B	500	DXG	3	0
4	C	604	IPA	5	0
2	D	502	DXG	6	0
2	A	499	DXG	5	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	444/446 (99%)	-0.12	12 (2%) 56 55	14, 33, 66, 100	1 (0%)
1	B	442/446 (99%)	0.11	4 (0%) 81 80	17, 43, 72, 100	0
1	C	443/446 (99%)	-0.29	8 (1%) 67 67	13, 31, 58, 100	1 (0%)
1	D	442/446 (99%)	-0.09	14 (3%) 50 49	18, 35, 70, 99	0
All	All	1771/1784 (99%)	-0.10	38 (2%) 63 63	13, 35, 68, 100	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	LEU	3.5
1	A	97	GLY	3.4
1	A	98	GLY	3.3
1	A	316	PHE	3.2
1	D	98	GLY	3.2
1	A	100	GLY	3.0
1	D	6	THR	2.9
1	D	434	GLY	2.9
1	D	100	GLY	2.8
1	D	92	ALA	2.7
1	A	431	LEU	2.6
1	D	95	ASP	2.6
1	C	104	PHE	2.6
1	C	92	ALA	2.6
1	C	101	LEU	2.6
1	B	104	PHE	2.5
1	A	92	ALA	2.5
1	D	104	PHE	2.5
1	C	98	GLY	2.5
1	C	97	GLY	2.4
1	D	101	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	97	GLY	2.4
1	C	316	PHE	2.3
1	D	420	GLY	2.2
1	B	92	ALA	2.1
1	C	96	ALA	2.1
1	A	101	LEU	2.1
1	B	106	LEU	2.1
1	A	103	THR	2.1
1	D	96	ALA	2.1
1	A	95	ASP	2.1
1	D	105	ASP	2.1
1	A	93	ASP	2.0
1	D	93	ASP	2.0
1	A	196	TYR	2.0
1	C	100	GLY	2.0
1	A	96	ALA	2.0
1	B	164	TYR	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	DXG	D	502	13/13	0.90	0.11	30,42,97,100	0
4	IPA	D	601	4/4	0.92	0.09	23,37,44,56	0
4	IPA	A	602	4/4	0.94	0.09	17,33,41,54	0
4	IPA	C	604	4/4	0.94	0.16	19,46,67,100	0
2	DXG	B	500	13/13	0.94	0.09	30,46,67,68	0
4	IPA	B	603	4/4	0.95	0.11	22,26,26,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DXG	A	499	13/13	0.95	0.08	19,38,62,81	0
2	DXG	C	501	13/13	0.95	0.09	25,35,70,100	0
3	MG	A	498	1/1	0.98	0.03	28,28,28,28	0
3	MG	C	498	1/1	0.99	0.02	29,29,29,29	0
3	MG	D	498	1/1	0.99	0.02	34,34,34,34	0
3	MG	B	498	1/1	0.99	0.03	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.