



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 AM UTC

PDB ID : 3NAZ / pdb_00003naz
Title : Basal state form of Yeast Glycogen Synthase
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2010-06-02
Resolution : 3.00 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

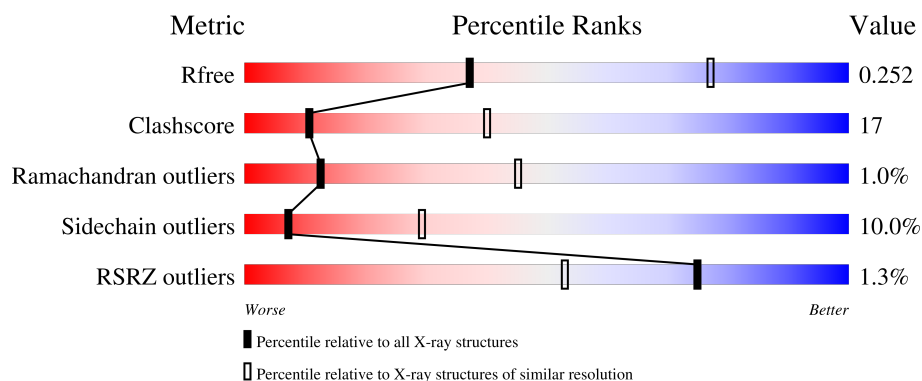
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	725	% 53% 27% • 16%
1	B	725	% 52% 28% 5% 16%
1	C	725	% 54% 26% • 15%
1	D	725	% 57% 23% 5% 15%
2	E	6	 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	6	 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19851 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	engineered mutation	UNP P27472
A	581	ALA	ARG	engineered mutation	UNP P27472
A	583	ALA	ARG	engineered mutation	UNP P27472
B	-19	MET	-	expression tag	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	engineered mutation	UNP P27472
B	581	ALA	ARG	engineered mutation	UNP P27472
B	583	ALA	ARG	engineered mutation	UNP P27472
C	-19	MET	-	expression tag	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	engineered mutation	UNP P27472
C	581	ALA	ARG	engineered mutation	UNP P27472
C	583	ALA	ARG	engineered mutation	UNP P27472
D	-19	MET	-	expression tag	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	engineered mutation	UNP P27472
D	581	ALA	ARG	engineered mutation	UNP P27472
D	583	ALA	ARG	engineered mutation	UNP P27472

- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	F	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

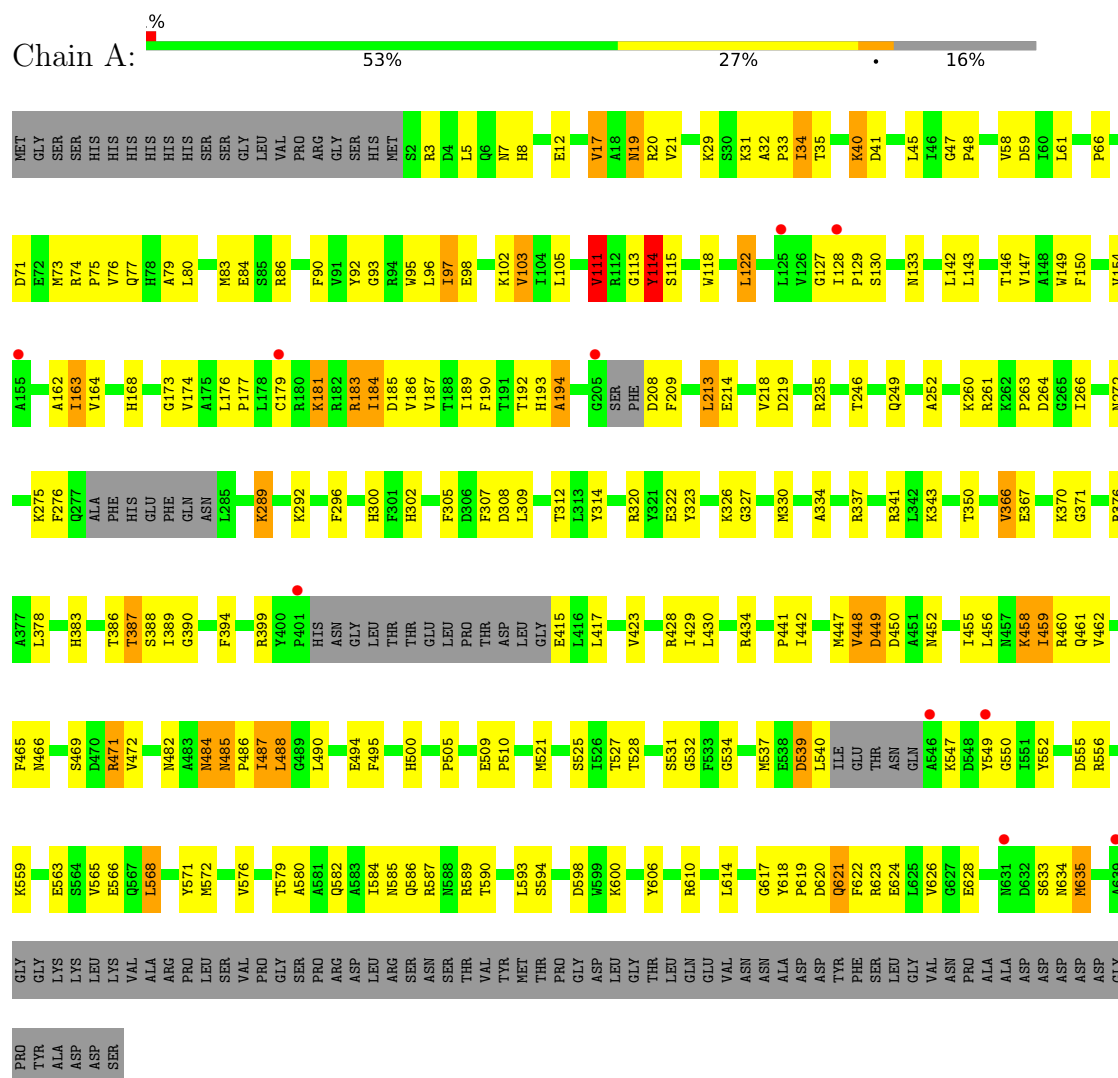
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

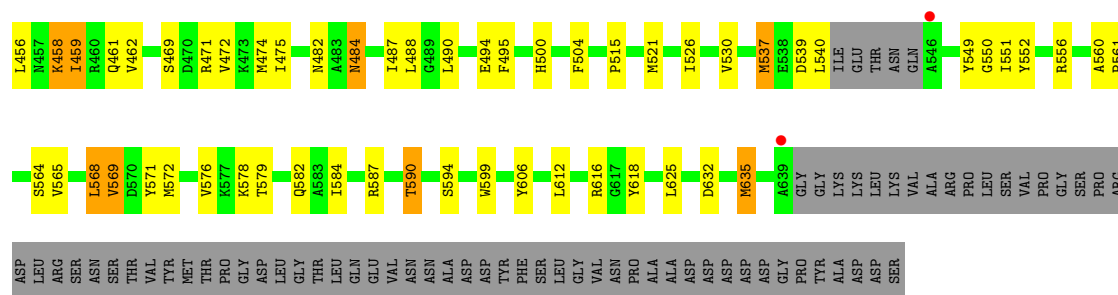
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glycogen [starch] synthase isoform 2

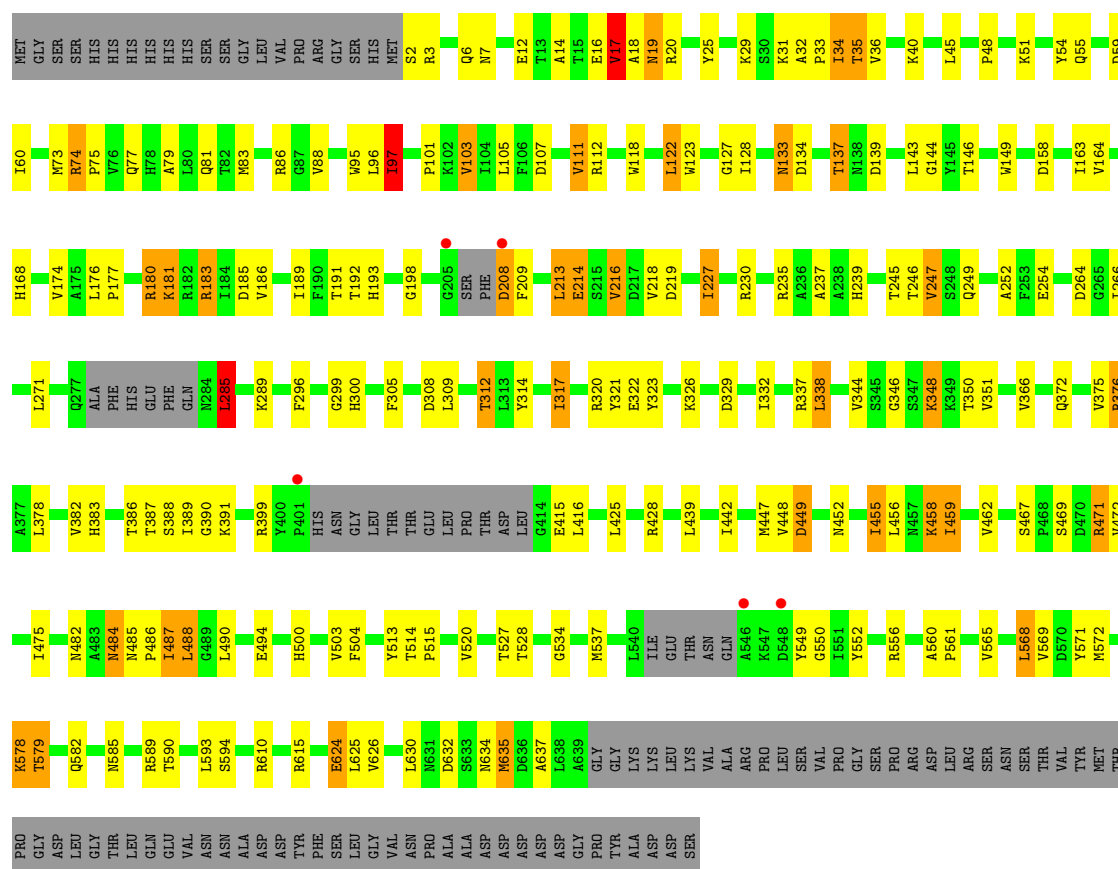


• Molecule 1: Glycogen [starch] synthase isoform 2

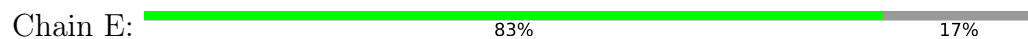




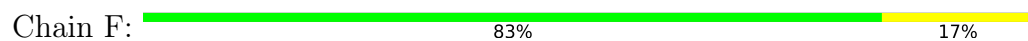
• Molecule 1: Glycogen [starch] synthase isoform 2



• Molecule 2: PEPTIDE



• Molecule 2: PEPTIDE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.53Å 166.15Å 121.03Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	48.03 – 3.00 48.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.03-3.00) 99.3 (48.03-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.203 , 0.254 0.205 , 0.252	Depositor DCC
R_{free} test set	3717 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19851	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	0/5038	0.86	7/6819 (0.1%)
1	B	0.47	0/5038	0.85	5/6819 (0.1%)
1	C	0.48	0/5050	0.84	10/6835 (0.1%)
1	D	0.52	0/5050	0.84	4/6835 (0.1%)
All	All	0.49	0/20176	0.85	26/27308 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ILE	N-CA-C	6.67	117.24	107.37
1	B	58	VAL	N-CA-C	6.10	116.65	108.11
1	C	126	VAL	N-CA-C	-6.03	107.41	113.20
1	C	58	VAL	N-CA-C	5.93	116.41	108.11
1	D	285	LEU	N-CA-C	5.84	123.24	110.80
1	A	485	ASN	CA-C-N	5.79	125.47	119.56
1	A	485	ASN	C-N-CA	5.79	125.47	119.56
1	B	128	ILE	N-CA-C	5.79	112.83	107.56
1	C	97	ILE	CB-CA-C	-5.73	103.31	111.34
1	C	285	LEU	N-CA-C	5.71	122.97	110.80
1	A	58	VAL	N-CA-C	5.70	116.07	107.75
1	B	267	LEU	CA-C-N	5.67	125.67	119.89
1	B	267	LEU	C-N-CA	5.67	125.67	119.89
1	A	509	GLU	CA-C-N	5.59	125.26	119.05
1	A	509	GLU	C-N-CA	5.59	125.26	119.05
1	A	21	VAL	N-CA-C	-5.58	108.06	113.53
1	C	17	VAL	CA-C-N	-5.57	113.84	123.25
1	C	17	VAL	C-N-CA	-5.57	113.84	123.25
1	D	97	ILE	CB-CA-C	-5.52	103.63	111.19
1	B	163	ILE	N-CA-C	5.15	115.47	107.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	434	ARG	CA-C-N	5.11	126.23	119.84
1	C	434	ARG	C-N-CA	5.11	126.23	119.84
1	C	47	GLY	CA-C-N	5.05	124.81	119.76
1	C	47	GLY	C-N-CA	5.05	124.81	119.76
1	D	17	VAL	CA-C-N	-5.00	114.64	122.95
1	D	17	VAL	C-N-CA	-5.00	114.64	122.95

There are no chirality outliers.

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	4923	0	4850	170	0
1	B	4923	0	4850	177	0
1	C	4935	0	4859	171	0
1	D	4935	0	4859	155	0
2	E	25	0	7	0	0
2	F	30	0	8	1	0
3	A	20	0	0	1	0
3	B	20	0	0	0	0
3	C	20	0	0	1	0
3	D	20	0	0	1	0
All	All	19851	0	19433	656	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 17.

All (656) 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:312:THR:HG22	1:C:350:THR:HB	1.35	1.06
1:D:314:TYR:H	1:D:500:HIS:HD2	1.03	1.00
1:C:29:LYS:HG3	1:C:97:ILE:HG21	1.45	0.98
1:B:29:LYS:HG3	1:B:97:ILE:HG21	1.46	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ILE:HD13	1:D:459:ILE:HG22	1.47	0.95
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.35	0.92
1:B:484:ASN:H	1:B:484:ASN:HD22	1.17	0.91
1:C:442:ILE:HD12	1:C:459:ILE:HD11	1.53	0.90
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.53	0.89
1:D:442:ILE:HD12	1:D:459:ILE:HD11	1.55	0.88
1:A:29:LYS:HG3	1:A:97:ILE:HG21	1.56	0.87
1:B:192:THR:HG22	1:B:246:THR:HG22	1.55	0.87
1:B:482:ASN:HB3	1:B:484:ASN:ND2	1.89	0.87
1:A:550:GLY:HA3	1:A:590:THR:HG22	1.57	0.85
1:C:443:VAL:CG2	1:C:456:LEU:HD21	2.05	0.85
1:C:284:ASN:N	1:C:284:ASN:HD22	1.75	0.84
1:D:29:LYS:HG3	1:D:97:ILE:HG21	1.57	0.84
1:A:482:ASN:HB3	1:A:484:ASN:HD21	1.42	0.84
1:B:266:ILE:HG22	1:B:268:PRO:HD3	1.60	0.83
1:C:484:ASN:HD22	1:C:484:ASN:H	1.20	0.82
1:B:314:TYR:H	1:B:500:HIS:HD2	1.29	0.81
1:A:552:TYR:HD1	1:A:571:TYR:CD2	1.98	0.81
1:D:314:TYR:H	1:D:500:HIS:CD2	1.95	0.80
1:A:95:TRP:CE3	1:A:97:ILE:HD11	2.16	0.80
1:B:95:TRP:CE3	1:B:97:ILE:HD11	2.17	0.80
1:C:133:ASN:HD22	1:C:133:ASN:H	1.28	0.80
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.65	0.79
1:A:95:TRP:CD2	1:A:97:ILE:HD11	2.17	0.79
1:C:95:TRP:CD2	1:C:97:ILE:HD11	2.18	0.79
1:C:443:VAL:HG21	1:C:456:LEU:HD21	1.63	0.79
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.13	0.79
1:B:442:ILE:HD12	1:B:459:ILE:HD11	1.65	0.78
1:A:442:ILE:HD12	1:A:459:ILE:HD11	1.64	0.78
1:B:448:VAL:O	1:B:449:ASP:HB2	1.84	0.78
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.13	0.77
1:D:579:THR:HG23	1:D:582:GLN:OE1	1.85	0.77
1:C:484:ASN:H	1:C:484:ASN:ND2	1.82	0.77
1:C:54:TYR:HE1	1:C:60:ILE:HD11	1.48	0.76
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.67	0.76
1:B:528:THR:HG22	1:B:530:VAL:H	1.51	0.76
1:B:549:TYR:O	1:B:590:THR:HG22	1.86	0.76
1:D:484:ASN:HD22	1:D:484:ASN:H	1.33	0.75
1:D:17:VAL:HG23	1:D:18:ALA:H	1.51	0.75
1:A:74:ARG:NH1	1:A:77:GLN:OE1	2.20	0.75
1:A:482:ASN:HB3	1:A:484:ASN:ND2	2.00	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:TYR:O	1:A:590:THR:HG22	1.87	0.74
1:A:308:ASP:O	1:A:312:THR:HG23	1.86	0.74
1:C:95:TRP:CE3	1:C:97:ILE:HD11	2.22	0.74
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.70	0.74
1:A:484:ASN:ND2	1:A:484:ASN:H	1.85	0.74
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.70	0.74
1:A:487:ILE:HG22	1:A:488:LEU:N	2.02	0.74
1:A:383:HIS:O	1:A:387:THR:HG23	1.88	0.74
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.70	0.73
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.68	0.73
1:C:314:TYR:H	1:C:500:HIS:HD2	1.33	0.73
1:A:484:ASN:H	1:A:484:ASN:HD22	1.35	0.73
1:D:264:ASP:O	1:D:635:MET:HG3	1.88	0.73
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.18	0.73
1:B:484:ASN:H	1:B:484:ASN:ND2	1.84	0.72
1:D:448:VAL:O	1:D:449:ASP:HB2	1.90	0.72
1:A:623:ARG:HG3	1:A:628:GLU:O	1.89	0.72
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.54	0.72
1:B:528:THR:CG2	1:B:530:VAL:HG22	2.20	0.72
1:B:17:VAL:HG21	1:B:47:GLY:HA3	1.72	0.71
1:B:311:ASN:HD21	1:B:348:LYS:HD2	1.55	0.71
1:D:192:THR:HG22	1:D:246:THR:HG22	1.71	0.71
1:B:482:ASN:HB3	1:B:484:ASN:HD21	1.53	0.70
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.72	0.70
1:C:448:VAL:O	1:C:449:ASP:HB2	1.92	0.69
1:D:133:ASN:H	1:D:133:ASN:HD22	1.38	0.69
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.71	0.69
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.75	0.69
1:A:174:VAL:O	1:A:177:PRO:HD2	1.93	0.69
1:A:181:LYS:HD3	1:A:181:LYS:C	2.17	0.69
1:A:323:TYR:OH	1:A:458:LYS:HG3	1.93	0.69
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.74	0.69
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.73	0.69
1:B:351:VAL:HB	1:B:472:VAL:HG12	1.75	0.69
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.76	0.68
1:A:314:TYR:H	1:A:500:HIS:HD2	1.41	0.68
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.73	0.68
1:C:192:THR:HG22	1:C:246:THR:HG22	1.73	0.68
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.24	0.68
1:B:567:GLN:HG2	1:B:571:TYR:CE1	2.30	0.67
1:C:17:VAL:HG23	1:C:18:ALA:H	1.57	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:HIS:O	1:C:387:THR:HG23	1.94	0.67
1:C:174:VAL:O	1:C:177:PRO:HD2	1.94	0.67
1:B:550:GLY:HA3	1:B:590:THR:HG22	1.76	0.67
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.26	0.67
1:A:320:ARG:NH1	1:A:322:GLU:OE2	2.27	0.67
1:C:484:ASN:HD22	1:C:484:ASN:N	1.92	0.67
1:C:443:VAL:HG12	1:C:445:HIS:H	1.60	0.66
1:D:549:TYR:O	1:D:590:THR:HG22	1.95	0.66
1:A:127:GLY:O	1:A:129:PRO:HD3	1.94	0.66
1:B:447:MET:HG3	1:B:456:LEU:HD11	1.78	0.66
1:D:213:LEU:HD12	1:D:213:LEU:C	2.22	0.65
1:A:80:LEU:HD22	1:A:90:PHE:CZ	2.31	0.65
1:B:17:VAL:CG2	1:B:47:GLY:HA3	2.27	0.65
1:B:264:ASP:O	1:B:635:MET:HG3	1.96	0.65
1:C:579:THR:HG23	1:C:582:GLN:OE1	1.97	0.65
1:B:320:ARG:NH1	1:B:322:GLU:OE2	2.30	0.65
1:B:586:GLN:O	1:B:590:THR:HG23	1.97	0.65
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.77	0.64
1:D:484:ASN:H	1:D:484:ASN:ND2	1.94	0.64
1:A:114:TYR:HD1	1:A:114:TYR:H	1.43	0.64
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.33	0.64
1:B:552:TYR:HD1	1:B:571:TYR:CD2	2.15	0.64
1:B:133:ASN:H	1:B:133:ASN:ND2	1.96	0.64
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.78	0.64
1:C:335:LEU:HD23	1:C:474:MET:HE1	1.80	0.64
1:A:429:ILE:HG12	1:C:397:ALA:HB1	1.80	0.63
1:D:74:ARG:NH1	1:D:77:GLN:OE1	2.30	0.63
1:B:133:ASN:H	1:B:133:ASN:HD22	1.47	0.63
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.81	0.63
1:D:271:LEU:HD13	1:D:520:VAL:HG21	1.80	0.63
1:B:487:ILE:HG22	1:B:488:LEU:N	2.13	0.63
1:C:549:TYR:O	1:C:590:THR:HG22	1.98	0.63
1:A:618:TYR:HB3	1:A:621:GLN:HG3	1.80	0.63
1:A:213:LEU:HD12	1:A:213:LEU:C	2.24	0.63
1:C:181:LYS:O	1:C:181:LYS:HD3	1.99	0.63
1:A:66:PRO:O	1:A:74:ARG:NH2	2.32	0.62
1:A:192:THR:CG2	1:A:246:THR:HG22	2.29	0.62
1:A:314:TYR:H	1:A:500:HIS:CD2	2.16	0.62
1:D:180:ARG:HH11	1:D:180:ARG:CG	2.12	0.62
1:D:383:HIS:O	1:D:387:THR:HG23	1.97	0.62
1:B:8:HIS:HB2	1:B:162:ALA:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.81	0.62
1:D:198:GLY:HA3	1:D:254:GLU:OE1	2.00	0.62
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.81	0.62
1:A:192:THR:HG22	1:A:246:THR:HG22	1.82	0.62
1:B:252:ALA:HB2	1:B:266:ILE:HD11	1.79	0.62
1:C:572:MET:O	1:C:576:VAL:HG23	2.00	0.62
1:D:168:HIS:HD2	1:D:193:HIS:NE2	1.97	0.62
1:D:181:LYS:HD3	1:D:181:LYS:C	2.25	0.62
1:C:322:GLU:HB2	1:C:326:LYS:HG2	1.81	0.61
1:D:314:TYR:N	1:D:500:HIS:HD2	1.87	0.61
1:D:585:ASN:HB3	1:D:589:ARG:NH2	2.15	0.61
1:A:580:ALA:O	1:A:584:ILE:HG13	2.01	0.61
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.36	0.60
1:D:634:ASN:HB2	1:D:637:ALA:H	1.66	0.60
1:D:299:GLY:HA2	1:D:375:VAL:HG21	1.82	0.60
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.31	0.60
1:B:528:THR:HG22	1:B:530:VAL:HG22	1.82	0.60
1:D:79:ALA:O	1:D:83:MET:HG2	2.02	0.60
1:C:482:ASN:HB3	1:C:484:ASN:ND2	2.16	0.59
1:A:320:ARG:NH2	3:A:802:SO4:O1	2.35	0.59
1:B:181:LYS:HD3	1:B:181:LYS:C	2.26	0.59
1:C:19:ASN:N	1:C:19:ASN:HD22	2.00	0.59
1:D:455:ILE:O	1:D:459:ILE:HG23	2.02	0.59
1:C:425:LEU:O	1:C:429:ILE:HG13	2.03	0.59
1:C:442:ILE:HG13	1:C:443:VAL:HG23	1.85	0.59
1:A:113:GLY:C	1:A:115:SER:H	2.11	0.59
1:A:252:ALA:HB2	1:A:266:ILE:HD11	1.85	0.59
1:A:448:VAL:O	1:A:449:ASP:HB2	2.02	0.59
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.37	0.59
1:B:309:LEU:HA	1:B:312:THR:HG23	1.84	0.59
1:C:458:LYS:HE3	1:C:461:GLN:OE1	2.03	0.59
1:C:612:LEU:HD21	1:C:616:ARG:HH21	1.68	0.58
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.38	0.58
1:C:389:ILE:HD11	1:C:417:LEU:HD21	1.83	0.58
1:A:307:PHE:O	1:C:399:ARG:NH2	2.36	0.58
1:A:235:ARG:HH21	1:A:260:LYS:CG	2.14	0.58
1:B:390:GLY:HA2	1:D:386:THR:HG21	1.85	0.58
1:B:626:VAL:HG12	1:B:628:GLU:HG2	1.86	0.58
1:C:54:TYR:CE1	1:C:60:ILE:HD11	2.35	0.58
1:D:180:ARG:HH11	1:D:180:ARG:HG3	1.69	0.58
1:A:19:ASN:N	1:A:19:ASN:HD22	2.01	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:C	1:B:115:SER:H	2.12	0.58
1:B:193:HIS:O	1:B:194:ALA:HB2	2.03	0.58
1:A:181:LYS:HD3	1:A:181:LYS:O	2.04	0.58
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.84	0.58
1:D:448:VAL:O	1:D:449:ASP:CB	2.52	0.58
1:C:181:LYS:HD3	1:C:181:LYS:C	2.29	0.58
1:A:606:TYR:O	1:A:610:ARG:HG3	2.04	0.57
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.85	0.57
1:C:487:ILE:HG22	1:C:488:LEU:N	2.20	0.57
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.04	0.57
1:B:181:LYS:HD3	1:B:181:LYS:O	2.04	0.57
1:A:302:HIS:O	1:A:434:ARG:HD2	2.05	0.57
1:C:210:TYR:CE1	1:C:250:ILE:HD11	2.39	0.57
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.86	0.57
1:C:134:ASP:OD2	1:C:137:THR:HG23	2.03	0.57
1:D:54:TYR:HE1	1:D:60:ILE:HD11	1.70	0.57
1:A:585:ASN:HB3	1:A:589:ARG:NH2	2.19	0.57
1:C:314:TYR:H	1:C:500:HIS:CD2	2.19	0.57
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.40	0.57
1:B:78:HIS:O	1:B:81:GLN:HB2	2.05	0.56
1:B:439:LEU:HD22	1:B:467:SER:HA	1.87	0.56
1:C:284:ASN:N	1:C:284:ASN:ND2	2.45	0.56
1:C:612:LEU:HD21	1:C:616:ARG:NH2	2.20	0.56
1:A:386:THR:HG21	1:C:390:GLY:CA	2.35	0.56
1:B:213:LEU:HD21	1:B:253:PHE:HE1	1.69	0.56
1:D:12:GLU:HB3	1:D:45:LEU:HD23	1.87	0.56
1:D:12:GLU:OE2	1:D:168:HIS:HE1	1.87	0.56
1:A:163:ILE:HB	1:A:186:VAL:HG12	1.88	0.56
1:D:309:LEU:HA	1:D:312:THR:HG23	1.88	0.56
1:A:208:ASP:OD1	1:A:209:PHE:N	2.38	0.56
1:B:580:ALA:O	1:B:584:ILE:HG13	2.06	0.56
1:D:227:ILE:HD12	1:D:230:ARG:HD2	1.87	0.56
1:D:95:TRP:CE3	1:D:97:ILE:HD11	2.41	0.56
1:C:218:VAL:HG23	1:C:219:ASP:N	2.20	0.56
1:A:168:HIS:HD2	1:A:193:HIS:NE2	2.04	0.56
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.71	0.55
1:C:16:GLU:O	1:C:17:VAL:C	2.49	0.55
1:B:213:LEU:C	1:B:213:LEU:HD12	2.32	0.55
1:C:113:GLY:C	1:C:115:SER:H	2.14	0.55
1:B:399:ARG:NH2	1:D:308:ASP:HA	2.21	0.55
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ARG:HG3	1:B:628:GLU:O	2.07	0.55
1:C:338:LEU:HD22	1:C:338:LEU:O	2.07	0.55
1:D:176:LEU:HD12	1:D:237:ALA:HB1	1.88	0.55
1:B:383:HIS:O	1:B:387:THR:HG23	2.07	0.55
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.72	0.55
1:D:134:ASP:CG	1:D:137:THR:HG23	2.32	0.55
1:D:448:VAL:O	1:D:448:VAL:HG12	2.07	0.55
1:A:92:TYR:OH	1:A:102:LYS:HD3	2.07	0.55
1:A:487:ILE:CG2	1:A:488:LEU:N	2.69	0.55
1:B:386:THR:HG21	1:D:390:GLY:CA	2.37	0.55
1:B:12:GLU:HB3	1:B:45:LEU:HD23	1.88	0.55
1:B:127:GLY:O	1:B:129:PRO:HD3	2.06	0.55
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.89	0.55
1:C:149:TRP:HD1	1:C:149:TRP:O	1.89	0.55
1:B:471:ARG:HA	1:B:471:ARG:NE	2.22	0.54
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.88	0.54
1:A:146:THR:O	1:A:149:TRP:HB3	2.06	0.54
1:B:447:MET:HG3	1:B:456:LEU:CD1	2.36	0.54
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.90	0.54
1:A:296:PHE:CE1	1:A:487:ILE:HG23	2.42	0.54
1:A:179:CYS:HA	1:A:184:ILE:HG13	1.88	0.54
1:C:321:TYR:CD1	1:C:321:TYR:C	2.86	0.54
1:C:458:LYS:HD3	1:C:458:LYS:O	2.07	0.54
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.39	0.54
1:C:504:PHE:CD2	1:C:515:PRO:HB3	2.43	0.54
1:A:622:PHE:CE1	1:A:626:VAL:HG21	2.43	0.53
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.90	0.53
1:C:218:VAL:HG23	1:C:219:ASP:H	1.74	0.53
1:C:254:GLU:HG3	1:C:258:LEU:HD12	1.89	0.53
1:D:181:LYS:HD3	1:D:181:LYS:O	2.08	0.53
1:D:252:ALA:HB2	1:D:266:ILE:HD11	1.90	0.53
1:A:307:PHE:HD1	1:A:312:THR:HG21	1.73	0.53
1:D:459:ILE:HA	1:D:462:VAL:HG22	1.91	0.53
1:D:565:VAL:O	1:D:569:VAL:HG23	2.09	0.53
1:A:449:ASP:OD2	1:A:452:ASN:HB2	2.08	0.53
1:C:112:ARG:O	1:C:115:SER:HB2	2.09	0.53
1:D:208:ASP:OD2	1:D:209:PHE:N	2.42	0.53
1:A:114:TYR:N	1:A:114:TYR:CD1	2.77	0.53
1:A:552:TYR:N	1:A:552:TYR:CD2	2.77	0.53
1:B:314:TYR:H	1:B:500:HIS:CD2	2.19	0.53
1:C:490:LEU:HD13	1:C:495:PHE:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:ASN:HB3	1:D:484:ASN:ND2	2.23	0.53
1:B:146:THR:O	1:B:149:TRP:HB3	2.09	0.53
1:B:338:LEU:O	1:B:338:LEU:HD22	2.08	0.53
1:D:17:VAL:HG23	1:D:18:ALA:N	2.23	0.53
1:B:528:THR:HG21	1:B:530:VAL:HG22	1.90	0.53
1:B:66:PRO:O	1:B:74:ARG:NH2	2.41	0.53
1:C:266:ILE:HG22	1:C:268:PRO:HG3	1.91	0.53
1:D:322:GLU:HB2	1:D:326:LYS:HG2	1.90	0.53
1:B:311:ASN:ND2	1:B:348:LYS:HD2	2.22	0.52
1:D:180:ARG:HG3	1:D:180:ARG:NH1	2.23	0.52
1:C:330:MET:CE	1:C:568:LEU:HD12	2.39	0.52
1:D:323:TYR:OH	1:D:458:LYS:HG3	2.10	0.52
1:A:150:PHE:O	1:A:154:VAL:HG23	2.09	0.52
1:D:568:LEU:HD22	1:D:572:MET:HE3	1.90	0.52
1:A:218:VAL:HG23	1:A:219:ASP:N	2.24	0.52
1:C:361:ASN:HA	1:C:448:VAL:HG23	1.92	0.52
1:D:490:LEU:HD22	1:D:494:GLU:HB3	1.91	0.52
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.92	0.52
1:A:341:ARG:NH2	1:A:566:GLU:OE1	2.43	0.52
1:A:527:THR:OG1	1:A:528:THR:N	2.39	0.52
1:B:61:LEU:HG	1:B:93:GLY:HA2	1.92	0.52
1:B:443:VAL:HG22	1:B:445:HIS:H	1.74	0.52
1:C:5:LEU:HD21	1:C:618:TYR:CD1	2.45	0.52
1:C:17:VAL:HG23	1:C:18:ALA:N	2.23	0.52
1:C:213:LEU:O	1:C:216:VAL:HG22	2.08	0.52
1:D:174:VAL:O	1:D:177:PRO:HD2	2.09	0.52
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.28	0.52
1:C:264:ASP:O	1:C:635:MET:HG3	2.10	0.52
1:C:315:PHE:CE2	1:C:572:MET:HG2	2.45	0.52
1:D:449:ASP:OD2	1:D:452:ASN:HB2	2.09	0.52
1:D:20:ARG:NH1	3:D:802:SO4:O3	2.43	0.52
1:B:449:ASP:OD1	1:B:452:ASN:HB2	2.10	0.51
1:D:180:ARG:HH11	1:D:180:ARG:CB	2.23	0.51
1:C:193:HIS:O	1:C:194:ALA:HB2	2.11	0.51
1:C:321:TYR:C	1:C:321:TYR:HD1	2.18	0.51
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.92	0.51
1:D:382:VAL:O	1:D:386:THR:HG23	2.10	0.51
1:A:389:ILE:HD11	1:A:417:LEU:HD21	1.93	0.51
1:C:332:ILE:HD13	1:C:459:ILE:HG22	1.91	0.51
1:D:550:GLY:HA3	1:D:590:THR:HG21	1.91	0.51
1:A:264:ASP:O	1:A:635:MET:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:CG	1:B:452:ASN:HB2	2.35	0.51
1:C:74:ARG:N	1:C:75:PRO:CD	2.73	0.51
1:A:598:ASP:OD2	1:A:600:LYS:HD2	2.10	0.51
1:B:333:GLU:OE2	1:B:337:ARG:HD2	2.10	0.51
1:C:565:VAL:O	1:C:569:VAL:HG23	2.11	0.51
1:D:51:LYS:HE3	1:D:107:ASP:OD1	2.11	0.51
1:A:549:TYR:HB3	1:A:593:LEU:HD11	1.90	0.51
1:C:378:LEU:HD22	1:C:382:VAL:HG23	1.92	0.51
1:C:103:VAL:HG13	1:C:105:LEU:HG	1.92	0.51
1:C:123:TRP:O	1:C:127:GLY:HA2	2.11	0.51
1:D:344:VAL:C	1:D:346:GLY:H	2.19	0.51
1:D:351:VAL:HB	1:D:472:VAL:HG12	1.93	0.51
1:B:499:CYS:O	1:B:587:ARG:NH2	2.44	0.51
1:A:143:LEU:O	1:A:147:VAL:HG23	2.10	0.50
1:B:29:LYS:HE3	1:B:97:ILE:CG2	2.41	0.50
1:C:372:GLN:O	1:C:376:ARG:HB2	2.12	0.50
1:C:389:ILE:HD11	1:C:417:LEU:CD2	2.42	0.50
1:A:447:MET:HG3	1:A:456:LEU:CD1	2.41	0.50
1:B:133:ASN:HD22	1:B:133:ASN:N	2.08	0.50
1:C:235:ARG:HH21	1:C:260:LYS:HG3	1.76	0.50
1:B:114:TYR:HD1	1:B:114:TYR:H	1.59	0.50
1:B:250:ILE:HG12	1:B:530:VAL:HA	1.92	0.50
1:A:430:LEU:HD13	1:D:55:GLN:O	2.12	0.50
1:B:361:ASN:HA	1:B:448:VAL:HG23	1.93	0.50
1:C:88:VAL:HG22	1:C:111:VAL:HG23	1.94	0.50
1:C:560:ALA:HB1	1:C:561:PRO:HD2	1.93	0.50
1:D:458:LYS:O	1:D:458:LYS:HD3	2.11	0.50
1:A:111:VAL:HG12	1:A:142:LEU:HD22	1.93	0.50
1:A:312:THR:HG22	1:A:350:THR:HB	1.93	0.50
1:A:399:ARG:NH2	1:C:307:PHE:O	2.45	0.50
1:B:266:ILE:HG22	1:B:268:PRO:CD	2.38	0.50
1:D:447:MET:HG3	1:D:456:LEU:HD11	1.93	0.50
1:A:394:PHE:HE1	1:C:379:GLU:HG3	1.76	0.50
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.11	0.50
1:D:487:ILE:HG22	1:D:488:LEU:N	2.26	0.50
1:D:442:ILE:CD1	1:D:459:ILE:HD11	2.36	0.50
1:C:286:HIS:ND1	1:C:587:ARG:NH2	2.60	0.50
1:B:179:CYS:HA	1:B:184:ILE:HG13	1.93	0.49
1:C:320:ARG:HB2	1:C:320:ARG:NH1	2.27	0.49
1:D:305:PHE:HZ	1:D:309:LEU:HG	1.76	0.49
1:A:61:LEU:HG	1:A:93:GLY:HA2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PHE:O	1:D:399:ARG:NH2	2.44	0.49
1:B:150:PHE:O	1:B:154:VAL:HG23	2.11	0.49
1:D:31:LYS:O	1:D:35:THR:HG23	2.12	0.49
1:A:399:ARG:NH2	1:C:308:ASP:HA	2.26	0.49
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.37	0.49
1:A:552:TYR:CD1	1:A:571:TYR:CD2	2.90	0.49
1:C:25:TYR:C	1:C:25:TYR:CD2	2.91	0.49
1:D:317:ILE:HG13	1:D:503:VAL:O	2.12	0.49
1:B:296:PHE:CE1	1:B:487:ILE:HG23	2.48	0.49
1:B:337:ARG:O	1:B:341:ARG:HG3	2.12	0.49
1:B:30:SER:O	1:B:599:TRP:CD1	2.66	0.49
1:B:555:ASP:OD1	1:B:555:ASP:C	2.56	0.49
1:D:300:HIS:CE1	1:D:475:ILE:CD1	2.96	0.49
1:A:113:GLY:O	1:A:115:SER:N	2.45	0.49
1:B:143:LEU:O	1:B:147:VAL:HG23	2.13	0.49
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.95	0.49
1:C:235:ARG:HG2	1:C:239:HIS:HD2	1.77	0.49
1:A:327:GLY:HA3	1:A:505:PRO:O	2.12	0.49
1:A:484:ASN:HD22	1:A:484:ASN:N	2.08	0.49
1:A:487:ILE:HG22	1:A:488:LEU:H	1.74	0.49
1:A:572:MET:O	1:A:576:VAL:HG23	2.12	0.48
1:C:252:ALA:HB2	1:C:266:ILE:HD11	1.95	0.48
1:B:385:VAL:CG1	1:B:417:LEU:HD21	2.43	0.48
1:D:19:ASN:HD22	1:D:19:ASN:N	2.11	0.48
1:A:133:ASN:H	1:A:133:ASN:ND2	2.11	0.48
1:A:289:LYS:HZ3	1:A:494:GLU:HG2	1.78	0.48
1:B:514:THR:OG1	1:B:515:PRO:CD	2.61	0.48
1:C:75:PRO:CB	1:C:158:ASP:HB2	2.42	0.48
1:C:490:LEU:HD22	1:C:494:GLU:HB3	1.95	0.48
1:D:29:LYS:HE3	1:D:97:ILE:CG2	2.43	0.48
1:A:289:LYS:NZ	1:A:494:GLU:HG2	2.29	0.48
1:C:482:ASN:HB3	1:C:484:ASN:HD21	1.79	0.48
1:A:307:PHE:CD1	1:A:312:THR:HG21	2.49	0.48
1:B:74:ARG:N	1:B:75:PRO:CD	2.77	0.48
1:B:133:ASN:ND2	1:B:133:ASN:N	2.62	0.48
1:C:34:ILE:HD12	1:C:34:ILE:HA	1.66	0.48
1:C:330:MET:HE2	1:C:568:LEU:HD12	1.96	0.48
1:B:322:GLU:HB2	1:B:326:LYS:HG2	1.95	0.48
1:B:34:ILE:HD11	1:B:600:LYS:HG3	1.95	0.48
1:C:176:LEU:HD12	1:C:237:ALA:HB1	1.96	0.48
1:A:111:VAL:HG13	1:A:118:TRP:CZ3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:C	1:C:346:GLY:H	2.22	0.48
1:D:180:ARG:HH11	1:D:180:ARG:HB2	1.79	0.48
1:A:458:LYS:HE3	1:A:461:GLN:OE1	2.14	0.47
1:B:125:LEU:O	1:B:126:VAL:HG22	2.14	0.47
1:D:48:PRO:HD3	1:D:143:LEU:HD22	1.96	0.47
1:D:308:ASP:O	1:D:312:THR:HG23	2.14	0.47
1:B:109:ASP:C	1:B:111:VAL:H	2.22	0.47
1:B:117:GLU:O	1:B:117:GLU:HG2	2.14	0.47
1:C:30:SER:O	1:C:599:TRP:CD1	2.67	0.47
1:C:146:THR:O	1:C:149:TRP:HB3	2.14	0.47
1:D:189:ILE:HD11	1:D:610:ARG:HA	1.96	0.47
1:D:442:ILE:HD12	1:D:459:ILE:CD1	2.33	0.47
1:B:572:MET:O	1:B:576:VAL:HG23	2.13	0.47
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.50	0.47
1:D:549:TYR:C	1:D:590:THR:HG22	2.38	0.47
1:A:449:ASP:CG	1:A:452:ASN:HB2	2.39	0.47
1:C:296:PHE:CE1	1:C:487:ILE:HG23	2.49	0.47
1:C:442:ILE:HD12	1:C:459:ILE:CD1	2.36	0.47
1:D:29:LYS:CG	1:D:97:ILE:HG21	2.38	0.47
1:B:386:THR:HG21	1:D:390:GLY:HA2	1.95	0.47
1:A:29:LYS:HE3	1:A:97:ILE:CG2	2.45	0.47
1:A:176:LEU:CD1	1:A:190:PHE:HB2	2.44	0.47
1:C:149:TRP:CD1	1:C:149:TRP:C	2.92	0.47
1:D:6:GLN:HE21	1:D:625:LEU:HD11	1.80	0.47
1:C:88:VAL:HG22	1:C:111:VAL:CG2	2.45	0.47
1:C:561:PRO:O	1:C:565:VAL:HG23	2.15	0.47
1:D:527:THR:HG21	1:D:534:GLY:HA2	1.97	0.47
1:A:550:GLY:CA	1:A:590:THR:HG22	2.39	0.47
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.48	0.47
1:D:578:LYS:HG2	1:D:582:GLN:HB3	1.97	0.47
1:B:32:ALA:HB3	1:B:33:PRO:CD	2.43	0.47
1:D:180:ARG:CG	1:D:180:ARG:NH1	2.76	0.47
1:A:176:LEU:HD11	1:A:190:PHE:HB2	1.96	0.46
1:A:183:ARG:HE	1:A:183:ARG:HB2	1.58	0.46
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.95	0.46
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.96	0.46
1:B:579:THR:HG23	1:B:582:GLN:OE1	2.16	0.46
1:A:187:VAL:HG21	1:A:614:LEU:HD23	1.97	0.46
1:A:300:HIS:HE1	1:A:441:PRO:O	1.98	0.46
1:A:334:ALA:CB	1:A:568:LEU:HD13	2.45	0.46
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HB3	1:C:41:ASP:H	1.47	0.46
1:A:76:VAL:O	1:A:79:ALA:HB3	2.15	0.46
1:A:484:ASN:ND2	1:A:484:ASN:N	2.59	0.46
1:B:308:ASP:O	1:B:312:THR:HG23	2.15	0.46
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.37	0.46
1:B:484:ASN:HD22	1:B:484:ASN:N	1.98	0.46
1:D:321:TYR:CD1	1:D:321:TYR:C	2.92	0.46
1:D:193:HIS:HA	1:D:247:VAL:HG22	1.97	0.46
1:A:448:VAL:O	1:A:448:VAL:HG12	2.16	0.46
1:B:272:ASN:O	1:B:275:LYS:HB3	2.15	0.46
1:C:7:ASN:O	1:C:7:ASN:CG	2.59	0.46
1:C:442:ILE:CD1	1:C:459:ILE:HD11	2.35	0.46
1:C:482:ASN:O	1:C:484:ASN:N	2.48	0.46
1:D:208:ASP:OD2	1:D:208:ASP:C	2.58	0.46
1:A:163:ILE:CG2	1:A:186:VAL:HG12	2.45	0.46
1:B:125:LEU:C	1:B:126:VAL:CG2	2.88	0.46
1:D:338:LEU:HD22	1:D:338:LEU:O	2.14	0.46
1:C:455:ILE:O	1:C:459:ILE:HG23	2.16	0.46
1:D:25:TYR:C	1:D:25:TYR:CD2	2.94	0.46
1:D:323:TYR:CE1	1:D:329:ASP:HB3	2.51	0.46
1:A:586:GLN:O	1:A:587:ARG:C	2.59	0.46
1:B:265:GLY:O	1:B:266:ILE:HD13	2.16	0.46
1:B:335:LEU:HD12	1:B:335:LEU:HA	1.76	0.46
1:A:623:ARG:HG3	1:A:628:GLU:C	2.41	0.45
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.46	0.45
1:C:564:SER:O	1:C:565:VAL:C	2.59	0.45
1:A:48:PRO:HD3	1:A:143:LEU:HD22	1.98	0.45
1:A:103:VAL:CG1	1:A:105:LEU:HG	2.46	0.45
1:A:510:PRO:O	1:A:532:GLY:HA3	2.16	0.45
1:C:265:GLY:HA3	1:C:635:MET:SD	2.55	0.45
1:C:333:GLU:OE2	1:C:337:ARG:HD2	2.17	0.45
1:B:95:TRP:CD2	1:B:97:ILE:HD11	2.52	0.45
1:A:83:MET:HE3	1:A:83:MET:HB3	1.83	0.45
1:B:448:VAL:O	1:B:448:VAL:HG12	2.17	0.45
1:D:439:LEU:HD22	1:D:467:SER:HA	1.97	0.45
1:A:40:LYS:HB3	1:A:41:ASP:H	1.62	0.45
1:B:136:GLU:OE1	1:B:136:GLU:N	2.46	0.45
1:C:131:PRO:HD2	1:C:229:HIS:CD2	2.52	0.45
1:C:300:HIS:CE1	1:C:475:ILE:CD1	2.99	0.45
1:A:74:ARG:N	1:A:75:PRO:CD	2.79	0.45
1:A:442:ILE:HD12	1:A:459:ILE:CD1	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:O	1:B:17:VAL:C	2.60	0.45
1:B:634:ASN:HB2	1:B:637:ALA:H	1.81	0.45
1:A:330:MET:CE	1:A:568:LEU:HD12	2.47	0.45
1:A:394:PHE:CE1	1:C:379:GLU:HG3	2.51	0.45
1:B:533:PHE:O	1:B:537:MET:HB2	2.17	0.45
1:B:547:LYS:HD2	1:B:571:TYR:HE2	1.82	0.45
1:D:95:TRP:CD2	1:D:97:ILE:HD11	2.52	0.45
1:D:112:ARG:NH2	1:D:139:ASP:OD1	2.50	0.44
1:D:218:VAL:HG23	1:D:219:ASP:H	1.81	0.44
1:A:471:ARG:NE	1:A:471:ARG:HA	2.32	0.44
1:C:315:PHE:HE2	1:C:572:MET:HG2	1.80	0.44
1:D:146:THR:O	1:D:149:TRP:HB3	2.18	0.44
1:A:289:LYS:HD2	1:A:289:LYS:N	2.31	0.44
1:A:465:PHE:O	1:A:466:ASN:HB2	2.16	0.44
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.52	0.44
1:C:133:ASN:H	1:C:133:ASN:ND2	2.06	0.44
1:C:539:ASP:O	1:C:540:LEU:HD23	2.18	0.44
1:D:176:LEU:HB2	1:D:177:PRO:HD3	1.98	0.44
1:A:8:HIS:HB2	1:A:162:ALA:O	2.17	0.44
1:A:73:MET:C	1:A:75:PRO:HD2	2.43	0.44
1:B:598:ASP:OD2	1:B:600:LYS:HB2	2.18	0.44
1:C:195:THR:O	1:C:196:LEU:C	2.60	0.44
1:D:425:LEU:HD23	1:D:425:LEU:HA	1.80	0.44
1:A:173:GLY:O	1:A:176:LEU:HB2	2.17	0.44
1:B:344:VAL:C	1:B:346:GLY:H	2.24	0.44
1:B:374:GLU:HA	1:B:374:GLU:OE1	2.17	0.44
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.82	0.44
1:A:3:ARG:HH12	1:A:185:ASP:HB3	1.81	0.44
1:B:73:MET:C	1:B:75:PRO:HD2	2.43	0.44
1:B:113:GLY:O	1:B:115:SER:N	2.50	0.44
1:B:334:ALA:CB	1:B:568:LEU:HD13	2.47	0.44
1:A:547:LYS:HD2	1:A:571:TYR:CE2	2.53	0.44
1:C:526:ILE:HG12	1:C:552:TYR:HB2	2.00	0.44
1:D:6:GLN:NE2	1:D:625:LEU:HD21	2.33	0.44
1:A:559:LYS:HB3	1:A:563:GLU:HB2	1.99	0.44
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.83	0.44
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.18	0.44
1:D:213:LEU:HD12	1:D:214:GLU:N	2.33	0.44
1:C:312:THR:HA	1:C:350:THR:O	2.18	0.44
1:D:218:VAL:HG23	1:D:219:ASP:N	2.32	0.44
1:A:34:ILE:HD12	1:A:34:ILE:HA	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:O	1:B:176:LEU:HB2	2.18	0.43
1:D:36:VAL:CG2	1:D:101:PRO:HB3	2.48	0.43
1:A:539:ASP:OD1	1:A:539:ASP:N	2.49	0.43
1:B:311:ASN:HD21	1:B:348:LYS:CD	2.28	0.43
1:C:183:ARG:HE	1:C:183:ARG:HB2	1.63	0.43
1:C:443:VAL:HG12	1:C:444:THR:N	2.33	0.43
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.36	0.43
1:D:54:TYR:CE1	1:D:60:ILE:HD11	2.52	0.43
1:A:31:LYS:O	1:A:32:ALA:C	2.61	0.43
1:B:322:GLU:O	1:B:323:TYR:C	2.62	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.76	0.43
1:C:264:ASP:CG	1:C:616:ARG:HH22	2.27	0.43
1:D:235:ARG:HG2	1:D:239:HIS:HD2	1.83	0.43
1:B:113:GLY:C	1:B:115:SER:N	2.76	0.43
1:B:340:TYR:O	1:B:341:ARG:C	2.62	0.43
1:C:276:PHE:CD2	1:C:521:MET:HE2	2.54	0.43
1:C:632:ASP:C	1:C:632:ASP:OD2	2.62	0.43
1:D:372:GLN:O	1:D:376:ARG:HB2	2.19	0.43
1:D:514:THR:OG1	1:D:515:PRO:CD	2.66	0.43
1:A:322:GLU:HB2	1:A:326:LYS:HG2	2.01	0.43
1:B:193:HIS:O	1:B:194:ALA:CB	2.65	0.43
1:B:210:TYR:CZ	1:B:530:VAL:HB	2.54	0.43
1:B:296:PHE:HE1	1:B:487:ILE:HG23	1.83	0.43
1:C:447:MET:HG3	1:C:456:LEU:CD1	2.47	0.43
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.53	0.43
1:D:560:ALA:HB1	1:D:561:PRO:CD	2.49	0.43
1:A:235:ARG:NH2	1:A:260:LYS:HG3	2.18	0.43
1:C:63:TRP:HZ3	1:C:81:GLN:HG2	1.83	0.43
1:D:320:ARG:HA	2:F:5:UNK:O	2.18	0.43
1:D:624:GLU:H	1:D:624:GLU:HG2	1.60	0.43
1:A:459:ILE:HA	1:A:462:VAL:HG22	2.00	0.43
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.53	0.43
1:B:529:ASN:HD21	1:B:557:ARG:HB3	1.84	0.43
1:B:560:ALA:HB1	1:B:561:PRO:HD2	2.01	0.43
1:A:272:ASN:O	1:A:275:LYS:HB3	2.19	0.43
1:B:19:ASN:N	1:B:19:ASN:HD22	2.16	0.43
1:C:537:MET:CG	1:C:551:ILE:HD13	2.49	0.43
1:D:16:GLU:O	1:D:17:VAL:C	2.61	0.43
1:D:77:GLN:O	1:D:81:GLN:HG3	2.18	0.43
1:D:183:ARG:HE	1:D:183:ARG:HB2	1.59	0.43
1:D:626:VAL:HG11	1:D:630:LEU:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASN:HA	1:A:486:PRO:HD3	1.81	0.43
1:A:579:THR:HG23	1:A:582:GLN:OE1	2.19	0.43
1:D:321:TYR:C	1:D:321:TYR:HD1	2.27	0.43
1:B:126:VAL:HG11	1:B:128:ILE:HD11	2.01	0.42
1:B:398:ILE:HD12	1:B:398:ILE:HA	1.90	0.42
1:C:113:GLY:C	1:C:115:SER:N	2.77	0.42
1:C:210:TYR:CZ	1:C:530:VAL:HB	2.54	0.42
1:D:74:ARG:HA	1:D:74:ARG:HD3	1.67	0.42
1:C:425:LEU:HA	1:C:425:LEU:HD23	1.77	0.42
1:A:261:ARG:O	1:A:263:PRO:HD3	2.19	0.42
1:A:366:VAL:HG12	1:A:367:GLU:N	2.33	0.42
1:A:547:LYS:HD2	1:A:571:TYR:HE2	1.84	0.42
1:D:123:TRP:O	1:D:127:GLY:HA2	2.19	0.42
1:A:5:LEU:HD21	1:A:618:TYR:CD1	2.54	0.42
1:A:617:GLY:C	1:A:619:PRO:HD3	2.45	0.42
1:B:126:VAL:HG12	1:B:126:VAL:O	2.19	0.42
1:B:180:ARG:HG3	1:B:180:ARG:HH11	1.84	0.42
1:B:390:GLY:CA	1:D:386:THR:HG21	2.48	0.42
1:B:76:VAL:O	1:B:79:ALA:HB3	2.18	0.42
1:B:425:LEU:O	1:B:429:ILE:HG13	2.18	0.42
1:A:555:ASP:C	1:A:555:ASP:OD1	2.63	0.42
1:D:88:VAL:HG22	1:D:111:VAL:HG23	2.02	0.42
1:D:504:PHE:CD2	1:D:515:PRO:HB3	2.54	0.42
1:D:73:MET:C	1:D:75:PRO:HD2	2.43	0.42
1:A:276:PHE:HD2	1:A:521:MET:HE2	1.85	0.42
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.52	0.42
1:A:490:LEU:HD13	1:A:495:PHE:HA	2.01	0.42
1:B:89:HIS:O	1:B:107:ASP:HB3	2.20	0.42
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.53	0.42
1:C:176:LEU:HD11	1:C:190:PHE:HB2	2.02	0.42
1:C:227:ILE:HG22	1:C:227:ILE:O	2.19	0.42
1:C:552:TYR:CD2	1:C:552:TYR:N	2.88	0.42
1:A:330:MET:HG2	1:A:565:VAL:HG22	2.01	0.42
1:A:330:MET:HE3	1:A:568:LEU:HD12	2.02	0.42
1:A:399:ARG:HH22	1:C:308:ASP:HA	1.84	0.42
1:B:300:HIS:HE1	1:B:441:PRO:O	2.03	0.42
1:C:326:LYS:NZ	3:C:706:SO4:O1	2.53	0.42
1:A:71:ASP:HA	1:A:74:ARG:HG2	2.00	0.41
1:B:3:ARG:HD3	1:B:162:ALA:HA	2.03	0.41
1:B:114:TYR:CD1	1:B:114:TYR:N	2.88	0.41
1:C:8:HIS:CE1	1:C:39:TYR:HE1	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:VAL:O	1:C:472:VAL:HG23	2.20	0.41
1:D:213:LEU:O	1:D:216:VAL:HG22	2.20	0.41
1:D:487:ILE:HD12	1:D:487:ILE:HA	1.82	0.41
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.81	0.41
1:B:316:PHE:CZ	1:B:496:VAL:HG22	2.56	0.41
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.83	0.41
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.83	0.41
1:B:341:ARG:NH2	1:B:566:GLU:OE1	2.50	0.41
1:C:184:ILE:H	1:C:184:ILE:HG12	1.73	0.41
1:C:210:TYR:HE1	1:C:250:ILE:HD11	1.82	0.41
1:C:332:ILE:HG21	1:C:459:ILE:HG22	2.02	0.41
1:C:448:VAL:O	1:C:448:VAL:HG12	2.20	0.41
1:D:34:ILE:HD12	1:D:34:ILE:HA	1.74	0.41
1:D:103:VAL:CG1	1:D:105:LEU:HG	2.50	0.41
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.35	0.41
1:C:149:TRP:O	1:C:149:TRP:CD1	2.71	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:D:456:LEU:HD23	1:D:456:LEU:HA	1.89	0.41
1:D:590:THR:O	1:D:593:LEU:HB2	2.21	0.41
1:B:51:LYS:HE3	1:B:107:ASP:OD1	2.20	0.41
1:B:125:LEU:C	1:B:126:VAL:HG23	2.46	0.41
1:C:459:ILE:HA	1:C:462:VAL:HG22	2.03	0.41
1:A:97:ILE:O	1:A:98:GLU:C	2.64	0.41
1:B:25:TYR:CD2	1:B:25:TYR:C	2.98	0.41
1:B:335:LEU:HD23	1:B:474:MET:HE1	2.02	0.41
1:B:423:VAL:HG12	1:B:424:MET:N	2.35	0.41
1:C:213:LEU:C	1:C:213:LEU:HD12	2.46	0.41
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.57	0.41
1:A:79:ALA:O	1:A:83:MET:HG2	2.21	0.41
1:A:193:HIS:O	1:A:194:ALA:HB2	2.21	0.41
1:A:370:LYS:O	1:A:371:GLY:C	2.63	0.41
1:A:415:GLU:HG2	1:A:417:LEU:O	2.21	0.41
1:B:40:LYS:HB3	1:B:41:ASP:H	1.64	0.41
1:B:331:PHE:CE1	1:B:503:VAL:HB	2.56	0.41
1:C:3:ARG:NH2	1:C:158:ASP:O	2.53	0.41
1:C:537:MET:HG2	1:C:551:ILE:HD13	2.03	0.41
1:D:111:VAL:HG13	1:D:118:TRP:CZ3	2.54	0.41
1:D:198:GLY:HA2	1:D:209:PHE:CZ	2.56	0.41
1:D:344:VAL:C	1:D:346:GLY:N	2.79	0.41
1:D:389:ILE:HG23	1:D:416:LEU:HD13	2.03	0.41
1:D:615:ARG:CZ	1:D:632:ASP:HB3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASP:O	1:A:624:GLU:HG2	2.21	0.41
1:C:330:MET:HE2	1:C:330:MET:HB3	1.90	0.41
1:D:191:THR:HG1	1:D:245:THR:HG1	1.67	0.41
1:A:74:ARG:HB2	1:A:75:PRO:HD3	2.03	0.40
1:A:213:LEU:C	1:A:213:LEU:CD1	2.94	0.40
1:A:337:ARG:O	1:A:341:ARG:HG3	2.20	0.40
1:B:69:PHE:CE2	1:B:77:GLN:HG3	2.56	0.40
1:B:174:VAL:O	1:B:177:PRO:HD2	2.21	0.40
1:B:528:THR:O	1:B:534:GLY:HA3	2.21	0.40
1:C:111:VAL:HG13	1:C:118:TRP:CZ3	2.56	0.40
1:B:289:LYS:HD2	1:B:289:LYS:N	2.36	0.40
1:D:133:ASN:H	1:D:133:ASN:ND2	2.14	0.40
1:D:158:ASP:C	1:D:158:ASP:OD1	2.64	0.40
1:D:447:MET:HG3	1:D:456:LEU:CD1	2.51	0.40
1:A:528:THR:O	1:A:534:GLY:HA3	2.21	0.40
1:A:539:ASP:O	1:A:540:LEU:HD23	2.22	0.40
1:B:125:LEU:O	1:B:126:VAL:CG2	2.69	0.40
1:B:227:ILE:HD13	1:B:227:ILE:HA	1.87	0.40
1:C:31:LYS:HE2	1:C:606:TYR:CE1	2.56	0.40
1:C:193:HIS:HA	1:C:247:VAL:HG22	2.03	0.40
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.56	0.40
1:C:320:ARG:HB2	1:C:320:ARG:HH11	1.87	0.40
1:D:296:PHE:CE1	1:D:487:ILE:HG23	2.57	0.40
1:D:527:THR:OG1	1:D:528:THR:N	2.51	0.40
1:A:19:ASN:N	1:A:19:ASN:ND2	2.68	0.40
1:B:66:PRO:HA	1:B:74:ARG:HH22	1.86	0.40
1:B:134:ASP:OD1	1:B:134:ASP:C	2.65	0.40
1:B:357:MET:HA	1:B:358:PRO:HD3	1.89	0.40
1:B:526:ILE:HG12	1:B:552:TYR:HB2	2.03	0.40
1:C:12:GLU:HG3	1:C:166:HIS:HB3	2.02	0.40
1:C:321:TYR:OH	1:C:455:ILE:HG12	2.21	0.40
1:B:623:ARG:HE	1:B:623:ARG:HB2	1.68	0.40
1:C:227:ILE:O	1:C:227:ILE:CG2	2.69	0.40
1:C:255:ALA:O	1:C:259:LEU:HB2	2.22	0.40
1:C:576:VAL:C	1:C:578:LYS:H	2.29	0.40
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.52	0.40
1:D:348:LYS:HD3	1:D:348:LYS:H	1.86	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	601/725 (83%)	548 (91%)	47 (8%)	6 (1%)	12	45
1	B	601/725 (83%)	543 (90%)	52 (9%)	6 (1%)	12	45
1	C	603/725 (83%)	553 (92%)	43 (7%)	7 (1%)	10	40
1	D	603/725 (83%)	561 (93%)	38 (6%)	4 (1%)	18	53
All	All	2408/2900 (83%)	2205 (92%)	180 (8%)	23 (1%)	12	45

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	449	ASP
1	B	114	TYR
1	B	126	VAL
1	B	449	ASP
1	C	285	LEU
1	C	415	GLU
1	C	449	ASP
1	D	17	VAL
1	D	285	LEU
1	D	449	ASP
1	A	20	ARG
1	B	194	ALA
1	C	17	VAL
1	C	194	ALA
1	D	415	GLU
1	C	114	TYR
1	A	194	ALA
1	A	448	VAL
1	B	210	TYR
1	B	17	VAL
1	C	448	VAL
1	A	111	VAL

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	526/622 (85%)	475 (90%)	51 (10%)	8	30
1	B	526/622 (85%)	472 (90%)	54 (10%)	7	28
1	C	527/622 (85%)	478 (91%)	49 (9%)	8	32
1	D	527/622 (85%)	471 (89%)	56 (11%)	6	27
All	All	2106/2488 (85%)	1896 (90%)	210 (10%)	7	29

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	17	VAL
1	A	19	ASN
1	A	34	ILE
1	A	35	THR
1	A	40	LYS
1	A	84	GLU
1	A	86	ARG
1	A	97	ILE
1	A	103	VAL
1	A	111	VAL
1	A	114	TYR
1	A	122	LEU
1	A	130	SER
1	A	164	VAL
1	A	181	LYS
1	A	183	ARG
1	A	184	ILE
1	A	213	LEU
1	A	214	GLU
1	A	249	GLN
1	A	289	LYS
1	A	292	LYS
1	A	343	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	366	VAL
1	A	376	ARG
1	A	378	LEU
1	A	387	THR
1	A	388	SER
1	A	423	VAL
1	A	428	ARG
1	A	455	ILE
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	472	VAL
1	A	484	ASN
1	A	487	ILE
1	A	488	LEU
1	A	525	SER
1	A	531	SER
1	A	537	MET
1	A	539	ASP
1	A	556	ARG
1	A	568	LEU
1	A	594	SER
1	A	621	GLN
1	A	633	SER
1	A	634	ASN
1	A	635	MET
1	B	7	ASN
1	B	17	VAL
1	B	19	ASN
1	B	34	ILE
1	B	35	THR
1	B	40	LYS
1	B	74	ARG
1	B	83	MET
1	B	84	GLU
1	B	86	ARG
1	B	97	ILE
1	B	103	VAL
1	B	111	VAL
1	B	114	TYR
1	B	122	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	133	ASN
1	B	164	VAL
1	B	181	LYS
1	B	183	ARG
1	B	184	ILE
1	B	192	THR
1	B	213	LEU
1	B	214	GLU
1	B	249	GLN
1	B	266	ILE
1	B	312	THR
1	B	335	LEU
1	B	338	LEU
1	B	343	LYS
1	B	363	SER
1	B	366	VAL
1	B	376	ARG
1	B	378	LEU
1	B	388	SER
1	B	423	VAL
1	B	427	ARG
1	B	428	ARG
1	B	450	ASP
1	B	455	ILE
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	484	ASN
1	B	487	ILE
1	B	488	LEU
1	B	517	GLU
1	B	537	MET
1	B	556	ARG
1	B	568	LEU
1	B	578	LYS
1	B	590	THR
1	B	633	SER
1	B	635	MET
1	C	7	ASN
1	C	9	LEU
1	C	19	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	34	ILE
1	C	40	LYS
1	C	53	THR
1	C	86	ARG
1	C	97	ILE
1	C	103	VAL
1	C	111	VAL
1	C	122	LEU
1	C	126	VAL
1	C	133	ASN
1	C	159	SER
1	C	164	VAL
1	C	180	ARG
1	C	181	LYS
1	C	183	ARG
1	C	214	GLU
1	C	227	ILE
1	C	247	VAL
1	C	249	GLN
1	C	271	LEU
1	C	284	ASN
1	C	289	LYS
1	C	335	LEU
1	C	337	ARG
1	C	338	LEU
1	C	348	LYS
1	C	366	VAL
1	C	376	ARG
1	C	378	LEU
1	C	381	THR
1	C	388	SER
1	C	428	ARG
1	C	458	LYS
1	C	459	ILE
1	C	469	SER
1	C	471	ARG
1	C	484	ASN
1	C	537	MET
1	C	556	ARG
1	C	568	LEU
1	C	569	VAL
1	C	584	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	590	THR
1	C	594	SER
1	C	625	LEU
1	C	635	MET
1	D	2	SER
1	D	7	ASN
1	D	17	VAL
1	D	19	ASN
1	D	34	ILE
1	D	35	THR
1	D	40	LYS
1	D	74	ARG
1	D	86	ARG
1	D	97	ILE
1	D	103	VAL
1	D	111	VAL
1	D	122	LEU
1	D	133	ASN
1	D	137	THR
1	D	164	VAL
1	D	180	ARG
1	D	181	LYS
1	D	183	ARG
1	D	208	ASP
1	D	213	LEU
1	D	214	GLU
1	D	216	VAL
1	D	227	ILE
1	D	247	VAL
1	D	249	GLN
1	D	285	LEU
1	D	289	LYS
1	D	312	THR
1	D	317	ILE
1	D	337	ARG
1	D	338	LEU
1	D	348	LYS
1	D	366	VAL
1	D	376	ARG
1	D	378	LEU
1	D	388	SER
1	D	391	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	428	ARG
1	D	455	ILE
1	D	458	LYS
1	D	459	ILE
1	D	469	SER
1	D	471	ARG
1	D	484	ASN
1	D	487	ILE
1	D	488	LEU
1	D	513	TYR
1	D	537	MET
1	D	556	ARG
1	D	568	LEU
1	D	578	LYS
1	D	579	THR
1	D	594	SER
1	D	624	GLU
1	D	635	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	ASN
1	A	8	HIS
1	A	19	ASN
1	A	78	HIS
1	A	81	GLN
1	A	133	ASN
1	A	168	HIS
1	A	300	HIS
1	A	484	ASN
1	A	500	HIS
1	A	567	GLN
1	A	621	GLN
1	B	6	GLN
1	B	8	HIS
1	B	19	ASN
1	B	78	HIS
1	B	81	GLN
1	B	133	ASN
1	B	168	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	HIS
1	B	300	HIS
1	B	311	ASN
1	B	362	ASN
1	B	484	ASN
1	B	500	HIS
1	B	567	GLN
1	B	586	GLN
1	C	6	GLN
1	C	7	ASN
1	C	8	HIS
1	C	19	ASN
1	C	78	HIS
1	C	81	GLN
1	C	133	ASN
1	C	239	HIS
1	C	257	HIS
1	C	300	HIS
1	C	484	ASN
1	C	500	HIS
1	C	567	GLN
1	C	621	GLN
1	D	6	GLN
1	D	8	HIS
1	D	19	ASN
1	D	133	ASN
1	D	168	HIS
1	D	239	HIS
1	D	257	HIS
1	D	300	HIS
1	D	362	ASN
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	804	-	4,4,4	0.73	0	6,6,6	0.49	0
3	SO4	B	804	-	4,4,4	0.79	0	6,6,6	1.05	0
3	SO4	B	706	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	D	801	-	4,4,4	0.41	0	6,6,6	0.29	0
3	SO4	B	801	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	A	801	-	4,4,4	0.27	0	6,6,6	0.13	0
3	SO4	A	803	-	4,4,4	0.29	0	6,6,6	0.28	0
3	SO4	A	802	-	4,4,4	0.32	0	6,6,6	0.34	0
3	SO4	C	804	-	4,4,4	0.78	0	6,6,6	0.79	0
3	SO4	C	803	-	4,4,4	0.31	0	6,6,6	0.21	0
3	SO4	D	804	-	4,4,4	0.76	0	6,6,6	0.96	0
3	SO4	C	801	-	4,4,4	0.28	0	6,6,6	0.16	0
3	SO4	C	706	-	4,4,4	0.30	0	6,6,6	0.19	0
3	SO4	D	802	-	4,4,4	0.27	0	6,6,6	0.24	0
3	SO4	B	802	-	4,4,4	0.39	0	6,6,6	0.32	0
3	SO4	D	803	-	4,4,4	0.27	0	6,6,6	0.22	0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	SO4	1	0
3	C	706	SO4	1	0
3	D	802	SO4	1	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	611/725 (84%)	-0.09	10 (1%)	70 47	39, 61, 87, 120	0
1	B	611/725 (84%)	-0.07	9 (1%)	72 49	48, 66, 91, 124	0
1	C	613/725 (84%)	-0.20	7 (1%)	78 57	38, 63, 88, 116	0
1	D	613/725 (84%)	-0.27	5 (0%)	82 64	36, 58, 85, 115	0
2	E	0/6	-	-	-	-	-
2	F	0/6	-	-	-	-	-
All	All	2448/2912 (84%)	-0.16	31 (1%)	75 53	36, 62, 88, 124	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	546	ALA	4.9
1	A	546	ALA	4.7
1	D	546	ALA	4.7
1	A	128	ILE	4.1
1	D	205	GLY	4.0
1	B	546	ALA	3.9
1	C	205	GLY	3.8
1	A	205	GLY	3.4
1	B	125	LEU	2.9
1	A	179	CYS	2.8
1	A	549	TYR	2.7
1	A	155	ALA	2.6
1	B	549	TYR	2.5
1	A	125	LEU	2.5
1	B	179	CYS	2.5
1	D	548	ASP	2.5
1	B	205	GLY	2.5
1	A	401	PRO	2.4
1	D	401	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	631	ASN	2.3
1	B	401	PRO	2.2
1	C	416	LEU	2.2
1	B	155	ALA	2.2
1	D	208	ASP	2.2
1	C	17	VAL	2.1
1	B	437	GLY	2.1
1	A	639	ALA	2.1
1	C	277	GLN	2.1
1	C	639	ALA	2.0
1	B	124	SER	2.0
1	C	401	PRO	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(Å ²)	Q<0.9
3	SO4	C	706	5/5	0.67	0.19	82,84,95,102	0
3	SO4	D	801	5/5	0.67	0.16	73,76,89,97	0
3	SO4	B	804	5/5	0.71	0.12	99,99,102,118	0
3	SO4	D	803	5/5	0.72	0.20	91,92,97,101	0
3	SO4	A	802	5/5	0.75	0.15	67,72,82,91	0
3	SO4	C	803	5/5	0.77	0.21	91,92,99,104	0
3	SO4	B	802	5/5	0.78	0.15	73,75,86,93	0
3	SO4	D	804	5/5	0.78	0.16	98,100,102,114	0
3	SO4	A	803	5/5	0.79	0.17	81,85,98,98	0
3	SO4	A	804	5/5	0.79	0.17	97,99,103,107	0
3	SO4	C	804	5/5	0.81	0.14	95,95,101,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	801	5/5	0.85	0.21	74,81,89,91	0
3	SO4	B	706	5/5	0.88	0.16	81,84,93,95	0
3	SO4	B	801	5/5	0.88	0.16	79,80,88,91	0
3	SO4	D	802	5/5	0.89	0.18	69,74,85,86	0
3	SO4	A	801	5/5	0.91	0.15	71,75,81,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.