



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:01 PM UTC

PDB ID : 3TMT / pdb_00003tmt
Title : IrisFP, distorted chromophore
Authors : Adam, V.; Carpentier, P.; Roy, A.; Field, M.; Bourgeois, D.
Deposited on : 2011-08-31
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

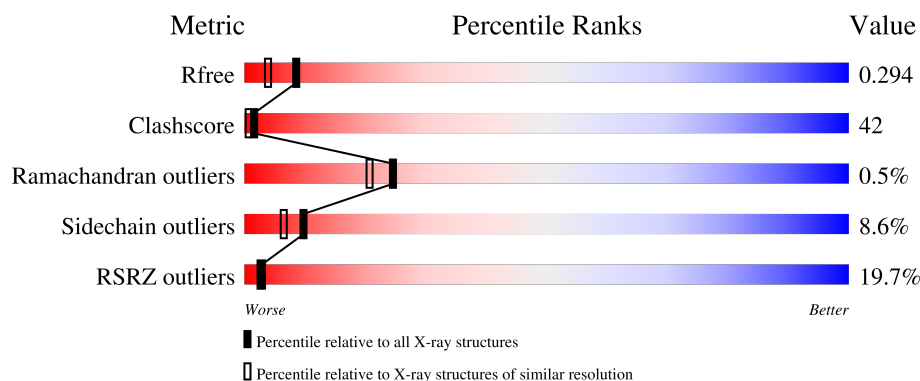
1 Overall quality at a glance

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))
R_{free}	180053	10052 (2.00-2.00)
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	230	21% 38% 49% 8% ...
1	B	230	9% 46% 46% 5% .
1	C	230	20% 40% 50% 5% ...
1	D	230	25% 40% 48% 7% ...

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	SO4	B	1225	-	-	X	-
2	SO4	B	227	-	-	X	-
2	SO4	C	1226	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9939 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 Green to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	3	4	0
			1808	1150	309	337	12			
1	B	221	Total	C	N	O	S	1	3	0
			1792	1141	305	335	11			
1	C	220	Total	C	N	O	S	1	2	0
			1779	1133	304	331	11			
1	D	221	Total	C	N	O	S	2	3	0
			1790	1140	305	333	12			

There are 44 discrepancies between the modelled and reference sequences:

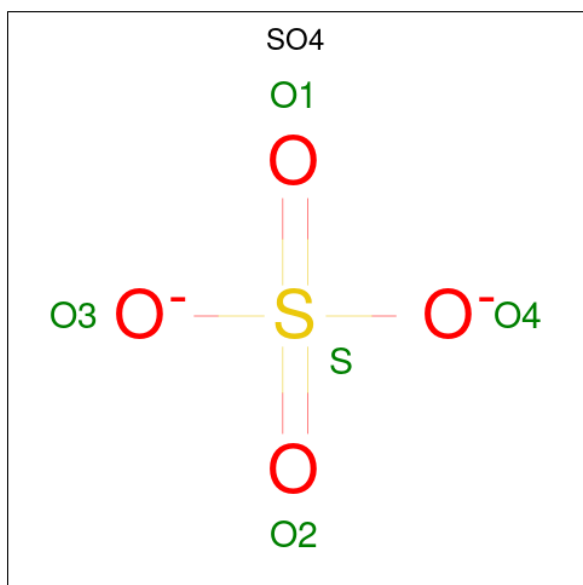
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q5S6Z9
A	-4	HIS	-	expression tag	UNP Q5S6Z9
A	-3	HIS	-	expression tag	UNP Q5S6Z9
A	-2	HIS	-	expression tag	UNP Q5S6Z9
A	-1	HIS	-	expression tag	UNP Q5S6Z9
A	0	HIS	-	expression tag	UNP Q5S6Z9
A	64	CR8	HIS	chromophore	UNP Q5S6Z9
A	64	CR8	TYR	chromophore	UNP Q5S6Z9
A	64	CR8	GLY	chromophore	UNP Q5S6Z9
A	173	SER	PHE	engineered mutation	UNP Q5S6Z9
A	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
B	-5	HIS	-	expression tag	UNP Q5S6Z9
B	-4	HIS	-	expression tag	UNP Q5S6Z9
B	-3	HIS	-	expression tag	UNP Q5S6Z9
B	-2	HIS	-	expression tag	UNP Q5S6Z9
B	-1	HIS	-	expression tag	UNP Q5S6Z9
B	0	HIS	-	expression tag	UNP Q5S6Z9
B	64	CR8	HIS	chromophore	UNP Q5S6Z9
B	64	CR8	TYR	chromophore	UNP Q5S6Z9
B	64	CR8	GLY	chromophore	UNP Q5S6Z9
B	173	SER	PHE	engineered mutation	UNP Q5S6Z9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
C	-5	HIS	-	expression tag	UNP Q5S6Z9
C	-4	HIS	-	expression tag	UNP Q5S6Z9
C	-3	HIS	-	expression tag	UNP Q5S6Z9
C	-2	HIS	-	expression tag	UNP Q5S6Z9
C	-1	HIS	-	expression tag	UNP Q5S6Z9
C	0	HIS	-	expression tag	UNP Q5S6Z9
C	64	CR8	HIS	chromophore	UNP Q5S6Z9
C	64	CR8	TYR	chromophore	UNP Q5S6Z9
C	64	CR8	GLY	chromophore	UNP Q5S6Z9
C	173	SER	PHE	engineered mutation	UNP Q5S6Z9
C	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
D	-5	HIS	-	expression tag	UNP Q5S6Z9
D	-4	HIS	-	expression tag	UNP Q5S6Z9
D	-3	HIS	-	expression tag	UNP Q5S6Z9
D	-2	HIS	-	expression tag	UNP Q5S6Z9
D	-1	HIS	-	expression tag	UNP Q5S6Z9
D	0	HIS	-	expression tag	UNP Q5S6Z9
D	64	CR8	HIS	chromophore	UNP Q5S6Z9
D	64	CR8	TYR	chromophore	UNP Q5S6Z9
D	64	CR8	GLY	chromophore	UNP Q5S6Z9
D	173	SER	PHE	engineered mutation	UNP Q5S6Z9
D	191	LEU	PHE	engineered mutation	UNP Q5S6Z9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	679	Total O 679 679	0	0
3	B	555	Total O 555 555	0	0
3	C	660	Total O 660 660	0	0

Continued on next page...

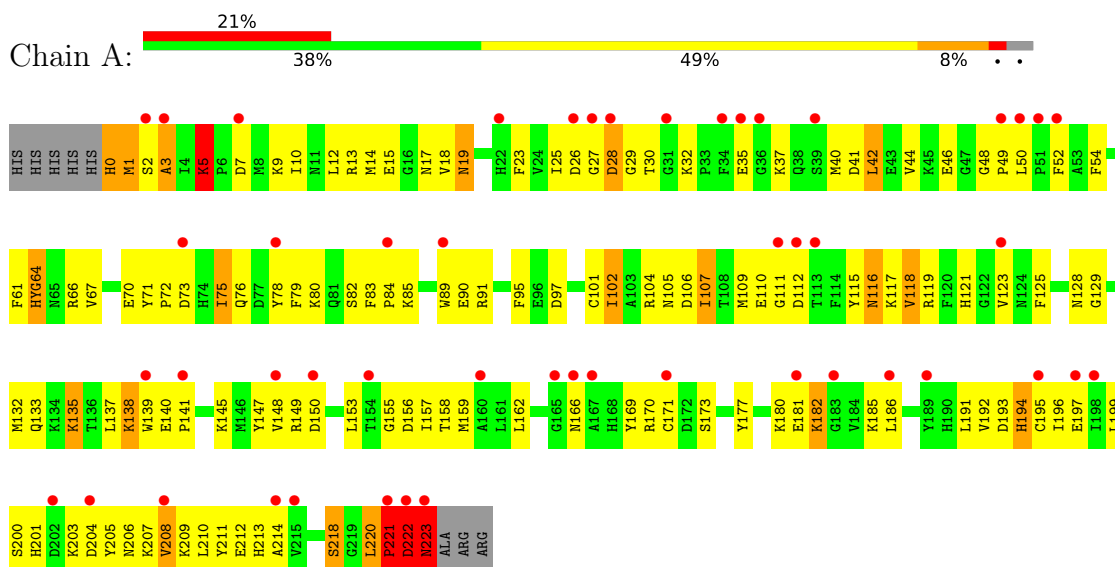
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	791	Total 791	O 791	0	0

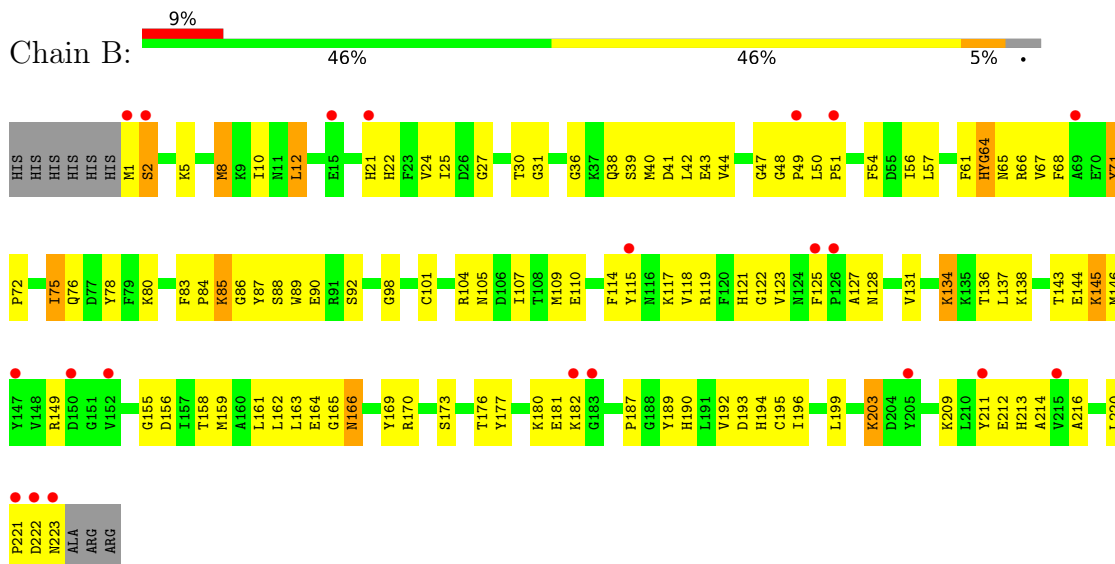
3 Residue-property plots

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.

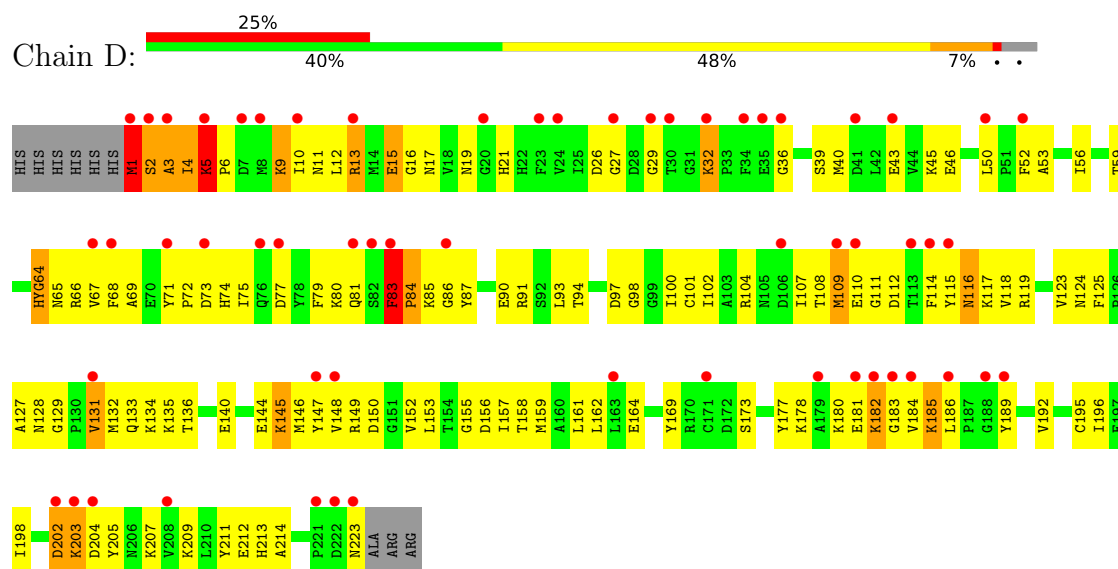
- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



- Molecule 1: Green to red photoconvertible GPF-like protein EosFP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.84Å 96.51Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.98 – 2.00 12.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.9 (12.98-2.00) 83.6 (12.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.295 , 0.295 0.294 , 0.294	Depositor DCC
R_{free} test set	3728 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	2.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9939	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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, CR8

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	1.10	17/1838 (0.9%)	1.12	23/2478 (0.9%)
1	B	0.50	0/1821	0.87	3/2455 (0.1%)
1	C	0.62	3/1805 (0.2%)	0.89	6/2434 (0.2%)
1	D	0.92	14/1819 (0.8%)	0.97	10/2452 (0.4%)
All	All	0.82	34/7283 (0.5%)	0.97	42/9819 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	C-O	-15.17	1.05	1.24
1	A	222	ASP	N-CA	-12.55	1.30	1.46
1	D	4	ILE	CA-CB	-12.15	1.35	1.53
1	A	221	PRO	CA-CB	-11.50	1.33	1.53
1	D	84	PRO	C-O	-10.82	1.09	1.24
1	A	2	SER	C-O	-10.75	1.11	1.24
1	A	3	ALA	C-O	-10.46	1.06	1.24
1	A	222	ASP	CA-C	-10.45	1.38	1.52
1	A	221	PRO	CG-CD	-10.25	1.24	1.51
1	C	2	SER	CB-OG	-10.09	1.22	1.42
1	A	221	PRO	CB-CG	-9.88	1.12	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	ILE	CB-CG2	-8.98	1.23	1.52
1	D	4	ILE	CG1-CD1	-8.57	1.18	1.51
1	D	83	PHE	CA-CB	-8.19	1.38	1.53
1	D	5	LYS	C-O	-8.00	1.15	1.23
1	A	1	MET	CG-SD	-7.92	1.60	1.80
1	D	3	ALA	N-CA	7.47	1.55	1.46
1	A	1	MET	CA-C	-7.28	1.44	1.52
1	D	4	ILE	CA-C	7.10	1.60	1.52
1	D	3	ALA	C-O	-7.08	1.15	1.23
1	A	3	ALA	CA-C	-7.04	1.42	1.52
1	A	220	LEU	N-CA	-6.76	1.37	1.45
1	D	84	PRO	CB-CG	-6.70	1.16	1.49
1	D	5	LYS	CA-C	6.61	1.62	1.52
1	D	3	ALA	CA-C	-6.49	1.44	1.53
1	A	3	ALA	CA-CB	6.41	1.63	1.53
1	A	2	SER	CA-CB	-6.25	1.43	1.53
1	D	84	PRO	C-N	-6.15	1.25	1.33
1	D	5	LYS	C-N	-6.12	1.28	1.33
1	A	223	ASN	CA-C	5.55	1.64	1.52
1	A	220	LEU	CG-CD2	-5.52	1.34	1.52
1	C	3	ALA	CA-CB	5.33	1.61	1.53
1	D	83	PHE	CE1-CZ	-5.07	1.23	1.38
1	A	223	ASN	C-O	5.03	1.33	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	SER	N-CA-C	16.78	131.63	111.33
1	C	4	ILE	CB-CA-C	-9.17	101.32	111.23
1	D	5	LYS	N-CA-C	8.42	120.41	110.31
1	A	1	MET	CA-C-N	7.72	130.96	120.38
1	A	1	MET	C-N-CA	7.72	130.96	120.38
1	D	83	PHE	CA-C-N	7.70	129.47	119.84
1	D	83	PHE	C-N-CA	7.70	129.47	119.84
1	C	3	ALA	N-CA-C	-7.65	102.98	112.47
1	A	2	SER	CA-CB-OG	-7.44	96.21	111.10
1	A	221	PRO	N-CD-CG	-6.96	95.44	103.80
1	D	1	MET	CG-SD-CE	6.61	115.45	100.90
1	A	221	PRO	CB-CA-C	-6.49	95.77	112.00
1	A	220	LEU	CA-C-O	6.39	126.81	120.17
1	A	107	ILE	N-CA-C	6.17	116.75	107.75
1	A	218	SER	CA-C-O	6.00	126.53	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	N-CA-C	-5.95	99.51	108.96
1	A	5	LYS	CA-C-N	5.93	125.63	119.82
1	A	5	LYS	C-N-CA	5.93	125.63	119.82
1	A	3	ALA	N-CA-CB	5.81	121.99	112.63
1	A	220	LEU	CA-CB-CG	5.75	136.44	116.30
1	D	84	PRO	CA-N-CD	-5.71	104.00	112.00
1	B	190	HIS	N-CA-C	5.67	116.04	108.38
1	A	223	ASN	CB-CA-C	5.55	120.65	110.10
1	C	58	THR	N-CA-C	5.53	117.39	111.36
1	D	83	PHE	N-CA-C	5.51	119.20	108.85
1	D	4	ILE	N-CA-CB	-5.44	104.24	110.49
1	A	0	HIS	CA-C-N	-5.38	115.04	122.30
1	A	0	HIS	C-N-CA	-5.38	115.04	122.30
1	A	221	PRO	CB-CG-CD	5.30	117.59	105.40
1	A	221	PRO	CA-N-CD	-5.25	104.14	111.50
1	D	4	ILE	N-CA-C	5.21	115.96	108.93
1	C	2	SER	CA-C-N	5.18	130.70	122.61
1	C	2	SER	C-N-CA	5.18	130.70	122.61
1	C	4	ILE	N-CA-CB	5.17	117.38	111.39
1	D	5	LYS	CB-CG-CD	5.12	123.07	111.30
1	A	2	SER	CA-C-N	5.11	131.28	123.47
1	A	2	SER	C-N-CA	5.11	131.28	123.47
1	A	129	GLY	CA-C-N	5.06	124.67	119.05
1	A	129	GLY	C-N-CA	5.06	124.67	119.05
1	D	16	GLY	N-CA-C	5.03	118.40	110.91
1	B	71	TYR	CA-C-N	5.01	125.40	119.99
1	B	71	TYR	C-N-CA	5.01	125.40	119.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	PRO	Peptide
1	C	2	SER	Peptide
1	D	1	MET	Peptide
1	D	83	PHE	Peptide

5.2 Too-close contacts

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1808	0	1730	159	0
1	B	1792	0	1719	143	1
1	C	1779	0	1703	150	1
1	D	1790	0	1720	150	0
2	A	20	0	0	1	0
2	B	15	0	0	5	0
2	C	25	0	0	4	0
2	D	25	0	0	1	0
3	A	679	0	0	79	5
3	B	555	0	0	68	6
3	C	660	0	0	66	3
3	D	791	0	0	70	5
All	All	9939	0	6872	596	11

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 42.

All (596) 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:B:5:LYS:NZ	3:B:662:HOH:O	1.83	1.09
1:A:135:LYS:NZ	3:A:723:HOH:O	1.86	1.06
2:B:1225:SO4:O4	3:B:595:HOH:O	1.75	1.03
1:C:197:GLU:OE2	3:C:1385:HOH:O	1.80	0.99
1:D:212:GLU:OE1	3:D:2145:HOH:O	1.81	0.97
1:A:221:PRO:O	1:A:221:PRO:HG2	1.58	0.96
1:C:2:SER:HA	1:C:4:ILE:HD12	1.46	0.95
1:C:204:ASP:OD1	3:C:266:HOH:O	1.83	0.95
1:B:85:LYS:HD2	3:B:2780:HOH:O	1.67	0.94
1:A:70:GLU:OE1	3:A:1896:HOH:O	1.85	0.94
1:B:180:LYS:NZ	3:B:3080:HOH:O	2.01	0.93
1:A:159:MET:SD	1:A:173:SER:HB2	2.10	0.91
1:D:64:CR8:H10	3:D:1799:HOH:O	1.70	0.91
1:D:87:TYR:CZ	1:D:107:ILE:HD13	2.07	0.89
1:A:80:LYS:NZ	3:A:1784:HOH:O	2.00	0.89
1:C:175:THR:HG23	3:C:1982:HOH:O	1.74	0.88
1:B:76:GLN:OE1	3:B:242:HOH:O	1.92	0.87
1:A:153:LEU:HB2	3:A:2117:HOH:O	1.73	0.87
1:B:50:LEU:O	1:B:134:LYS:NZ	2.08	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:O	3:B:284:HOH:O	1.92	0.86
1:B:85:LYS:HD3	1:B:181:GLU:HB2	1.57	0.86
1:A:0:HIS:HA	3:A:3332:HOH:O	1.75	0.86
1:B:27:GLY:HA3	1:B:40:MET:HE2	1.58	0.85
2:B:1224:SO4:O2	3:B:2277:HOH:O	1.95	0.85
1:A:125:PHE:HB2	1:A:132:MET:HE3	1.57	0.84
1:A:186:LEU:HD22	3:A:2117:HOH:O	1.77	0.84
1:B:146:MET:HE3	3:B:876:HOH:O	1.75	0.84
1:B:10:ILE:HD12	3:B:312:HOH:O	1.76	0.82
1:C:104:ARG:HG3	1:C:119:ARG:HB2	1.61	0.82
1:D:148:VAL:HG22	3:D:2062:HOH:O	1.77	0.82
1:A:72:PRO:O	3:A:846:HOH:O	1.95	0.82
1:A:220:LEU:HB3	1:A:221:PRO:HB3	1.61	0.82
1:A:182:LYS:HB2	3:A:2689:HOH:O	1.78	0.82
1:C:112:ASP:OD1	3:C:292:HOH:O	1.98	0.81
2:C:1226:SO4:O2	3:C:2751:HOH:O	1.98	0.81
1:C:2:SER:CB	1:C:4:ILE:H	1.94	0.80
1:C:2:SER:CA	1:C:4:ILE:H	1.93	0.80
2:B:227:SO4:O2	3:B:241:HOH:O	1.97	0.80
1:C:159:MET:SD	1:C:173:SER:HB3	2.21	0.80
1:A:109:MET:O	3:A:2045:HOH:O	1.98	0.80
1:C:25:ILE:O	3:C:791:HOH:O	2.00	0.80
1:D:83:PHE:CE2	1:D:86:GLY:HA2	2.16	0.80
1:A:72:PRO:HG2	1:A:75:ILE:HG13	1.62	0.80
1:B:75:ILE:HD12	3:B:3176:HOH:O	1.81	0.79
1:A:76:GLN:NE2	3:A:530:HOH:O	1.81	0.79
1:B:180:LYS:O	3:B:962:HOH:O	1.98	0.79
1:D:27:GLY:O	3:D:904:HOH:O	2.00	0.79
1:D:223:ASN:O	3:D:1975:HOH:O	2.00	0.79
1:C:116:ASN:O	3:C:2138:HOH:O	2.00	0.79
1:C:77:ASP:HB2	3:C:3204:HOH:O	1.83	0.79
1:C:85:LYS:HG2	1:C:181:GLU:HG2	1.62	0.79
2:C:1224:SO4:O1	3:C:1898:HOH:O	2.00	0.78
1:A:73:ASP:OD1	3:A:1925:HOH:O	2.00	0.78
1:B:110:GLU:OE2	3:B:740:HOH:O	2.00	0.78
1:C:222:ASP:OD2	1:C:222:ASP:N	2.17	0.78
1:D:73:ASP:OD2	3:D:563:HOH:O	2.02	0.77
1:A:106[A]:ASP:OD1	3:A:3046:HOH:O	2.03	0.77
1:D:128:ASN:O	3:D:1940:HOH:O	2.01	0.77
1:C:91:ARG:NH2	3:C:2773:HOH:O	2.16	0.77
1:B:104:ARG:HG2	3:B:2118:HOH:O	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:NZ	1:A:181:GLU:OE1	2.18	0.76
1:A:194:HIS:HB3	1:A:212:GLU:OE1	1.84	0.76
1:A:110:GLU:HB2	1:A:115:TYR:CE1	2.20	0.76
1:A:209:LYS:HG3	3:A:260:HOH:O	1.86	0.75
1:B:49:PRO:HB2	3:B:2124:HOH:O	1.84	0.75
1:B:203:LYS:O	3:B:267:HOH:O	2.05	0.75
1:D:64:CR8:H23	1:D:212:GLU:HB2	1.68	0.75
1:C:83:PHE:O	3:C:3135:HOH:O	2.03	0.75
1:A:106[B]:ASP:OD2	3:A:515:HOH:O	2.05	0.75
1:C:130:PRO:O	3:C:1876:HOH:O	2.04	0.75
1:A:37:LYS:HE2	3:A:2795:HOH:O	1.86	0.75
1:C:117:LYS:HE3	1:C:119:ARG:CZ	2.17	0.75
1:C:121:HIS:NE2	3:C:466:HOH:O	2.20	0.75
1:D:64:CR8:C23	1:D:212:GLU:HB2	2.17	0.75
1:D:202:ASP:OD2	1:D:207:LYS:HB2	1.87	0.75
1:A:222:ASP:C	1:A:222:ASP:OD1	2.29	0.74
1:B:144:GLU:CD	1:B:146:MET:HE2	2.11	0.74
1:A:66:ARG:HD2	1:A:192:VAL:HG11	1.69	0.74
1:B:30:THR:HB	3:B:2029:HOH:O	1.87	0.74
1:C:161:LEU:HD12	1:C:169:TYR:HD2	1.52	0.74
2:B:1225:SO4:O3	3:B:3330:HOH:O	2.06	0.73
2:A:227:SO4:O3	3:A:1682:HOH:O	2.05	0.73
1:C:85:LYS:HE2	3:C:3104:HOH:O	1.88	0.73
1:A:196:ILE:HG12	3:A:2116:HOH:O	1.87	0.73
1:D:132:MET:HE1	3:D:2130:HOH:O	1.88	0.73
1:A:185:LYS:HE3	3:A:3326:HOH:O	1.88	0.73
1:C:7:ASP:OD1	3:C:2148:HOH:O	2.06	0.73
1:A:199:LEU:O	3:A:738:HOH:O	2.06	0.73
1:B:199:LEU:O	3:B:299:HOH:O	2.04	0.73
1:B:220:LEU:O	3:B:2154:HOH:O	2.05	0.73
1:D:10:ILE:HB	3:D:1432:HOH:O	1.88	0.73
1:B:117:LYS:NZ	3:B:2103:HOH:O	2.22	0.73
1:D:45:LYS:HD3	3:D:3229:HOH:O	1.86	0.73
1:D:162:LEU:HD21	3:D:2141:HOH:O	1.87	0.73
1:A:201:HIS:NE2	3:A:1805:HOH:O	2.22	0.72
1:D:13:ARG:HG2	3:D:3130:HOH:O	1.89	0.72
1:D:181:GLU:OE2	3:D:683:HOH:O	2.06	0.72
1:C:2:SER:HB2	3:C:762:HOH:O	1.88	0.72
1:D:135:LYS:HE2	3:D:951:HOH:O	1.88	0.71
1:C:2:SER:HB3	1:C:4:ILE:H	1.54	0.71
1:C:170:ARG:NH1	3:C:314:HOH:O	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:HB2	1:D:101:CYS:HB2	1.72	0.71
1:A:135:LYS:HB2	3:A:2678:HOH:O	1.89	0.71
1:D:195[A]:CYS:SG	1:D:213:HIS:HB3	2.31	0.70
1:D:11:ASN:OD1	3:D:904:HOH:O	2.09	0.70
1:B:222:ASP:OD2	3:B:1363:HOH:O	2.10	0.70
1:A:10:ILE:HD13	3:A:3119:HOH:O	1.89	0.70
1:C:6:PRO:O	3:C:447:HOH:O	2.08	0.70
1:B:209:LYS:NZ	3:B:1429:HOH:O	2.23	0.70
1:C:70:GLU:OE1	3:C:577:HOH:O	2.09	0.70
2:D:1226:SO4:O3	3:D:3132:HOH:O	2.08	0.70
1:A:148:VAL:O	3:A:294:HOH:O	2.10	0.69
1:A:28:ASP:OD1	1:A:28:ASP:N	2.26	0.69
1:D:56:ILE:HG12	3:D:809:HOH:O	1.89	0.69
1:C:202:ASP:OD2	1:C:207:LYS:HB2	1.92	0.69
1:C:31:GLY:HA3	1:C:68:PHE:CE2	2.28	0.69
1:B:50:LEU:HD22	3:B:2976:HOH:O	1.93	0.69
1:A:203:LYS:NZ	3:A:722:HOH:O	2.17	0.69
1:C:149:ARG:NH1	3:C:1745:HOH:O	2.25	0.69
1:D:53:ALA:O	3:D:809:HOH:O	2.10	0.69
1:C:2:SER:C	1:C:4:ILE:H	1.99	0.68
1:C:165:GLY:N	3:C:1379:HOH:O	2.25	0.68
1:D:128:ASN:O	3:D:2781:HOH:O	2.11	0.68
1:C:174:ARG:HG2	1:D:124:ASN:ND2	2.09	0.68
1:C:80:LYS:O	3:C:3135:HOH:O	2.12	0.68
1:B:67:VAL:HG11	1:B:83:PHE:CE1	2.29	0.68
1:A:110:GLU:HB2	1:A:115:TYR:HE1	1.57	0.67
1:A:91:ARG:NH1	3:A:353:HOH:O	2.27	0.67
1:C:95:PHE:CD2	1:C:171:CYS:HB2	2.30	0.67
1:D:26:ASP:HB2	1:D:45:LYS:HE3	1.75	0.67
1:D:87:TYR:CE1	1:D:107:ILE:HD13	2.30	0.67
1:C:97:ASP:OD2	3:C:1981:HOH:O	2.12	0.67
1:B:72:PRO:HG2	1:B:75:ILE:HG13	1.76	0.67
1:C:87:TYR:CZ	1:C:107:ILE:HD12	2.29	0.67
1:B:64:CR8:O13	3:B:270:HOH:O	2.12	0.67
2:C:1226:SO4:O2	3:C:948:HOH:O	2.13	0.67
1:A:35:GLU:OE1	3:A:268:HOH:O	2.13	0.67
1:A:104:ARG:NH1	1:B:122:GLY:O	2.28	0.67
1:B:24:VAL:HG12	3:B:2066:HOH:O	1.94	0.67
1:C:49:PRO:HA	3:C:248:HOH:O	1.95	0.67
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.77	0.67
1:D:136:THR:HG21	1:D:161:LEU:HD13	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:HB3	3:A:846:HOH:O	1.93	0.66
1:C:158:THR:HG23	1:C:170:ARG:CZ	2.25	0.66
1:A:64:CR8:O13	3:A:458:HOH:O	2.13	0.66
1:C:64:CR8:O2	3:C:2773:HOH:O	2.14	0.66
1:B:90:GLU:OE1	3:B:1686:HOH:O	2.13	0.66
1:C:117:LYS:HE3	1:C:119:ARG:NH1	2.11	0.66
1:B:144:GLU:OE2	1:B:177:TYR:OH	2.14	0.65
1:C:96:GLU:OE2	1:C:170:ARG:N	2.27	0.65
1:A:7:ASP:O	3:A:965:HOH:O	2.14	0.65
1:C:220:LEU:O	3:C:2633:HOH:O	2.14	0.65
1:A:180:LYS:O	3:A:797:HOH:O	2.14	0.65
1:B:189:TYR:CE2	1:D:140:GLU:HB3	2.32	0.65
1:D:147:TYR:CE2	3:D:2129:HOH:O	2.50	0.65
1:B:78:TYR:HE2	3:B:2201:HOH:O	1.79	0.64
1:C:10:ILE:HD11	1:C:68:PHE:CZ	2.33	0.64
1:D:150:ASP:HA	3:D:1857:HOH:O	1.97	0.64
1:A:112:ASP:HB3	3:A:3122:HOH:O	1.96	0.64
1:C:58:THR:CG2	3:C:2054:HOH:O	2.45	0.64
1:D:149:ARG:HG3	3:D:2175:HOH:O	1.97	0.64
1:C:26:ASP:OD1	3:C:791:HOH:O	2.15	0.64
1:A:64:CR8:C1	3:A:1929:HOH:O	2.45	0.64
1:A:194:HIS:CB	1:A:212:GLU:OE1	2.45	0.64
1:A:64:CR8:H23	1:A:212:GLU:HB2	1.79	0.64
3:C:269:HOH:O	1:D:98:GLY:HA3	1.97	0.64
1:B:87:TYR:CZ	1:B:107:ILE:HD13	2.33	0.64
1:C:40:MET:HE3	1:C:64:CR8:H10	1.79	0.64
1:D:15:GLU:HG3	1:D:119:ARG:CZ	2.29	0.63
1:D:72:PRO:HG2	1:D:75:ILE:HD12	1.78	0.63
1:B:223:ASN:O	3:B:2653:HOH:O	2.14	0.63
1:A:150:ASP:OD2	3:A:253:HOH:O	2.14	0.63
1:C:174:ARG:NH1	3:C:252:HOH:O	2.30	0.63
1:D:109:MET:HE2	1:D:114:PHE:CE1	2.32	0.63
1:D:186:LEU:HD22	3:D:2062:HOH:O	1.98	0.63
1:D:4:ILE:HD11	1:D:83:PHE:HB2	1.80	0.63
1:A:90:GLU:OE2	1:A:104:ARG:NE	2.28	0.62
1:C:151:GLY:N	3:C:283:HOH:O	2.09	0.62
3:C:482:HOH:O	1:D:127:ALA:HB2	1.98	0.62
1:C:2:SER:HB3	1:C:4:ILE:N	2.14	0.62
1:C:196:ILE:HG21	3:C:3179:HOH:O	1.98	0.62
1:C:184:VAL:O	3:C:2627:HOH:O	2.16	0.61
1:B:12:LEU:HD23	1:B:12:LEU:C	2.24	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:HE3	3:B:1625:HOH:O	2.00	0.61
3:A:2622:HOH:O	1:B:22:HIS:HB2	2.01	0.61
1:C:16:GLY:HA3	1:C:23:PHE:CE1	2.34	0.61
1:A:46:GLU:OE2	3:A:838:HOH:O	2.16	0.61
1:A:110:GLU:HG3	3:A:3041:HOH:O	1.99	0.61
1:A:133:GLN:HB2	3:A:2678:HOH:O	2.00	0.61
1:D:19:ASN:ND2	3:D:241:HOH:O	2.13	0.61
1:A:138:LYS:HE2	1:A:162:LEU:HD22	1.83	0.60
1:D:40:MET:HB2	3:D:1799:HOH:O	2.01	0.60
1:B:143:THR:H	1:D:145:LYS:HZ1	1.46	0.60
1:B:199:LEU:HD12	1:B:209:LYS:HG2	1.82	0.60
1:D:144:GLU:CD	1:D:146:MET:HE2	2.26	0.60
1:D:59:THR:HG23	3:D:273:HOH:O	2.02	0.60
1:A:210:LEU:HB2	3:A:2777:HOH:O	2.02	0.60
1:B:56:ILE:HA	3:B:2791:HOH:O	2.02	0.60
1:C:174:ARG:NH2	3:C:269:HOH:O	2.11	0.60
1:D:77:ASP:OD2	1:D:80:LYS:HD2	2.00	0.60
1:B:2:SER:OG	3:B:1953:HOH:O	1.97	0.60
1:B:25:ILE:HD12	1:B:61:PHE:HZ	1.66	0.60
1:C:8:MET:O	1:C:31:GLY:N	2.29	0.60
1:A:78:TYR:O	1:A:82:SER:OG	2.16	0.59
1:C:111:GLY:O	3:C:721:HOH:O	2.17	0.59
1:C:133:GLN:OE1	3:C:836:HOH:O	2.17	0.59
1:D:147:TYR:HA	3:D:2132:HOH:O	2.02	0.59
1:C:31:GLY:HA3	1:C:68:PHE:HE2	1.67	0.59
1:C:203:LYS:HB3	3:C:1848:HOH:O	2.03	0.59
1:C:145:LYS:O	1:C:155:GLY:HA2	2.03	0.59
1:A:67:VAL:HG23	1:A:80:LYS:HG2	1.85	0.59
1:A:220:LEU:HD23	1:A:223:ASN:HD21	1.67	0.59
1:B:80:LYS:NZ	3:B:245:HOH:O	2.34	0.59
1:C:184:VAL:O	3:C:257:HOH:O	2.16	0.59
1:D:156:ASP:N	3:D:2129:HOH:O	2.36	0.59
1:A:158:THR:HG23	1:A:170:ARG:NH1	2.18	0.59
1:B:72:PRO:HD2	3:B:3176:HOH:O	2.03	0.59
1:D:125:PHE:CE1	1:D:131:VAL:HG21	2.38	0.58
1:D:110:GLU:HB2	1:D:115:TYR:CE1	2.38	0.58
1:C:40:MET:HB2	3:C:2069:HOH:O	2.03	0.58
1:C:66:ARG:HG2	1:C:79:PHE:CE1	2.38	0.58
1:C:2:SER:C	1:C:4:ILE:N	2.55	0.58
1:A:197:GLU:HG3	3:A:2704:HOH:O	2.03	0.58
1:A:14:MET:HE3	1:A:61:PHE:CE1	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:654:HOH:O	1:C:221:PRO:HG3	2.03	0.58
1:D:108:THR:HB	3:D:244:HOH:O	2.04	0.58
1:A:54:PHE:CZ	1:A:208:VAL:HG21	2.38	0.57
1:C:136:THR:HG21	1:C:161:LEU:HD13	1.84	0.57
1:B:89:TRP:NE1	1:B:105:ASN:HB3	2.18	0.57
1:D:1:MET:HB3	3:D:1063:HOH:O	2.04	0.57
1:C:125:PHE:CE1	1:C:131:VAL:HG21	2.39	0.57
1:A:13:ARG:NH1	3:A:2674:HOH:O	2.37	0.57
1:B:12:LEU:HB3	1:B:40:MET:HE1	1.87	0.57
1:B:64:CR8:C23	1:B:212:GLU:HB2	2.35	0.57
1:A:23:PHE:CE2	1:A:52:PHE:HZ	2.23	0.56
1:A:140:GLU:HB3	1:C:189:TYR:CE2	2.40	0.56
1:B:220:LEU:CD2	1:B:221:PRO:HA	2.34	0.56
1:A:7:ASP:OD1	3:A:3171:HOH:O	2.17	0.56
1:A:140:GLU:HB3	1:A:141:PRO:HD2	1.86	0.56
1:C:4:ILE:HG22	1:C:4:ILE:O	1.90	0.56
1:A:37:LYS:HE3	1:A:213:HIS:CE1	2.41	0.56
1:B:193:ASP:O	1:B:214:ALA:HA	2.06	0.56
1:C:79:PHE:HE2	1:C:177:TYR:CD1	2.23	0.56
1:B:44:VAL:HG12	3:B:833:HOH:O	2.04	0.56
1:A:118:VAL:O	1:A:119:ARG:NH2	2.37	0.56
1:A:123:VAL:HB	1:B:90:GLU:HB3	1.87	0.56
1:C:25:ILE:HG12	1:C:44:VAL:HG22	1.87	0.56
1:B:158:THR:HG23	1:B:170:ARG:CZ	2.36	0.56
1:D:203:LYS:HD2	3:D:2762:HOH:O	2.06	0.56
1:C:7:ASP:OD1	1:C:32:LYS:NZ	2.36	0.56
1:C:49:PRO:HB3	1:C:204:ASP:HB3	1.88	0.56
1:B:71:TYR:O	3:B:2162:HOH:O	2.18	0.56
1:B:30:THR:HG23	3:B:288:HOH:O	2.06	0.55
1:B:145:LYS:O	1:B:155:GLY:HA2	2.06	0.55
1:B:156:ASP:HB3	3:D:1813:HOH:O	2.06	0.55
1:C:13:ARG:HA	3:C:791:HOH:O	2.06	0.55
1:B:181:GLU:HG2	1:B:182:LYS:O	2.07	0.55
1:D:29:GLY:HA2	3:D:1759:HOH:O	2.05	0.55
1:A:210:LEU:HD13	3:A:2777:HOH:O	2.06	0.55
1:B:84:PRO:HB3	1:B:109:MET:CE	2.37	0.55
1:B:66:ARG:HB2	3:B:1907:HOH:O	2.05	0.55
1:B:66:ARG:N	3:B:1907:HOH:O	2.20	0.54
1:D:161:LEU:HB2	1:D:169:TYR:HB3	1.89	0.54
1:A:30:THR:O	3:A:2120:HOH:O	2.18	0.54
1:D:13:ARG:NH1	3:D:2258:HOH:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:LYS:HE2	3:D:2176:HOH:O	2.08	0.54
1:A:149:ARG:NH2	1:C:96:GLU:OE1	2.40	0.54
1:C:136:THR:CG2	1:C:161:LEU:HD13	2.38	0.54
1:A:32:LYS:HG2	3:A:3171:HOH:O	2.06	0.54
1:A:207:LYS:HG2	3:A:247:HOH:O	2.08	0.54
1:B:76:GLN:N	3:B:1415:HOH:O	2.41	0.54
1:B:101:CYS:HA	1:B:121:HIS:O	2.07	0.54
1:C:32:LYS:HB3	1:C:35:GLU:HB2	1.90	0.54
1:C:58:THR:HG22	3:C:2054:HOH:O	2.05	0.54
1:C:161:LEU:HD12	1:C:169:TYR:CD2	2.38	0.53
1:D:111:GLY:HA3	3:D:1406:HOH:O	2.07	0.53
1:A:19:ASN:ND2	3:A:1806:HOH:O	1.91	0.53
1:C:130:PRO:HG3	3:C:506:HOH:O	2.08	0.53
1:A:3:ALA:HB3	1:A:109:MET:HE3	1.91	0.53
1:A:149:ARG:NH2	3:A:496:HOH:O	2.05	0.53
1:D:3:ALA:HA	3:D:1778:HOH:O	2.08	0.53
1:D:146:MET:HE1	1:D:177:TYR:CE2	2.43	0.53
1:C:123:VAL:HG12	1:D:90:GLU:OE2	2.09	0.53
1:D:65:ASN:HD22	1:D:68:PHE:HE1	1.57	0.53
1:D:157:ILE:HB	1:D:173:SER:HB3	1.90	0.53
1:A:46:GLU:HG2	3:A:751:HOH:O	2.09	0.53
1:C:58:THR:HG23	3:C:2054:HOH:O	2.06	0.53
1:D:136:THR:CG2	1:D:161:LEU:HD13	2.38	0.53
1:A:128:ASN:OD1	3:A:2169:HOH:O	2.18	0.53
1:B:119:ARG:NH1	3:B:1952:HOH:O	2.27	0.52
1:B:196:ILE:HB	1:B:212:GLU:HG2	1.90	0.52
1:D:69:ALA:O	1:D:80:LYS:NZ	2.42	0.52
1:D:72:PRO:HB2	1:D:74:HIS:CE1	2.45	0.52
1:B:166:ASN:HB2	3:B:1984:HOH:O	2.08	0.52
1:D:9:LYS:HB3	3:D:2761:HOH:O	2.09	0.52
1:A:197:GLU:HB2	3:A:917:HOH:O	2.08	0.52
1:B:39[B]:SER:HG	1:B:211:TYR:HD1	1.57	0.52
1:B:51:PRO:HA	1:B:134:LYS:HZ2	1.75	0.52
1:B:162:LEU:HD21	3:B:719:HOH:O	2.10	0.52
1:C:38:GLN:NE2	3:C:1637:HOH:O	2.05	0.52
1:B:39[A]:SER:HG	1:B:211:TYR:HD1	1.57	0.52
1:B:182:LYS:N	3:B:1814:HOH:O	2.42	0.52
1:B:220:LEU:C	3:B:2749:HOH:O	2.53	0.52
1:B:48:GLY:O	3:B:930:HOH:O	2.18	0.52
1:A:101:CYS:HA	1:A:121:HIS:O	2.10	0.51
1:C:90:GLU:C	3:C:1982:HOH:O	2.52	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:PHE:CD1	1:D:131:VAL:HG21	2.46	0.51
1:D:156:ASP:HB2	3:D:1836:HOH:O	2.11	0.51
1:B:67:VAL:CG1	1:B:83:PHE:HE1	2.23	0.51
1:C:49:PRO:CB	1:C:204:ASP:HB3	2.40	0.51
1:D:145:LYS:O	1:D:155:GLY:HA2	2.10	0.51
1:A:3:ALA:O	1:A:5:LYS:HE3	2.11	0.51
1:A:23:PHE:CE2	1:A:52:PHE:CZ	2.98	0.51
1:A:111:GLY:O	3:A:711:HOH:O	2.19	0.51
1:A:204:ASP:O	1:A:205:TYR:HB2	2.09	0.51
1:C:197:GLU:O	1:C:210:LEU:HD12	2.10	0.51
1:A:102:ILE:HD12	1:A:102:ILE:C	2.36	0.51
1:A:207:LYS:HE3	3:A:1348:HOH:O	2.11	0.51
1:D:204:ASP:O	1:D:205:TYR:HB2	2.10	0.51
1:C:139:TRP:CH2	1:C:159:MET:HE2	2.45	0.51
1:D:72:PRO:HB2	1:D:74:HIS:ND1	2.25	0.51
1:B:110:GLU:CG	1:B:115:TYR:CE1	2.94	0.50
1:B:159:MET:SD	1:B:173:SER:HB2	2.52	0.50
1:D:152:VAL:HA	3:D:256:HOH:O	2.10	0.50
1:D:178:LYS:HD3	3:D:2991:HOH:O	2.10	0.50
1:A:112:ASP:HA	3:A:711:HOH:O	2.11	0.50
1:C:136:THR:HG23	3:C:1876:HOH:O	2.12	0.50
1:A:12:LEU:C	1:A:12:LEU:HD23	2.37	0.50
1:A:218:SER:HB2	3:A:465:HOH:O	2.11	0.50
1:D:156:ASP:CG	3:D:2129:HOH:O	2.55	0.50
1:B:195:CYS:SG	1:B:213:HIS:HB3	2.51	0.50
1:C:14:MET:HA	1:C:118:VAL:O	2.11	0.50
1:D:5:LYS:HB3	1:D:6:PRO:HD2	1.93	0.50
1:A:40:MET:HB2	1:A:64:CR8:H10	1.94	0.50
1:A:64:CR8:C23	1:A:212:GLU:HB2	2.41	0.50
1:D:209:LYS:HE2	3:D:2744:HOH:O	2.12	0.50
1:A:25:ILE:HG12	1:A:44:VAL:HG22	1.94	0.50
1:A:137:LEU:HD12	1:A:162:LEU:HG	1.93	0.50
1:B:136:THR:HG21	1:B:161:LEU:HD13	1.93	0.50
1:D:66:ARG:NH2	3:D:252:HOH:O	2.44	0.50
1:B:85:LYS:HB2	3:B:235:HOH:O	2.12	0.49
1:C:39:SER:HA	1:C:210:LEU:O	2.11	0.49
1:C:144:GLU:HA	1:C:157:ILE:HG12	1.94	0.49
1:D:13:ARG:NH2	3:D:642:HOH:O	2.44	0.49
1:B:41:ASP:OD1	1:B:209:LYS:HE3	2.11	0.49
1:C:17:ASN:HA	1:C:21:HIS:O	2.12	0.49
1:C:37:LYS:HD3	1:C:211:TYR:OH	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:N	1:A:107:ILE:HD12	2.28	0.49
1:C:104:ARG:CG	1:C:119:ARG:HB2	2.39	0.49
1:C:144:GLU:CD	1:C:146:MET:HE2	2.36	0.49
1:A:26:ASP:O	1:A:42:LEU:HA	2.13	0.49
1:C:57:LEU:O	1:C:60:ALA:HB3	2.12	0.49
1:C:105:ASN:CG	1:C:118:VAL:HG22	2.37	0.49
1:C:91:ARG:HB2	3:C:1982:HOH:O	2.11	0.49
1:D:45:LYS:C	1:D:46:GLU:HG3	2.37	0.49
1:C:93:LEU:HB2	1:C:101:CYS:HB2	1.94	0.49
1:D:129:GLY:O	1:D:133:GLN:HB2	2.13	0.49
1:B:84:PRO:HB3	1:B:109:MET:HE2	1.95	0.49
1:D:2:SER:HB2	3:D:1966:HOH:O	2.13	0.49
1:D:50:LEU:HD13	1:D:52:PHE:CZ	2.47	0.49
1:B:21:HIS:CE1	1:B:47:GLY:O	2.66	0.49
1:B:220:LEU:HG	3:D:2778:HOH:O	2.11	0.49
1:C:182:LYS:HD2	3:C:2403:HOH:O	2.12	0.49
1:A:0:HIS:CA	3:A:3332:HOH:O	2.48	0.48
1:A:138:LYS:HE2	1:A:162:LEU:CD2	2.42	0.48
1:B:68:PHE:HB3	3:B:884:HOH:O	2.13	0.48
1:B:145:LYS:HD3	1:D:158:THR:HB	1.94	0.48
1:B:67:VAL:HG11	1:B:83:PHE:HE1	1.75	0.48
1:B:145:LYS:N	1:B:145:LYS:HD2	2.28	0.48
1:C:89:TRP:CE2	1:C:105:ASN:HB3	2.47	0.48
1:C:98:GLY:HA2	3:C:1946:HOH:O	2.12	0.48
1:D:182:LYS:HD3	3:D:725:HOH:O	2.12	0.48
1:B:163:LEU:HD11	1:B:169:TYR:HB2	1.96	0.48
1:D:39[B]:SER:HG	1:D:211:TYR:HD1	1.61	0.48
1:D:83:PHE:CD2	1:D:86:GLY:HA2	2.48	0.48
1:B:31:GLY:HA3	1:B:68:PHE:CE1	2.48	0.48
1:D:110:GLU:HG2	3:D:2083:HOH:O	2.12	0.48
1:D:185:LYS:HB2	3:D:1964:HOH:O	2.14	0.48
1:A:37:LYS:HB2	3:A:1983:HOH:O	2.13	0.48
1:A:32:LYS:HD2	3:A:1983:HOH:O	2.14	0.48
1:C:14:MET:HG2	3:C:3175:HOH:O	2.12	0.48
1:C:66:ARG:NH1	1:C:177:TYR:OH	2.43	0.48
1:A:95:PHE:CD1	1:A:171:CYS:HB2	2.49	0.48
1:C:111:GLY:HA3	3:C:2235:HOH:O	2.14	0.48
1:B:182:LYS:HB2	3:B:1814:HOH:O	2.13	0.48
1:C:54:PHE:CE2	1:C:208:VAL:HG11	2.48	0.48
1:D:104:ARG:HG3	1:D:119:ARG:HB2	1.95	0.48
1:D:149:ARG:NH1	3:D:1852:HOH:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:CZ	3:A:2674:HOH:O	2.62	0.47
1:A:27:GLY:HA2	1:A:41:ASP:O	2.13	0.47
1:A:145:LYS:O	1:A:155:GLY:HA2	2.14	0.47
1:D:94:THR:HG23	1:D:100:ILE:CD1	2.44	0.47
1:D:153:LEU:HA	3:D:2062:HOH:O	2.13	0.47
1:D:183:GLY:O	1:D:184:VAL:C	2.55	0.47
1:A:67:VAL:O	1:A:80:LYS:HE3	2.13	0.47
1:B:27:GLY:CA	1:B:40:MET:HE2	2.38	0.47
1:C:202:ASP:HB2	2:C:1226:SO4:O1	2.14	0.47
1:D:198:ILE:HD13	1:D:205:TYR:HE2	1.78	0.47
1:D:69:ALA:HA	1:D:214:ALA:HB3	1.96	0.47
1:B:123:VAL:HG22	3:B:2050:HOH:O	2.13	0.47
1:B:149:ARG:HD2	3:B:1995:HOH:O	2.14	0.47
1:C:10:ILE:N	1:C:29:GLY:O	2.45	0.47
1:C:73:ASP:OD2	3:C:2686:HOH:O	2.19	0.47
1:D:12:LEU:HD23	1:D:12:LEU:C	2.39	0.47
1:A:220:LEU:HD23	1:A:223:ASN:ND2	2.30	0.47
1:B:66:ARG:NH2	3:B:256:HOH:O	2.47	0.47
1:B:143:THR:H	1:D:145:LYS:NZ	2.12	0.47
1:D:185:LYS:HB3	1:D:185:LYS:HE3	1.54	0.47
1:A:220:LEU:HB3	1:A:221:PRO:CB	2.38	0.47
1:C:202:ASP:HB3	3:C:1902:HOH:O	2.14	0.47
1:A:12:LEU:HD23	1:A:13:ARG:N	2.30	0.47
1:D:32:LYS:HE3	3:D:1880:HOH:O	2.15	0.47
1:D:66:ARG:HG2	1:D:79:PHE:CE1	2.50	0.47
1:B:21:HIS:HE1	1:B:47:GLY:O	1.97	0.46
1:B:98:GLY:HA3	3:B:234:HOH:O	2.14	0.46
1:D:132:MET:HE3	3:D:1689:HOH:O	2.15	0.46
1:C:206:ASN:OD1	3:C:248:HOH:O	2.20	0.46
1:D:10:ILE:N	3:D:2761:HOH:O	2.49	0.46
1:A:125:PHE:HB2	1:A:132:MET:CE	2.39	0.46
1:D:117:LYS:HD3	3:D:2052:HOH:O	2.16	0.46
1:A:18:VAL:HB	1:A:52:PHE:CE2	2.51	0.46
1:B:12:LEU:HB3	1:B:40:MET:CE	2.45	0.46
1:C:90:GLU:OE2	1:D:19:ASN:HA	2.16	0.46
1:A:13:ARG:HG3	3:A:645:HOH:O	2.16	0.46
1:B:39[A]:SER:OG	1:B:211:TYR:HD1	1.98	0.46
1:B:39[B]:SER:OG	1:B:211:TYR:HD1	1.98	0.46
1:D:117:LYS:HE2	3:D:1998:HOH:O	2.14	0.46
1:B:144:GLU:CD	1:B:146:MET:CE	2.86	0.46
1:A:32:LYS:HE2	3:A:555:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD11	1:A:210:LEU:HD22	1.98	0.46
1:A:54:PHE:CE1	1:A:208:VAL:HG21	2.50	0.46
1:B:89:TRP:CE2	1:B:105:ASN:HB3	2.51	0.46
1:B:220:LEU:HD22	1:B:221:PRO:HA	1.96	0.46
1:C:76:GLN:NE2	1:C:81:GLN:HG3	2.29	0.46
1:D:45:LYS:HD2	3:D:1721:HOH:O	2.15	0.46
1:C:2:SER:OG	1:C:4:ILE:HB	2.16	0.46
1:A:147:TYR:CZ	1:A:149:ARG:HD2	2.50	0.46
1:D:56:ILE:CG1	3:D:809:HOH:O	2.56	0.46
1:D:85:LYS:HE2	3:D:2966:HOH:O	2.16	0.46
1:A:35:GLU:HB3	3:A:2017:HOH:O	2.16	0.45
1:A:90:GLU:HB3	1:B:123:VAL:HB	1.99	0.45
1:D:85:LYS:HD2	1:D:181:GLU:OE2	2.16	0.45
1:D:91:ARG:O	1:D:102:ILE:HA	2.16	0.45
1:C:102:ILE:HD12	1:C:102:ILE:C	2.42	0.45
1:B:64:CR8:H23	1:B:212:GLU:HB2	1.99	0.45
1:C:196:ILE:HG22	3:C:2981:HOH:O	2.15	0.45
1:D:85:LYS:HD2	1:D:181:GLU:HB2	1.98	0.45
1:D:116:ASN:ND2	1:D:116:ASN:N	2.64	0.45
1:D:180:LYS:HD2	1:D:180:LYS:HA	1.84	0.45
1:B:64:CR8:C1	3:B:1781:HOH:O	2.64	0.45
1:B:76:GLN:HB3	1:B:187:PRO:HA	1.98	0.45
1:A:85:LYS:HD3	1:A:181:GLU:OE2	2.17	0.45
1:D:153:LEU:HB3	1:D:177:TYR:HB2	1.97	0.45
1:A:13:ARG:HD2	1:A:13:ARG:HA	1.77	0.45
1:A:97:ASP:OD1	1:A:169:TYR:OH	2.31	0.45
1:B:164:GLU:O	3:B:934:HOH:O	2.21	0.45
1:D:159:MET:SD	1:D:173:SER:HB2	2.57	0.45
1:A:89:TRP:CE2	1:A:105:ASN:HB3	2.52	0.45
1:A:195[A]:CYS:SG	1:A:213:HIS:HB3	2.57	0.45
1:B:165:GLY:C	3:B:1984:HOH:O	2.59	0.45
1:C:202:ASP:CB	3:C:1902:HOH:O	2.65	0.45
1:D:147:TYR:HE2	3:D:2129:HOH:O	1.93	0.45
1:C:112:ASP:OD2	3:C:1997:HOH:O	2.21	0.44
1:A:37:LYS:CE	3:A:2795:HOH:O	2.55	0.44
1:B:65:ASN:OD1	1:B:67:VAL:HG22	2.17	0.44
1:B:144:GLU:OE1	1:B:146:MET:HE2	2.16	0.44
1:D:53:ALA:N	1:D:134:LYS:HG2	2.32	0.44
1:A:37:LYS:NZ	3:A:510:HOH:O	2.11	0.44
1:A:208:VAL:HG12	3:A:2777:HOH:O	2.16	0.44
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HB2	3:C:2138:HOH:O	2.15	0.44
1:C:124:ASN:N	3:D:653:HOH:O	2.50	0.44
1:D:9:LYS:HD3	1:D:112:ASP:OD2	2.18	0.44
1:D:66:ARG:O	1:D:66:ARG:HG3	2.18	0.44
1:A:66:ARG:CZ	1:A:66:ARG:HB2	2.47	0.44
1:A:13:ARG:NH1	3:A:2360:HOH:O	2.50	0.44
1:C:105:ASN:HA	1:C:117:LYS:O	2.18	0.44
1:C:121:HIS:HB3	1:D:102:ILE:HD11	1.99	0.44
1:D:81:GLN:HG3	3:D:2057:HOH:O	2.17	0.44
1:D:164:GLU:O	3:D:1362:HOH:O	2.21	0.44
1:C:192:VAL:HG12	1:C:193:ASP:O	2.18	0.44
1:C:223:ASN:OD1	1:C:223:ASN:C	2.61	0.44
1:D:66:ARG:HD2	1:D:192:VAL:HG11	1.99	0.44
1:A:110:GLU:CG	3:A:3041:HOH:O	2.63	0.44
1:A:28:ASP:OD2	3:A:946:HOH:O	2.20	0.44
1:B:87:TYR:CE1	1:B:107:ILE:HD13	2.53	0.43
1:A:0:HIS:NE2	1:A:83:PHE:O	2.41	0.43
1:A:84:PRO:O	1:A:85:LYS:C	2.59	0.43
1:A:135:LYS:HD2	3:A:2678:HOH:O	2.17	0.43
1:C:222:ASP:O	1:C:223:ASN:C	2.60	0.43
1:D:119:ARG:HD3	1:D:119:ARG:HA	1.74	0.43
1:B:83:PHE:CZ	1:B:114:PHE:HE1	2.36	0.43
1:B:105:ASN:CG	1:B:118:VAL:HG22	2.43	0.43
1:B:123:VAL:HG13	3:B:2050:HOH:O	2.17	0.43
1:D:29:GLY:CA	3:D:1432:HOH:O	2.67	0.43
1:D:36:GLY:HA2	1:D:68:PHE:C	2.43	0.43
1:D:43:GLU:HG2	1:D:45:LYS:HE2	2.00	0.43
1:D:117:LYS:HG3	1:D:119:ARG:HH22	1.82	0.43
1:A:5:LYS:HD2	3:A:711:HOH:O	2.18	0.43
1:A:67:VAL:CG2	1:A:80:LYS:HG2	2.48	0.43
3:A:289:HOH:O	1:B:127:ALA:HB3	2.19	0.43
1:C:38:GLN:HB2	3:C:1637:HOH:O	2.18	0.43
1:D:196:ILE:HB	1:D:212:GLU:HG2	2.00	0.43
1:A:137:LEU:HD11	3:A:3243:HOH:O	2.17	0.43
1:B:110:GLU:HG2	1:B:115:TYR:CE1	2.52	0.43
1:C:65:ASN:CG	1:C:107:ILE:HD13	2.44	0.43
1:B:8:MET:HG3	3:B:2240:HOH:O	2.17	0.43
1:D:144:GLU:HB3	1:D:192:VAL:HB	2.01	0.43
1:C:139:TRP:CZ3	1:C:159:MET:HE2	2.54	0.43
1:D:15:GLU:HG3	1:D:119:ARG:NH1	2.33	0.43
1:D:131:VAL:HB	3:D:233:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:HB3	3:A:1386:HOH:O	2.19	0.43
1:D:43:GLU:OE1	1:D:207:LYS:HG2	2.18	0.43
1:D:87:TYR:CZ	1:D:107:ILE:CD1	2.93	0.43
1:A:72:PRO:HB3	3:A:1589:HOH:O	2.19	0.43
1:A:123:VAL:HG12	1:B:90:GLU:OE2	2.19	0.43
1:B:36:GLY:HA2	1:B:68:PHE:C	2.44	0.43
1:A:10:ILE:N	1:A:29:GLY:O	2.49	0.42
1:A:48:GLY:HA2	1:A:49:PRO:C	2.44	0.42
1:D:9:LYS:HE3	1:D:112:ASP:OD2	2.19	0.42
1:A:83:PHE:HA	1:A:84:PRO:C	2.43	0.42
1:B:51:PRO:HA	1:B:134:LYS:NZ	2.34	0.42
1:B:196:ILE:HB	1:B:212:GLU:CG	2.49	0.42
1:D:13:ARG:NH2	3:D:3051:HOH:O	2.51	0.42
1:D:145:LYS:HG3	1:D:189:TYR:OH	2.19	0.42
1:B:170:ARG:CZ	1:B:170:ARG:HB3	2.49	0.42
1:A:166:ASN:ND2	3:A:3220:HOH:O	2.10	0.42
1:B:22:HIS:CE1	3:B:2211:HOH:O	2.72	0.42
1:A:17:ASN:OD1	1:A:17:ASN:C	2.61	0.42
1:A:116:ASN:N	1:A:116:ASN:ND2	2.67	0.42
1:B:137:LEU:HD22	3:B:2796:HOH:O	2.19	0.42
1:C:134:LYS:NZ	3:C:630:HOH:O	2.53	0.42
1:B:38:GLN:NE2	3:B:323:HOH:O	2.07	0.42
1:B:136:THR:CG2	1:B:161:LEU:HD13	2.49	0.42
1:C:10:ILE:HG21	1:C:40:MET:HE2	2.01	0.42
1:C:217:HIS:ND1	1:C:223:ASN:HB3	2.34	0.42
1:B:85:LYS:NZ	3:B:704:HOH:O	2.16	0.42
1:B:92:SER:O	1:B:173:SER:HA	2.20	0.42
1:C:205:TYR:N	1:C:205:TYR:CD1	2.88	0.42
1:A:15:GLU:OE2	3:A:569:HOH:O	2.21	0.42
1:A:18:VAL:HG12	1:A:132:MET:HE1	2.01	0.42
1:C:83:PHE:CB	1:C:84:PRO:HA	2.45	0.42
1:C:120:PHE:CD1	1:C:120:PHE:C	2.98	0.42
1:A:193:ASP:O	1:A:214:ALA:HA	2.19	0.42
1:B:89:TRP:HA	1:B:176:THR:O	2.20	0.42
1:C:49:PRO:HB3	1:C:204:ASP:CB	2.50	0.42
1:C:89:TRP:HB2	3:C:1982:HOH:O	2.20	0.42
1:A:139:TRP:CZ3	1:A:159:MET:HB3	2.55	0.42
1:B:125:PHE:CE1	1:B:131:VAL:HG21	2.55	0.42
1:A:79:PHE:HE1	1:A:177:TYR:CD1	2.37	0.41
1:B:220:LEU:HB3	1:D:195[A]:CYS:SG	2.60	0.41
1:C:41:ASP:OD1	1:C:209:LYS:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:PHE:CD2	3:C:2054:HOH:O	2.72	0.41
1:C:130:PRO:C	3:C:1876:HOH:O	2.55	0.41
1:C:196:ILE:HB	1:C:212:GLU:CG	2.50	0.41
1:D:135:LYS:NZ	3:D:3105:HOH:O	2.13	0.41
1:B:84:PRO:HB3	1:B:109:MET:HE1	2.02	0.41
1:B:88[A]:SER:OG	3:B:2907:HOH:O	2.08	0.41
1:B:220:LEU:HA	1:B:221:PRO:HA	1.74	0.41
2:B:227:SO4:O3	3:B:2729:HOH:O	2.21	0.41
1:C:89:TRP:HA	3:C:2085:HOH:O	2.19	0.41
1:A:199:LEU:HD11	1:A:211:TYR:HB2	2.03	0.41
1:B:203:LYS:HD3	3:B:3325:HOH:O	2.21	0.41
1:C:126:PRO:HB3	3:D:2175:HOH:O	2.18	0.41
1:C:148:VAL:HG11	1:C:186:LEU:HD13	2.02	0.41
1:D:5:LYS:HD3	1:D:5:LYS:N	2.35	0.41
1:D:144:GLU:OE1	1:D:146:MET:HE2	2.19	0.41
1:A:50:LEU:HD13	1:A:52:PHE:CE1	2.55	0.41
1:A:66:ARG:NE	1:A:194:HIS:HE1	2.17	0.41
1:A:156:ASP:HA	1:A:173:SER:O	2.21	0.41
1:B:194:HIS:HB3	1:B:212:GLU:OE1	2.20	0.41
1:C:217:HIS:CE1	1:C:219:GLY:HA2	2.55	0.41
1:D:85:LYS:HD2	1:D:181:GLU:CD	2.45	0.41
1:B:83:PHE:CE2	1:B:86:GLY:HA2	2.56	0.41
1:A:203:LYS:HB3	3:A:806:HOH:O	2.19	0.41
1:A:204:ASP:O	3:A:264:HOH:O	2.21	0.41
1:B:203:LYS:HE3	3:B:2516:HOH:O	2.20	0.41
1:C:90:GLU:HB3	1:D:123:VAL:HB	2.02	0.41
1:A:18:VAL:CG1	1:A:132:MET:HE1	2.50	0.41
1:A:125:PHE:CB	1:A:132:MET:HE3	2.40	0.41
1:D:135:LYS:NZ	3:D:2684:HOH:O	2.47	0.41
1:C:163:LEU:HD11	1:C:169:TYR:HB2	2.03	0.41
1:A:106[A]:ASP:C	1:A:107:ILE:HD12	2.46	0.40
1:D:66:ARG:CZ	1:D:66:ARG:HB2	2.50	0.40
1:D:71:TYR:HA	1:D:72:PRO:HD3	1.81	0.40
1:B:43:GLU:HG3	3:B:3206:HOH:O	2.20	0.40
1:C:26:ASP:OD2	1:C:45:LYS:HG3	2.21	0.40
1:C:60:ALA:O	1:C:118:VAL:HG11	2.21	0.40
1:C:137:LEU:HA	1:C:137:LEU:HD23	1.75	0.40
1:D:97:ASP:OD1	1:D:169:TYR:OH	2.31	0.40
1:A:83:PHE:HB3	1:A:109:MET:HE2	2.03	0.40
1:A:111:GLY:HA2	3:A:681:HOH:O	2.21	0.40
1:B:192:VAL:HA	1:B:216:ALA:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASN:HA	1:D:21:HIS:O	2.21	0.40
1:B:54:PHE:HB2	3:B:421:HOH:O	2.20	0.40
1:D:94:THR:HG23	1:D:100:ILE:HD13	2.04	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASN:ND2	3:B:322:HOH:O[3_554]	1.89	0.31
3:A:3106:HOH:O	3:D:2715:HOH:O[4_445]	1.99	0.21
3:B:2380:HOH:O	3:D:2944:HOH:O[3_554]	2.02	0.18
3:A:453:HOH:O	3:B:301:HOH:O[3_554]	2.04	0.16
3:C:1436:HOH:O	3:D:2068:HOH:O[2_555]	2.05	0.15
3:B:2134:HOH:O	3:C:638:HOH:O[2_554]	2.06	0.14
3:A:710:HOH:O	3:D:2307:HOH:O[3_554]	2.07	0.13
1:C:41:ASP:OD2	3:A:752:HOH:O[4_555]	2.07	0.13
3:A:308:HOH:O	3:B:522:HOH:O[3_554]	2.08	0.12
3:B:771:HOH:O	3:B:1414:HOH:O[3_554]	2.09	0.11
3:C:552:HOH:O	3:D:2030:HOH:O[2_555]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/230 (96%)	208 (94%)	11 (5%)	2 (1%)	14	9
1	B	219/230 (95%)	216 (99%)	3 (1%)	0	100	100
1	C	217/230 (94%)	209 (96%)	8 (4%)	0	100	100
1	D	219/230 (95%)	210 (96%)	7 (3%)	2 (1%)	14	9
All	All	876/920 (95%)	843 (96%)	29 (3%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	222	ASP
1	D	84	PRO
1	D	131	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	194/197 (98%)	173 (89%)	21 (11%)	6	3
1	B	192/197 (98%)	179 (93%)	13 (7%)	14	11
1	C	190/197 (96%)	175 (92%)	15 (8%)	11	8
1	D	192/197 (98%)	176 (92%)	16 (8%)	10	7
All	All	768/788 (98%)	703 (92%)	65 (8%)	10	7

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LYS
1	A	9	LYS
1	A	19	ASN
1	A	28	ASP
1	A	42	LEU
1	A	75	ILE
1	A	102	ILE
1	A	116	ASN
1	A	117	LYS
1	A	118	VAL
1	A	135	LYS
1	A	138	LYS
1	A	157	ILE
1	A	182	LYS
1	A	191	LEU
1	A	194	HIS
1	A	206	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	208	VAL
1	A	222	ASP
1	A	223	ASN
1	B	1	MET
1	B	2	SER
1	B	8	MET
1	B	12	LEU
1	B	42	LEU
1	B	57	LEU
1	B	75	ILE
1	B	85	LYS
1	B	134	LYS
1	B	138	LYS
1	B	145	LYS
1	B	166	ASN
1	B	203	LYS
1	C	4	ILE
1	C	10	ILE
1	C	13	ARG
1	C	28	ASP
1	C	67	VAL
1	C	85	LYS
1	C	100	ILE
1	C	110	GLU
1	C	116	ASN
1	C	145	LYS
1	C	174	ARG
1	C	182	LYS
1	C	196	ILE
1	C	205	TYR
1	C	222	ASP
1	D	1	MET
1	D	2	SER
1	D	5	LYS
1	D	9	LYS
1	D	13	ARG
1	D	15	GLU
1	D	32	LYS
1	D	67	VAL
1	D	109	MET
1	D	116	ASN
1	D	118	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	145	LYS
1	D	182	LYS
1	D	185	LYS
1	D	202	ASP
1	D	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	B	21	HIS
1	B	22	HIS
1	B	121	HIS
1	B	166	ASN
1	B	223	ASN
1	D	11	ASN
1	D	81	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CR8	D	64	1	25,27,28	1.75	5 (20%)	24,37,39	1.33	3 (12%)
1	CR8	B	64	1	25,27,28	1.79	5 (20%)	24,37,39	1.35	2 (8%)
1	CR8	C	64	1	25,27,28	1.74	6 (24%)	24,37,39	1.54	6 (25%)
1	CR8	A	64	1	25,27,28	1.77	5 (20%)	24,37,39	1.43	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	D	64	1	-	6/12/25/26	0/3/3/3
1	CR8	B	64	1	-	8/12/25/26	0/3/3/3
1	CR8	C	64	1	-	6/12/25/26	0/3/3/3
1	CR8	A	64	1	-	8/12/25/26	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	CR8	C1-N2	4.20	1.38	1.32
1	B	64	CR8	C8-C7	4.08	1.49	1.39
1	A	64	CR8	C8-C7	4.01	1.49	1.39
1	D	64	CR8	C1-N2	3.79	1.37	1.32
1	A	64	CR8	C1-N2	3.70	1.37	1.32
1	C	64	CR8	C1-N2	3.67	1.37	1.32
1	B	64	CR8	C8-CA2	3.60	1.48	1.40
1	D	64	CR8	C8-C7	3.58	1.47	1.39
1	C	64	CR8	C8-C7	3.57	1.47	1.39
1	A	64	CR8	C8-CA2	3.51	1.48	1.40
1	D	64	CR8	C8-CA2	3.49	1.48	1.40
1	C	64	CR8	C8-CA2	3.12	1.47	1.40
1	B	64	CR8	C4-C11	-2.82	1.38	1.46
1	D	64	CR8	C4-C11	-2.82	1.38	1.46
1	C	64	CR8	C12-C11	-2.80	1.39	1.46
1	B	64	CR8	C12-C11	-2.75	1.39	1.46
1	A	64	CR8	C4-C11	-2.60	1.39	1.46
1	D	64	CR8	C12-C11	-2.60	1.39	1.46
1	A	64	CR8	C12-C11	-2.43	1.39	1.46
1	C	64	CR8	C4-C11	-2.35	1.40	1.46
1	C	64	CR8	CA2-N2	-2.32	1.33	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CR8	CA1-C20-C21	-3.59	107.26	113.23
1	C	64	CR8	C3-CA3-N3	-3.54	104.37	112.43
1	D	64	CR8	C12-C6-C7	-3.41	118.87	122.10
1	C	64	CR8	C4-C5-C7	-2.89	119.36	122.10
1	C	64	CR8	CA1-C20-C21	-2.68	108.78	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	C1-N3-C2	-2.30	104.93	107.83
1	C	64	CR8	C12-C6-C7	-2.24	119.98	122.10
1	B	64	CR8	C12-C6-C7	-2.16	120.06	122.10
1	D	64	CR8	C23-C21-N22	2.13	108.17	105.65
1	C	64	CR8	C1-N3-C2	-2.09	105.19	107.83
1	C	64	CR8	C6-C7-C5	2.04	120.27	115.81
1	B	64	CR8	C23-C21-N22	2.04	108.06	105.65

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C6-C7-C8-CA2
1	A	64	CR8	C7-C8-CA2-N2
1	A	64	CR8	C3-CA3-N3-C2
1	A	64	CR8	CA1-C20-C21-N22
1	A	64	CR8	CA1-C20-C21-C23
1	B	64	CR8	C5-C7-C8-CA2
1	B	64	CR8	C6-C7-C8-CA2
1	B	64	CR8	C7-C8-CA2-N2
1	B	64	CR8	C3-CA3-N3-C2
1	B	64	CR8	CA1-C20-C21-N22
1	B	64	CR8	CA1-C20-C21-C23
1	C	64	CR8	C5-C7-C8-CA2
1	C	64	CR8	C6-C7-C8-CA2
1	C	64	CR8	C7-C8-CA2-N2
1	C	64	CR8	CA1-C20-C21-N22
1	C	64	CR8	CA1-C20-C21-C23
1	D	64	CR8	C5-C7-C8-CA2
1	D	64	CR8	C6-C7-C8-CA2
1	D	64	CR8	C7-C8-CA2-N2
1	D	64	CR8	CA1-C20-C21-N22
1	D	64	CR8	CA1-C20-C21-C23
1	A	64	CR8	C5-C7-C8-CA2
1	B	64	CR8	C3-CA3-N3-C1
1	C	64	CR8	C7-C8-CA2-C2
1	D	64	CR8	C7-C8-CA2-C2
1	A	64	CR8	C3-CA3-N3-C1
1	A	64	CR8	C7-C8-CA2-C2
1	B	64	CR8	C7-C8-CA2-C2

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	64	CR8	3	0
1	B	64	CR8	4	0
1	C	64	CR8	2	0
1	A	64	CR8	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	1224	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	227	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	C	1226	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	D	1227	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	B	227	-	4,4,4	0.26	0	6,6,6	0.40	0
2	SO4	B	1224	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	A	1225	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	B	1225	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	1224	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	C	1225	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	C	1227	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	227	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	1225	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	D	227	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	D	228	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	A	228	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	D	1226	-	4,4,4	0.24	0	6,6,6	0.07	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.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1224	SO4	1	0
2	A	227	SO4	1	0
2	C	1226	SO4	3	0
2	B	227	SO4	2	0
2	B	1224	SO4	1	0
2	B	1225	SO4	2	0
2	D	1226	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	221/230 (96%)	1.48	49 (22%) 2 2	8, 20, 30, 38	6 (2%)
1	B	220/230 (95%)	1.17	21 (9%) 14 12	11, 18, 26, 40	4 (1%)
1	C	219/230 (95%)	1.45	45 (20%) 2 2	13, 21, 30, 37	4 (1%)
1	D	220/230 (95%)	1.55	58 (26%) 1 1	11, 22, 34, 49	6 (2%)
All	All	880/920 (95%)	1.41	173 (19%) 3 3	8, 20, 31, 49	20 (2%)

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	5.4
1	B	1	MET	4.6
1	D	2	SER	4.5
1	D	184	VAL	4.0
1	B	69	ALA	3.9
1	C	223	ASN	3.8
1	A	3	ALA	3.6
1	C	86	GLY	3.6
1	D	7	ASP	3.5
1	A	7	ASP	3.4
1	D	115	TYR	3.4
1	A	39[A]	SER	3.4
1	D	186	LEU	3.4
1	D	3	ALA	3.4
1	A	166	ASN	3.3
1	C	12	LEU	3.3
1	C	81	GLN	3.3
1	A	222	ASP	3.3
1	C	2	SER	3.2
1	C	84	PRO	3.2
1	D	29	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	43	GLU	3.2
1	A	171	CYS	3.2
1	A	150	ASP	3.1
1	A	36	GLY	3.1
1	D	182	LYS	3.1
1	A	183	GLY	3.1
1	C	202	ASP	3.1
1	C	222	ASP	3.1
1	C	83	PHE	3.0
1	C	3	ALA	3.0
1	A	165	GLY	3.0
1	A	214	ALA	2.9
1	D	77	ASP	2.9
1	C	214	ALA	2.9
1	C	150	ASP	2.9
1	C	184	VAL	2.9
1	D	222	ASP	2.9
1	A	198	ILE	2.9
1	A	84	PRO	2.9
1	C	23	PHE	2.9
1	D	24	VAL	2.8
1	D	221	PRO	2.8
1	C	204	ASP	2.8
1	C	118	VAL	2.8
1	D	13	ARG	2.8
1	A	208	VAL	2.8
1	A	223	ASN	2.7
1	B	222	ASP	2.7
1	C	48	GLY	2.7
1	D	179	ALA	2.7
1	D	67	VAL	2.7
1	A	2	SER	2.7
1	D	202	ASP	2.7
1	A	52	PHE	2.7
1	A	49	PRO	2.7
1	A	221	PRO	2.7
1	B	211	TYR	2.7
1	A	73	ASP	2.7
1	D	181	GLU	2.6
1	C	125	PHE	2.6
1	A	78	TYR	2.6
1	B	152	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	215	VAL	2.6
1	C	13	ARG	2.6
1	D	8	MET	2.6
1	B	21	HIS	2.6
1	D	83	PHE	2.6
1	C	211	TYR	2.6
1	D	30	THR	2.6
1	C	49	PRO	2.6
1	B	150	ASP	2.6
1	A	35	GLU	2.6
1	A	154	THR	2.6
1	B	221	PRO	2.6
1	A	50	LEU	2.6
1	A	27	GLY	2.5
1	D	223	ASN	2.5
1	B	51	PRO	2.5
1	D	109	MET	2.5
1	D	114	PHE	2.5
1	A	202	ASP	2.5
1	A	113	THR	2.5
1	B	49	PRO	2.5
1	B	126	PRO	2.5
1	A	148	VAL	2.4
1	B	205	TYR	2.4
1	A	111	GLY	2.4
1	B	183	GLY	2.4
1	A	123	VAL	2.4
1	C	39	SER	2.4
1	C	221	PRO	2.4
1	A	34	PHE	2.4
1	A	197	GLU	2.4
1	A	26	ASP	2.4
1	C	92	SER	2.4
1	D	71	TYR	2.4
1	D	147	TYR	2.4
1	C	151	GLY	2.4
1	D	73	ASP	2.4
1	C	54	PHE	2.4
1	D	1	MET	2.4
1	D	208	VAL	2.4
1	A	22	HIS	2.4
1	A	141	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	130	PRO	2.4
1	D	203	LYS	2.3
1	C	142	SER	2.3
1	C	21	HIS	2.3
1	C	164	GLU	2.3
1	A	139	TRP	2.3
1	D	81	GLN	2.3
1	B	115	TYR	2.3
1	D	189	TYR	2.3
1	C	42	LEU	2.3
1	C	10	ILE	2.3
1	A	167	ALA	2.3
1	A	31	GLY	2.3
1	A	89	TRP	2.3
1	D	36	GLY	2.3
1	D	35	GLU	2.3
1	C	51	PRO	2.3
1	C	36	GLY	2.3
1	D	23	PHE	2.2
1	D	68	PHE	2.2
1	A	189	TYR	2.2
1	D	52	PHE	2.2
1	C	117	LYS	2.2
1	C	16	GLY	2.2
1	D	183	GLY	2.2
1	A	181	GLU	2.2
1	D	110	GLU	2.2
1	C	182	LYS	2.2
1	D	86	GLY	2.2
1	D	76	GLN	2.2
1	C	203	LYS	2.2
1	B	15	GLU	2.1
1	A	215	VAL	2.1
1	D	131	VAL	2.1
1	D	20	GLY	2.1
1	A	186	LEU	2.1
1	D	163	LEU	2.1
1	D	171	CYS	2.1
1	B	2	SER	2.1
1	D	5	LYS	2.1
1	C	87	TYR	2.1
1	D	10	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	67	VAL	2.1
1	D	148	VAL	2.1
1	A	160	ALA	2.1
1	D	82	SER	2.1
1	A	28	ASP	2.1
1	D	41	ASP	2.1
1	D	204	ASP	2.1
1	C	56	ILE	2.1
1	D	188	GLY	2.1
1	B	125	PHE	2.1
1	D	50	LEU	2.1
1	A	112	ASP	2.1
1	D	106	ASP	2.1
1	A	51	PRO	2.1
1	D	34	PHE	2.1
1	C	69	ALA	2.1
1	B	223	ASN	2.0
1	A	195[A]	CYS	2.0
1	A	204	ASP	2.0
1	C	33	PRO	2.0
1	D	113	THR	2.0
1	B	182	LYS	2.0
1	C	90	GLU	2.0
1	C	167	ALA	2.0
1	D	32	LYS	2.0
1	B	147	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR8	A	64	25/26	0.79	0.13	9,18,26,34	0
1	CR8	C	64	25/26	0.79	0.15	6,17,24,32	0
1	CR8	D	64	25/26	0.84	0.11	11,19,25,27	0
1	CR8	B	64	25/26	0.88	0.12	11,17,21,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1226	5/5	0.53	0.21	29,36,44,51	5
2	SO4	C	1226	5/5	0.54	0.19	25,25,29,40	5
2	SO4	C	227	5/5	0.57	0.20	36,38,55,74	0
2	SO4	B	1224	5/5	0.68	0.20	34,40,51,62	0
2	SO4	A	228	5/5	0.71	0.20	31,34,54,59	0
2	SO4	C	1227	5/5	0.74	0.13	24,27,39,45	5
2	SO4	A	1225	5/5	0.75	0.19	11,11,22,35	5
2	SO4	D	1225	5/5	0.79	0.17	29,30,35,37	0
2	SO4	D	227	5/5	0.79	0.16	32,35,45,55	0
2	SO4	A	1224	5/5	0.80	0.14	21,30,35,46	0
2	SO4	B	1225	5/5	0.82	0.14	8,13,20,27	5
2	SO4	B	227	5/5	0.82	0.15	17,26,28,42	0
2	SO4	D	1227	5/5	0.83	0.17	18,27,33,39	5
2	SO4	C	1224	5/5	0.84	0.11	22,27,39,49	0
2	SO4	C	1225	5/5	0.85	0.20	23,23,39,51	0
2	SO4	D	228	5/5	0.85	0.12	28,28,33,41	0
2	SO4	A	227	5/5	0.88	0.11	29,30,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.