



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:40 pm BST

PDB ID : 3IEM
Title : Crystal Structure of TTHA0252 from *Thermus thermophilus* HB8 complexed with RNA analog
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.
Deposited on : 2009-07-23
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

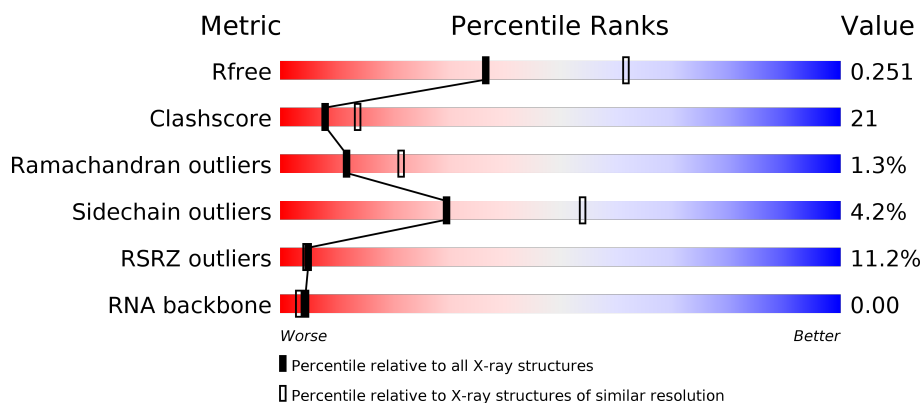
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



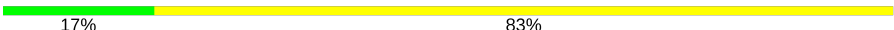
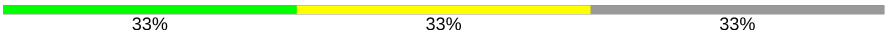
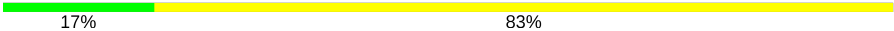


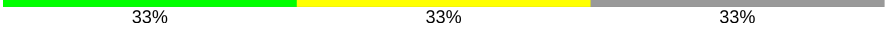




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 on 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	431	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
1	B	431	<div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	C	431	<div> <div>23%</div> <div>54%</div> <div>45%</div> <div>.</div> </div>
1	D	431	<div> <div>20%</div> <div>52%</div> <div>44%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	6	 17% 83%
2	H	6	 33% 33% 33%
2	I	6	 17% 83%
2	J	6	 17% 33% 50%
2	K	6	 50% 50%
2	L	6	 33% 33% 33%
2	M	6	 33% 67%
2	N	6	 17% 33% 50%
2	O	6	 33% 67%
2	P	6	 17% 17% 67%

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	SSU	G	3	-	-	X	-
2	SSU	M	2	-	-	X	-
3	SO4	A	439	-	-	-	X
3	SO4	A	446	-	-	X	X
3	SO4	B	443	-	-	-	X
3	SO4	B	445	-	-	X	X
3	SO4	B	448	-	-	X	-
3	SO4	C	439	-	-	X	-
3	SO4	D	436	-	-	X	-
3	SO4	D	439	-	-	X	-
5	FLC	B	450	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14354 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 Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3326	2127	597	594	8			

- Molecule 2 is a RNA chain called RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	6	Total 101	C 45	N 10	O 36	P 5	S 5	0	0	1
2	H	4	Total 61	C 27	N 6	O 22	P 3	S 3	0	0	1
2	I	6	Total 85	C 36	N 8	O 31	P 5	S 5	0	0	1
2	J	3	Total 41	C 18	N 4	O 15	P 2	S 2	0	0	1
2	K	3	Total 57	C 27	N 6	O 20	P 2	S 2	0	0	0
2	L	4	Total 45	C 18	N 4	O 17	P 3	S 3	0	0	1
2	M	2	Total 21	C 9	N 2	O 8	P 1	S 1	0	0	0
2	N	3	Total 41	C 18	N 4	O 15	P 2	S 2	0	0	1
2	O	2	Total 37	C 18	N 4	O 13	P 1	S 1	0	0	0
2	P	2	Total 21	C 9	N 2	O 8	P 1	S 1	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: 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	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	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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	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	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	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	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	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	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

Continued on next page...

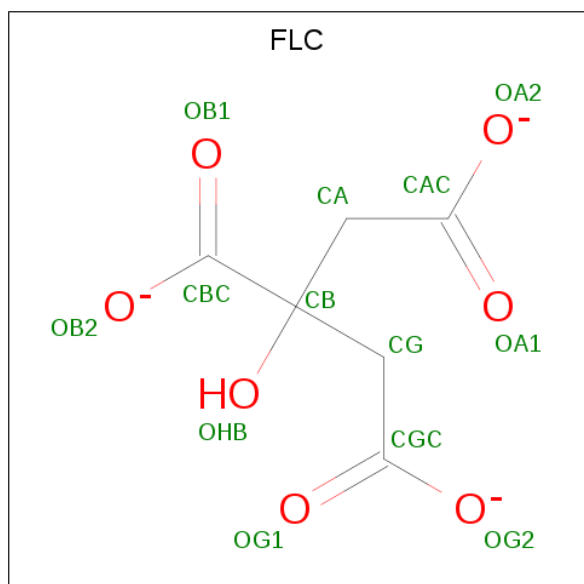
Continued from previous page...

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	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



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

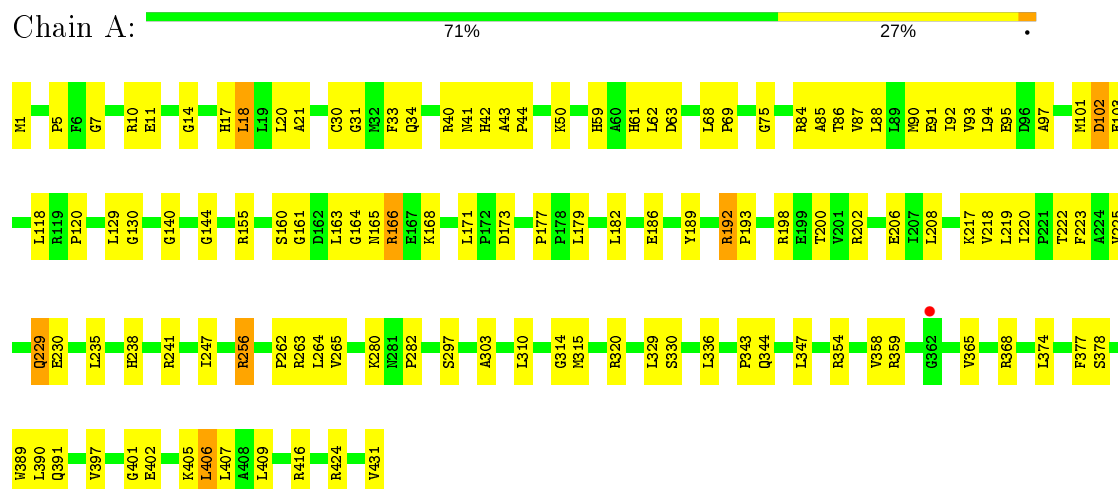
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	B	71	Total 71	O 71	0	0
6	C	22	Total 22	O 22	0	0
6	D	37	Total 37	O 37	0	0
6	G	1	Total 1	O 1	0	0
6	J	2	Total 2	O 2	0	0
6	K	2	Total 2	O 2	0	0
6	L	2	Total 2	O 2	0	0
6	M	1	Total 1	O 1	0	0
6	O	2	Total 2	O 2	0	0

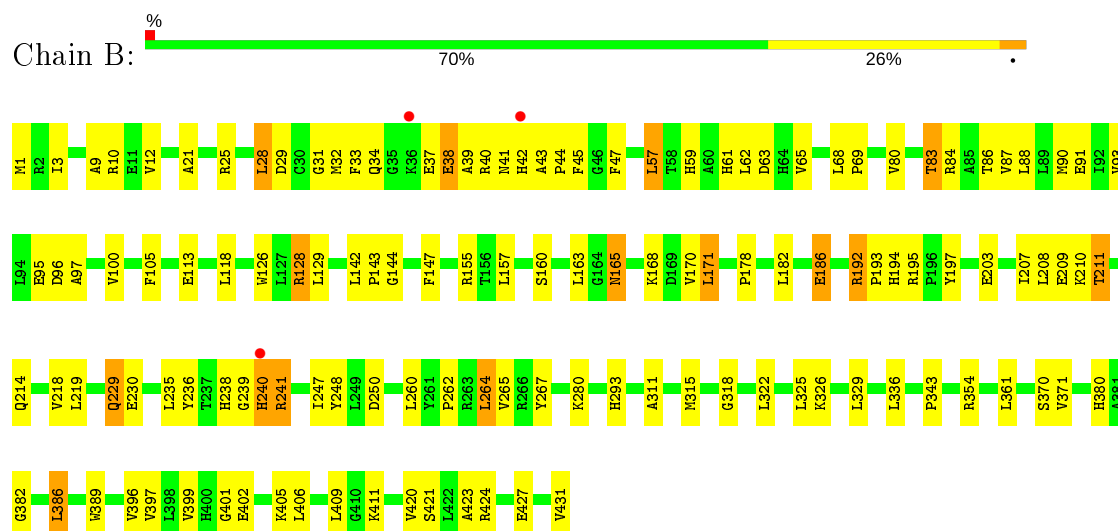
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Ribonuclease TTHA0252

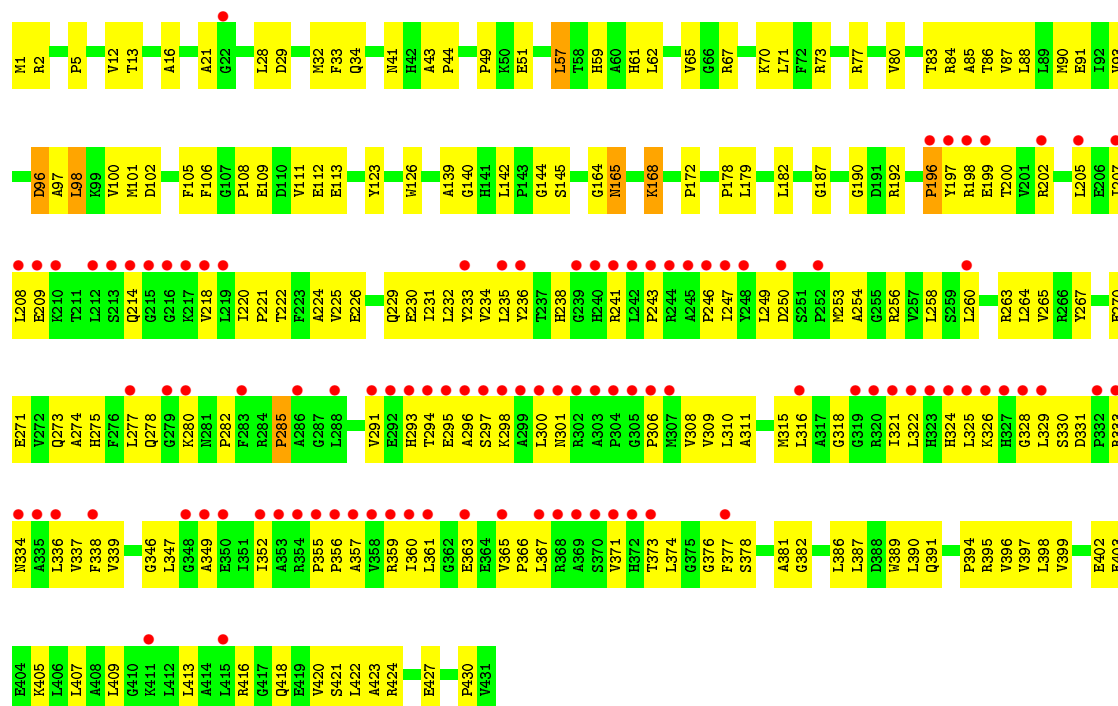


• Molecule 1: Ribonuclease TTHA0252



• Molecule 1: Ribonuclease TTHA0252



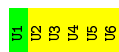


• Molecule 1: Ribonuclease TTHA0252

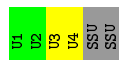


• Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

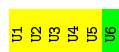




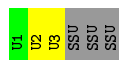
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



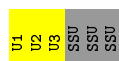
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



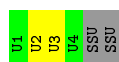
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



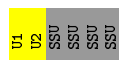
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



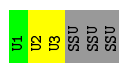
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

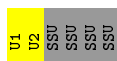


- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')



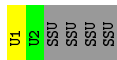
- Molecule 2: RNA (5'-R*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')





- Molecule 2: RNA (5'-R>(* (SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3')

Chain P:  17% 17% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.69Å 146.44Å 119.97Å 90.00° 110.37° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 45.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.50) 94.0 (45.93-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.257 0.207 , 0.251	Depositor DCC
R_{free} test set	8060 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	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	14354	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SSU, FLC, ZN, 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	0.37	0/3407	0.66	2/4621 (0.0%)
1	B	0.38	0/3407	0.66	1/4621 (0.0%)
1	C	0.31	0/3407	0.59	0/4621
1	D	0.31	0/3407	0.59	1/4621 (0.0%)
All	All	0.35	0/13628	0.62	4/18484 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLY	N-CA-C	-5.81	98.58	113.10
1	B	386	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	225	VAL	CA-C-N	5.17	128.58	117.20
1	D	161	GLY	N-CA-C	-5.08	100.41	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3326	0	3351	90	0
1	B	3326	0	3351	117	0
1	C	3326	0	3351	171	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3326	0	3351	196	0
2	G	101	0	51	20	0
2	H	61	0	31	4	0
2	I	85	0	40	14	0
2	J	41	0	21	1	0
2	K	57	0	31	7	0
2	L	45	0	20	1	0
2	M	21	0	10	7	0
2	N	41	0	21	2	0
2	O	37	0	21	5	0
2	P	21	0	10	2	0
3	A	80	0	0	5	0
3	B	90	0	0	4	0
3	C	60	0	0	2	0
3	D	55	0	0	5	0
3	J	5	0	0	0	0
3	K	5	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	13	0	5	4	0
6	A	84	0	0	6	0
6	B	71	0	0	1	0
6	C	22	0	0	0	0
6	D	37	0	0	0	0
6	G	1	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
6	M	1	0	0	0	0
6	O	2	0	0	1	0
All	All	14354	0	13665	596	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 21.

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)
2:M:1:SSU:H1'	2:M:2:SSU:S1P	1.56	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:H	1:D:368:ARG:HB2	1.21	1.03
1:D:47:PHE:HA	2:M:2:SSU:S1P	1.99	1.03
2:M:1:SSU:C1'	2:M:2:SSU:S1P	2.47	1.03
1:C:98:LEU:HD11	1:C:108:PRO:HA	1.39	1.01
1:B:370:SER:HA	3:B:448:SO4:O4	1.60	1.00
1:A:33:PHE:H	1:A:41:ASN:HD21	1.08	0.98
1:D:34:GLN:HE22	2:I:3:SSU:H2'	1.24	0.98
1:D:168:LYS:HE3	1:D:230:GLU:OE1	1.65	0.97
1:B:33:PHE:N	1:B:41:ASN:HD21	1.66	0.94
1:D:244:ARG:H	1:D:244:ARG:HD2	1.32	0.94
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.29	0.94
1:C:172:PRO:HA	3:C:439:SO4:O2	1.69	0.92
1:C:220:ILE:HG12	1:C:337:VAL:HB	1.52	0.92
1:B:33:PHE:H	1:B:41:ASN:ND2	1.66	0.92
1:B:380:HIS:NE2	2:K:1:SSU:H5'	1.85	0.92
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.52	0.91
1:C:33:PHE:H	1:C:41:ASN:HD21	0.91	0.90
1:D:301:ASN:HB3	1:D:327:HIS:HB3	1.52	0.89
1:D:325:LEU:HD23	1:D:329:LEU:HD22	1.55	0.87
1:A:256:ARG:HD3	3:A:443:SO4:O1	1.74	0.87
2:G:3:SSU:H4'	2:G:4:SSU:OP2	1.72	0.87
1:C:336:LEU:HD22	1:C:371:VAL:HG13	1.57	0.86
1:C:140:GLY:O	1:C:164:GLY:HA3	1.77	0.85
1:B:10:ARG:HH12	1:B:424:ARG:HG2	1.41	0.85
1:D:250:ASP:HB3	1:D:311:ALA:HB2	1.59	0.84
1:D:298:LYS:HA	1:D:301:ASN:ND2	1.91	0.84
1:C:33:PHE:H	1:C:41:ASN:ND2	1.75	0.83
1:B:10:ARG:NH1	1:B:424:ARG:HG2	1.94	0.82
1:C:62:LEU:HD13	1:C:93:VAL:HG12	1.62	0.81
1:D:34:GLN:HE22	2:I:3:SSU:C2'	1.91	0.81
1:A:168:LYS:HE3	1:A:230:GLU:OE1	1.78	0.81
1:C:33:PHE:N	1:C:41:ASN:HD21	1.74	0.81
1:B:10:ARG:HH12	1:B:424:ARG:CG	1.93	0.81
2:I:3:SSU:H6	2:I:3:SSU:H5''	1.63	0.81
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.62	0.80
1:D:331:ASP:N	1:D:368:ARG:HB2	1.97	0.79
1:D:34:GLN:NE2	2:I:3:SSU:H2'	1.97	0.79
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.64	0.78
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.65	0.77
1:C:330:SER:HA	1:C:366:PRO:HB2	1.65	0.77
3:A:446:SO4:O1	1:B:248:TYR:CE2	2.38	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:VAL:HB	1:C:308:VAL:HG22	1.66	0.76
1:C:249:LEU:HD11	1:C:254:ALA:HB3	1.68	0.76
3:A:444:SO4:O2	2:G:6:SSU:H5	1.84	0.76
1:A:155:ARG:HD3	1:A:431:VAL:O	1.85	0.76
1:D:216:GLY:HA3	1:D:333:ARG:O	1.85	0.75
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.65	0.75
1:C:298:LYS:HA	1:C:301:ASN:ND2	2.02	0.75
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.68	0.75
1:D:355:PRO:HB2	1:D:356:PRO:HD2	1.69	0.74
1:C:250:ASP:HA	1:C:291:VAL:HB	1.69	0.74
1:C:391:GLN:HA	1:C:416:ARG:NH2	2.02	0.74
2:J:2:SSU:O2'	2:J:3:SSU:H3'	1.87	0.74
1:A:220:ILE:HB	1:A:310:LEU:HD23	1.70	0.73
1:D:10:ARG:CZ	1:D:424:ARG:HE	2.01	0.73
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.70	0.73
1:D:217:LYS:HB2	1:D:334:ASN:ND2	2.03	0.73
1:C:424:ARG:HD3	1:C:427:GLU:OE2	1.89	0.73
1:B:411:LYS:HB2	5:B:450:FLC:HG2	1.70	0.73
2:H:4:SSU:H6	2:H:4:SSU:S1P	2.28	0.73
1:B:236:TYR:OH	1:B:280:LYS:HE3	1.88	0.72
3:A:446:SO4:O1	1:B:248:TYR:HE2	1.72	0.72
1:D:231:ILE:O	1:D:234:VAL:HG22	1.88	0.72
1:A:91:GLU:O	1:A:95:GLU:HG2	1.89	0.72
1:D:5:PRO:HA	1:D:17:HIS:HD2	1.55	0.72
1:D:62:LEU:HD13	1:D:93:VAL:CG1	2.18	0.72
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.71	0.72
1:D:344:GLN:CD	1:D:344:GLN:H	1.92	0.72
1:B:37:GLU:O	1:B:40:ARG:HG2	1.90	0.72
1:C:250:ASP:HB3	1:C:311:ALA:HB2	1.71	0.72
1:D:33:PHE:H	1:D:41:ASN:HD21	1.36	0.72
1:A:34:GLN:HE22	2:G:3:SSU:H2'	1.56	0.71
1:C:234:VAL:O	1:C:238:HIS:HB2	1.90	0.71
1:D:8:ALA:O	1:D:399:VAL:HG22	1.90	0.71
1:C:280:LYS:HE2	1:C:280:LYS:HA	1.73	0.71
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.71	0.70
1:A:5:PRO:HA	1:A:17:HIS:HD2	1.56	0.70
1:D:240:HIS:HE1	1:D:241:ARG:HH21	1.38	0.70
1:B:260:LEU:HG	1:B:264:LEU:HD21	1.74	0.70
1:A:34:GLN:NE2	2:G:3:SSU:H2'	2.06	0.70
1:A:92:ILE:HG12	1:A:256:ARG:HH11	1.56	0.70
1:C:347:LEU:HD11	1:C:360:ILE:HG12	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PHE:HB2	1:C:373:THR:HA	1.75	0.69
1:D:204:PHE:O	1:D:208:LEU:HG	1.91	0.69
1:D:347:LEU:HG	1:D:351:ILE:HD11	1.75	0.68
1:D:229:GLN:HG3	1:D:261:TYR:CE1	2.29	0.68
1:C:62:LEU:HD13	1:C:93:VAL:CG1	2.24	0.67
1:C:57:LEU:HG	1:C:65:VAL:HG12	1.74	0.67
1:D:313:SER:HB2	2:I:5:SSU:O2	1.95	0.67
1:D:244:ARG:H	1:D:244:ARG:CD	2.06	0.67
1:D:47:PHE:CA	2:M:2:SSU:S1P	2.81	0.67
1:A:368:ARG:HH11	1:A:368:ARG:HG3	1.60	0.67
1:D:157:LEU:HD12	1:D:158:VAL:H	1.60	0.67
1:A:222:THR:HG21	1:A:310:LEU:HD22	1.77	0.67
1:C:275:HIS:ND1	1:C:282:PRO:HB3	2.09	0.66
1:C:270:GLU:HG2	3:C:439:SO4:O4	1.95	0.66
1:B:57:LEU:HG	1:B:65:VAL:HG12	1.77	0.66
1:A:280:LYS:O	1:A:282:PRO:HD3	1.95	0.66
1:B:229:GLN:H	1:B:229:GLN:NE2	1.94	0.66
1:D:127:LEU:HG	1:D:129:LEU:CD1	2.26	0.66
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.77	0.66
1:C:381:ALA:HB3	1:C:386:LEU:HD13	1.78	0.66
1:D:296:ALA:O	1:D:300:LEU:HG	1.96	0.65
2:N:2:SSU:C3'	2:N:3:SSU:H5'	2.27	0.65
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.78	0.65
1:C:32:MET:HA	1:C:67:ARG:HG3	1.79	0.65
1:B:44:PRO:HB2	2:H:4:SSU:O4	1.97	0.65
1:C:205:LEU:HD23	1:C:208:LEU:HD12	1.79	0.64
1:C:86:THR:HG22	1:C:90:MET:HE3	1.79	0.64
1:A:160:SER:HB2	1:A:163:LEU:HD21	1.79	0.64
1:C:274:ALA:O	1:C:277:LEU:HB3	1.98	0.64
1:D:33:PHE:CD2	1:D:40:ARG:HB2	2.33	0.64
1:B:163:LEU:HD21	1:B:389:TRP:CG	2.33	0.64
2:O:1:SSU:H5''	6:O:468:HOH:O	1.97	0.63
1:B:326:LYS:HD2	1:B:361:LEU:HB2	1.80	0.63
1:A:33:PHE:H	1:A:41:ASN:ND2	1.90	0.63
1:A:62:LEU:HD13	1:A:93:VAL:CG1	2.27	0.63
1:B:170:VAL:HG12	1:B:171:LEU:HD13	1.81	0.63
2:I:3:SSU:H5''	2:I:3:SSU:C6	2.28	0.63
1:B:86:THR:HG22	1:B:90:MET:CE	2.29	0.62
1:A:33:PHE:N	1:A:41:ASN:HD21	1.90	0.62
1:D:355:PRO:O	1:D:367:LEU:HD21	1.99	0.62
1:D:274:ALA:O	1:D:278:GLN:HG2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ILE:O	1:C:325:LEU:HD13	2.00	0.62
1:D:240:HIS:HE1	1:D:241:ARG:NH2	1.97	0.62
1:D:354:ARG:NH1	1:D:371:VAL:HG23	2.15	0.62
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.81	0.61
1:B:83:THR:HG22	1:B:86:THR:H	1.64	0.61
1:D:225:VAL:O	1:D:257:VAL:HG11	2.00	0.61
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.80	0.61
1:D:197:TYR:O	1:D:201:VAL:HG23	2.01	0.61
1:D:297:SER:OG	1:D:320:ARG:HD3	2.00	0.61
1:C:253:MET:HA	1:C:256:ARG:HH21	1.65	0.61
1:C:416:ARG:HE	1:C:418:GLN:NE2	1.99	0.60
1:C:280:LYS:O	1:C:282:PRO:HD3	2.00	0.60
1:D:296:ALA:HA	1:D:299:ALA:HB3	1.82	0.60
1:B:33:PHE:HB3	1:B:37:GLU:HB2	1.82	0.60
1:C:220:ILE:HB	1:C:310:LEU:HD23	1.84	0.60
1:C:49:PRO:HB3	1:C:71:LEU:HD12	1.83	0.60
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.83	0.60
1:A:97:ALA:O	1:A:101:MET:HB2	2.02	0.60
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.82	0.60
1:C:209:GLU:HG2	1:C:243:PRO:CD	2.31	0.60
1:D:157:LEU:HD12	1:D:158:VAL:N	2.17	0.60
1:A:208:LEU:HD21	1:A:218:VAL:HG11	1.84	0.60
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.83	0.60
1:A:330:SER:O	1:A:368:ARG:HG3	2.02	0.59
1:C:209:GLU:HG2	1:C:243:PRO:HD2	1.84	0.59
1:D:358:VAL:HG12	1:D:359:ARG:N	2.17	0.59
1:B:83:THR:HG21	1:B:144:GLY:CA	2.33	0.59
1:C:224:ALA:HB1	1:C:254:ALA:N	2.17	0.59
1:A:34:GLN:OE1	2:G:3:SSU:H2'	2.02	0.59
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.85	0.59
1:D:220:ILE:HG22	1:D:222:THR:HG23	1.83	0.59
6:B:498:HOH:O	2:K:2:SSU:H3'	2.03	0.59
1:D:101:MET:SD	1:D:104:PRO:HA	2.43	0.59
1:C:357:ALA:HB1	1:C:365:VAL:O	2.02	0.59
1:A:34:GLN:HE22	2:G:3:SSU:C2'	2.17	0.58
1:A:103:GLU:HG3	1:A:103:GLU:O	2.03	0.58
1:C:265:VAL:HG12	1:C:273:GLN:HG2	1.86	0.58
1:C:382:GLY:O	1:C:386:LEU:HB2	2.02	0.58
2:O:1:SSU:H1'	2:O:2:SSU:H6	1.85	0.58
1:C:97:ALA:O	1:C:101:MET:HB2	2.04	0.57
1:D:324:HIS:C	1:D:325:LEU:HD12	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:NH1	1:A:198:ARG:HB3	2.20	0.57
1:C:221:PRO:HA	1:C:311:ALA:O	2.05	0.57
1:B:293:HIS:HB3	3:B:445:SO4:O2	2.04	0.57
1:C:315:MET:O	1:C:316:LEU:HB2	2.04	0.57
1:C:100:VAL:HG11	2:O:2:SSU:H2'	1.86	0.57
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.40	0.57
1:A:202:ARG:O	1:A:206:GLU:HG3	2.05	0.56
1:B:207:ILE:O	1:B:211:THR:HG22	2.04	0.56
1:C:221:PRO:HD2	1:C:337:VAL:O	2.04	0.56
1:C:57:LEU:HD22	1:C:80:VAL:CG1	2.35	0.56
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.40	0.56
1:D:12:VAL:HG23	1:D:13:THR:HG23	1.87	0.56
1:C:165:ASN:HB3	1:C:168:LYS:HD3	1.87	0.56
1:C:338:PHE:HD2	1:C:373:THR:HG1	1.53	0.56
1:D:330:SER:O	1:D:331:ASP:HB2	2.05	0.56
1:D:229:GLN:H	1:D:229:GLN:CD	2.07	0.56
1:D:331:ASP:H	1:D:368:ARG:CB	2.07	0.56
1:D:411:LYS:HE2	1:D:415:LEU:HD11	1.87	0.56
1:A:416:ARG:HD2	6:A:454:HOH:O	2.04	0.56
1:B:39:ALA:O	1:B:42:HIS:HD2	1.89	0.56
1:B:370:SER:CA	3:B:448:SO4:O4	2.47	0.56
1:A:378:SER:OG	2:G:2:SSU:S1P	2.58	0.56
1:D:360:ILE:C	1:D:362:GLY:H	2.09	0.56
1:C:168:LYS:HG2	1:C:197:TYR:CD2	2.41	0.55
1:C:88:LEU:O	1:C:91:GLU:HB3	2.07	0.55
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.87	0.55
1:A:34:GLN:CD	2:G:3:SSU:H2'	2.27	0.55
1:C:12:VAL:HG23	1:C:13:THR:HG23	1.87	0.55
1:B:29:ASP:HA	1:B:57:LEU:HD12	1.89	0.55
1:C:86:THR:O	1:C:90:MET:HB2	2.07	0.55
1:D:98:LEU:HD11	1:D:108:PRO:HA	1.89	0.55
1:D:212:LEU:HB3	1:D:243:PRO:HG3	1.89	0.55
1:D:80:VAL:HB	1:D:118:LEU:HD23	1.89	0.55
1:D:168:LYS:HE3	1:D:230:GLU:CD	2.27	0.55
1:C:346:GLY:H	1:C:349:ALA:HB3	1.71	0.54
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.43	0.54
1:B:411:LYS:HB2	5:B:450:FLC:HA2	1.89	0.54
1:C:168:LYS:HG2	1:C:197:TYR:CE2	2.42	0.54
1:D:357:ALA:HB1	1:D:365:VAL:O	2.07	0.54
1:A:320:ARG:HD3	2:G:6:SSU:H3'	1.88	0.54
1:C:41:ASN:O	1:C:70:LYS:HE3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:CG	1:A:103:GLU:H	2.10	0.54
1:D:358:VAL:HG12	1:D:359:ARG:H	1.73	0.54
1:D:381:ALA:HB3	1:D:386:LEU:CD1	2.38	0.54
1:B:163:LEU:HD21	1:B:389:TRP:CD2	2.42	0.54
1:B:33:PHE:HB3	1:B:37:GLU:CB	2.37	0.54
1:D:240:HIS:CE1	1:D:241:ARG:HH21	2.22	0.54
1:D:301:ASN:HB3	1:D:327:HIS:CB	2.32	0.54
1:B:39:ALA:O	1:B:42:HIS:CD2	2.61	0.54
1:C:198:ARG:HG3	1:C:198:ARG:HH21	1.72	0.54
1:D:244:ARG:HD2	1:D:244:ARG:N	2.13	0.54
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.07	0.54
1:C:77:ARG:HG2	1:C:77:ARG:HH11	1.72	0.54
1:A:120:PRO:HB2	3:D:436:SO4:O4	2.08	0.54
1:A:424:ARG:HD3	6:A:517:HOH:O	2.08	0.54
1:D:414:ALA:C	1:D:416:ARG:H	2.10	0.54
1:B:192:ARG:HB2	1:B:193:PRO:HD2	1.90	0.53
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.21	0.53
1:C:1:MET:HG3	1:C:21:ALA:HB2	1.90	0.53
1:C:386:LEU:O	1:C:390:LEU:HD23	2.09	0.53
1:B:318:GLY:HA2	1:B:322:LEU:HD11	1.90	0.53
1:D:420:VAL:HG22	1:D:421:SER:N	2.23	0.53
1:B:91:GLU:O	1:B:95:GLU:HG2	2.08	0.53
1:C:205:LEU:C	1:C:207:ILE:H	2.11	0.53
1:D:70:LYS:NZ	1:D:74:GLU:OE1	2.37	0.53
1:C:12:VAL:HG21	2:P:1:SSU:O2	2.09	0.53
1:C:409:LEU:O	1:C:409:LEU:HD23	2.08	0.53
1:C:96:ASP:O	1:C:100:VAL:HG23	2.09	0.53
1:A:208:LEU:CD2	1:A:218:VAL:HG11	2.39	0.52
1:D:10:ARG:NH2	1:D:424:ARG:HH21	2.07	0.52
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.91	0.52
1:D:374:LEU:C	1:D:376:GLY:H	2.11	0.52
1:B:210:LYS:O	1:B:214:GLN:HG2	2.10	0.52
1:D:360:ILE:O	1:D:361:LEU:HB2	2.10	0.52
1:B:382:GLY:O	1:B:386:LEU:HD22	2.10	0.52
1:C:249:LEU:HD11	1:C:254:ALA:CB	2.37	0.52
1:D:221:PRO:HD2	1:D:337:VAL:O	2.09	0.52
1:A:87:VAL:HG13	1:A:118:LEU:HD13	1.91	0.52
1:C:396:VAL:O	1:C:420:VAL:HA	2.10	0.52
1:A:262:PRO:O	1:A:265:VAL:HG23	2.08	0.52
1:A:168:LYS:NZ	1:A:377:PHE:O	2.38	0.52
1:C:231:ILE:O	1:C:235:LEU:HG	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:LYS:CB	5:B:450:FLC:HG2	2.37	0.52
1:D:410:GLY:O	1:D:420:VAL:HG11	2.10	0.52
1:B:318:GLY:HA2	1:B:322:LEU:CD1	2.40	0.52
1:B:34:GLN:HE21	1:B:63:ASP:HB3	1.74	0.52
1:D:147:PHE:HB2	1:D:160:SER:HA	1.92	0.52
1:D:220:ILE:HB	1:D:310:LEU:CD2	2.40	0.52
2:N:2:SSU:H3'	2:N:3:SSU:H5'	1.90	0.51
1:A:88:LEU:HD12	1:A:264:LEU:HD21	1.91	0.51
1:D:127:LEU:HG	1:D:129:LEU:HD11	1.92	0.51
1:D:409:LEU:HD13	1:D:409:LEU:O	2.10	0.51
1:C:12:VAL:HG23	1:C:13:THR:N	2.25	0.51
1:D:191:ASP:OD1	1:D:405:LYS:HE3	2.11	0.51
1:A:358:VAL:HG12	1:A:359:ARG:N	2.26	0.51
1:D:216:GLY:O	1:D:306:PRO:HA	2.11	0.51
1:A:314:GLY:N	2:G:5:SSU:S1P	2.66	0.51
1:B:411:LYS:CA	5:B:450:FLC:HG2	2.41	0.51
1:A:18:LEU:HD13	1:A:20:LEU:HD21	1.92	0.51
1:B:88:LEU:HD12	1:B:264:LEU:HD11	1.92	0.51
1:D:411:LYS:O	1:D:415:LEU:HG	2.11	0.51
1:B:87:VAL:HG13	1:B:118:LEU:HD13	1.93	0.50
1:B:208:LEU:HD23	1:B:218:VAL:HG21	1.92	0.50
1:D:332:PRO:HA	1:D:368:ARG:O	2.11	0.50
1:D:348:GLY:O	1:D:352:ILE:HG13	2.11	0.50
1:D:325:LEU:HA	1:D:329:LEU:HB2	1.93	0.50
2:O:1:SSU:O2'	2:O:2:SSU:H5'	2.11	0.50
1:D:420:VAL:HG22	1:D:421:SER:H	1.75	0.50
1:D:358:VAL:HB	1:D:365:VAL:CG1	2.41	0.50
1:C:325:LEU:HA	1:C:329:LEU:HD11	1.93	0.50
1:D:220:ILE:HB	1:D:310:LEU:HD23	1.94	0.50
1:D:326:LYS:HD3	3:D:439:SO4:O3	2.11	0.50
1:D:47:PHE:CB	2:M:2:SSU:S1P	2.99	0.50
1:A:166:ARG:HB2	1:A:166:ARG:NH2	2.27	0.50
1:A:354:ARG:NH1	6:A:522:HOH:O	2.44	0.50
1:D:85:ALA:HB3	1:D:144:GLY:HA3	1.93	0.50
2:I:5:SSU:O4'	2:I:5:SSU:O2	2.28	0.50
1:B:420:VAL:HG22	1:B:421:SER:N	2.27	0.50
1:C:202:ARG:HH11	1:C:202:ARG:HG3	1.77	0.50
1:A:165:ASN:HB3	1:A:168:LYS:HD3	1.94	0.50
1:B:147:PHE:HB2	1:B:160:SER:HA	1.94	0.50
1:B:260:LEU:HG	1:B:264:LEU:CD2	2.39	0.50
1:C:298:LYS:HD3	1:C:301:ASN:ND2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PRO:HG2	1:C:357:ALA:H	1.76	0.50
1:D:11:GLU:OE1	1:D:33:PHE:HE1	1.95	0.50
1:A:61:HIS:HD2	2:G:4:SSU:S1P	2.34	0.49
1:B:207:ILE:O	1:B:211:THR:CG2	2.60	0.49
1:C:398:LEU:HD12	1:C:398:LEU:N	2.27	0.49
1:C:409:LEU:O	1:C:413:LEU:HG	2.12	0.49
1:B:83:THR:HG21	1:B:144:GLY:HA3	1.92	0.49
1:C:65:VAL:HG11	1:C:90:MET:HE1	1.94	0.49
1:D:325:LEU:CB	1:D:329:LEU:HB2	2.42	0.49
1:D:207:ILE:HD13	1:D:372:HIS:CG	2.47	0.49
1:A:86:THR:HG22	1:A:90:MET:HE2	1.94	0.49
1:D:298:LYS:HE2	1:D:323:HIS:HB3	1.94	0.49
2:M:1:SSU:C2'	2:M:2:SSU:S1P	3.01	0.49
2:K:2:SSU:O5'	2:K:2:SSU:H6	2.13	0.49
1:D:326:LYS:HB2	1:D:360:ILE:HG21	1.93	0.49
1:A:1:MET:HG3	1:A:21:ALA:HB2	1.94	0.49
1:B:10:ARG:HH12	1:B:424:ARG:HG3	1.74	0.49
1:B:86:THR:O	1:B:90:MET:HB2	2.12	0.49
1:C:2:ARG:HH22	1:C:430:PRO:HB3	1.78	0.49
1:D:1:MET:HG3	1:D:21:ALA:CB	2.38	0.49
1:D:347:LEU:HG	1:D:351:ILE:CD1	2.41	0.49
1:B:128:ARG:O	1:B:129:LEU:HD23	2.12	0.49
1:B:293:HIS:HD2	3:B:445:SO4:O3	1.95	0.49
1:C:168:LYS:HE3	1:C:230:GLU:OE1	2.13	0.49
1:C:229:GLN:NE2	1:C:258:LEU:HD13	2.28	0.49
1:C:402:GLU:HB2	1:C:405:LYS:HG2	1.95	0.49
1:D:354:ARG:HH11	1:D:371:VAL:HG23	1.77	0.49
1:C:209:GLU:HA	1:C:243:PRO:HG3	1.95	0.48
1:D:291:VAL:HG21	1:D:300:LEU:HD11	1.95	0.48
1:B:97:ALA:HA	2:K:3:SSU:H5	1.93	0.48
1:A:200:THR:HG23	1:A:374:LEU:HB3	1.94	0.48
1:C:318:GLY:HA2	1:C:322:LEU:HD11	1.94	0.48
1:D:192:ARG:HH11	1:D:192:ARG:HG3	1.78	0.48
1:D:325:LEU:HD12	1:D:325:LEU:N	2.28	0.48
1:B:396:VAL:O	1:B:420:VAL:HA	2.14	0.48
1:C:199:GLU:O	1:C:202:ARG:HB3	2.13	0.48
1:C:360:ILE:O	1:C:361:LEU:HB2	2.12	0.48
1:D:113:GLU:OE2	1:D:117:HIS:HE1	1.96	0.48
1:D:331:ASP:OD2	1:D:332:PRO:HD2	2.13	0.48
1:C:355:PRO:HB2	1:C:356:PRO:HD2	1.96	0.48
1:C:83:THR:O	1:C:87:VAL:HG23	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:SER:HA	2:I:1:SSU:O3'	2.13	0.48
1:A:61:HIS:HA	2:G:4:SSU:S1P	2.52	0.48
1:C:236:TYR:CD2	1:C:282:PRO:HA	2.49	0.48
1:C:309:VAL:HG11	1:C:324:HIS:CD2	2.49	0.48
1:D:380:HIS:CD2	2:I:2:SSU:H3'	2.49	0.48
1:B:195:ARG:NH1	1:B:203:GLU:OE2	2.43	0.48
1:C:325:LEU:HA	1:C:329:LEU:CD1	2.43	0.48
1:C:355:PRO:O	1:C:367:LEU:HD23	2.13	0.48
1:C:396:VAL:HG12	1:C:398:LEU:HD12	1.95	0.48
1:D:170:VAL:HG12	1:D:171:LEU:HD13	1.94	0.48
1:B:9:ALA:O	1:B:10:ARG:HB2	2.14	0.48
1:B:10:ARG:NH1	1:B:424:ARG:CG	2.64	0.48
1:C:230:GLU:O	1:C:234:VAL:HG23	2.14	0.48
1:B:84:ARG:HB3	1:B:267:TYR:OH	2.14	0.48
1:D:33:PHE:H	1:D:41:ASN:ND2	2.09	0.48
1:A:320:ARG:HH11	2:G:6:SSU:H5''	1.79	0.48
1:A:320:ARG:NH1	2:G:6:SSU:H5''	2.29	0.47
1:B:250:ASP:HB3	1:B:311:ALA:HB2	1.96	0.47
1:B:354:ARG:NH1	1:B:371:VAL:HG23	2.29	0.47
1:C:192:ARG:HD2	1:C:192:ARG:O	2.14	0.47
1:D:186:GLU:HA	1:D:399:VAL:O	2.14	0.47
1:D:1:MET:HE1	1:D:152:GLY:N	2.29	0.47
1:D:366:PRO:HG2	3:D:433:SO4:O2	2.14	0.47
1:B:155:ARG:HD2	1:B:431:VAL:O	2.14	0.47
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.49	0.47
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.49	0.47
1:C:298:LYS:HD3	1:C:301:ASN:HD21	1.78	0.47
1:C:381:ALA:HB3	1:C:386:LEU:CD1	2.45	0.47
1:D:225:VAL:HG21	2:I:4:SSU:S1P	2.54	0.47
1:D:315:MET:O	1:D:316:LEU:HB2	2.15	0.47
1:A:402:GLU:HB2	1:A:405:LYS:HD3	1.96	0.47
1:D:355:PRO:CB	1:D:356:PRO:HD2	2.43	0.47
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.95	0.47
1:D:384:ASP:OD2	1:D:384:ASP:N	2.48	0.47
1:D:5:PRO:HG2	1:D:423:ALA:HB1	1.95	0.47
1:C:209:GLU:HG2	1:C:243:PRO:HD3	1.96	0.47
1:C:274:ALA:O	1:C:278:GLN:HG2	2.15	0.47
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.97	0.47
1:D:336:LEU:HD21	1:D:338:PHE:CE1	2.49	0.47
1:B:401:GLY:HA3	1:B:406:LEU:HD13	1.96	0.47
1:C:51:GLU:OE2	1:C:51:GLU:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLN:H	1:A:229:GLN:NE2	2.13	0.47
1:B:168:LYS:HE3	1:B:230:GLU:OE1	2.15	0.47
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.50	0.47
1:B:262:PRO:O	1:B:265:VAL:HG23	2.15	0.47
1:C:139:ALA:HB3	1:C:145:SER:OG	2.15	0.47
1:C:399:VAL:HG12	1:C:423:ALA:HB3	1.97	0.47
1:D:214:GLN:O	1:D:216:GLY:N	2.48	0.47
2:G:5:SSU:O3'	2:G:6:SSU:H4'	2.14	0.47
1:D:259:SER:O	1:D:262:PRO:HD2	2.15	0.46
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.49	0.46
1:D:109:GLU:N	1:D:109:GLU:OE2	2.43	0.46
1:D:221:PRO:HB3	1:D:321:ILE:HG12	1.97	0.46
1:C:275:HIS:N	1:C:275:HIS:CD2	2.83	0.46
1:D:223:PHE:CE2	1:D:315:MET:HG2	2.50	0.46
1:C:403:GLU:O	1:C:407:LEU:HG	2.16	0.46
1:D:12:VAL:HG12	1:D:401:GLY:CA	2.39	0.46
1:B:31:GLY:HA3	1:B:63:ASP:C	2.35	0.46
1:B:402:GLU:HB2	1:B:405:LYS:HG2	1.97	0.46
1:C:398:LEU:HD13	1:C:420:VAL:HG23	1.98	0.46
1:D:291:VAL:HG13	1:D:296:ALA:HB3	1.98	0.46
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.97	0.46
1:B:86:THR:HG22	1:B:90:MET:HE2	1.96	0.46
1:C:246:PRO:HD2	1:C:306:PRO:O	2.16	0.46
1:D:327:HIS:CD2	3:D:439:SO4:O2	2.69	0.46
1:D:316:LEU:O	1:D:322:LEU:HD21	2.16	0.46
1:D:182:LEU:HD11	1:D:397:VAL:HG23	1.98	0.46
1:A:140:GLY:O	1:A:164:GLY:HA3	2.15	0.46
1:A:42:HIS:NE2	1:A:103:GLU:HG3	2.31	0.46
1:A:50:LYS:HE2	1:A:75:GLY:HA3	1.98	0.46
1:D:224:ALA:HB1	1:D:254:ALA:CA	2.46	0.46
1:A:11:GLU:OE2	1:A:40:ARG:NH1	2.48	0.46
1:B:37:GLU:O	1:B:38:GLU:C	2.55	0.46
1:C:421:SER:C	1:C:422:LEU:HD12	2.36	0.46
1:B:47:PHE:HA	2:H:3:SSU:OP2	2.16	0.45
1:C:356:PRO:O	1:C:367:LEU:HB3	2.16	0.45
1:C:422:LEU:N	1:C:422:LEU:HD12	2.32	0.45
1:A:297:SER:OG	1:A:320:ARG:HG2	2.16	0.45
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.51	0.45
1:D:380:HIS:HD2	2:I:2:SSU:H5"	1.81	0.45
3:A:446:SO4:O1	1:B:248:TYR:CD2	2.69	0.45
1:D:326:LYS:NZ	1:D:361:LEU:HD12	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.51	0.45
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.98	0.45
1:B:142:LEU:HG	1:B:143:PRO:HD2	1.97	0.45
1:C:165:ASN:HB3	1:C:168:LYS:CD	2.47	0.45
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.51	0.45
1:D:326:LYS:HD2	1:D:360:ILE:HG12	1.99	0.45
1:D:163:LEU:HD11	1:D:389:TRP:CE3	2.52	0.45
1:C:263:ARG:C	1:C:264:LEU:HD12	2.36	0.45
1:D:89:LEU:O	1:D:93:VAL:HG23	2.16	0.45
1:A:238:HIS:O	1:A:241:ARG:HG2	2.17	0.45
1:C:109:GLU:HA	1:C:112:GLU:HG2	1.97	0.45
1:D:209:GLU:OE2	1:D:243:PRO:HD3	2.17	0.45
1:D:214:GLN:O	1:D:333:ARG:HD2	2.17	0.45
2:M:1:SSU:O2'	2:M:2:SSU:P	2.73	0.45
1:B:157:LEU:HD12	1:B:182:LEU:O	2.18	0.44
1:B:260:LEU:O	1:B:264:LEU:HD22	2.17	0.44
1:B:83:THR:HG21	1:B:144:GLY:HA2	1.99	0.44
1:C:100:VAL:HG12	1:C:100:VAL:O	2.17	0.44
1:C:387:LEU:HB3	1:C:416:ARG:NH1	2.32	0.44
2:K:3:SSU:H3'	3:K:36:SO4:S	2.57	0.44
1:A:31:GLY:HA3	1:A:63:ASP:C	2.37	0.44
1:B:32:MET:HE2	1:B:105:PHE:HZ	1.81	0.44
1:A:7:GLY:HA3	1:A:14:GLY:O	2.18	0.44
1:C:232:LEU:O	1:C:285:PRO:HD3	2.18	0.44
1:C:394:PRO:HG2	1:C:395:ARG:H	1.81	0.44
1:D:9:ALA:O	1:D:11:GLU:HG2	2.18	0.44
1:D:321:ILE:HG23	1:D:322:LEU:N	2.33	0.44
1:B:194:HIS:NE2	1:B:380:HIS:O	2.48	0.44
1:B:186:GLU:HA	1:B:399:VAL:O	2.18	0.44
1:B:59:HIS:HD2	1:B:61:HIS:H	1.64	0.44
1:C:225:VAL:HG23	2:O:2:SSU:S1P	2.58	0.44
1:D:182:LEU:HD23	1:D:431:VAL:HG22	1.98	0.44
1:D:31:GLY:HA3	1:D:63:ASP:O	2.18	0.44
1:A:68:LEU:N	1:A:69:PRO:HD2	2.32	0.44
1:C:190:GLY:HA3	1:C:409:LEU:HD12	1.99	0.44
1:C:5:PRO:HG2	1:C:423:ALA:HB1	2.00	0.44
1:A:217:LYS:HE2	1:A:303:ALA:O	2.18	0.44
1:B:10:ARG:NH1	1:B:423:ALA:O	2.50	0.44
1:B:239:GLY:C	1:B:241:ARG:H	2.20	0.44
1:C:142:LEU:HD22	1:C:226:GLU:HB2	1.99	0.44
1:D:165:ASN:HB3	1:D:168:LYS:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:487:HOH:O	1:D:179:LEU:HB2	2.18	0.44
1:B:128:ARG:HD2	1:C:179:LEU:H	1.83	0.43
1:B:160:SER:HB2	1:B:163:LEU:CD1	2.48	0.43
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.99	0.43
1:B:84:ARG:NH1	1:B:88:LEU:HD21	2.32	0.43
1:C:389:TRP:HE3	1:C:390:LEU:HD22	1.83	0.43
1:A:177:PRO:HB3	1:A:389:TRP:CZ2	2.52	0.43
1:B:113:GLU:OE1	1:B:113:GLU:HA	2.18	0.43
1:B:315:MET:CE	1:B:343:PRO:HD3	2.48	0.43
1:C:214:GLN:NE2	1:C:333:ARG:HA	2.33	0.43
1:C:271:GLU:O	1:C:274:ALA:HB3	2.18	0.43
1:D:234:VAL:HG23	1:D:235:LEU:N	2.33	0.43
1:A:189:TYR:CE1	2:G:2:SSU:S1P	3.12	0.43
1:C:336:LEU:HD23	1:C:336:LEU:C	2.38	0.43
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.45	0.43
1:D:234:VAL:O	1:D:238:HIS:HB2	2.18	0.43
1:D:295:GLU:N	1:D:295:GLU:OE2	2.51	0.43
1:C:165:ASN:HB2	1:C:378:SER:O	2.18	0.43
1:C:391:GLN:HA	1:C:416:ARG:HH21	1.78	0.43
1:D:325:LEU:CD2	1:D:329:LEU:HD22	2.39	0.43
1:D:246:PRO:HG2	1:D:307:MET:HB2	1.99	0.43
1:D:285:PRO:HD2	1:D:288:LEU:HD22	2.00	0.43
1:D:221:PRO:HA	1:D:311:ALA:O	2.19	0.43
1:A:129:LEU:O	1:A:130:GLY:C	2.57	0.43
1:A:166:ARG:HH22	1:A:173:ASP:CG	2.22	0.43
1:A:344:GLN:O	1:A:344:GLN:HG3	2.17	0.43
1:B:32:MET:CE	1:B:105:PHE:HZ	2.30	0.43
1:C:294:THR:O	1:C:297:SER:HB3	2.19	0.43
2:I:2:SSU:S1P	2:I:2:SSU:H4'	2.59	0.43
1:C:73:ARG:HG3	1:C:73:ARG:HH21	1.83	0.43
1:D:298:LYS:HD3	1:D:301:ASN:ND2	2.34	0.43
1:D:313:SER:O	1:D:321:ILE:HG21	2.19	0.43
1:D:59:HIS:HD2	1:D:142:LEU:HD12	1.84	0.43
1:A:223:PHE:HD2	2:G:5:SSU:S1P	2.42	0.43
2:L:2:SSU:H4'	2:L:3:SSU:S1P	2.57	0.43
1:A:401:GLY:HA3	1:A:406:LEU:HD13	2.00	0.43
1:B:31:GLY:HA3	1:B:63:ASP:O	2.19	0.43
1:B:3:ILE:HG23	1:B:3:ILE:O	2.19	0.43
1:C:109:GLU:O	1:C:112:GLU:HG2	2.19	0.43
1:C:331:ASP:HB3	1:C:334:ASN:OD1	2.19	0.43
1:D:2:ARG:HH22	1:D:430:PRO:HD3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:ND1	1:B:241:ARG:NH2	2.67	0.42
1:B:37:GLU:OE2	1:B:40:ARG:HD3	2.18	0.42
2:K:1:SSU:C2'	2:K:1:SSU:O2	2.67	0.42
1:C:198:ARG:HG3	1:C:198:ARG:NH2	2.34	0.42
1:C:316:LEU:HD23	1:C:321:ILE:HG21	2.02	0.42
1:D:224:ALA:HB1	1:D:254:ALA:HA	2.01	0.42
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.54	0.42
1:B:420:VAL:CG2	1:B:421:SER:N	2.82	0.42
1:C:235:LEU:CD1	1:C:247:ILE:HD13	2.47	0.42
1:C:77:ARG:NH1	1:C:77:ARG:HG2	2.33	0.42
1:D:325:LEU:CA	1:D:329:LEU:HB2	2.50	0.42
1:D:346:GLY:O	1:D:349:ALA:HB3	2.19	0.42
1:D:326:LYS:HD2	1:D:360:ILE:CG1	2.49	0.42
2:K:2:SSU:O3'	2:K:3:SSU:C4'	2.67	0.42
1:C:229:GLN:HE22	1:C:258:LEU:HB2	1.84	0.42
1:C:296:ALA:O	1:C:300:LEU:HG	2.19	0.42
1:D:31:GLY:HA3	1:D:63:ASP:C	2.39	0.42
1:A:347:LEU:HD11	1:A:358:VAL:HG11	2.01	0.42
1:D:298:LYS:HE2	1:D:323:HIS:CB	2.49	0.42
1:D:10:ARG:NH1	1:D:424:ARG:HE	2.17	0.42
1:A:391:GLN:HA	1:A:416:ARG:NH2	2.35	0.42
1:B:96:ASP:O	1:B:100:VAL:HG23	2.20	0.42
1:D:100:VAL:HG13	2:I:5:SSU:C5	2.49	0.42
1:D:202:ARG:O	1:D:206:GLU:HG3	2.19	0.42
1:D:24:ARG:HG2	1:D:24:ARG:HH21	1.85	0.42
1:D:177:PRO:HB3	1:D:389:TRP:CZ2	2.55	0.42
1:D:336:LEU:C	1:D:336:LEU:HD23	2.40	0.42
1:D:37:GLU:HA	1:D:37:GLU:OE1	2.20	0.42
1:D:190:GLY:HA3	1:D:409:LEU:HB2	2.00	0.42
1:A:198:ARG:HH11	1:A:198:ARG:HB3	1.83	0.42
1:C:13:THR:HG21	1:C:34:GLN:HB2	2.02	0.42
2:G:3:SSU:C4'	2:G:4:SSU:OP2	2.56	0.42
1:B:128:ARG:HD2	1:C:179:LEU:N	2.35	0.42
1:B:424:ARG:NE	1:B:427:GLU:OE2	2.50	0.42
1:C:298:LYS:HA	1:C:301:ASN:HD22	1.81	0.42
1:C:398:LEU:N	1:C:398:LEU:CD1	2.83	0.42
1:D:233:TYR:HE1	1:D:282:PRO:HB2	1.84	0.42
1:D:28:LEU:O	1:D:29:ASP:HB2	2.20	0.42
1:C:326:LYS:HD2	1:C:361:LEU:HD22	2.02	0.42
1:C:361:LEU:C	1:C:363:GLU:H	2.24	0.42
1:B:28:LEU:O	1:B:29:ASP:HB2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD13	1:B:93:VAL:HG12	2.02	0.41
1:C:105:PHE:CE1	1:C:106:PHE:HD1	2.38	0.41
1:D:374:LEU:C	1:D:376:GLY:N	2.73	0.41
1:D:409:LEU:C	1:D:409:LEU:HD13	2.41	0.41
1:A:84:ARG:HD2	3:D:436:SO4:O3	2.20	0.41
1:A:166:ARG:HB2	1:A:166:ARG:HH21	1.84	0.41
1:A:192:ARG:HB2	1:A:193:PRO:HD2	2.00	0.41
1:B:57:LEU:HD22	1:B:80:VAL:CG1	2.50	0.41
1:C:108:PRO:O	1:C:111:VAL:HB	2.20	0.41
1:D:280:LYS:O	1:D:282:PRO:HD3	2.19	0.41
1:D:325:LEU:HB3	1:D:329:LEU:HB2	2.02	0.41
1:B:240:HIS:HE1	1:B:241:ARG:CZ	2.33	0.41
1:C:359:ARG:HH11	1:C:359:ARG:HG2	1.85	0.41
1:D:168:LYS:HG2	1:D:197:TYR:CE2	2.55	0.41
1:D:299:ALA:HA	1:D:302:ARG:CD	2.50	0.41
1:C:200:THR:HG22	1:C:377:PHE:HE1	1.85	0.41
1:C:396:VAL:HG12	1:C:398:LEU:CD1	2.51	0.41
1:D:420:VAL:O	1:D:421:SER:HB3	2.21	0.41
1:A:378:SER:CB	2:G:2:SSU:S1P	3.08	0.41
1:B:25:ARG:NH2	2:H:3:SSU:H5	2.35	0.41
1:C:416:ARG:NE	1:C:418:GLN:NE2	2.66	0.41
1:C:112:GLU:HG3	1:C:113:GLU:N	2.36	0.41
1:C:220:ILE:HG22	1:C:222:THR:HG23	2.02	0.41
1:C:318:GLY:HA2	1:C:322:LEU:CD1	2.51	0.41
1:B:34:GLN:NE2	1:B:63:ASP:HB3	2.36	0.41
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.56	0.41
1:C:59:HIS:HD2	1:C:61:HIS:HB2	1.85	0.41
1:D:20:LEU:CD2	1:D:25:ARG:HG2	2.51	0.41
1:A:97:ALA:HA	2:G:4:SSU:H5	2.03	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.94	0.41
1:A:17:HIS:HE1	6:A:482:HOH:O	2.04	0.41
1:B:68:LEU:N	1:B:69:PRO:HD2	2.35	0.41
1:C:123:TYR:OH	1:C:144:GLY:HA2	2.21	0.41
1:D:205:LEU:HD13	1:D:241:ARG:HD2	2.02	0.41
1:D:59:HIS:CD2	1:D:142:LEU:HD12	2.55	0.41
1:D:220:ILE:HD12	1:D:310:LEU:HD21	2.03	0.41
1:D:358:VAL:HB	1:D:365:VAL:HG13	2.02	0.41
2:P:1:SSU:O5'	2:P:1:SSU:H6	2.21	0.41
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.51	0.41
1:C:280:LYS:HE2	1:C:280:LYS:CA	2.48	0.41
1:A:256:ARG:CZ	6:A:468:HOH:O	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:C	1:B:165:ASN:HD22	2.23	0.41
1:B:32:MET:HB3	1:B:32:MET:HE2	1.92	0.41
1:B:33:PHE:HD2	1:B:41:ASN:HD22	1.68	0.41
1:B:424:ARG:HD3	1:B:427:GLU:OE1	2.21	0.40
1:D:387:LEU:HD11	1:D:412:LEU:HD13	2.02	0.40
1:D:32:MET:HA	1:D:67:ARG:HG3	2.02	0.40
2:I:3:SSU:HO2'	2:I:4:SSU:P	2.45	0.40
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.56	0.40
1:A:315:MET:HE2	1:A:343:PRO:HG3	2.03	0.40
1:C:349:ALA:HA	1:C:352:ILE:CD1	2.51	0.40
1:D:12:VAL:HG23	1:D:13:THR:N	2.36	0.40
1:D:61:HIS:CE1	1:D:142:LEU:HD11	2.57	0.40
1:D:215:GLY:HA2	1:D:306:PRO:HD3	2.02	0.40
1:D:84:ARG:HH11	1:D:84:ARG:HG3	1.86	0.40
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.57	0.40
1:C:329:LEU:HD12	1:C:329:LEU:N	2.36	0.40
1:C:374:LEU:C	1:C:376:GLY:H	2.25	0.40
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.57	0.40
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.36	0.40
1:D:208:LEU:O	1:D:212:LEU:HG	2.20	0.40
1:D:68:LEU:N	1:D:69:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	410 (96%)	17 (4%)	2 (0%)	29	48
1	B	429/431 (100%)	405 (94%)	21 (5%)	3 (1%)	22	39
1	C	429/431 (100%)	369 (86%)	50 (12%)	10 (2%)	6	10
1	D	429/431 (100%)	377 (88%)	44 (10%)	8 (2%)	8	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1716/1724 (100%)	1561 (91%)	132 (8%)	23 (1%)	12	21

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	241	ARG
1	A	102	ASP
1	B	240	HIS
1	B	241	ARG
1	C	168	LYS
1	C	196	PRO
1	C	295	GLU
1	D	215	GLY
1	D	241	ARG
1	D	331	ASP
1	C	328	GLY
1	D	291	VAL
1	D	328	GLY
1	D	347	LEU
1	B	38	GLU
1	C	16	ALA
1	C	29	ASP
1	C	102	ASP
1	A	30	CYS
1	C	285	PRO
1	D	38	GLU
1	D	356	PRO
1	C	187	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/342 (100%)	324 (95%)	18 (5%)	22	43
1	B	342/342 (100%)	325 (95%)	17 (5%)	24	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	342/342 (100%)	335 (98%)	7 (2%)	55	79
1	D	342/342 (100%)	327 (96%)	15 (4%)	28	52
All	All	1368/1368 (100%)	1311 (96%)	57 (4%)	30	54

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	18	LEU
1	A	94	LEU
1	A	166	ARG
1	A	171	LEU
1	A	186	GLU
1	A	192	ARG
1	A	219	LEU
1	A	229	GLN
1	A	256	ARG
1	A	263	ARG
1	A	329	LEU
1	A	336	LEU
1	A	365	VAL
1	A	390	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU
1	B	28	LEU
1	B	57	LEU
1	B	83	THR
1	B	128	ARG
1	B	165	ASN
1	B	171	LEU
1	B	186	GLU
1	B	192	ARG
1	B	209	GLU
1	B	211	THR
1	B	219	LEU
1	B	229	GLN
1	B	264	LEU
1	B	325	LEU
1	B	329	LEU
1	B	336	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	LEU
1	C	28	LEU
1	C	57	LEU
1	C	96	ASP
1	C	98	LEU
1	C	165	ASN
1	C	196	PRO
1	C	293	HIS
1	D	94	LEU
1	D	96	ASP
1	D	165	ASN
1	D	171	LEU
1	D	179	LEU
1	D	186	GLU
1	D	192	ARG
1	D	229	GLN
1	D	244	ARG
1	D	264	LEU
1	D	360	ILE
1	D	367	LEU
1	D	386	LEU
1	D	398	LEU
1	D	407	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	41	ASN
1	A	229	GLN
1	A	293	HIS
1	A	383	GLN
1	A	391	GLN
1	B	41	ASN
1	B	42	HIS
1	B	165	ASN
1	B	229	GLN
1	B	240	HIS
1	B	293	HIS
1	B	383	GLN
1	C	34	GLN
1	C	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	165	ASN
1	C	214	GLN
1	C	229	GLN
1	C	278	GLN
1	C	301	ASN
1	C	418	GLN
1	D	17	HIS
1	D	34	GLN
1	D	41	ASN
1	D	151	GLN
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	240	HIS
1	D	301	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	0/6	-	-
2	H	0/6	-	-
2	I	0/6	-	-
2	J	0/6	-	-
2	K	0/6	-	-
2	L	0/6	-	-
2	M	0/6	-	-
2	N	0/6	-	-
2	O	0/6	-	-
2	P	0/6	-	-
All	All	0/60	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

Of 35 non-standard protein/DNA/RNA residues modelled in this entry, 6 are modelled with single atom - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SSU	I	3	2	14,21,22	1.14	2 (14%)	14,30,33	1.40	1 (7%)
2	SSU	M	2	2	0,3,22	0.00	-	0,3,33	0.00	-
2	SSU	L	2	2	14,21,22	1.12	1 (7%)	14,30,33	1.22	1 (7%)
2	SSU	J	3	2	14,21,22	1.14	2 (14%)	14,30,33	1.19	1 (7%)
2	SSU	I	6	2	0,3,22	0.00	-	0,3,33	0.00	-
2	SSU	K	2	2	14,21,22	1.14	1 (7%)	14,30,33	1.10	1 (7%)
2	SSU	J	2	2	14,21,22	1.12	1 (7%)	14,30,33	1.17	1 (7%)
2	SSU	M	1	2	14,18,22	1.09	1 (7%)	14,26,33	1.37	2 (14%)
2	SSU	P	2	2	0,3,22	0.00	-	0,3,33	0.00	-
2	SSU	I	4	2	14,21,22	1.12	1 (7%)	14,30,33	1.14	1 (7%)
2	SSU	L	3	2	14,21,22	1.29	2 (14%)	14,30,33	1.18	1 (7%)
2	SSU	O	2	2	14,21,22	1.11	1 (7%)	14,30,33	1.18	1 (7%)
2	SSU	I	2	2	14,21,22	1.13	1 (7%)	14,30,33	1.17	1 (7%)
2	SSU	O	1	2	14,18,22	1.09	1 (7%)	14,26,33	1.11	1 (7%)
2	SSU	G	2	2	14,21,22	1.21	2 (14%)	14,30,33	1.18	1 (7%)
2	SSU	I	5	2	14,21,22	1.10	1 (7%)	14,30,33	1.23	1 (7%)
2	SSU	G	4	2	14,21,22	1.16	1 (7%)	14,30,33	1.14	1 (7%)
2	SSU	L	4	2	0,3,22	0.00	-	0,3,33	0.00	-
2	SSU	N	3	2	14,21,22	1.18	1 (7%)	14,30,33	1.15	1 (7%)
2	SSU	H	3	2	14,21,22	1.17	1 (7%)	14,30,33	1.13	1 (7%)
2	SSU	H	2	2	14,21,22	1.12	1 (7%)	14,30,33	1.11	1 (7%)
2	SSU	G	3	2	14,21,22	1.23	2 (14%)	14,30,33	1.24	1 (7%)
2	SSU	P	1	2	14,18,22	1.12	2 (14%)	14,26,33	1.21	1 (7%)
2	SSU	K	1	2	14,18,22	1.13	2 (14%)	14,26,33	1.15	1 (7%)
2	SSU	G	6	2	14,21,22	1.12	1 (7%)	14,30,33	1.22	1 (7%)
2	SSU	K	3	2	14,21,22	1.14	1 (7%)	14,30,33	1.13	1 (7%)
2	SSU	N	2	2	14,21,22	1.15	1 (7%)	14,30,33	1.16	1 (7%)
2	SSU	G	5	2	14,21,22	1.11	1 (7%)	14,30,33	1.18	1 (7%)
2	SSU	H	4	2	14,21,22	1.17	1 (7%)	14,30,33	1.12	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SSU	I	3	2	-	4/5/25/26	0/2/2/2
2	SSU	L	2	2	-	0/5/25/26	0/2/2/2
2	SSU	J	3	2	-	2/5/25/26	0/2/2/2
2	SSU	K	2	2	-	4/5/25/26	0/2/2/2
2	SSU	J	2	2	-	2/5/25/26	0/2/2/2
2	SSU	M	1	2	-	2/4/22/26	0/2/2/2
2	SSU	I	4	2	-	3/5/25/26	0/2/2/2
2	SSU	L	3	2	-	0/5/25/26	0/2/2/2
2	SSU	O	2	2	-	2/5/25/26	0/2/2/2
2	SSU	I	2	2	-	5/5/25/26	0/2/2/2
2	SSU	O	1	2	-	3/4/22/26	0/2/2/2
2	SSU	G	2	2	-	4/5/25/26	0/2/2/2
2	SSU	I	5	2	-	3/5/25/26	0/2/2/2
2	SSU	G	4	2	-	3/5/25/26	0/2/2/2
2	SSU	N	3	2	-	1/5/25/26	0/2/2/2
2	SSU	H	3	2	-	3/5/25/26	0/2/2/2
2	SSU	H	2	2	-	0/5/25/26	0/2/2/2
2	SSU	G	3	2	-	0/5/25/26	0/2/2/2
2	SSU	P	1	2	-	2/4/22/26	0/2/2/2
2	SSU	K	1	2	-	1/4/22/26	0/2/2/2
2	SSU	G	6	2	-	2/5/25/26	0/2/2/2
2	SSU	K	3	2	-	5/5/25/26	0/2/2/2
2	SSU	N	2	2	-	4/5/25/26	0/2/2/2
2	SSU	G	5	2	-	0/5/25/26	0/2/2/2
2	SSU	H	4	2	-	3/5/25/26	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	3	SSU	C4-N3	3.63	1.39	1.33
2	H	3	SSU	C4-N3	3.35	1.38	1.33
2	G	2	SSU	C4-N3	3.34	1.38	1.33
2	G	3	SSU	C4-N3	3.33	1.38	1.33
2	H	4	SSU	C4-N3	3.28	1.38	1.33
2	N	3	SSU	C4-N3	3.27	1.38	1.33
2	L	2	SSU	C4-N3	3.27	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	SSU	C4-N3	3.23	1.38	1.33
2	G	6	SSU	C4-N3	3.21	1.38	1.33
2	G	5	SSU	C4-N3	3.20	1.38	1.33
2	K	3	SSU	C4-N3	3.20	1.38	1.33
2	I	2	SSU	C4-N3	3.18	1.38	1.33
2	N	2	SSU	C4-N3	3.16	1.38	1.33
2	P	1	SSU	C4-N3	3.14	1.38	1.33
2	O	2	SSU	C4-N3	3.13	1.38	1.33
2	I	3	SSU	C4-N3	3.13	1.38	1.33
2	G	4	SSU	C4-N3	3.12	1.38	1.33
2	J	3	SSU	C4-N3	3.07	1.38	1.33
2	M	1	SSU	C4-N3	3.06	1.38	1.33
2	J	2	SSU	C4-N3	3.05	1.38	1.33
2	K	1	SSU	C4-N3	3.04	1.38	1.33
2	K	2	SSU	C4-N3	3.02	1.38	1.33
2	I	5	SSU	C4-N3	2.99	1.38	1.33
2	O	1	SSU	C4-N3	2.99	1.38	1.33
2	I	4	SSU	C4-N3	2.98	1.38	1.33
2	L	3	SSU	C6-N1	2.26	1.38	1.35
2	G	2	SSU	C6-N1	2.11	1.38	1.35
2	K	1	SSU	C6-N1	2.09	1.38	1.35
2	J	3	SSU	C6-N1	2.06	1.38	1.35
2	G	3	SSU	C6-N1	2.04	1.38	1.35
2	I	3	SSU	C6-N1	2.04	1.38	1.35
2	P	1	SSU	C6-N1	2.02	1.38	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	SSU	C5-C4-N3	-4.01	114.49	123.31
2	H	3	SSU	C5-C4-N3	-3.99	114.52	123.31
2	P	1	SSU	C5-C4-N3	-3.98	114.55	123.31
2	G	5	SSU	C5-C4-N3	-3.97	114.57	123.31
2	N	3	SSU	C5-C4-N3	-3.97	114.58	123.31
2	K	1	SSU	C5-C4-N3	-3.96	114.60	123.31
2	O	2	SSU	C5-C4-N3	-3.95	114.62	123.31
2	I	3	SSU	C5-C4-N3	-3.95	114.63	123.31
2	I	2	SSU	C5-C4-N3	-3.95	114.63	123.31
2	G	4	SSU	C5-C4-N3	-3.94	114.63	123.31
2	G	3	SSU	C5-C4-N3	-3.94	114.63	123.31
2	N	2	SSU	C5-C4-N3	-3.94	114.64	123.31
2	K	2	SSU	C5-C4-N3	-3.94	114.65	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	SSU	C5-C4-N3	-3.94	114.65	123.31
2	O	1	SSU	C5-C4-N3	-3.94	114.65	123.31
2	I	4	SSU	C5-C4-N3	-3.93	114.66	123.31
2	H	2	SSU	C5-C4-N3	-3.93	114.66	123.31
2	G	6	SSU	C5-C4-N3	-3.92	114.68	123.31
2	H	4	SSU	C5-C4-N3	-3.91	114.71	123.31
2	J	3	SSU	C5-C4-N3	-3.90	114.72	123.31
2	L	2	SSU	C5-C4-N3	-3.90	114.72	123.31
2	M	1	SSU	C5-C4-N3	-3.90	114.72	123.31
2	K	3	SSU	C5-C4-N3	-3.90	114.73	123.31
2	J	2	SSU	C5-C4-N3	-3.89	114.75	123.31
2	G	2	SSU	C5-C4-N3	-3.88	114.77	123.31
2	M	1	SSU	O4'-C1'-C2'	-2.06	103.92	106.93

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	SSU	C2'-C1'-N1-C6
2	I	3	SSU	O4'-C1'-N1-C6
2	J	3	SSU	O4'-C4'-C5'-O5'
2	K	2	SSU	C2'-C1'-N1-C6
2	K	2	SSU	O4'-C1'-N1-C6
2	I	4	SSU	O4'-C1'-N1-C6
2	I	4	SSU	C3'-C4'-C5'-O5'
2	G	6	SSU	C4'-C5'-O5'-P
2	I	2	SSU	C2'-C1'-N1-C6
2	I	2	SSU	O4'-C1'-N1-C6
2	O	1	SSU	C2'-C1'-N1-C6
2	G	2	SSU	C2'-C1'-N1-C6
2	G	2	SSU	O4'-C1'-N1-C6
2	I	5	SSU	C2'-C1'-N1-C6
2	G	4	SSU	C2'-C1'-N1-C6
2	G	4	SSU	O4'-C1'-N1-C6
2	H	3	SSU	O4'-C1'-N1-C6
2	K	1	SSU	C2'-C1'-N1-C6
2	K	3	SSU	C2'-C1'-N1-C6
2	K	3	SSU	O4'-C1'-N1-C6
2	K	3	SSU	O4'-C4'-C5'-O5'
2	K	3	SSU	C3'-C4'-C5'-O5'
2	K	3	SSU	C4'-C5'-O5'-P
2	N	2	SSU	C2'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	N	2	SSU	O4'-C1'-N1-C6
2	N	2	SSU	O4'-C4'-C5'-O5'
2	M	1	SSU	C3'-C4'-C5'-O5'
2	M	1	SSU	O4'-C4'-C5'-O5'
2	O	1	SSU	C3'-C4'-C5'-O5'
2	O	2	SSU	C3'-C4'-C5'-O5'
2	N	2	SSU	C3'-C4'-C5'-O5'
2	J	3	SSU	C3'-C4'-C5'-O5'
2	P	1	SSU	O4'-C4'-C5'-O5'
2	O	1	SSU	O4'-C4'-C5'-O5'
2	I	4	SSU	O4'-C4'-C5'-O5'
2	I	2	SSU	C3'-C4'-C5'-O5'
2	H	4	SSU	C3'-C4'-C5'-O5'
2	I	5	SSU	C3'-C4'-C5'-O5'
2	P	1	SSU	C3'-C4'-C5'-O5'
2	O	2	SSU	O4'-C4'-C5'-O5'
2	I	3	SSU	C4'-C5'-O5'-P
2	I	2	SSU	C4'-C5'-O5'-P
2	I	5	SSU	C4'-C5'-O5'-P
2	I	3	SSU	O4'-C4'-C5'-O5'
2	K	2	SSU	O4'-C4'-C5'-O5'
2	G	2	SSU	O4'-C4'-C5'-O5'
2	G	6	SSU	O4'-C4'-C5'-O5'
2	J	2	SSU	O4'-C4'-C5'-O5'
2	J	2	SSU	C3'-C4'-C5'-O5'
2	G	2	SSU	C3'-C4'-C5'-O5'
2	G	4	SSU	C4'-C5'-O5'-P
2	N	3	SSU	C4'-C5'-O5'-P
2	H	3	SSU	C4'-C5'-O5'-P
2	H	4	SSU	C4'-C5'-O5'-P
2	I	2	SSU	O4'-C4'-C5'-O5'
2	H	4	SSU	O4'-C4'-C5'-O5'
2	K	2	SSU	C3'-C4'-C5'-O5'
2	H	3	SSU	O4'-C4'-C5'-O5'

There are no ring outliers.

25 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	SSU	6	0
2	M	2	SSU	7	0
2	L	2	SSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	3	SSU	1	0
2	K	2	SSU	3	0
2	J	2	SSU	1	0
2	M	1	SSU	4	0
2	I	4	SSU	2	0
2	L	3	SSU	1	0
2	O	2	SSU	4	0
2	I	2	SSU	3	0
2	O	1	SSU	3	0
2	G	2	SSU	3	0
2	I	5	SSU	3	0
2	G	4	SSU	5	0
2	N	3	SSU	2	0
2	H	3	SSU	2	0
2	G	3	SSU	7	0
2	P	1	SSU	2	0
2	K	1	SSU	2	0
2	G	6	SSU	5	0
2	K	3	SSU	3	0
2	N	2	SSU	2	0
2	G	5	SSU	3	0
2	H	4	SSU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 8 are monoatomic - leaving 60 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	443	-	4,4,4	1.02	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	441	-	4,4,4	1.02	0	6,6,6	0.65	0
3	SO4	B	445	-	4,4,4	1.05	0	6,6,6	0.62	0
3	SO4	D	437	-	4,4,4	1.00	0	6,6,6	0.66	0
3	SO4	B	433	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	432	-	4,4,4	1.01	0	6,6,6	0.64	0
3	SO4	C	436	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	A	439	-	4,4,4	1.02	0	6,6,6	0.64	0
3	SO4	B	440	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	C	442	-	4,4,4	0.98	0	6,6,6	0.64	0
3	SO4	C	441	-	4,4,4	1.04	0	6,6,6	0.65	0
3	SO4	J	40	-	4,4,4	1.00	0	6,6,6	0.65	0
3	SO4	D	435	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	B	439	-	4,4,4	1.02	0	6,6,6	0.64	0
3	SO4	D	432	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	B	435	-	4,4,4	1.03	0	6,6,6	0.66	0
3	SO4	A	440	-	4,4,4	1.03	0	6,6,6	0.66	0
3	SO4	B	444	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	B	449	-	4,4,4	0.94	0	6,6,6	0.71	0
3	SO4	C	433	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	C	434	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	D	440	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	B	443	-	4,4,4	1.03	0	6,6,6	0.65	0
3	SO4	D	434	-	4,4,4	0.99	0	6,6,6	0.66	0
3	SO4	C	432	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	C	438	-	4,4,4	1.01	0	6,6,6	0.65	0
3	SO4	A	442	-	4,4,4	0.99	0	6,6,6	0.66	0
3	SO4	B	442	-	4,4,4	1.00	0	6,6,6	0.67	0
3	SO4	B	438	-	4,4,4	1.03	0	6,6,6	0.63	0
3	SO4	B	446	-	4,4,4	1.03	0	6,6,6	0.64	0
3	SO4	B	436	-	4,4,4	0.99	0	6,6,6	0.65	0
3	SO4	B	441	-	4,4,4	1.02	0	6,6,6	0.65	0
3	SO4	A	434	-	4,4,4	1.01	0	6,6,6	0.67	0
3	SO4	B	437	-	4,4,4	1.01	0	6,6,6	0.64	0
3	SO4	B	434	-	4,4,4	1.03	0	6,6,6	0.66	0
3	SO4	A	441	-	4,4,4	1.00	0	6,6,6	0.65	0
3	SO4	B	447	-	4,4,4	0.94	0	6,6,6	0.71	0
3	SO4	C	439	-	4,4,4	1.03	0	6,6,6	0.65	0
5	FLC	B	450	-	3,12,12	1.21	0	3,17,17	0.26	0
3	SO4	A	435	-	4,4,4	1.04	0	6,6,6	0.65	0
3	SO4	D	442	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	A	436	-	4,4,4	1.03	0	6,6,6	0.68	0
3	SO4	A	447	-	4,4,4	1.00	0	6,6,6	0.65	0
3	SO4	D	439	-	4,4,4	1.02	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	432	-	4,4,4	1.06	0	6,6,6	0.63	0
3	SO4	D	436	-	4,4,4	1.03	0	6,6,6	0.62	0
3	SO4	C	437	-	4,4,4	1.02	0	6,6,6	0.65	0
3	SO4	A	437	-	4,4,4	0.96	0	6,6,6	0.66	0
3	SO4	A	444	-	4,4,4	0.99	0	6,6,6	0.68	0
3	SO4	A	443	-	4,4,4	0.99	0	6,6,6	0.67	0
3	SO4	A	433	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	B	448	-	4,4,4	1.03	0	6,6,6	0.65	0
3	SO4	C	440	-	4,4,4	1.02	0	6,6,6	0.66	0
3	SO4	K	36	-	4,4,4	1.02	0	6,6,6	0.65	0
3	SO4	D	433	-	4,4,4	1.02	0	6,6,6	0.67	0
3	SO4	A	445	-	4,4,4	1.01	0	6,6,6	0.66	0
3	SO4	D	438	-	4,4,4	1.04	0	6,6,6	0.67	0
3	SO4	C	435	-	4,4,4	1.03	0	6,6,6	0.67	0
3	SO4	A	446	-	4,4,4	0.99	0	6,6,6	0.67	0
3	SO4	A	438	-	4,4,4	1.03	0	6,6,6	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FLC	B	450	-	-	0/6/16/16	-

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.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	445	SO4	2	0
3	C	439	SO4	2	0
5	B	450	FLC	4	0
3	D	439	SO4	2	0
3	D	436	SO4	2	0
3	A	444	SO4	1	0
3	A	443	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	448	SO4	2	0
3	K	36	SO4	1	0
3	D	433	SO4	1	0
3	A	446	SO4	3	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	431/431 (100%)	-0.11	1 (0%) 95 95	14, 29, 51, 67	0
1	B	431/431 (100%)	-0.16	3 (0%) 87 89	14, 29, 52, 69	0
1	C	431/431 (100%)	1.11	101 (23%) 0 0	21, 63, 117, 137	0
1	D	431/431 (100%)	0.96	88 (20%) 1 0	22, 51, 111, 134	0
2	G	0/6	-	-	-	-
2	H	0/6	-	-	-	-
2	I	0/6	-	-	-	-
2	J	0/6	-	-	-	-
2	K	0/6	-	-	-	-
2	L	0/6	-	-	-	-
2	M	0/6	-	-	-	-
2	N	0/6	-	-	-	-
2	O	0/6	-	-	-	-
2	P	0/6	-	-	-	-
All	All	1724/1784 (96%)	0.45	193 (11%) 5 4	14, 39, 111, 137	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	361	LEU	10.6
1	C	216	GLY	8.4
1	C	242	LEU	7.8
1	C	354	ARG	7.2
1	D	362	GLY	7.1
1	C	322	LEU	7.0
1	C	244	ARG	6.9
1	D	330	SER	6.7
1	C	213	SER	6.6
1	C	329	LEU	6.3
1	C	218	VAL	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	361	LEU	6.1
1	D	365	VAL	6.0
1	C	335	ALA	5.8
1	D	333	ARG	5.7
1	D	371	VAL	5.7
1	C	306	PRO	5.7
1	D	332	PRO	5.5
1	D	293	HIS	5.4
1	C	295	GLU	5.4
1	C	208	LEU	5.2
1	D	356	PRO	5.2
1	C	212	LEU	5.2
1	D	369	ALA	5.2
1	C	369	ALA	5.1
1	C	353	ALA	5.0
1	C	239	GLY	5.0
1	C	370	SER	5.0
1	C	323	HIS	4.9
1	D	291	VAL	4.9
1	D	286	ALA	4.9
1	D	358	VAL	4.9
1	C	241	ARG	4.8
1	D	359	ARG	4.8
1	C	215	GLY	4.7
1	C	336	LEU	4.7
1	C	333	ARG	4.6
1	C	300	LEU	4.6
1	D	322	LEU	4.6
1	D	242	LEU	4.6
1	C	245	ALA	4.5
1	D	218	VAL	4.5
1	C	296	ALA	4.4
1	C	338	PHE	4.4
1	D	216	GLY	4.4
1	D	326	LYS	4.3
1	C	248	TYR	4.3
1	C	334	ASN	4.3
1	D	355	PRO	4.3
1	C	207	ILE	4.2
1	D	300	LEU	4.2
1	C	326	LYS	4.2
1	D	368	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	415	LEU	4.1
1	D	366	PRO	4.1
1	C	307	MET	4.1
1	D	303	ALA	4.1
1	C	209	GLU	4.1
1	D	306	PRO	4.1
1	C	304	PRO	4.1
1	C	371	VAL	4.1
1	C	235	LEU	4.0
1	C	358	VAL	4.0
1	D	240	HIS	4.0
1	C	324	HIS	4.0
1	C	305	GLY	4.0
1	D	241	ARG	3.9
1	C	321	ILE	3.9
1	C	292	GLU	3.9
1	B	42	HIS	3.8
1	C	277	LEU	3.8
1	D	316	LEU	3.8
1	C	319	GLY	3.8
1	C	372	HIS	3.8
1	D	210	LYS	3.8
1	D	328	GLY	3.8
1	D	238	HIS	3.7
1	C	348	GLY	3.7
1	C	217	LYS	3.7
1	D	338	PHE	3.7
1	C	365	VAL	3.7
1	D	352	ILE	3.7
1	C	301	ASN	3.6
1	C	373	THR	3.6
1	D	297	SER	3.5
1	C	294	THR	3.5
1	C	303	ALA	3.5
1	C	214	GLN	3.5
1	C	299	ALA	3.4
1	C	377	PHE	3.4
1	D	360	ILE	3.4
1	C	415	LEU	3.4
1	C	247	ILE	3.4
1	C	233	TYR	3.4
1	C	210	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	307	MET	3.3
1	D	295	GLU	3.3
1	C	327	HIS	3.3
1	D	239	GLY	3.3
1	C	332	PRO	3.3
1	C	302	ARG	3.3
1	C	243	PRO	3.2
1	C	356	PRO	3.2
1	D	321	ILE	3.2
1	C	411	LYS	3.2
1	C	359	ARG	3.2
1	A	362	GLY	3.2
1	D	302	ARG	3.2
1	D	292	GLU	3.2
1	D	207	ILE	3.2
1	C	240	HIS	3.2
1	C	363	GLU	3.1
1	D	325	LEU	3.1
1	C	286	ALA	3.1
1	D	235	LEU	3.1
1	C	298	LYS	3.1
1	D	290	VAL	3.0
1	C	198	ARG	2.9
1	D	246	PRO	2.9
1	C	280	LYS	2.9
1	C	199	GLU	2.9
1	D	287	GLY	2.9
1	D	336	LEU	2.9
1	D	250	ASP	2.9
1	D	364	GLU	2.8
1	D	327	HIS	2.8
1	C	205	LEU	2.8
1	D	347	LEU	2.8
1	D	101	MET	2.8
1	C	352	ILE	2.8
1	C	320	ARG	2.8
1	D	247	ILE	2.8
1	D	373	THR	2.8
1	D	249	LEU	2.8
1	C	293	HIS	2.7
1	C	297	SER	2.7
1	D	243	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	260	LEU	2.7
1	D	324	HIS	2.7
1	C	197	TYR	2.7
1	D	341	TYR	2.7
1	D	208	LEU	2.6
1	D	363	GLU	2.6
1	D	308	VAL	2.6
1	D	329	LEU	2.6
1	D	252	PRO	2.6
1	C	283	PHE	2.6
1	C	360	ILE	2.5
1	D	323	HIS	2.5
1	D	337	VAL	2.5
1	C	357	ALA	2.5
1	D	296	ALA	2.5
1	C	325	LEU	2.5
1	C	350	GLU	2.5
1	D	234	VAL	2.5
1	C	355	PRO	2.5
1	C	367	LEU	2.4
1	D	357	ALA	2.4
1	D	258	LEU	2.4
1	C	288	LEU	2.4
1	D	251	SER	2.4
1	D	213	SER	2.4
1	C	279	GLY	2.4
1	D	225	VAL	2.4
1	D	305	GLY	2.4
1	D	298	LYS	2.4
1	D	370	SER	2.4
1	C	196	PRO	2.3
1	D	108	PRO	2.3
1	C	22	GLY	2.3
1	D	205	LEU	2.3
1	C	368	ARG	2.3
1	C	250	ASP	2.3
1	D	353	ALA	2.3
1	D	211	THR	2.3
1	D	294	THR	2.3
1	C	219	LEU	2.3
1	B	36	LYS	2.2
1	C	291	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	236	TYR	2.2
1	D	99	LYS	2.2
1	D	209	GLU	2.2
1	C	202	ARG	2.1
1	C	328	GLY	2.1
1	C	316	LEU	2.1
1	D	344	GLN	2.1
1	D	149	VAL	2.1
1	C	246	PRO	2.1
1	C	252	PRO	2.0
1	C	349	ALA	2.0
1	D	104	PRO	2.0
1	D	244	ARG	2.0
1	B	240	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SSU	M	1	17/21	0.57	0.28	84,91,92,92	0
2	SSU	N	2	20/21	0.60	0.25	91,99,107,107	0
2	SSU	M	2	4/21	0.62	0.30	86,88,88,93	0
2	SSU	G	6	20/21	0.68	0.38	104,111,112,112	0
2	SSU	N	3	20/21	0.69	0.36	107,112,114,114	0
2	SSU	O	2	20/21	0.70	0.22	136,137,137,138	0
2	SSU	O	1	17/21	0.73	0.28	136,136,137,137	0
2	SSU	G	5	20/21	0.76	0.24	93,95,100,103	0
2	SSU	K	1	17/21	0.77	0.31	87,90,95,95	0
2	SSU	J	3	20/21	0.77	0.27	72,77,79,79	0
2	SSU	I	3	20/21	0.77	0.21	101,102,106,107	0
2	SSU	K	2	20/21	0.78	0.27	93,95,98,99	0
2	SSU	G	3	20/21	0.79	0.20	77,81,84,85	0
2	SSU	P	1	17/21	0.80	0.30	131,132,133,133	0
2	SSU	I	5	20/21	0.80	0.21	102,104,106,107	0
2	SSU	H	4	20/21	0.82	0.36	88,92,95,96	0
2	SSU	J	1	1/21	0.84	0.30	73,73,73,73	0
2	SSU	I	2	20/21	0.86	0.40	96,108,113,113	0
2	SSU	G	4	20/21	0.86	0.19	86,90,91,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SSU	I	6	4/21	0.86	0.30	108,108,108,108	0
2	SSU	P	2	4/21	0.88	0.34	131,131,132,132	0
2	SSU	J	2	20/21	0.88	0.19	56,66,73,73	0
2	SSU	L	1	1/21	0.89	0.35	53,53,53,53	0
2	SSU	L	3	20/21	0.89	0.20	46,60,68,69	0
2	SSU	L	4	4/21	0.89	0.17	61,62,63,67	0
2	SSU	K	3	20/21	0.89	0.21	96,98,100,101	0
2	SSU	I	4	20/21	0.90	0.18	98,99,100,101	0
2	SSU	H	3	20/21	0.90	0.26	76,88,91,91	0
2	SSU	H	2	20/21	0.92	0.22	64,69,76,79	0
2	SSU	H	1	1/21	0.93	0.18	77,77,77,77	0
2	SSU	G	2	20/21	0.93	0.20	33,63,67,73	0
2	SSU	L	2	20/21	0.96	0.13	39,44,56,56	0
2	SSU	I	1	1/21	0.97	0.32	97,97,97,97	0
2	SSU	N	1	1/21	0.97	0.16	106,106,106,106	0
2	SSU	G	1	1/21	0.99	0.18	36,36,36,36	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
3	SO4	A	433	5/5	0.57	0.25	134,134,135,135	0
3	SO4	D	432	5/5	0.67	0.23	138,138,138,138	0
3	SO4	A	445	5/5	0.67	0.27	150,150,150,150	0
3	SO4	C	441	5/5	0.69	0.26	122,122,123,123	0
3	SO4	B	439	5/5	0.70	0.37	113,113,114,114	0
3	SO4	A	443	5/5	0.71	0.31	126,126,126,127	0
3	SO4	A	439	5/5	0.75	0.42	173,173,173,173	0
3	SO4	C	436	5/5	0.75	0.21	114,114,115,115	0
3	SO4	B	437	5/5	0.75	0.34	168,168,169,169	0
3	SO4	A	446	5/5	0.75	0.42	115,115,115,116	0
3	SO4	B	443	5/5	0.76	0.55	131,131,131,132	0
3	SO4	D	433	5/5	0.76	0.22	103,103,103,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FLC	B	450	13/13	0.77	0.46	86,91,93,93	0
3	SO4	B	445	5/5	0.78	0.42	121,121,122,122	0
3	SO4	A	441	5/5	0.78	0.36	144,144,144,144	0
3	SO4	A	440	5/5	0.79	0.27	106,106,107,107	0
3	SO4	A	447	5/5	0.80	0.21	133,133,133,134	0
3	SO4	B	446	5/5	0.80	0.32	122,122,122,122	0
3	SO4	C	438	5/5	0.80	0.19	112,112,113,113	0
3	SO4	D	439	5/5	0.81	0.14	135,136,136,136	0
3	SO4	B	434	5/5	0.81	0.17	117,117,118,118	0
3	SO4	D	437	5/5	0.81	0.18	126,126,127,127	0
3	SO4	B	432	5/5	0.82	0.18	99,99,100,100	0
3	SO4	A	432	5/5	0.82	0.16	123,123,123,123	0
3	SO4	D	441	5/5	0.83	0.22	136,136,136,136	0
3	SO4	A	435	5/5	0.83	0.20	100,100,101,101	0
3	SO4	B	433	5/5	0.84	0.21	122,122,122,122	0
3	SO4	C	433	5/5	0.84	0.32	130,131,131,131	0
3	SO4	K	36	5/5	0.85	0.25	112,112,112,113	0
3	SO4	D	442	5/5	0.85	0.30	100,101,101,101	0
3	SO4	B	444	5/5	0.85	0.35	122,122,122,122	0
3	SO4	D	440	5/5	0.85	0.15	121,121,122,122	0
3	SO4	B	441	5/5	0.86	0.30	134,134,134,134	0
3	SO4	D	434	5/5	0.86	0.21	117,117,117,117	0
3	SO4	C	435	5/5	0.88	0.16	92,93,94,94	0
3	SO4	C	437	5/5	0.88	0.14	118,118,118,119	0
3	SO4	J	40	5/5	0.89	0.29	133,133,133,134	0
3	SO4	D	436	5/5	0.89	0.24	105,105,105,106	0
3	SO4	C	432	5/5	0.90	0.33	121,121,121,122	0
3	SO4	B	447	5/5	0.90	0.48	162,162,162,162	5
3	SO4	C	439	5/5	0.90	0.15	99,99,100,100	0
3	SO4	C	440	5/5	0.91	0.12	120,120,120,121	0
3	SO4	C	442	5/5	0.91	0.19	75,77,77,78	0
3	SO4	A	444	5/5	0.92	0.24	85,85,85,86	0
3	SO4	B	448	5/5	0.92	0.34	111,111,111,111	0
3	SO4	B	435	5/5	0.92	0.15	111,111,111,111	0
4	ZN	A	449	1/1	0.93	0.06	73,73,73,73	0
3	SO4	A	436	5/5	0.94	0.27	84,84,85,85	0
3	SO4	B	440	5/5	0.94	0.20	99,99,100,100	0
3	SO4	B	442	5/5	0.94	0.17	61,62,63,64	0
3	SO4	C	443	5/5	0.94	0.11	87,87,88,88	0
3	SO4	D	435	5/5	0.94	0.12	76,76,76,77	0
3	SO4	C	434	5/5	0.95	0.13	77,77,78,78	0
4	ZN	B	452	1/1	0.95	0.05	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	438	5/5	0.95	0.11	73,74,74,75	0
3	SO4	A	437	5/5	0.96	0.15	49,50,51,52	0
3	SO4	B	438	5/5	0.96	0.11	73,73,73,74	0
3	SO4	D	438	5/5	0.96	0.13	60,61,62,63	0
4	ZN	C	444	1/1	0.97	0.09	75,75,75,75	0
4	ZN	C	445	1/1	0.97	0.12	81,81,81,81	0
3	SO4	B	449	5/5	0.97	0.18	43,43,45,45	0
3	SO4	A	434	5/5	0.98	0.08	83,83,83,83	0
4	ZN	B	451	1/1	0.98	0.04	56,56,56,56	0
4	ZN	D	444	1/1	0.99	0.08	69,69,69,69	0
4	ZN	D	443	1/1	0.99	0.13	70,70,70,70	0
3	SO4	B	436	5/5	0.99	0.15	35,35,37,37	0
3	SO4	A	442	5/5	0.99	0.14	32,33,33,35	0
4	ZN	A	448	1/1	0.99	0.04	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.