Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:25 AM GMT

PDB ID	:	3IE2
Title	:	Crystal Structure of H400V mutant TTHA0252 from Thermus thermophilus HB8
Authors	:	Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2009-07-22
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

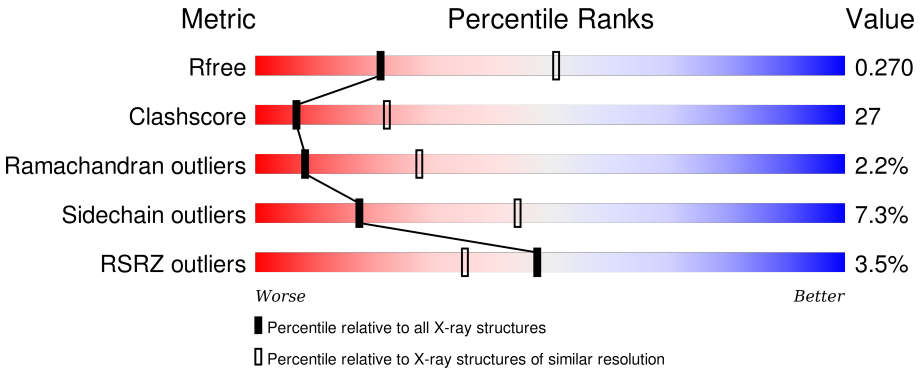
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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 <=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	% 60% 37% •
1	B	431	58% 36% 5%
1	C	431	3% 50% 46% •
1	D	431	10% 44% 50% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	440	-	-	-	X
2	SO4	A	443	-	-	-	X
2	SO4	A	449	-	-	-	X
2	SO4	A	453	-	-	-	X
2	SO4	B	440	-	-	-	X
2	SO4	C	441	-	-	-	X
2	SO4	C	444	-	-	-	X
3	BTB	A	456	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13713 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.

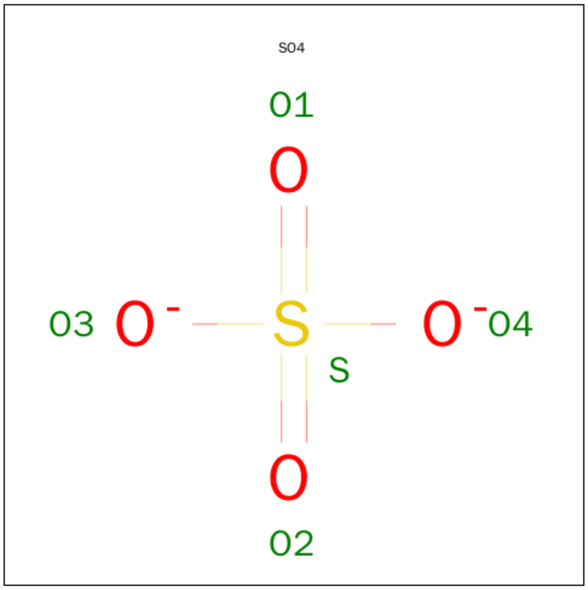
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3323	2126	595	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3323	2126	595	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3323	2126	595	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3323	2126	595	594	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	VAL	HIS	ENGINEERED	UNP Q5SLP1
B	400	VAL	HIS	ENGINEERED	UNP Q5SLP1
C	400	VAL	HIS	ENGINEERED	UNP Q5SLP1
D	400	VAL	HIS	ENGINEERED	UNP Q5SLP1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	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	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	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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	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	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	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	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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

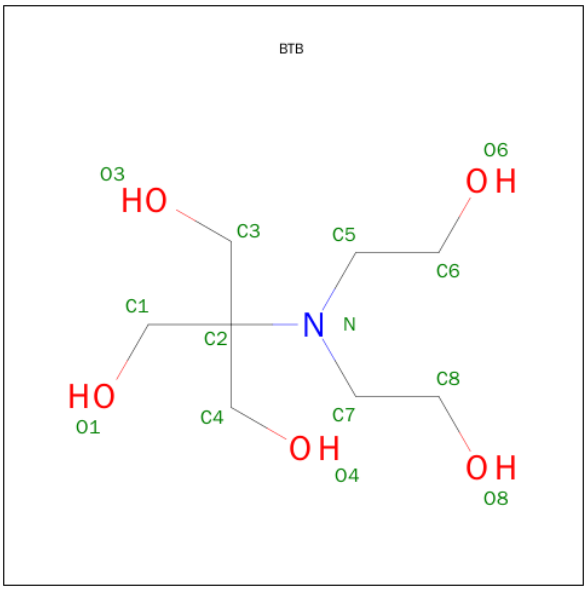
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is water.

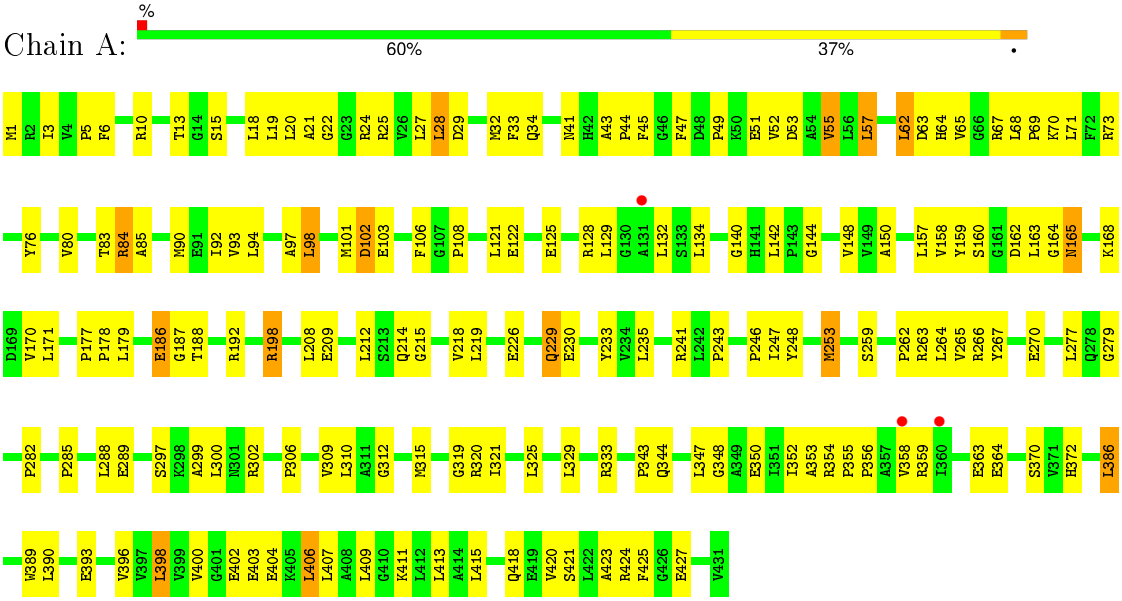
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	B	14	Total O 14 14	0	0
5	C	18	Total O 18 18	0	0
5	D	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

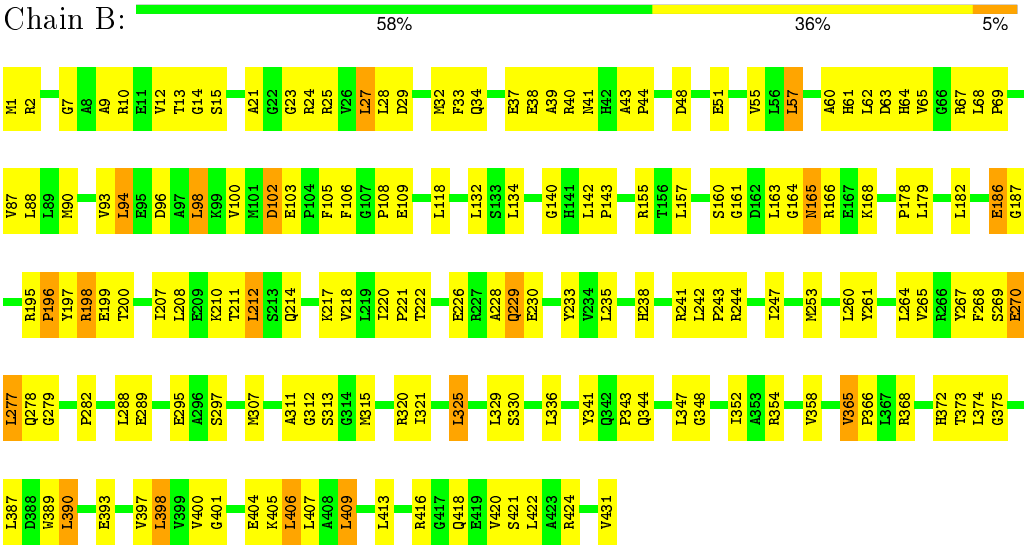
- Molecule 1: Ribonuclease TTHA0252

Chain A:



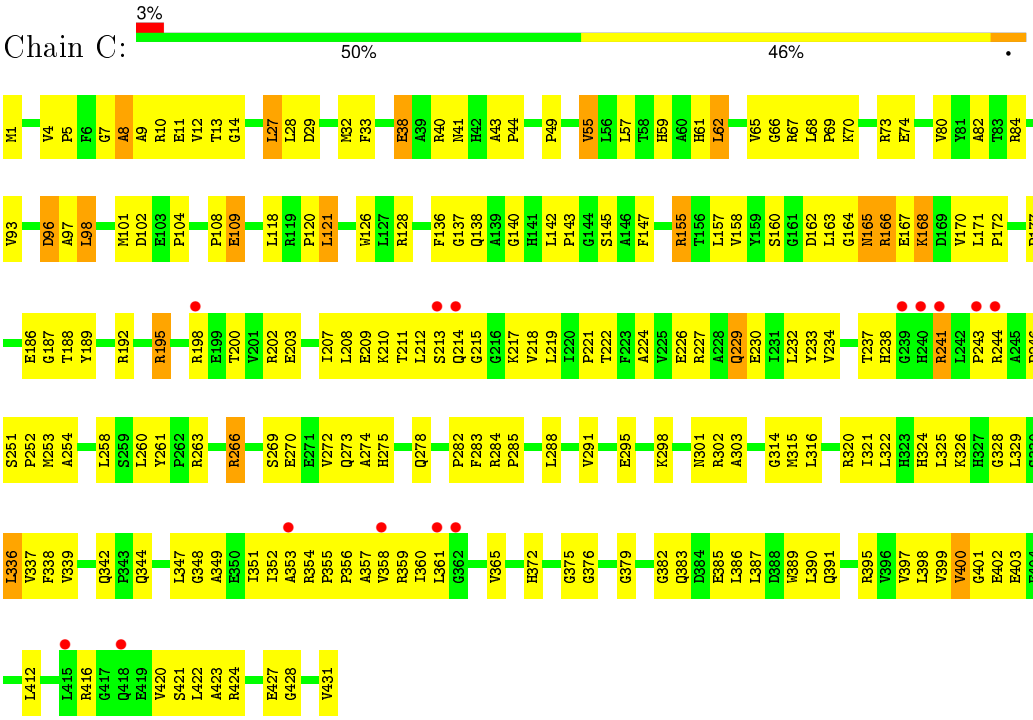
- Molecule 1: Ribonuclease TTHA0252

Chain B:



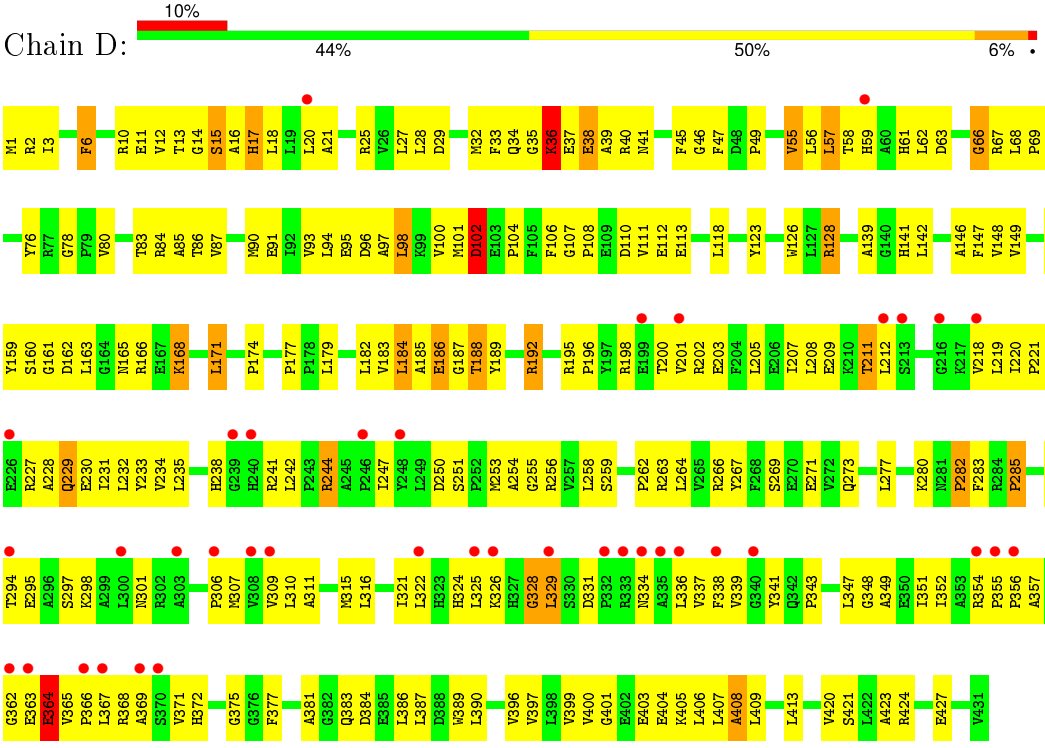
- Molecule 1: Ribonuclease TTHA0252

Chain C:



• Molecule 1: Ribonuclease TTHA0252

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.44Å 149.74Å 122.12Å 90.00° 110.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 41.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.80) 89.3 (41.94-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.01 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.275 0.214 , 0.270	Depositor DCC
R_{free} test set	5345 reflections (10.11%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 55276 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13713	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, SO4, BTB

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	0.42	0/3403	0.68	0/4616
1	B	0.41	0/3403	0.67	0/4616
1	C	0.34	0/3403	0.61	0/4616
1	D	0.32	0/3403	0.58	0/4616
All	All	0.37	0/13612	0.64	0/18464

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3323	0	3353	129	0
1	B	3323	0	3353	158	0
1	C	3323	0	3353	202	0
1	D	3323	0	3353	244	0
2	A	120	0	0	0	0
2	B	95	0	0	3	0
2	C	70	0	0	2	0
2	D	40	0	0	1	0
3	A	14	0	19	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	27	0	0	0	0
5	B	14	0	0	0	0
5	C	18	0	0	3	0
5	D	19	0	0	5	0
All	All	13713	0	13431	720	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 27.

All (720) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:PHE:N	1:C:41:ASN:HD21	1.60	0.99
1:C:33:PHE:H	1:C:41:ASN:ND2	1.61	0.98
1:C:298:LYS:HA	1:C:301:ASN:ND2	1.77	0.97
1:C:298:LYS:HA	1:C:301:ASN:HD22	1.28	0.96
1:D:220:ILE:HG12	1:D:337:VAL:HB	1.49	0.95
1:D:198:ARG:NH2	1:D:202:ARG:HH21	1.65	0.94
1:C:10:ARG:HH22	1:C:424:ARG:HE	0.96	0.91
1:D:211:THR:HG23	1:D:212:LEU:H	1.34	0.91
1:B:160:SER:HB2	1:B:163:LEU:HD21	1.52	0.89
1:B:208:LEU:HD23	1:B:218:VAL:HG21	1.52	0.89
1:B:33:PHE:H	1:B:41:ASN:HD21	1.23	0.87
1:C:207:ILE:O	1:C:211:THR:HG22	1.75	0.87
1:D:221:PRO:HB3	1:D:321:ILE:HG12	1.57	0.86
1:C:168:LYS:HE3	1:C:230:GLU:OE1	1.75	0.86
1:C:10:ARG:NH2	1:C:424:ARG:HE	1.74	0.85
1:C:232:LEU:HD11	1:C:249:LEU:HD22	1.56	0.85
1:B:208:LEU:O	1:B:212:LEU:HB2	1.79	0.83
1:D:228:ALA:HB3	1:D:229:GLN:NE2	1.95	0.81
1:D:13:THR:HG21	1:D:34:GLN:HB2	1.64	0.80
1:B:37:GLU:HB3	1:B:40:ARG:HG3	1.64	0.79
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.63	0.79
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.63	0.79
1:C:202:ARG:HG2	1:C:202:ARG:HH21	1.50	0.77
1:D:207:ILE:O	1:D:211:THR:HG22	1.84	0.77
1:A:320:ARG:HH11	3:A:456:BTB:H31	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD21	1:D:68:LEU:HD22	1.69	0.75
1:D:17:HIS:HD2	1:D:184:LEU:HD21	1.52	0.75
1:D:359:ARG:NH1	1:D:362:GLY:HA2	2.00	0.75
1:D:227:ARG:HG2	1:D:227:ARG:HH21	1.51	0.74
1:D:20:LEU:CD2	1:D:25:ARG:HG2	2.17	0.74
1:A:160:SER:HB2	1:A:163:LEU:HD21	1.69	0.74
1:A:1:MET:HG3	1:A:21:ALA:HB2	1.70	0.73
1:B:192:ARG:HH11	1:B:192:ARG:HG3	1.54	0.73
1:D:195:ARG:NH2	1:D:375:GLY:H	1.87	0.73
1:C:101:MET:SD	1:C:104:PRO:HA	2.29	0.73
1:D:331:ASP:HB3	1:D:334:ASN:ND2	2.02	0.73
1:B:33:PHE:H	1:B:41:ASN:ND2	1.86	0.72
1:A:33:PHE:H	1:A:41:ASN:HD21	1.37	0.72
1:B:33:PHE:N	1:B:41:ASN:HD21	1.86	0.72
1:D:315:MET:SD	1:D:343:PRO:HD3	2.29	0.72
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.24	0.72
1:D:97:ALA:O	1:D:101:MET:HB2	1.89	0.71
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.71	0.71
1:D:17:HIS:CD2	1:D:184:LEU:HD21	2.25	0.71
1:C:12:VAL:HG23	1:C:13:THR:HG23	1.72	0.71
1:D:36:LYS:H	1:D:36:LYS:HD2	1.56	0.71
1:B:179:LEU:HD13	1:C:128:ARG:HH12	1.56	0.71
1:A:309:VAL:C	1:A:310:LEU:HD12	2.11	0.71
1:D:250:ASP:HB3	1:D:311:ALA:HB2	1.72	0.70
1:C:10:ARG:HH22	1:C:424:ARG:NE	1.81	0.70
1:B:195:ARG:NH2	1:B:375:GLY:H	1.88	0.70
1:D:195:ARG:HH21	1:D:375:GLY:H	1.39	0.69
1:B:315:MET:HE2	1:B:343:PRO:HD3	1.73	0.69
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.08	0.69
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.75	0.69
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.76	0.68
1:A:98:LEU:HD11	1:A:108:PRO:HA	1.75	0.68
1:A:320:ARG:HD3	3:A:456:BTB:H81	1.75	0.68
1:A:219:LEU:HD23	1:A:325:LEU:HD12	1.74	0.68
1:C:360:ILE:HG22	1:C:361:LEU:HD12	1.76	0.68
1:B:179:LEU:HD13	1:C:128:ARG:NH1	2.09	0.68
1:C:160:SER:HB2	1:C:163:LEU:HD11	1.75	0.68
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.76	0.68
1:B:32:MET:HA	1:B:67:ARG:HG3	1.76	0.67
1:D:263:ARG:HG2	1:D:263:ARG:O	1.93	0.67
1:A:102:ASP:CG	1:A:103:GLU:H	1.98	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:GLY:O	1:C:352:ILE:HG13	1.94	0.67
1:D:244:ARG:H	1:D:244:ARG:HD2	1.59	0.66
1:C:229:GLN:NE2	1:C:229:GLN:H	1.94	0.66
1:B:98:LEU:HD11	1:B:108:PRO:HA	1.77	0.66
1:D:187:GLY:HA2	1:D:386:LEU:HD21	1.77	0.66
1:B:37:GLU:O	1:B:39:ALA:N	2.30	0.65
1:D:168:LYS:HE2	1:D:230:GLU:OE1	1.96	0.65
1:D:171:LEU:HD22	1:D:171:LEU:H	1.62	0.65
1:A:3:ILE:HD12	1:A:19:LEU:HA	1.76	0.65
1:B:315:MET:CE	1:B:343:PRO:HD3	2.26	0.65
1:C:285:PRO:HD2	1:C:288:LEU:HD22	1.79	0.65
1:D:183:VAL:HG12	1:D:183:VAL:O	1.97	0.65
1:C:355:PRO:HB2	1:C:356:PRO:HD2	1.78	0.65
1:C:59:HIS:CE1	1:C:162:ASP:HB2	2.32	0.65
1:A:128:ARG:HH12	1:D:179:LEU:HD13	1.61	0.65
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.33	0.64
1:C:230:GLU:O	1:C:234:VAL:HG23	1.97	0.64
1:A:413:LEU:HD22	1:A:418:GLN:OE1	1.97	0.64
1:A:319:GLY:HA2	3:A:456:BTB:H82	1.77	0.64
1:B:179:LEU:HB2	1:C:128:ARG:HH11	1.62	0.64
1:C:420:VAL:HG22	1:C:421:SER:N	2.13	0.64
1:D:355:PRO:O	1:D:367:LEU:HD23	1.98	0.64
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.79	0.64
1:A:424:ARG:HD3	1:A:427:GLU:OE1	1.97	0.64
1:D:37:GLU:O	1:D:39:ALA:N	2.31	0.64
1:D:33:PHE:H	1:D:41:ASN:HD21	1.45	0.64
1:D:155:ARG:HG2	1:D:155:ARG:HH11	1.63	0.64
1:C:326:LYS:HA	1:C:365:VAL:HG11	1.79	0.63
1:C:252:PRO:HD2	5:C:457:HOH:O	1.99	0.63
1:C:219:LEU:HD12	1:C:219:LEU:N	2.14	0.63
1:C:10:ARG:CZ	1:C:424:ARG:HG2	2.29	0.63
1:A:32:MET:HA	1:A:67:ARG:HG3	1.81	0.63
1:C:10:ARG:NH1	1:C:424:ARG:HG2	2.13	0.63
1:D:37:GLU:HB3	1:D:40:ARG:HG3	1.81	0.63
1:C:195:ARG:NH2	1:C:375:GLY:H	1.97	0.63
1:D:3:ILE:HD12	1:D:18:LEU:O	1.99	0.62
1:C:163:LEU:HD12	1:C:163:LEU:N	2.15	0.62
1:D:12:VAL:HG23	1:D:13:THR:N	2.15	0.62
1:B:168:LYS:HE2	1:B:230:GLU:OE1	1.99	0.62
1:D:186:GLU:HA	1:D:399:VAL:O	1.99	0.62
1:C:140:GLY:O	1:C:164:GLY:HA3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASP:O	1:D:104:PRO:HD3	1.99	0.62
1:D:17:HIS:N	1:D:17:HIS:ND1	2.46	0.62
1:B:189:TYR:OH	1:B:341:TYR:HB2	1.99	0.62
1:C:260:LEU:HD12	1:C:263:ARG:HD3	1.80	0.62
1:D:231:ILE:HG21	1:D:310:LEU:HD21	1.80	0.62
1:A:97:ALA:O	1:A:101:MET:HB2	2.00	0.62
1:B:404:GLU:H	1:B:404:GLU:CD	2.02	0.61
1:B:195:ARG:HH11	1:B:195:ARG:HG3	1.64	0.61
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.82	0.61
1:C:316:LEU:HD11	1:C:338:PHE:HE1	1.65	0.61
1:B:295:GLU:OE2	1:B:295:GLU:N	2.23	0.61
1:D:359:ARG:CA	1:D:364:GLU:HG3	2.29	0.61
1:C:90:MET:HE1	1:C:118:LEU:HD21	1.82	0.61
1:C:214:GLN:NE2	1:C:333:ARG:HA	2.15	0.61
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.80	0.61
1:D:250:ASP:HA	1:D:291:VAL:HB	1.82	0.61
1:C:359:ARG:HH11	1:C:359:ARG:HG2	1.65	0.61
1:C:202:ARG:HG2	1:C:202:ARG:NH2	2.12	0.60
1:B:68:LEU:N	1:B:69:PRO:HD2	2.16	0.60
1:B:200:THR:HG23	1:B:374:LEU:HB3	1.82	0.60
1:D:357:ALA:HB1	1:D:365:VAL:O	2.00	0.60
1:B:192:ARG:HH11	1:B:192:ARG:CG	2.14	0.60
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.37	0.60
1:C:269:SER:O	1:C:273:GLN:HG3	2.00	0.60
1:D:211:THR:HG21	1:D:218:VAL:HG22	1.83	0.60
1:A:68:LEU:N	1:A:69:PRO:HD2	2.17	0.60
1:D:208:LEU:HD23	1:D:218:VAL:HG11	1.84	0.60
1:D:36:LYS:HD2	1:D:36:LYS:N	2.15	0.60
1:B:28:LEU:O	1:B:29:ASP:HB2	2.01	0.60
1:D:139:ALA:O	1:D:174:PRO:HG3	2.02	0.60
1:C:360:ILE:HD12	1:C:365:VAL:HG21	1.84	0.59
1:C:322:LEU:HB3	1:C:361:LEU:HD11	1.84	0.59
1:D:163:LEU:HD11	1:D:389:TRP:CE2	2.37	0.59
1:C:155:ARG:HD3	1:C:431:VAL:O	2.02	0.59
1:D:309:VAL:O	1:D:310:LEU:HD12	2.02	0.59
1:D:198:ARG:HH22	1:D:202:ARG:HH21	1.47	0.59
1:C:32:MET:HA	1:C:67:ARG:HG3	1.84	0.59
1:B:192:ARG:HG2	2:B:441:SO4:S	2.41	0.59
1:C:316:LEU:HD11	1:C:338:PHE:CE1	2.37	0.59
1:C:62:LEU:HD13	1:C:93:VAL:CG1	2.32	0.59
1:C:157:LEU:HD12	1:C:182:LEU:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TYR:HE1	1:D:146:ALA:HB2	1.67	0.59
1:D:219:LEU:HD23	1:D:325:LEU:HD12	1.84	0.59
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.85	0.59
1:B:88:LEU:HD13	1:B:260:LEU:HD11	1.85	0.59
1:A:198:ARG:NH2	1:A:198:ARG:HG2	2.16	0.59
1:D:309:VAL:C	1:D:310:LEU:HD12	2.22	0.58
1:C:11:GLU:OE1	1:C:33:PHE:HE1	1.87	0.58
1:D:285:PRO:HD2	1:D:288:LEU:HD22	1.84	0.58
1:C:97:ALA:O	1:C:101:MET:HB2	2.04	0.58
1:D:91:GLU:O	1:D:95:GLU:HG2	2.03	0.58
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.84	0.58
1:A:157:LEU:HG	1:A:158:VAL:N	2.17	0.58
1:A:310:LEU:N	1:A:310:LEU:HD12	2.19	0.58
1:D:61:HIS:HB3	1:D:63:ASP:OD1	2.03	0.58
1:C:251:SER:HB3	1:C:254:ALA:HB3	1.84	0.58
1:D:45:PHE:HB3	1:D:47:PHE:CE1	2.38	0.58
1:C:195:ARG:CZ	1:C:375:GLY:H	2.16	0.58
1:B:398:LEU:HB3	1:B:406:LEU:HG	1.85	0.58
1:B:23:GLY:O	1:B:24:ARG:HD3	2.04	0.58
1:B:188:THR:HG22	1:B:189:TYR:CD1	2.38	0.58
1:D:171:LEU:N	1:D:171:LEU:HD22	2.19	0.58
1:C:7:GLY:HA3	1:C:14:GLY:O	2.03	0.58
1:B:57:LEU:HG	1:B:65:VAL:HG22	1.85	0.58
1:B:182:LEU:HD11	1:B:397:VAL:CG2	2.31	0.58
1:D:363:GLU:O	1:D:365:VAL:HG13	2.04	0.58
1:B:210:LYS:O	1:B:214:GLN:HG2	2.04	0.58
1:B:221:PRO:HA	1:B:311:ALA:O	2.03	0.57
1:D:195:ARG:NH2	1:D:375:GLY:N	2.51	0.57
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.39	0.57
1:A:128:ARG:NH1	1:D:179:LEU:HB2	2.19	0.57
1:D:396:VAL:HG12	1:D:397:VAL:N	2.19	0.57
1:D:33:PHE:HB3	1:D:37:GLU:HB2	1.86	0.57
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.38	0.57
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.69	0.57
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.39	0.57
1:D:49:PRO:HB3	1:D:71:LEU:HD12	1.87	0.57
1:B:315:MET:HE2	1:B:341:TYR:O	2.05	0.57
1:C:171:LEU:HD21	1:C:226:GLU:OE1	2.04	0.57
1:A:262:PRO:O	1:A:265:VAL:HG23	2.04	0.57
1:D:258:LEU:HD11	1:D:283:PHE:HB3	1.87	0.57
1:B:191:ASP:OD1	1:B:405:LYS:HE2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLY:HA2	1:C:379:GLY:O	2.04	0.57
1:A:55:VAL:HG13	1:A:80:VAL:HG22	1.85	0.57
1:C:211:THR:HG21	1:C:218:VAL:HG22	1.87	0.57
1:D:16:ALA:C	1:D:17:HIS:ND1	2.57	0.57
1:C:229:GLN:CD	1:C:229:GLN:H	2.06	0.57
1:A:122:GLU:O	1:A:125:GLU:HB2	2.04	0.56
1:D:266:ARG:HG3	1:D:267:TYR:N	2.20	0.56
1:B:409:LEU:HD22	1:B:413:LEU:HG	1.87	0.56
1:D:16:ALA:HA	1:D:29:ASP:O	2.04	0.56
1:C:90:MET:HE1	1:C:118:LEU:CD2	2.35	0.56
1:A:266:ARG:HG3	1:A:267:TYR:N	2.21	0.56
1:B:61:HIS:HB3	1:B:63:ASP:OD1	2.06	0.56
1:A:263:ARG:HG2	1:D:277:LEU:HD21	1.88	0.56
1:D:329:LEU:HD13	1:D:369:ALA:HB3	1.88	0.56
1:A:170:VAL:HG21	1:A:230:GLU:HG3	1.88	0.56
1:D:6:PHE:HB2	1:D:16:ALA:O	2.06	0.56
1:D:359:ARG:HA	1:D:364:GLU:HA	1.87	0.56
1:D:20:LEU:HD23	1:D:25:ARG:HG2	1.87	0.56
1:C:230:GLU:O	1:C:233:TYR:HB3	2.05	0.56
1:D:28:LEU:O	1:D:29:ASP:HB2	2.05	0.56
1:D:55:VAL:HG22	1:D:80:VAL:HG13	1.87	0.56
1:B:48:ASP:OD2	1:B:51:GLU:HG2	2.05	0.56
1:B:100:VAL:HG12	1:B:100:VAL:O	2.05	0.56
1:C:422:LEU:N	1:C:422:LEU:HD12	2.21	0.56
1:B:297:SER:OG	1:B:320:ARG:HG2	2.06	0.56
1:D:192:ARG:NH1	5:D:456:HOH:O	2.38	0.56
1:C:171:LEU:N	1:C:171:LEU:HD22	2.21	0.55
1:D:383:GLN:O	1:D:387:LEU:HG	2.05	0.55
1:D:183:VAL:O	1:D:185:ALA:N	2.39	0.55
1:C:314:GLY:O	1:C:342:GLN:NE2	2.40	0.55
1:B:33:PHE:HB2	1:B:41:ASN:ND2	2.22	0.55
1:C:168:LYS:HE3	1:C:230:GLU:CD	2.27	0.55
1:D:229:GLN:H	1:D:229:GLN:NE2	2.04	0.55
1:D:12:VAL:HG23	1:D:13:THR:H	1.71	0.55
1:B:98:LEU:HD11	1:B:108:PRO:CA	2.36	0.55
1:B:161:GLY:O	1:B:186:GLU:HG2	2.06	0.55
1:D:69:PRO:HB3	1:D:111:VAL:HA	1.88	0.55
1:A:348:GLY:O	1:A:352:ILE:HG13	2.05	0.55
1:A:198:ARG:HH21	1:A:198:ARG:HG2	1.70	0.55
1:D:87:VAL:HA	1:D:90:MET:CE	2.37	0.55
1:A:404:GLU:CD	1:A:404:GLU:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:SER:HB2	1:D:163:LEU:HD21	1.88	0.55
1:D:359:ARG:HA	1:D:364:GLU:HG3	1.88	0.55
1:B:13:THR:HG21	1:B:34:GLN:HB2	1.88	0.55
1:B:229:GLN:H	1:B:229:GLN:CD	2.08	0.55
1:D:155:ARG:HG2	1:D:155:ARG:NH1	2.22	0.55
1:C:214:GLN:HE21	1:C:333:ARG:HA	1.72	0.55
1:D:107:GLY:O	1:D:111:VAL:HG23	2.08	0.54
1:D:20:LEU:HD22	1:D:25:ARG:HG2	1.90	0.54
1:B:10:ARG:HH12	1:B:424:ARG:NH2	2.04	0.54
1:D:208:LEU:CD2	1:D:218:VAL:HG11	2.38	0.54
1:D:326:LYS:HE3	1:D:363:GLU:HG2	1.90	0.54
1:C:420:VAL:HG22	1:C:421:SER:H	1.72	0.54
1:B:265:VAL:HG23	1:B:276:PHE:CD2	2.42	0.54
1:B:55:VAL:CG1	1:B:80:VAL:HG22	2.38	0.54
1:B:393:GLU:O	1:B:418:GLN:HG2	2.07	0.54
1:C:98:LEU:HD11	1:C:108:PRO:HA	1.90	0.54
1:A:420:VAL:HG22	1:A:421:SER:N	2.22	0.54
1:D:205:LEU:HD11	1:D:238:HIS:CG	2.43	0.54
1:A:288:LEU:HD12	1:A:289:GLU:H	1.73	0.54
1:B:160:SER:HB2	1:B:163:LEU:CD2	2.33	0.54
1:C:211:THR:HG23	1:C:212:LEU:H	1.72	0.54
1:B:195:ARG:HG3	1:B:195:ARG:NH1	2.22	0.54
1:D:354:ARG:HD2	1:D:367:LEU:HD21	1.90	0.54
1:D:141:HIS:O	1:D:142:LEU:HD23	2.07	0.54
1:B:348:GLY:O	1:B:352:ILE:HG13	2.08	0.54
1:D:83:THR:O	1:D:87:VAL:HG23	2.08	0.53
1:D:211:THR:HG23	1:D:212:LEU:N	2.14	0.53
1:B:208:LEU:HD21	1:B:218:VAL:HG11	1.89	0.53
1:C:211:THR:HG23	1:C:212:LEU:N	2.24	0.53
1:C:406:LEU:HB3	1:C:422:LEU:HD21	1.91	0.53
1:D:225:VAL:HB	5:D:448:HOH:O	2.08	0.53
1:B:277:LEU:C	1:B:279:GLY:H	2.12	0.53
1:C:182:LEU:HB2	1:C:395:ARG:NH1	2.24	0.53
1:A:229:GLN:H	1:A:229:GLN:CD	2.12	0.53
1:C:247:ILE:O	1:C:288:LEU:HA	2.08	0.53
1:B:207:ILE:HD13	1:B:372:HIS:CG	2.44	0.53
1:A:57:LEU:HG	1:A:65:VAL:HG22	1.91	0.53
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.39	0.53
1:A:297:SER:OG	1:A:320:ARG:HG2	2.08	0.53
1:A:24:ARG:HA	1:A:53:ASP:OD2	2.07	0.53
1:C:27:LEU:HD22	1:C:29:ASP:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:VAL:HA	1:D:90:MET:HE2	1.91	0.53
1:B:165:ASN:C	1:B:165:ASN:HD22	2.12	0.53
1:B:347:LEU:CD1	1:B:358:VAL:HG11	2.39	0.53
1:C:84:ARG:HD3	2:C:435:SO4:O2	2.09	0.52
1:B:155:ARG:HD3	1:B:431:VAL:O	2.09	0.52
1:A:142:LEU:CD2	1:A:226:GLU:HB2	2.40	0.52
1:C:382:GLY:O	1:C:386:LEU:HD13	2.09	0.52
1:B:330:SER:O	1:B:368:ARG:HD2	2.10	0.52
1:D:381:ALA:HB3	1:D:386:LEU:CD1	2.40	0.52
1:C:210:LYS:O	1:C:214:GLN:HG2	2.09	0.52
1:D:55:VAL:C	1:D:56:LEU:HD12	2.29	0.52
1:A:178:PRO:HB3	1:D:126:TRP:CE3	2.44	0.52
1:D:405:LYS:O	1:D:408:ALA:HB3	2.10	0.52
1:C:208:LEU:CD2	1:C:218:VAL:HG11	2.38	0.52
1:B:80:VAL:HB	1:B:118:LEU:HD23	1.91	0.52
1:C:28:LEU:O	1:C:29:ASP:HB2	2.10	0.52
1:B:238:HIS:ND1	1:B:241:ARG:NH1	2.51	0.52
1:D:266:ARG:HD2	1:D:267:TYR:CE2	2.45	0.52
1:C:138:GLN:NE2	1:C:172:PRO:HG2	2.25	0.52
1:C:241:ARG:HH11	1:C:241:ARG:HG2	1.74	0.52
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.44	0.52
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.92	0.52
1:B:420:VAL:HG22	1:B:421:SER:N	2.25	0.52
1:D:205:LEU:HD13	1:D:241:ARG:HH21	1.75	0.52
1:B:217:LYS:HG2	1:B:307:MET:HG2	1.91	0.52
1:B:179:LEU:HB2	1:C:128:ARG:NH1	2.25	0.52
1:A:355:PRO:HB2	1:A:356:PRO:HD2	1.91	0.52
1:D:221:PRO:HA	1:D:311:ALA:O	2.09	0.51
1:C:70:LYS:O	1:C:73:ARG:HB3	2.10	0.51
1:A:359:ARG:HD3	1:A:364:GLU:OE1	2.10	0.51
1:A:398:LEU:HB3	1:A:406:LEU:HG	1.92	0.51
1:C:203:GLU:O	1:C:207:ILE:HG13	2.10	0.51
1:D:221:PRO:HB3	1:D:321:ILE:CG1	2.35	0.51
1:B:61:HIS:CD2	1:B:142:LEU:HD11	2.45	0.51
1:D:32:MET:HG2	1:D:66:GLY:HA3	1.91	0.51
1:D:294:THR:O	1:D:297:SER:HB3	2.10	0.51
1:D:227:ARG:NH2	1:D:227:ARG:HG2	2.25	0.51
1:C:59:HIS:HE1	1:C:162:ASP:HB2	1.75	0.51
1:B:109:GLU:H	1:B:109:GLU:CD	2.14	0.51
1:C:195:ARG:HB2	5:C:453:HOH:O	2.09	0.51
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.46	0.51
1:A:259:SER:O	1:A:262:PRO:HD2	2.11	0.51
1:B:33:PHE:HB3	1:B:37:GLU:HB2	1.92	0.51
1:D:298:LYS:HE2	5:D:451:HOH:O	2.10	0.51
1:D:182:LEU:HD12	1:D:183:VAL:H	1.75	0.51
1:D:269:SER:HB2	2:D:435:SO4:O1	2.10	0.51
1:D:12:VAL:HG23	1:D:13:THR:HG23	1.92	0.51
1:C:27:LEU:HB3	1:C:55:VAL:HB	1.93	0.51
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.93	0.51
1:A:270:GLU:CD	1:D:266:ARG:HH12	2.13	0.51
1:D:57:LEU:HD21	1:D:68:LEU:CD2	2.39	0.51
1:D:354:ARG:HA	1:D:367:LEU:HD21	1.92	0.51
1:C:217:LYS:HE2	1:C:303:ALA:O	2.11	0.51
1:D:159:TYR:CD2	1:D:160:SER:N	2.79	0.51
1:C:170:VAL:HA	1:C:272:VAL:HG21	1.93	0.51
1:C:315:MET:HA	1:C:342:GLN:HE22	1.76	0.50
1:A:229:GLN:NE2	1:A:229:GLN:H	2.09	0.50
1:C:321:ILE:HG23	1:C:322:LEU:N	2.26	0.50
1:D:232:LEU:HD13	1:D:288:LEU:HD21	1.92	0.50
1:C:387:LEU:HB3	1:C:416:ARG:NH1	2.26	0.50
1:B:274:ALA:O	1:B:278:GLN:HG2	2.12	0.50
1:B:33:PHE:HB2	1:B:41:ASN:HD21	1.77	0.50
1:D:363:GLU:HG3	1:D:363:GLU:O	2.10	0.50
1:B:57:LEU:HD22	1:B:80:VAL:HG12	1.93	0.50
1:B:86:THR:HG22	1:B:90:MET:HE2	1.93	0.50
1:C:59:HIS:CD2	1:C:61:HIS:HB2	2.47	0.50
1:A:288:LEU:HD12	1:A:289:GLU:N	2.27	0.50
1:C:344:GLN:HG3	1:C:349:ALA:CB	2.41	0.50
1:B:7:GLY:HA3	1:B:14:GLY:O	2.11	0.50
1:D:1:MET:HA	1:D:21:ALA:HB2	1.94	0.50
1:C:80:VAL:HB	1:C:118:LEU:HD23	1.94	0.50
1:B:9:ALA:O	1:B:10:ARG:HB2	2.10	0.50
1:B:192:ARG:H	1:B:192:ARG:HD2	1.77	0.50
1:D:399:VAL:HG12	1:D:423:ALA:HB3	1.94	0.50
1:A:98:LEU:HG	1:A:106:PHE:HE2	1.76	0.49
1:D:3:ILE:HD12	1:D:18:LEU:C	2.31	0.49
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.42	0.49
1:D:187:GLY:HA2	1:D:386:LEU:CD2	2.42	0.49
1:C:98:LEU:HD11	1:C:108:PRO:HB3	1.95	0.49
1:A:140:GLY:O	1:A:164:GLY:HA3	2.10	0.49
1:C:246:PRO:HB2	1:C:248:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:SER:O	1:D:262:PRO:HD2	2.12	0.49
1:A:55:VAL:CG1	1:A:80:VAL:HG22	2.42	0.49
1:C:229:GLN:HG3	1:C:261:TYR:CZ	2.46	0.49
1:A:6:PHE:HA	1:A:425:PHE:CE1	2.47	0.49
1:D:203:GLU:O	1:D:207:ILE:HG13	2.13	0.49
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.48	0.49
1:D:17:HIS:HD2	1:D:184:LEU:CD2	2.23	0.49
1:D:227:ARG:CG	1:D:227:ARG:HH21	2.24	0.49
1:B:10:ARG:HH12	1:B:424:ARG:HH21	1.59	0.49
1:B:387:LEU:HB3	1:B:416:ARG:NH1	2.27	0.49
1:A:212:LEU:HB2	1:A:243:PRO:CG	2.42	0.49
1:A:1:MET:HG3	1:A:21:ALA:CB	2.41	0.49
1:C:170:VAL:HB	1:C:171:LEU:HD22	1.95	0.49
1:D:200:THR:HG22	1:D:377:PHE:CE1	2.48	0.49
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.48	0.49
1:D:321:ILE:HG23	1:D:322:LEU:N	2.27	0.49
1:D:189:TYR:OH	1:D:341:TYR:HB2	2.12	0.49
1:C:198:ARG:HG2	1:C:198:ARG:HH21	1.77	0.49
1:C:221:PRO:HD2	1:C:337:VAL:O	2.13	0.49
1:A:170:VAL:CG2	1:A:230:GLU:HG3	2.43	0.49
1:C:209:GLU:OE2	1:C:243:PRO:HD3	2.13	0.49
1:D:220:ILE:HB	1:D:310:LEU:HG	1.93	0.49
1:B:86:THR:HG22	1:B:90:MET:CE	2.43	0.49
1:D:396:VAL:CG1	1:D:397:VAL:N	2.76	0.49
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.93	0.49
1:A:63:ASP:OD1	1:A:64:HIS:HD2	1.96	0.49
1:D:182:LEU:HD12	1:D:183:VAL:N	2.28	0.48
1:C:325:LEU:O	1:C:329:LEU:HB2	2.13	0.48
1:D:349:ALA:HA	1:D:352:ILE:HD12	1.95	0.48
1:B:198:ARG:HH21	1:B:198:ARG:HG2	1.78	0.48
1:D:195:ARG:HH21	1:D:375:GLY:N	2.08	0.48
1:B:178:PRO:HD3	1:C:126:TRP:CD1	2.48	0.48
1:B:196:PRO:O	1:B:199:GLU:HG2	2.14	0.48
1:C:274:ALA:O	1:C:278:GLN:HG2	2.13	0.48
1:C:163:LEU:H	1:C:163:LEU:HD12	1.78	0.48
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.78	0.48
1:C:398:LEU:N	1:C:398:LEU:HD22	2.29	0.48
1:D:160:SER:HB2	1:D:163:LEU:CD2	2.42	0.48
1:D:348:GLY:O	1:D:352:ILE:HG13	2.13	0.48
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.78	0.48
1:B:163:LEU:HD11	1:B:389:TRP:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:PHE:CD2	1:D:111:VAL:HG22	2.49	0.48
1:A:63:ASP:CG	1:A:64:HIS:CD2	2.87	0.48
1:D:128:ARG:HD2	5:D:442:HOH:O	2.13	0.48
1:C:298:LYS:CA	1:C:301:ASN:HD22	2.13	0.48
1:A:177:PRO:HB3	1:A:389:TRP:CZ2	2.49	0.48
1:A:396:VAL:O	1:A:420:VAL:HA	2.13	0.48
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.95	0.48
1:A:215:GLY:HA2	1:A:306:PRO:HB3	1.96	0.48
1:C:207:ILE:HD13	1:C:372:HIS:CD2	2.49	0.48
1:A:350:GLU:O	1:A:353:ALA:HB3	2.14	0.48
1:B:344:GLN:OE1	1:B:344:GLN:HA	2.14	0.48
1:A:98:LEU:HD11	1:A:108:PRO:CA	2.42	0.48
1:B:269:SER:O	1:B:273:GLN:HG3	2.14	0.48
1:C:10:ARG:HH12	1:C:424:ARG:NE	2.12	0.48
1:B:228:ALA:HB3	1:B:229:GLN:NE2	2.29	0.48
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.95	0.48
1:A:62:LEU:HD13	1:A:93:VAL:CG1	2.44	0.48
1:A:45:PHE:CE2	1:A:70:LYS:HG2	2.49	0.47
1:B:57:LEU:HD22	1:B:80:VAL:CG1	2.44	0.47
1:A:212:LEU:HB2	1:A:243:PRO:HG2	1.96	0.47
1:D:208:LEU:HD23	1:D:218:VAL:HG21	1.96	0.47
1:C:387:LEU:HD11	1:C:412:LEU:HD13	1.96	0.47
1:A:18:LEU:HG	1:A:20:LEU:HD21	1.96	0.47
1:A:163:LEU:N	1:A:163:LEU:HD22	2.28	0.47
1:D:86:THR:O	1:D:90:MET:HG3	2.15	0.47
1:C:258:LEU:HD11	1:C:283:PHE:HB3	1.96	0.47
1:B:62:LEU:HD13	1:B:93:VAL:HG12	1.96	0.47
1:D:90:MET:HE1	1:D:118:LEU:HD22	1.96	0.47
1:D:73:ARG:HG3	1:D:110:ASP:OD2	2.15	0.47
1:A:13:THR:HG21	1:A:34:GLN:HB2	1.96	0.47
1:C:208:LEU:HD21	1:C:218:VAL:HG11	1.97	0.47
1:C:224:ALA:HB3	1:C:253:MET:CE	2.45	0.47
1:C:166:ARG:HG2	1:C:385:GLU:OE1	2.14	0.47
1:D:359:ARG:HH12	1:D:362:GLY:HA2	1.77	0.47
1:C:219:LEU:O	1:C:336:LEU:HD23	2.13	0.47
1:C:195:ARG:CB	5:C:453:HOH:O	2.63	0.47
1:B:132:LEU:HD21	1:B:134:LEU:HD21	1.96	0.47
1:D:280:LYS:HD2	5:D:453:HOH:O	2.15	0.47
1:D:389:TRP:HE3	1:D:390:LEU:CD1	2.28	0.47
1:C:391:GLN:HA	1:C:416:ARG:NH2	2.29	0.47
1:C:250:ASP:OD1	1:C:320:ARG:NH1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LEU:HD11	1:D:338:PHE:HE1	1.80	0.47
1:D:98:LEU:O	1:D:101:MET:HB3	2.15	0.47
1:B:384:ASP:OD2	1:B:384:ASP:N	2.47	0.47
1:D:6:PHE:CZ	1:D:47:PHE:HB3	2.50	0.46
1:D:336:LEU:C	1:D:336:LEU:HD23	2.36	0.46
1:A:33:PHE:H	1:A:41:ASN:ND2	2.10	0.46
1:C:389:TRP:HE3	1:C:390:LEU:CD1	2.28	0.46
1:A:320:ARG:CD	3:A:456:BTB:H81	2.44	0.46
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.97	0.46
1:C:406:LEU:HB3	1:C:422:LEU:CD2	2.45	0.46
1:D:73:ARG:CG	1:D:73:ARG:HH21	2.28	0.46
1:C:224:ALA:HB1	1:C:254:ALA:N	2.30	0.46
1:C:347:LEU:O	1:C:351:ILE:HG13	2.15	0.46
1:B:2:ARG:NH2	2:B:446:SO4:S	2.89	0.46
1:B:389:TRP:HE3	1:B:390:LEU:HD13	1.81	0.46
1:C:353:ALA:HB3	1:C:355:PRO:HD3	1.98	0.46
1:C:1:MET:HG2	1:C:431:VAL:CG2	2.44	0.46
1:A:285:PRO:HD2	1:A:288:LEU:HD22	1.98	0.46
1:B:105:PHE:CD1	1:B:106:PHE:HD1	2.33	0.46
1:C:295:GLU:OE2	1:C:295:GLU:N	2.48	0.46
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.80	0.46
1:C:10:ARG:HB3	1:C:403:GLU:HG3	1.96	0.46
1:D:35:GLY:O	1:D:36:LYS:C	2.54	0.46
1:C:219:LEU:CD1	1:C:219:LEU:N	2.78	0.46
1:D:90:MET:O	1:D:91:GLU:C	2.53	0.46
1:A:63:ASP:CG	1:A:64:HIS:HD2	2.18	0.46
1:D:409:LEU:CD2	1:D:413:LEU:HG	2.46	0.46
1:C:266:ARG:HA	1:C:273:GLN:OE1	2.16	0.46
1:D:266:ARG:HD2	1:D:267:TYR:CZ	2.51	0.46
1:C:27:LEU:O	1:C:55:VAL:HA	2.16	0.46
1:B:140:GLY:O	1:B:164:GLY:HA3	2.16	0.46
1:D:404:GLU:CD	1:D:404:GLU:H	2.18	0.46
1:A:214:GLN:NE2	1:A:333:ARG:HA	2.31	0.46
1:B:33:PHE:CG	1:B:40:ARG:HB2	2.51	0.46
1:D:13:THR:CB	1:D:34:GLN:H	2.28	0.46
1:D:14:GLY:O	1:D:15:SER:C	2.54	0.46
1:C:213:SER:C	1:C:215:GLY:H	2.19	0.46
1:D:11:GLU:C	1:D:401:GLY:H	2.20	0.46
1:B:157:LEU:HD12	1:B:182:LEU:O	2.16	0.46
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.46	0.46
1:B:270:GLU:HB2	2:B:438:SO4:O4	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LEU:HD13	1:C:136:PHE:CE2	2.51	0.46
1:C:402:GLU:O	1:C:403:GLU:C	2.54	0.45
1:B:33:PHE:HD2	1:B:41:ASN:HD22	1.64	0.45
1:D:45:PHE:CE1	1:D:67:ARG:HD2	2.51	0.45
1:B:189:TYR:HH	1:B:341:TYR:HB2	1.80	0.45
1:D:147:PHE:HB2	1:D:159:TYR:O	2.16	0.45
1:C:359:ARG:NH1	1:C:359:ARG:HG2	2.30	0.45
1:C:49:PRO:HG3	1:C:74:GLU:HB2	1.98	0.45
1:D:157:LEU:HD12	1:D:158:VAL:H	1.82	0.45
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.82	0.45
1:D:62:LEU:HD13	1:D:93:VAL:CG1	2.44	0.45
1:C:61:HIS:NE2	1:C:142:LEU:HD11	2.32	0.45
1:A:92:ILE:HG22	1:A:253:MET:CE	2.46	0.45
1:C:4:VAL:HG22	1:C:428:GLY:CA	2.46	0.45
1:A:148:VAL:HB	1:A:159:TYR:HB3	1.97	0.45
1:B:27:LEU:O	1:B:55:VAL:HA	2.16	0.45
1:A:212:LEU:CB	1:A:243:PRO:HG2	2.47	0.45
1:D:306:PRO:O	1:D:307:MET:HB3	2.16	0.45
1:D:360:ILE:O	1:D:361:LEU:HB2	2.16	0.45
1:A:165:ASN:C	1:A:165:ASN:HD22	2.18	0.45
1:D:62:LEU:O	1:D:66:GLY:N	2.47	0.45
1:D:49:PRO:HB3	1:D:71:LEU:CD1	2.46	0.45
1:B:265:VAL:HA	1:B:268:PHE:CD2	2.52	0.45
1:C:166:ARG:HH11	1:C:166:ARG:HG3	1.81	0.45
1:D:351:ILE:CG2	1:D:371:VAL:HG21	2.46	0.45
1:A:393:GLU:OE2	1:A:393:GLU:HA	2.17	0.45
1:B:102:ASP:CG	1:B:103:GLU:H	2.20	0.45
1:B:41:ASN:HD22	1:B:41:ASN:N	2.15	0.45
1:A:320:ARG:HD3	3:A:456:BTB:C8	2.46	0.45
1:D:35:GLY:O	1:D:38:GLU:HB2	2.16	0.45
1:C:57:LEU:HD23	1:C:90:MET:SD	2.57	0.45
1:B:398:LEU:HD22	1:B:420:VAL:CG2	2.46	0.45
1:D:205:LEU:CD1	1:D:241:ARG:HH21	2.29	0.45
1:D:331:ASP:HB3	1:D:334:ASN:HD22	1.78	0.45
1:C:358:VAL:HG12	1:C:359:ARG:N	2.32	0.45
1:D:241:ARG:O	1:D:242:LEU:HD23	2.17	0.45
1:D:347:LEU:O	1:D:351:ILE:HG13	2.17	0.45
1:C:405:LYS:O	1:C:408:ALA:HB3	2.17	0.45
1:C:158:VAL:HG23	1:C:180:ALA:HB2	1.98	0.45
1:A:246:PRO:HG2	1:A:248:TYR:HE1	1.80	0.45
1:A:299:ALA:HA	1:A:302:ARG:HH11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ASN:C	1:C:165:ASN:HD22	2.20	0.45
1:D:201:VAL:HG13	1:D:234:VAL:HG11	1.99	0.45
1:C:200:THR:HG21	1:C:376:GLY:HA3	1.99	0.45
1:D:15:SER:HA	1:D:17:HIS:HE1	1.82	0.44
1:D:363:GLU:O	1:D:364:GLU:C	2.54	0.44
1:A:420:VAL:CG2	1:A:421:SER:N	2.80	0.44
1:C:241:ARG:NH1	1:C:241:ARG:HG2	2.32	0.44
1:A:49:PRO:HB3	1:A:71:LEU:HD12	1.99	0.44
1:B:382:GLY:O	1:B:386:LEU:HB2	2.16	0.44
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.98	0.44
1:B:365:VAL:HA	1:B:366:PRO:HD3	1.86	0.44
1:C:208:LEU:HA	1:C:211:THR:CG2	2.48	0.44
3:A:456:BTB:H71	3:A:456:BTB:O3	2.16	0.44
1:A:102:ASP:CG	1:A:103:GLU:N	2.68	0.44
1:D:84:ARG:HB2	1:D:267:TYR:OH	2.18	0.44
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.53	0.44
1:D:200:THR:HG22	1:D:377:PHE:HE1	1.81	0.44
1:D:420:VAL:HG22	1:D:421:SER:N	2.32	0.44
1:C:233:TYR:CD1	1:C:282:PRO:HB2	2.53	0.44
1:D:263:ARG:C	1:D:264:LEU:HD12	2.38	0.44
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.99	0.44
1:D:253:MET:C	1:D:255:GLY:N	2.71	0.44
1:A:52:VAL:HB	1:A:76:TYR:CD2	2.52	0.44
1:C:420:VAL:CG2	1:C:421:SER:N	2.80	0.44
1:B:63:ASP:OD1	1:B:64:HIS:HD2	1.99	0.44
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.81	0.44
1:D:90:MET:HE3	1:D:118:LEU:HD13	2.00	0.44
1:B:420:VAL:CG2	1:B:421:SER:N	2.81	0.44
1:B:142:LEU:O	1:B:143:PRO:C	2.55	0.44
1:C:9:ALA:O	1:C:10:ARG:HB2	2.17	0.44
1:C:32:MET:HB3	1:C:66:GLY:HA3	2.00	0.44
1:B:208:LEU:CD2	1:B:218:VAL:HG21	2.37	0.44
1:B:387:LEU:HB3	1:B:416:ARG:HH12	1.83	0.44
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.99	0.44
1:B:373:THR:O	1:B:374:LEU:HD23	2.18	0.44
1:B:25:ARG:HH11	1:B:51:GLU:HB3	1.83	0.44
1:A:312:GLY:O	1:A:321:ILE:HG22	2.18	0.44
1:D:32:MET:HA	1:D:67:ARG:HG3	1.99	0.43
1:D:62:LEU:HD21	1:D:97:ALA:HB2	2.00	0.43
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.83	0.43
1:B:155:ARG:NH1	1:B:431:VAL:OXT	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PRO:HB3	1:D:126:TRP:CD2	2.53	0.43
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.99	0.43
1:B:312:GLY:HA2	1:B:313:SER:C	2.38	0.43
1:C:401:GLY:HA3	1:C:406:LEU:CD1	2.47	0.43
1:A:248:TYR:CE2	1:A:300:LEU:HD21	2.53	0.43
1:A:28:LEU:O	1:A:29:ASP:HB2	2.18	0.43
1:B:288:LEU:HD12	1:B:289:GLU:H	1.83	0.43
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.33	0.43
1:B:229:GLN:HG3	1:B:261:TYR:CZ	2.53	0.43
1:D:316:LEU:HD11	1:D:338:PHE:CE1	2.53	0.43
1:A:179:LEU:HD12	1:A:393:GLU:OE2	2.18	0.43
1:A:162:ASP:HA	1:A:186:GLU:OE1	2.19	0.43
1:A:370:SER:OG	1:A:372:HIS:HE1	2.01	0.43
1:A:315:MET:SD	1:A:343:PRO:HD3	2.58	0.43
1:C:167:GLU:O	1:C:168:LYS:O	2.36	0.43
1:A:198:ARG:HH21	1:A:198:ARG:CG	2.31	0.43
1:A:129:LEU:O	1:A:132:LEU:HB3	2.19	0.43
1:C:284:ARG:HA	1:C:288:LEU:HD23	1.99	0.43
1:C:59:HIS:NE2	1:C:61:HIS:HB2	2.33	0.43
1:D:251:SER:HB3	1:D:254:ALA:HB3	2.01	0.43
1:A:41:ASN:O	1:A:70:LYS:HE3	2.19	0.43
1:D:232:LEU:O	1:D:285:PRO:HD3	2.19	0.43
1:A:68:LEU:N	1:A:69:PRO:CD	2.82	0.43
1:B:358:VAL:O	1:B:365:VAL:HG13	2.18	0.43
1:C:4:VAL:HA	1:C:5:PRO:HD3	1.90	0.43
1:D:229:GLN:H	1:D:229:GLN:CD	2.18	0.43
1:C:321:ILE:O	1:C:325:LEU:HD13	2.19	0.43
1:D:187:GLY:O	1:D:189:TYR:N	2.52	0.43
1:C:182:LEU:HD11	1:C:397:VAL:CG2	2.49	0.43
1:D:10:ARG:NH2	1:D:424:ARG:NH2	2.66	0.43
1:B:229:GLN:H	1:B:229:GLN:NE2	2.16	0.43
1:A:22:GLY:C	1:A:24:ARG:H	2.21	0.43
1:D:148:VAL:HG12	1:D:149:VAL:N	2.33	0.43
1:A:3:ILE:HD12	1:A:19:LEU:CA	2.44	0.43
1:C:356:PRO:HG2	1:C:357:ALA:H	1.84	0.43
1:B:84:ARG:HB2	1:B:267:TYR:OH	2.18	0.43
1:D:207:ILE:HD13	1:D:372:HIS:CG	2.54	0.43
1:A:1:MET:HE2	1:A:132:LEU:HD13	2.01	0.43
1:C:325:LEU:O	1:C:329:LEU:N	2.47	0.43
1:D:171:LEU:CD2	1:D:171:LEU:H	2.30	0.43
1:C:354:ARG:N	1:C:355:PRO:CD	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:VAL:HG13	1:B:80:VAL:HG13	2.01	0.43
1:D:10:ARG:HB3	1:D:403:GLU:HG3	2.00	0.43
1:C:383:GLN:O	1:C:387:LEU:HG	2.19	0.43
1:A:134:LEU:HD23	1:A:150:ALA:HA	2.01	0.43
1:C:275:HIS:ND1	1:C:282:PRO:HB3	2.33	0.42
1:D:85:ALA:HB2	1:D:267:TYR:CE2	2.54	0.42
1:C:401:GLY:HA3	1:C:406:LEU:HD11	2.00	0.42
1:D:211:THR:HG21	1:D:218:VAL:CG2	2.49	0.42
1:A:226:GLU:C	1:A:229:GLN:HE21	2.22	0.42
1:D:224:ALA:HB3	1:D:253:MET:CE	2.49	0.42
1:D:291:VAL:HG11	1:D:297:SER:HB2	2.01	0.42
1:D:253:MET:O	1:D:256:ARG:N	2.53	0.42
1:A:277:LEU:C	1:A:279:GLY:H	2.23	0.42
1:C:399:VAL:HG12	1:C:423:ALA:HB3	2.00	0.42
1:C:59:HIS:HB3	1:C:145:SER:HA	2.02	0.42
1:D:219:LEU:HD21	1:D:324:HIS:O	2.20	0.42
1:B:354:ARG:HG3	1:B:354:ARG:NH1	2.34	0.42
1:A:163:LEU:HD11	1:A:389:TRP:CE2	2.55	0.42
1:D:424:ARG:O	1:D:427:GLU:HB2	2.19	0.42
1:A:25:ARG:HD3	1:A:51:GLU:O	2.20	0.42
1:C:270:GLU:HG2	2:C:433:SO4:O3	2.19	0.42
1:D:12:VAL:CG2	1:D:13:THR:N	2.82	0.42
1:D:6:PHE:HE1	1:D:46:GLY:HA3	1.85	0.42
1:C:57:LEU:HG	1:C:65:VAL:HG22	2.01	0.42
1:D:403:GLU:O	1:D:407:LEU:HD23	2.20	0.42
1:A:57:LEU:HD23	1:A:90:MET:SD	2.59	0.42
1:C:1:MET:HG2	1:C:431:VAL:HG21	2.02	0.42
1:D:91:GLU:O	1:D:95:GLU:CG	2.66	0.42
1:B:86:THR:O	1:B:90:MET:HB2	2.19	0.42
1:C:320:ARG:O	1:C:324:HIS:HD2	2.02	0.42
1:D:112:GLU:HG3	1:D:113:GLU:N	2.34	0.42
1:C:331:ASP:HA	1:C:332:PRO:HD2	1.90	0.42
1:A:233:TYR:CE1	1:A:282:PRO:HB2	2.54	0.42
1:C:7:GLY:O	1:C:9:ALA:N	2.53	0.42
1:C:214:GLN:HE21	1:C:333:ARG:CA	2.31	0.42
1:C:138:GLN:NE2	1:C:172:PRO:CG	2.83	0.42
1:C:387:LEU:O	1:C:416:ARG:NH2	2.46	0.42
1:B:33:PHE:CB	1:B:41:ASN:HD21	2.33	0.42
1:B:192:ARG:NH1	1:B:192:ARG:CG	2.76	0.42
1:C:163:LEU:CD1	1:C:163:LEU:N	2.83	0.42
1:D:367:LEU:HG	1:D:367:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:N	1:D:56:LEU:HD12	2.35	0.42
1:B:7:GLY:O	1:B:9:ALA:N	2.53	0.42
1:C:137:GLY:HA3	1:C:147:PHE:CZ	2.55	0.42
1:D:76:TYR:CZ	1:D:78:GLY:HA3	2.55	0.42
1:C:187:GLY:O	1:C:189:TYR:N	2.53	0.42
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.54	0.42
1:C:422:LEU:N	1:C:422:LEU:CD1	2.82	0.42
1:B:165:ASN:C	1:B:165:ASN:ND2	2.72	0.42
1:C:109:GLU:H	1:C:109:GLU:HG3	1.59	0.42
1:D:41:ASN:O	1:D:70:LYS:HE3	2.20	0.41
1:D:68:LEU:N	1:D:69:PRO:HD2	2.35	0.41
1:D:98:LEU:HD11	1:D:108:PRO:HB3	2.02	0.41
1:B:68:LEU:N	1:B:69:PRO:CD	2.82	0.41
1:C:403:GLU:O	1:C:407:LEU:CD2	2.68	0.41
1:C:165:ASN:C	1:C:167:GLU:H	2.23	0.41
1:D:228:ALA:HB3	1:D:229:GLN:HE22	1.83	0.41
1:D:359:ARG:CB	1:D:364:GLU:HG3	2.50	0.41
1:C:284:ARG:HA	1:C:288:LEU:CD2	2.50	0.41
1:D:399:VAL:CG1	1:D:423:ALA:HB3	2.49	0.41
1:D:147:PHE:HB2	1:D:160:SER:HA	2.02	0.41
1:C:344:GLN:HA	1:C:349:ALA:HB2	2.02	0.41
1:A:73:ARG:HG3	1:A:73:ARG:O	2.20	0.41
1:A:413:LEU:CD2	1:A:418:GLN:OE1	2.67	0.41
1:A:168:LYS:HE2	1:A:230:GLU:OE1	2.20	0.41
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.56	0.41
1:C:237:THR:O	1:C:238:HIS:CG	2.73	0.41
1:D:220:ILE:HG22	1:D:222:THR:HG23	2.02	0.41
1:D:336:LEU:HD23	1:D:337:VAL:N	2.35	0.41
1:D:11:GLU:OE1	1:D:37:GLU:HG3	2.20	0.41
1:A:85:ALA:HB3	1:A:144:GLY:HA3	2.02	0.41
1:B:87:VAL:HG13	1:B:118:LEU:CD1	2.51	0.41
1:C:250:ASP:HA	1:C:291:VAL:HB	2.03	0.41
1:A:411:LYS:O	1:A:415:LEU:HG	2.20	0.41
1:C:68:LEU:N	1:C:69:PRO:HD2	2.35	0.41
1:D:177:PRO:HB3	1:D:389:TRP:CZ2	2.55	0.41
1:D:351:ILE:HG22	1:D:371:VAL:HG21	2.01	0.41
1:B:233:TYR:CE1	1:B:282:PRO:HB2	2.55	0.41
1:A:310:LEU:CD1	1:A:310:LEU:N	2.84	0.41
1:D:355:PRO:HB2	1:D:356:PRO:HD2	2.03	0.41
1:A:424:ARG:HD3	1:A:427:GLU:CD	2.41	0.41
1:D:141:HIS:CD2	1:D:162:ASP:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:CA	1:A:229:GLN:HE21	2.34	0.41
1:D:269:SER:O	1:D:273:GLN:HG3	2.21	0.41
1:D:187:GLY:O	1:D:188:THR:C	2.59	0.41
1:D:325:LEU:HB3	1:D:329:LEU:HD23	2.01	0.41
1:B:65:VAL:HG11	1:B:90:MET:CG	2.50	0.41
1:B:90:MET:O	1:B:94:LEU:HB2	2.21	0.41
1:C:96:ASP:C	1:C:98:LEU:N	2.74	0.41
1:D:58:THR:HG21	1:D:161:GLY:HA3	2.02	0.41
1:D:36:LYS:HB3	1:D:36:LYS:HE3	1.95	0.41
1:A:128:ARG:NH1	1:D:179:LEU:HD13	2.32	0.41
1:A:235:LEU:HD13	1:A:247:ILE:CD1	2.51	0.41
1:B:421:SER:C	1:B:422:LEU:HD12	2.41	0.41
1:B:63:ASP:CG	1:B:64:HIS:HD2	2.24	0.41
1:D:384:ASP:N	1:D:384:ASP:OD2	2.54	0.41
1:B:187:GLY:O	1:B:188:THR:C	2.60	0.41
1:B:277:LEU:C	1:B:279:GLY:N	2.74	0.41
1:A:402:GLU:O	1:A:403:GLU:C	2.60	0.41
1:B:33:PHE:HD2	1:B:41:ASN:ND2	2.18	0.40
1:C:67:ARG:O	1:C:70:LYS:HB3	2.20	0.40
1:B:265:VAL:HA	1:B:268:PHE:HD2	1.84	0.40
1:A:83:THR:HA	1:A:121:LEU:O	2.21	0.40
1:A:84:ARG:HB2	1:A:84:ARG:HE	1.63	0.40
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.78	0.40
1:D:106:PHE:CE2	1:D:111:VAL:HG22	2.56	0.40
1:A:187:GLY:O	1:A:188:THR:C	2.59	0.40
1:D:366:PRO:HG2	1:D:368:ARG:HH12	1.85	0.40
1:A:1:MET:CE	1:A:132:LEU:HD13	2.51	0.40
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.91	0.40
1:B:98:LEU:HA	1:B:98:LEU:HD23	1.91	0.40
1:C:182:LEU:HB3	1:C:431:VAL:HG13	2.03	0.40
1:D:326:LYS:C	1:D:328:GLY:H	2.24	0.40
1:B:142:LEU:HD22	1:B:226:GLU:HB2	2.03	0.40
1:C:8:ALA:HB1	1:C:400:VAL:H	1.86	0.40
1:C:227:ARG:O	1:C:230:GLU:HB3	2.21	0.40
1:C:386:LEU:HD12	1:C:386:LEU:N	2.36	0.40
1:D:233:TYR:OH	1:D:271:GLU:HG2	2.22	0.40
1:B:242:LEU:HD22	1:B:243:PRO:HD2	2.04	0.40
1:B:400:VAL:O	1:B:400:VAL:HG12	2.21	0.40
1:C:82:ALA:O	1:C:120:PRO:HA	2.22	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%)	394 (92%)	32 (8%)	3 (1%)	26 62
1	B	429/431 (100%)	398 (93%)	26 (6%)	5 (1%)	16 47
1	C	429/431 (100%)	367 (86%)	53 (12%)	9 (2%)	9 29
1	D	429/431 (100%)	354 (82%)	55 (13%)	20 (5%)	3 9
All	All	1716/1724 (100%)	1513 (88%)	166 (10%)	37 (2%)	8 28

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	GLU
1	B	102	ASP
1	C	8	ALA
1	C	168	LYS
1	D	38	GLU
1	C	166	ARG
1	D	6	PHE
1	D	15	SER
1	D	36	LYS
1	D	102	ASP
1	D	184	LEU
1	D	211	THR
1	A	102	ASP
1	A	400	VAL
1	B	60	ALA
1	C	188	THR
1	C	244	ARG
1	D	188	THR
1	D	209	GLU
1	D	224	ALA
1	D	328	GLY
1	D	408	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	188	THR
1	C	38	GLU
1	D	100	VAL
1	D	168	LYS
1	D	364	GLU
1	B	196	PRO
1	C	328	GLY
1	D	282	PRO
1	D	400	VAL
1	A	354	ARG
1	C	400	VAL
1	D	66	GLY
1	D	196	PRO
1	D	285	PRO
1	C	143	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/342 (100%)	313 (92%)	29 (8%)	13	36
1	B	342/342 (100%)	314 (92%)	28 (8%)	14	38
1	C	342/342 (100%)	322 (94%)	20 (6%)	25	57
1	D	342/342 (100%)	319 (93%)	23 (7%)	20	50
All	All	1368/1368 (100%)	1268 (93%)	100 (7%)	17	44

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	15	SER
1	A	27	LEU
1	A	28	LEU
1	A	55	VAL
1	A	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	LEU
1	A	84	ARG
1	A	94	LEU
1	A	98	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	192	ARG
1	A	198	ARG
1	A	209	GLU
1	A	229	GLN
1	A	241	ARG
1	A	253	MET
1	A	264	LEU
1	A	329	LEU
1	A	344	GLN
1	A	363	GLU
1	A	386	LEU
1	A	390	LEU
1	A	398	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU
1	B	15	SER
1	B	27	LEU
1	B	57	LEU
1	B	84	ARG
1	B	94	LEU
1	B	96	ASP
1	B	98	LEU
1	B	165	ASN
1	B	186	GLU
1	B	192	ARG
1	B	198	ARG
1	B	211	THR
1	B	212	LEU
1	B	229	GLN
1	B	244	ARG
1	B	253	MET
1	B	264	LEU
1	B	270	GLU
1	B	277	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	325	LEU
1	B	329	LEU
1	B	336	LEU
1	B	365	VAL
1	B	390	LEU
1	B	398	LEU
1	B	406	LEU
1	B	407	LEU
1	B	409	LEU
1	C	27	LEU
1	C	38	GLU
1	C	55	VAL
1	C	62	LEU
1	C	96	ASP
1	C	98	LEU
1	C	102	ASP
1	C	109	GLU
1	C	121	LEU
1	C	155	ARG
1	C	165	ASN
1	C	186	GLU
1	C	192	ARG
1	C	195	ARG
1	C	229	GLN
1	C	241	ARG
1	C	266	ARG
1	C	302	ARG
1	C	336	LEU
1	C	427	GLU
1	D	2	ARG
1	D	17	HIS
1	D	27	LEU
1	D	36	LYS
1	D	55	VAL
1	D	57	LEU
1	D	73	ARG
1	D	94	LEU
1	D	96	ASP
1	D	98	LEU
1	D	102	ASP
1	D	128	ARG
1	D	165	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	166	ARG
1	D	171	LEU
1	D	186	GLU
1	D	192	ARG
1	D	229	GLN
1	D	244	ARG
1	D	295	GLU
1	D	329	LEU
1	D	364	GLU
1	D	406	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	165	ASN
1	A	214	GLN
1	A	229	GLN
1	A	293	HIS
1	A	344	GLN
1	A	372	HIS
1	A	380	HIS
1	B	34	GLN
1	B	41	ASN
1	B	165	ASN
1	B	229	GLN
1	B	240	HIS
1	B	293	HIS
1	B	380	HIS
1	B	383	GLN
1	C	34	GLN
1	C	41	ASN
1	C	59	HIS
1	C	117	HIS
1	C	151	GLN
1	C	165	ASN
1	C	214	GLN
1	C	229	GLN
1	C	301	ASN
1	C	323	HIS
1	D	34	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	41	ASN
1	D	165	ASN
1	D	229	GLN
1	D	323	HIS
1	D	324	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 70 ligands modelled in this entry, 4 are monoatomic - leaving 66 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	SO4	A	432	-	4,4,4	1.41	0	6,6,6	0.88	0
2	SO4	A	433	-	4,4,4	1.51	0	6,6,6	0.96	0
2	SO4	A	434	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	A	435	-	4,4,4	1.50	0	6,6,6	0.94	0
2	SO4	A	436	-	4,4,4	1.48	0	6,6,6	0.97	0
2	SO4	A	437	-	4,4,4	1.52	0	6,6,6	0.93	0
2	SO4	A	438	-	4,4,4	1.45	0	6,6,6	0.96	0
2	SO4	A	439	-	4,4,4	1.56	0	6,6,6	0.92	0
2	SO4	A	440	-	4,4,4	1.59	0	6,6,6	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	441	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	A	442	-	4,4,4	1.50	0	6,6,6	0.96	0
2	SO4	A	443	-	4,4,4	1.53	0	6,6,6	0.93	0
2	SO4	A	444	-	4,4,4	1.64	0	6,6,6	0.87	0
2	SO4	A	445	-	4,4,4	1.51	0	6,6,6	0.93	0
2	SO4	A	446	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	A	447	-	4,4,4	1.50	0	6,6,6	0.96	0
2	SO4	A	448	-	4,4,4	1.35	0	6,6,6	1.06	1 (16%)
2	SO4	A	449	-	4,4,4	1.50	0	6,6,6	0.96	0
2	SO4	A	450	-	4,4,4	1.53	0	6,6,6	0.91	0
2	SO4	A	451	-	4,4,4	1.57	0	6,6,6	0.90	0
2	SO4	A	452	-	4,4,4	1.58	0	6,6,6	0.89	0
2	SO4	A	453	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	A	454	-	4,4,4	1.49	0	6,6,6	0.93	0
2	SO4	A	455	-	4,4,4	1.51	0	6,6,6	0.96	0
3	BTB	A	456	-	12,13,13	1.76	4 (33%)	8,16,16	1.55	1 (12%)
2	SO4	B	432	-	4,4,4	1.50	0	6,6,6	0.96	0
2	SO4	B	433	-	4,4,4	1.49	0	6,6,6	0.97	0
2	SO4	B	434	-	4,4,4	1.41	0	6,6,6	1.01	0
2	SO4	B	435	-	4,4,4	1.47	0	6,6,6	0.97	0
2	SO4	B	436	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	B	437	-	4,4,4	1.58	0	6,6,6	0.90	0
2	SO4	B	438	-	4,4,4	1.62	0	6,6,6	0.85	0
2	SO4	B	439	-	4,4,4	1.57	0	6,6,6	0.93	0
2	SO4	B	440	-	4,4,4	1.53	0	6,6,6	0.93	0
2	SO4	B	441	-	4,4,4	1.49	0	6,6,6	0.98	0
2	SO4	B	442	-	4,4,4	1.55	0	6,6,6	0.93	0
2	SO4	B	443	-	4,4,4	1.51	0	6,6,6	0.94	0
2	SO4	B	444	-	4,4,4	1.52	0	6,6,6	0.96	0
2	SO4	B	445	-	4,4,4	1.58	0	6,6,6	0.92	0
2	SO4	B	446	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	B	447	-	4,4,4	1.54	0	6,6,6	0.92	0
2	SO4	B	448	-	4,4,4	1.52	0	6,6,6	0.91	0
2	SO4	B	449	-	4,4,4	1.48	0	6,6,6	0.96	0
2	SO4	B	450	-	4,4,4	1.67	0	6,6,6	0.92	0
2	SO4	C	432	-	4,4,4	1.57	0	6,6,6	0.92	0
2	SO4	C	433	-	4,4,4	1.50	0	6,6,6	0.97	0
2	SO4	C	434	-	4,4,4	1.47	0	6,6,6	0.96	0
2	SO4	C	435	-	4,4,4	1.47	0	6,6,6	0.98	0
2	SO4	C	436	-	4,4,4	1.50	0	6,6,6	0.95	0
2	SO4	C	437	-	4,4,4	1.43	0	6,6,6	0.97	0
2	SO4	C	438	-	4,4,4	1.48	0	6,6,6	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	439	-	4,4,4	1.54	0	6,6,6	0.92	0
2	SO4	C	440	-	4,4,4	1.48	0	6,6,6	0.97	0
2	SO4	C	441	-	4,4,4	1.48	0	6,6,6	0.98	0
2	SO4	C	442	-	4,4,4	1.49	0	6,6,6	0.94	0
2	SO4	C	443	-	4,4,4	1.56	0	6,6,6	0.92	0
2	SO4	C	444	-	4,4,4	1.48	0	6,6,6	0.97	0
2	SO4	C	445	-	4,4,4	1.49	0	6,6,6	0.96	0
2	SO4	D	432	-	4,4,4	1.51	0	6,6,6	0.96	0
2	SO4	D	433	-	4,4,4	1.51	0	6,6,6	0.95	0
2	SO4	D	434	-	4,4,4	1.49	0	6,6,6	0.94	0
2	SO4	D	435	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	D	436	-	4,4,4	1.47	0	6,6,6	0.96	0
2	SO4	D	437	-	4,4,4	1.49	0	6,6,6	0.95	0
2	SO4	D	438	-	4,4,4	1.53	0	6,6,6	0.92	0
2	SO4	D	439	-	4,4,4	1.52	0	6,6,6	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	432	-	-	0/0/0/0	0/0/0/0
2	SO4	A	433	-	-	0/0/0/0	0/0/0/0
2	SO4	A	434	-	-	0/0/0/0	0/0/0/0
2	SO4	A	435	-	-	0/0/0/0	0/0/0/0
2	SO4	A	436	-	-	0/0/0/0	0/0/0/0
2	SO4	A	437	-	-	0/0/0/0	0/0/0/0
2	SO4	A	438	-	-	0/0/0/0	0/0/0/0
2	SO4	A	439	-	-	0/0/0/0	0/0/0/0
2	SO4	A	440	-	-	0/0/0/0	0/0/0/0
2	SO4	A	441	-	-	0/0/0/0	0/0/0/0
2	SO4	A	442	-	-	0/0/0/0	0/0/0/0
2	SO4	A	443	-	-	0/0/0/0	0/0/0/0
2	SO4	A	444	-	-	0/0/0/0	0/0/0/0
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	A	446	-	-	0/0/0/0	0/0/0/0
2	SO4	A	447	-	-	0/0/0/0	0/0/0/0
2	SO4	A	448	-	-	0/0/0/0	0/0/0/0
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0
2	SO4	A	450	-	-	0/0/0/0	0/0/0/0
2	SO4	A	451	-	-	0/0/0/0	0/0/0/0
2	SO4	A	452	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	453	-	-	0/0/0/0	0/0/0/0
2	SO4	A	454	-	-	0/0/0/0	0/0/0/0
2	SO4	A	455	-	-	0/0/0/0	0/0/0/0
3	BTB	A	456	-	-	0/21/21/21	0/0/0/0
2	SO4	B	432	-	-	0/0/0/0	0/0/0/0
2	SO4	B	433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	434	-	-	0/0/0/0	0/0/0/0
2	SO4	B	435	-	-	0/0/0/0	0/0/0/0
2	SO4	B	436	-	-	0/0/0/0	0/0/0/0
2	SO4	B	437	-	-	0/0/0/0	0/0/0/0
2	SO4	B	438	-	-	0/0/0/0	0/0/0/0
2	SO4	B	439	-	-	0/0/0/0	0/0/0/0
2	SO4	B	440	-	-	0/0/0/0	0/0/0/0
2	SO4	B	441	-	-	0/0/0/0	0/0/0/0
2	SO4	B	442	-	-	0/0/0/0	0/0/0/0
2	SO4	B	443	-	-	0/0/0/0	0/0/0/0
2	SO4	B	444	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	446	-	-	0/0/0/0	0/0/0/0
2	SO4	B	447	-	-	0/0/0/0	0/0/0/0
2	SO4	B	448	-	-	0/0/0/0	0/0/0/0
2	SO4	B	449	-	-	0/0/0/0	0/0/0/0
2	SO4	B	450	-	-	0/0/0/0	0/0/0/0
2	SO4	C	432	-	-	0/0/0/0	0/0/0/0
2	SO4	C	433	-	-	0/0/0/0	0/0/0/0
2	SO4	C	434	-	-	0/0/0/0	0/0/0/0
2	SO4	C	435	-	-	0/0/0/0	0/0/0/0
2	SO4	C	436	-	-	0/0/0/0	0/0/0/0
2	SO4	C	437	-	-	0/0/0/0	0/0/0/0
2	SO4	C	438	-	-	0/0/0/0	0/0/0/0
2	SO4	C	439	-	-	0/0/0/0	0/0/0/0
2	SO4	C	440	-	-	0/0/0/0	0/0/0/0
2	SO4	C	441	-	-	0/0/0/0	0/0/0/0
2	SO4	C	442	-	-	0/0/0/0	0/0/0/0
2	SO4	C	443	-	-	0/0/0/0	0/0/0/0
2	SO4	C	444	-	-	0/0/0/0	0/0/0/0
2	SO4	C	445	-	-	0/0/0/0	0/0/0/0
2	SO4	D	432	-	-	0/0/0/0	0/0/0/0
2	SO4	D	433	-	-	0/0/0/0	0/0/0/0
2	SO4	D	434	-	-	0/0/0/0	0/0/0/0
2	SO4	D	435	-	-	0/0/0/0	0/0/0/0
2	SO4	D	436	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	437	-	-	0/0/0/0	0/0/0/0
2	SO4	D	438	-	-	0/0/0/0	0/0/0/0
2	SO4	D	439	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	456	BTB	C3-C2	2.42	1.56	1.53
3	A	456	BTB	C4-C2	2.70	1.56	1.53
3	A	456	BTB	C1-C2	2.84	1.56	1.53
3	A	456	BTB	C5-N	3.69	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	456	BTB	C7-N-C5	-3.12	102.58	112.52
2	A	448	SO4	O2-S-O1	-2.06	102.98	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	456	BTB	6	0
2	B	438	SO4	1	0
2	B	441	SO4	1	0
2	B	446	SO4	1	0
2	C	433	SO4	1	0
2	C	435	SO4	1	0
2	D	435	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.39	3 (0%) 89 84	20, 38, 59, 82	0
1	B	431/431 (100%)	-0.35	0 100 100	22, 40, 65, 83	0
1	C	431/431 (100%)	0.08	14 (3%) 51 39	17, 68, 102, 115	0
1	D	431/431 (100%)	0.57	44 (10%) 9 4	35, 78, 132, 146	0
All	All	1724/1724 (100%)	-0.02	61 (3%) 48 35	17, 50, 113, 146	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	366	PRO	6.4
1	D	356	PRO	4.8
1	D	360	ILE	4.4
1	D	361	LEU	4.4
1	D	306	PRO	4.3
1	D	332	PRO	4.2
1	D	239	GLY	4.1
1	D	367	LEU	3.9
1	D	216	GLY	3.9
1	C	361	LEU	3.8
1	D	358	VAL	3.8
1	C	241	ARG	3.6
1	D	294	THR	3.6
1	D	212	LEU	3.6
1	C	415	LEU	3.4
1	C	213	SER	3.4
1	D	329	LEU	3.4
1	D	213	SER	3.3
1	D	363	GLU	3.3
1	C	240	HIS	3.2
1	C	239	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	334	ASN	3.1
1	C	214	GLN	2.9
1	D	326	LYS	2.9
1	D	226	GLU	2.8
1	D	288	LEU	2.8
1	D	223	PHE	2.7
1	D	300	LEU	2.7
1	C	243	PRO	2.7
1	D	240	HIS	2.6
1	D	322	LEU	2.5
1	D	308	VAL	2.5
1	D	354	ARG	2.5
1	C	198	ARG	2.5
1	D	201	VAL	2.5
1	C	362	GLY	2.5
1	D	199	GLU	2.4
1	D	325	LEU	2.4
1	D	333	ARG	2.4
1	D	340	GLY	2.4
1	C	358	VAL	2.4
1	D	309	VAL	2.4
1	D	362	GLY	2.4
1	D	335	ALA	2.3
1	D	59	HIS	2.3
1	D	218	VAL	2.3
1	D	369	ALA	2.3
1	D	246	PRO	2.2
1	C	244	ARG	2.2
1	D	303	ALA	2.2
1	A	358	VAL	2.2
1	D	355	PRO	2.2
1	D	20	LEU	2.2
1	D	336	LEU	2.2
1	A	131	ALA	2.2
1	C	353	ALA	2.1
1	D	248	TYR	2.1
1	D	338	PHE	2.1
1	A	360	ILE	2.1
1	C	418	GLN	2.1
1	D	370	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	443	5/5	0.93	0.29	7.09	96,96,97,97	0
2	SO4	A	453	5/5	0.67	0.47	6.10	153,153,153,153	0
2	SO4	C	441	5/5	0.75	0.47	5.46	133,134,134,134	0
3	BTB	A	456	14/14	0.78	0.30	5.09	60,67,70,70	0
2	SO4	A	449	5/5	0.95	0.18	3.21	84,84,85,85	0
2	SO4	A	440	5/5	0.89	0.30	3.15	99,100,101,101	0
2	SO4	B	440	5/5	0.79	0.28	2.76	140,141,141,141	0
2	SO4	C	444	5/5	0.92	0.37	2.30	127,128,128,128	0
2	SO4	B	450	5/5	0.97	0.21	1.79	51,52,54,56	0
2	SO4	A	452	5/5	0.84	0.20	1.51	129,129,129,129	0
2	SO4	B	439	5/5	0.96	0.17	0.76	62,63,64,64	0
2	SO4	D	434	5/5	0.75	0.26	0.71	151,151,152,152	0
2	SO4	D	435	5/5	0.93	0.16	0.28	97,98,99,99	0
2	SO4	A	432	5/5	0.99	0.15	0.09	36,37,38,42	0
2	SO4	C	432	5/5	0.92	0.26	-0.00	84,85,86,87	0
2	SO4	B	437	5/5	0.92	0.16	-0.18	97,98,98,98	0
2	SO4	B	438	5/5	0.96	0.16	-0.28	70,70,71,71	0
4	ZN	B	451	1/1	0.95	0.17	-0.29	76,76,76,76	0
2	SO4	A	444	5/5	0.98	0.12	-0.40	47,49,50,50	0
4	ZN	A	457	1/1	0.98	0.16	-0.59	50,50,50,50	0
2	SO4	D	436	5/5	0.89	0.17	-0.62	119,119,120,120	0
4	ZN	D	440	1/1	0.98	0.26	-1.06	86,86,86,86	0
4	ZN	C	446	1/1	0.97	0.12	-1.84	76,76,76,76	0
2	SO4	A	448	5/5	0.96	0.12	-1.87	70,71,72,73	0
2	SO4	D	432	5/5	0.97	0.21	-2.69	80,81,81,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	445	5/5	0.84	0.27	-	127,127,127,127	0
2	SO4	A	437	5/5	0.83	0.24	-	126,126,126,126	0
2	SO4	D	437	5/5	0.90	0.31	-	135,135,135,136	0
2	SO4	C	433	5/5	0.91	0.16	-	98,100,100,100	0
2	SO4	A	435	5/5	0.77	0.34	-	171,171,172,172	0
2	SO4	C	437	5/5	0.93	0.16	-	126,126,126,126	0
2	SO4	A	434	5/5	0.91	0.19	-	127,127,127,127	0
2	SO4	C	442	5/5	0.94	0.10	-	90,90,91,91	0
2	SO4	A	454	5/5	0.92	0.28	-	110,110,111,111	0
2	SO4	C	443	5/5	0.91	0.15	-	93,93,94,94	0
2	SO4	B	445	5/5	0.87	0.22	-	104,104,105,105	0
2	SO4	B	448	5/5	0.84	0.33	-	131,131,132,132	0
2	SO4	B	435	5/5	0.89	0.25	-	112,112,112,112	0
2	SO4	C	438	5/5	0.81	0.21	-	137,137,138,138	0
2	SO4	C	440	5/5	0.86	0.34	-	132,132,132,133	0
2	SO4	C	435	5/5	0.96	0.13	-	90,90,90,90	0
2	SO4	A	451	5/5	0.72	0.34	-	145,145,146,146	0
2	SO4	C	436	5/5	0.94	0.17	-	117,117,117,117	0
2	SO4	B	444	5/5	0.69	0.32	-	149,150,150,150	0
2	SO4	B	443	5/5	0.90	0.13	-	117,117,118,118	0
2	SO4	C	439	5/5	0.97	0.11	-	63,64,65,65	0
2	SO4	A	438	5/5	0.90	0.28	-	114,114,115,115	0
2	SO4	A	455	5/5	0.86	0.27	-	136,136,136,136	0
2	SO4	A	436	5/5	0.83	0.21	-	135,135,135,136	0
2	SO4	C	445	5/5	0.86	0.21	-	120,121,121,121	0
2	SO4	B	433	5/5	0.89	0.17	-	114,114,115,115	0
2	SO4	A	450	5/5	0.85	0.19	-	123,123,124,124	0
2	SO4	D	439	5/5	0.81	0.17	-	139,139,139,139	0
2	SO4	B	434	5/5	0.94	0.12	-	75,75,76,76	0
2	SO4	C	434	5/5	0.96	0.16	-	93,93,93,93	0
2	SO4	B	442	5/5	0.91	0.24	-	119,119,119,120	0
2	SO4	A	442	5/5	0.88	0.19	-	104,104,104,104	0
2	SO4	A	446	5/5	0.82	0.27	-	144,144,144,144	0
2	SO4	A	441	5/5	0.90	0.23	-	110,111,111,111	0
2	SO4	B	436	5/5	0.87	0.17	-	125,125,125,125	0
2	SO4	D	433	5/5	0.94	0.11	-	99,100,100,101	0
2	SO4	A	433	5/5	0.82	0.21	-	130,131,131,131	0
2	SO4	B	432	5/5	0.92	0.23	-	92,93,93,94	0
2	SO4	B	441	5/5	0.86	0.25	-	138,138,138,138	0
2	SO4	A	447	5/5	0.81	0.21	-	129,129,130,130	0
2	SO4	D	438	5/5	0.69	0.25	-	146,146,147,147	0
2	SO4	B	449	5/5	0.88	0.24	-	112,112,112,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	446	5/5	0.96	0.14	-	96,96,97,97	0
2	SO4	B	447	5/5	0.87	0.27	-	130,131,131,131	0
2	SO4	A	439	5/5	0.74	0.26	-	134,134,135,135	0

6.5 Other polymers (i)

There are no such residues in this entry.