



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:07 AM EDT

PDB ID : 1KH1  
Title : Crystal Structure of Thermus thermophilus HB8 Argininosuccinate Synthetase  
Authors : Goto, M.; Nakajima, Y.; Hirotsu, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2001-11-29  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.36.2  
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) : 2.36.2

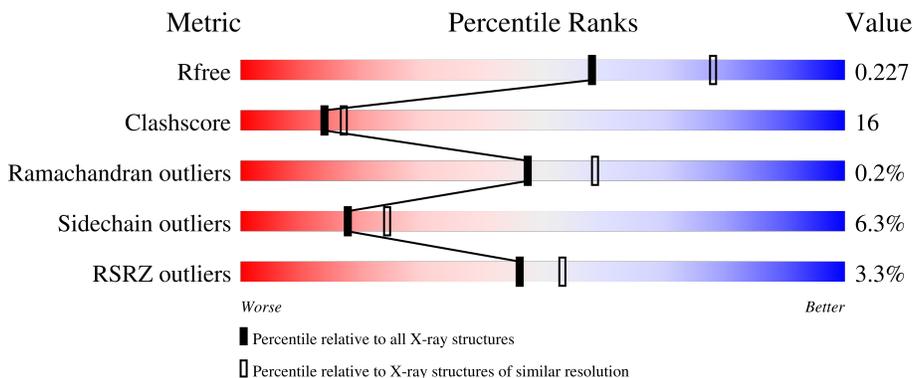
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	400	
1	B	400	
1	C	400	
1	D	400	

## 2 Entry composition [i](#)

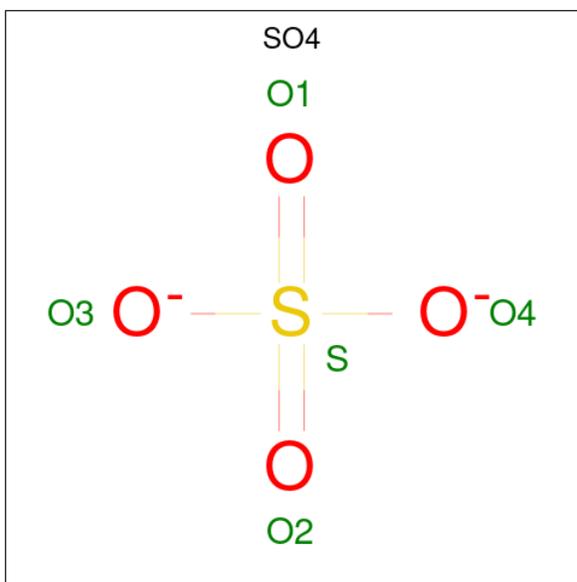
There are 3 unique types of molecules in this entry. The entry contains 12650 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Argininosuccinate Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	Total 3017	C 1931	N 526	O 551	S 9	0	0	0
1	B	382	Total 3034	C 1940	N 529	O 556	S 9	0	0	0
1	C	386	Total 3066	C 1963	N 533	O 561	S 9	0	0	0
1	D	385	Total 3055	C 1954	N 532	O 560	S 9	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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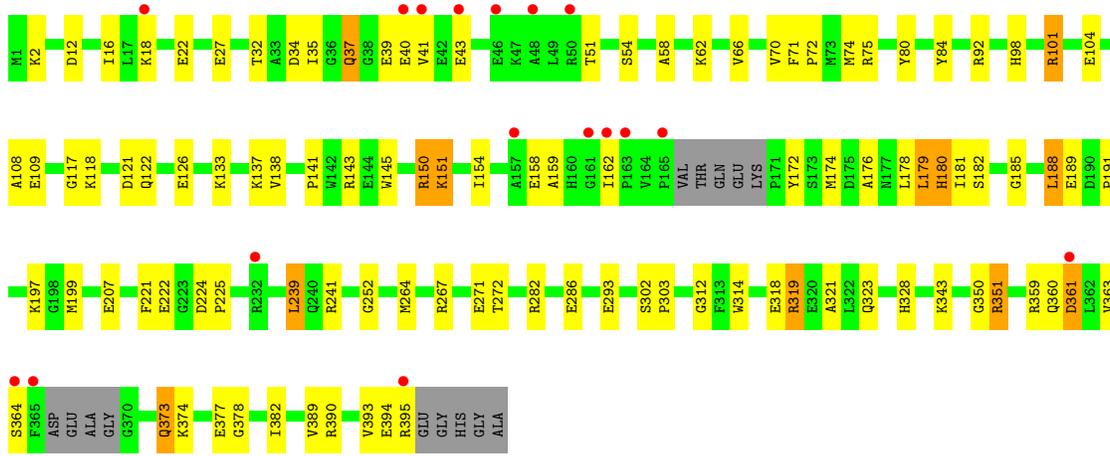
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

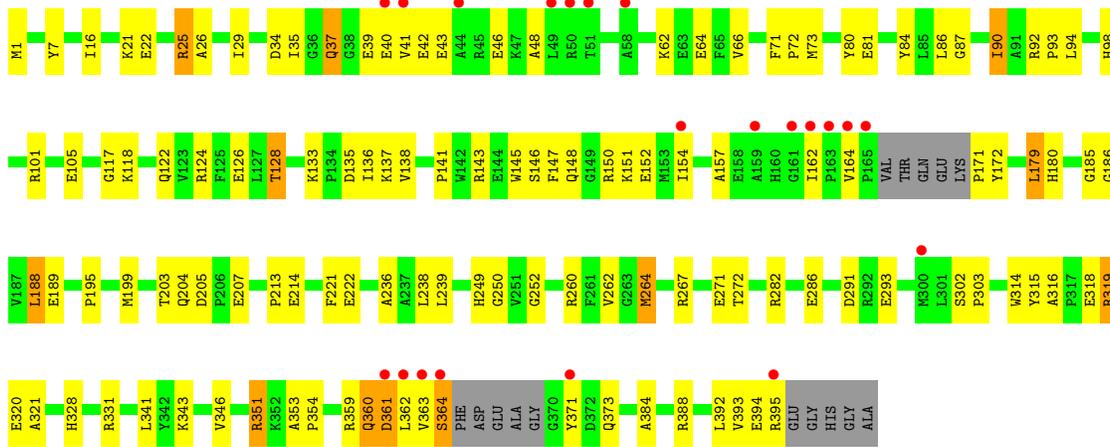
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	124	Total	O	0	0
			124	124		
3	C	105	Total	O	0	0
			105	105		
3	D	97	Total	O	0	0
			97	97		





● Molecule 1: Argininosuccinate Synthetase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	228.41Å 228.41Å 161.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 48.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 89.2 (48.70-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.229 0.199 , 0.227	Depositor DCC
$R_{free}$ test set	12404 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.39	0/3085	0.66	4/4169 (0.1%)
1	B	0.39	0/3102	0.67	2/4192 (0.0%)
1	C	0.40	0/3135	0.66	3/4237 (0.1%)
1	D	0.39	0/3123	0.67	3/4221 (0.1%)
All	All	0.39	0/12445	0.66	12/16819 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	CB-CA-C	-12.49	85.42	110.40
1	C	221	PHE	CB-CA-C	-11.59	87.22	110.40
1	A	221	PHE	CB-CA-C	-10.84	88.72	110.40
1	D	221	PHE	CB-CA-C	-10.63	89.13	110.40
1	C	222	GLU	N-CA-C	7.83	132.15	111.00
1	A	222	GLU	N-CA-C	7.54	131.35	111.00
1	D	222	GLU	N-CA-C	7.32	130.76	111.00
1	A	221	PHE	N-CA-C	-6.07	94.60	111.00
1	B	222	GLU	N-CA-C	5.94	127.03	111.00
1	C	221	PHE	N-CA-C	-5.72	95.54	111.00
1	D	221	PHE	N-CA-C	-5.68	95.66	111.00
1	A	257	VAL	N-CA-C	-5.13	97.15	111.00

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	3017	0	3006	114	0
1	B	3034	0	3018	103	0
1	C	3066	0	3052	104	0
1	D	3055	0	3043	108	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	132	0	0	9	0
3	B	124	0	0	3	0
3	C	105	0	0	6	0
3	D	97	0	0	2	0
All	All	12650	0	12119	384	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 16.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:H	1:B:151:LYS:HD2	1.08	1.08
1:C:37:GLN:H	1:C:37:GLN:NE2	1.53	1.07
1:D:151:LYS:H	1:D:151:LYS:HD2	1.11	1.07
1:C:151:LYS:H	1:C:151:LYS:HD2	1.18	1.04
1:D:35:ILE:H	1:D:37:GLN:NE2	1.59	1.01
1:C:37:GLN:N	1:C:37:GLN:HE21	1.60	0.99
1:A:349:VAL:HG13	1:B:194:GLU:HB2	1.47	0.96
1:D:35:ILE:H	1:D:37:GLN:HE22	1.07	0.96
1:C:395:ARG:HG3	1:C:395:ARG:HH11	1.31	0.92
1:B:35:ILE:H	1:B:37:GLN:NE2	1.67	0.90
1:C:319:ARG:HH21	1:C:323:GLN:HE21	1.20	0.89
1:C:151:LYS:H	1:C:151:LYS:CD	1.83	0.89
1:D:393:VAL:C	1:D:395:ARG:H	1.75	0.88
1:A:150:ARG:HB3	1:A:151:LYS:HE3	1.55	0.88
1:C:37:GLN:H	1:C:37:GLN:HE21	0.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HD2	1:C:151:LYS:N	1.91	0.86
1:B:151:LYS:H	1:B:151:LYS:CD	1.84	0.86
1:A:123:VAL:HG22	1:B:380:ILE:HD11	1.57	0.85
1:A:390:ARG:O	1:A:394:GLU:HG2	1.79	0.83
1:B:34:ASP:HB2	1:B:41:VAL:HG21	1.61	0.82
1:D:151:LYS:HD2	1:D:151:LYS:N	1.95	0.82
1:C:122:GLN:NE2	1:C:143:ARG:HH11	1.78	0.81
1:B:37:GLN:NE2	1:B:37:GLN:H	1.79	0.80
1:D:351:ARG:HD2	1:D:351:ARG:N	1.97	0.79
1:A:151:LYS:HE3	1:A:151:LYS:H	1.48	0.79
1:D:151:LYS:H	1:D:151:LYS:CD	1.90	0.78
1:B:1:MET:O	1:B:26:ALA:HB1	1.84	0.78
1:B:126:GLU:HG2	1:B:138:VAL:HG11	1.66	0.78
1:D:361:ASP:HA	1:D:364:SER:HB2	1.64	0.78
1:A:41:VAL:HG12	1:A:58:ALA:HB1	1.67	0.76
1:A:293:GLU:HB3	1:C:318:GLU:HG2	1.67	0.76
1:D:42:GLU:O	1:D:46:GLU:HG3	1.86	0.76
1:A:318:GLU:HG2	1:C:293:GLU:CB	2.16	0.76
1:A:293:GLU:CB	1:C:318:GLU:HG2	2.15	0.76
1:B:151:LYS:HD2	1:B:151:LYS:N	1.94	0.75
1:C:351:ARG:HD2	1:C:351:ARG:N	2.01	0.74
1:A:70:VAL:O	1:A:74:MET:HG3	1.86	0.74
1:A:318:GLU:HG2	1:C:293:GLU:HB3	1.68	0.74
1:A:373:GLN:H	1:A:373:GLN:NE2	1.86	0.74
1:C:122:GLN:HE21	1:C:143:ARG:HH11	1.34	0.73
1:D:171:PRO:O	1:D:186:GLY:HA3	1.87	0.73
1:B:351:ARG:HD2	1:B:351:ARG:N	2.02	0.73
1:B:359:ARG:HB3	1:B:361:ASP:OD1	1.88	0.73
1:A:98:HIS:HD2	1:A:101:ARG:NH1	1.85	0.73
1:D:393:VAL:C	1:D:395:ARG:N	2.40	0.73
1:C:319:ARG:HH21	1:C:323:GLN:NE2	1.87	0.72
1:A:351:ARG:HD2	1:A:351:ARG:N	2.04	0.72
1:A:109:GLU:O	1:A:137:LYS:HE2	1.88	0.72
1:D:35:ILE:N	1:D:37:GLN:HE22	1.85	0.71
1:B:100:VAL:O	1:B:104:GLU:HG3	1.90	0.71
1:B:293:GLU:HB3	1:D:318:GLU:HG2	1.71	0.70
1:D:126:GLU:HG2	1:D:138:VAL:HG11	1.73	0.70
1:D:395:ARG:NH1	1:D:395:ARG:HB3	2.06	0.70
1:B:293:GLU:CB	1:D:318:GLU:HG2	2.21	0.70
1:C:18:LYS:HG3	1:C:162:ILE:HD11	1.72	0.70
1:C:18:LYS:CG	1:C:162:ILE:HD11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HE3	3:C:1356:HOH:O	1.90	0.70
1:C:395:ARG:HH11	1:C:395:ARG:CG	2.04	0.70
1:A:123:VAL:HG22	1:B:380:ILE:CD1	2.20	0.69
1:D:179:LEU:O	1:D:272:THR:HG23	1.93	0.69
1:C:74:MET:HE2	3:C:1315:HOH:O	1.93	0.68
1:B:122:GLN:HE21	1:B:143:ARG:HH11	1.41	0.68
1:A:67:ARG:NH1	1:A:68:ASP:OD1	2.27	0.67
1:B:35:ILE:H	1:B:37:GLN:HE22	1.41	0.67
1:A:27:GLU:HG3	1:A:54:SER:CB	2.24	0.67
1:C:264:MET:HB2	1:D:362:LEU:HD13	1.76	0.67
1:B:41:VAL:HG12	1:B:58:ALA:HB1	1.77	0.67
1:B:314:TRP:O	1:B:319:ARG:HD3	1.94	0.67
1:D:282:ARG:O	1:D:286:GLU:HG3	1.95	0.67
1:A:93:PRO:HA	1:A:128:THR:HG21	1.77	0.66
1:D:40:GLU:HG3	1:D:43:GLU:HG3	1.76	0.66
1:D:40:GLU:CG	1:D:43:GLU:HG3	2.26	0.66
1:D:98:HIS:HD2	1:D:101:ARG:HH12	1.44	0.66
1:D:395:ARG:HB3	1:D:395:ARG:CZ	2.26	0.66
1:B:32:THR:HG22	1:B:41:VAL:HG13	1.76	0.66
1:B:318:GLU:HG2	1:D:293:GLU:HB3	1.78	0.66
1:C:32:THR:CG2	1:C:41:VAL:HG13	2.27	0.65
1:D:124:ARG:O	1:D:128:THR:HG23	1.96	0.65
1:A:151:LYS:H	1:A:151:LYS:CE	2.08	0.65
1:A:293:GLU:HB2	1:C:318:GLU:CG	2.25	0.65
1:D:98:HIS:HD2	1:D:101:ARG:NH1	1.95	0.65
1:A:349:VAL:CG1	1:B:194:GLU:HB2	2.25	0.64
1:B:37:GLN:H	1:B:37:GLN:HE21	1.44	0.64
1:B:393:VAL:C	1:B:395:ARG:H	2.01	0.64
1:A:133:LYS:HG2	1:A:136:ILE:HB	1.79	0.63
1:B:35:ILE:N	1:B:37:GLN:NE2	2.42	0.63
1:D:98:HIS:CD2	1:D:101:ARG:NH1	2.66	0.63
1:A:21:LYS:HD3	3:A:1313:HOH:O	1.99	0.63
1:A:151:LYS:H	1:A:151:LYS:CD	2.12	0.63
1:C:118:LYS:HG2	3:D:1428:HOH:O	1.98	0.63
1:D:117:GLY:HA2	1:D:122:GLN:HE22	1.63	0.63
1:D:133:LYS:HD3	1:D:136:ILE:HB	1.80	0.63
1:C:41:VAL:HG12	1:C:58:ALA:HB1	1.79	0.62
1:C:35:ILE:H	1:C:37:GLN:NE2	1.98	0.62
1:D:1:MET:O	1:D:26:ALA:HB1	2.00	0.61
1:A:126:GLU:HG2	1:A:138:VAL:HG11	1.81	0.61
1:C:302:SER:HB2	1:C:303:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLU:O	1:C:191:PRO:HD3	2.00	0.60
1:B:293:GLU:HB2	1:D:318:GLU:CG	2.31	0.60
1:A:41:VAL:CG1	1:A:58:ALA:HB1	2.30	0.60
1:A:214:GLU:OE1	1:A:249:HIS:HE1	1.84	0.60
1:B:1:MET:HB3	1:B:26:ALA:HB2	1.82	0.60
1:D:90:ILE:HD11	1:D:179:LEU:HD12	1.83	0.60
1:D:360:GLN:HA	1:D:363:VAL:HG22	1.84	0.60
1:C:16:ILE:HG23	1:C:141:PRO:HG2	1.84	0.59
1:B:97:LYS:NZ	3:B:1116:HOH:O	2.35	0.59
1:D:117:GLY:HA2	1:D:122:GLN:NE2	2.17	0.59
1:A:331:ARG:CB	1:A:331:ARG:HH11	2.16	0.59
1:B:359:ARG:O	1:B:361:ASP:N	2.35	0.59
1:A:318:GLU:CG	1:C:293:GLU:HB2	2.32	0.59
1:D:37:GLN:NE2	1:D:37:GLN:H	2.00	0.58
1:A:370:GLY:N	3:A:1105:HOH:O	2.35	0.58
1:B:314:TRP:CE3	1:B:319:ARG:HD2	2.38	0.58
1:A:249:HIS:HD2	3:A:1155:HOH:O	1.85	0.58
1:B:32:THR:CG2	1:B:41:VAL:HG13	2.33	0.58
1:B:376:ALA:O	1:B:380:ILE:HG12	2.02	0.58
1:D:124:ARG:O	1:D:128:THR:CG2	2.51	0.58
1:C:12:ASP:OD1	1:C:150:ARG:NH2	2.37	0.58
1:D:314:TRP:O	1:D:319:ARG:HD3	2.04	0.57
1:C:185:GLY:O	1:C:188:LEU:HB2	2.04	0.57
1:A:282:ARG:HD2	3:A:1115:HOH:O	2.04	0.57
1:B:35:ILE:N	1:B:37:GLN:HE22	2.00	0.57
1:A:395:ARG:NH1	3:A:1301:HOH:O	2.37	0.57
1:A:349:VAL:HG12	3:A:1418:HOH:O	2.05	0.57
1:D:395:ARG:NH1	1:D:395:ARG:CB	2.68	0.57
1:A:393:VAL:C	1:A:395:ARG:H	2.07	0.57
1:B:318:GLU:HG2	1:D:293:GLU:CB	2.35	0.57
1:D:122:GLN:HE21	1:D:143:ARG:HH11	1.53	0.57
1:D:35:ILE:N	1:D:37:GLN:NE2	2.43	0.56
1:B:171:PRO:O	1:B:186:GLY:HA3	2.04	0.56
1:C:122:GLN:HE22	1:C:143:ARG:HD3	1.70	0.56
1:B:214:GLU:OE1	1:B:249:HIS:HE1	1.89	0.56
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.11	0.56
1:C:32:THR:HG22	1:C:41:VAL:HG13	1.87	0.56
1:A:90:ILE:HD11	1:A:179:LEU:HD12	1.86	0.56
1:C:282:ARG:O	1:C:286:GLU:HG3	2.06	0.56
1:B:42:GLU:O	1:B:46:GLU:HG3	2.06	0.56
1:B:282:ARG:O	1:B:286:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:HG2	1:C:293:GLU:HB2	1.84	0.56
1:D:162:ILE:O	1:D:164:VAL:HG13	2.06	0.56
1:B:93:PRO:HA	1:B:128:THR:HG21	1.88	0.56
1:B:122:GLN:NE2	1:B:143:ARG:HH11	2.02	0.56
1:D:21:LYS:O	1:D:25:ARG:HA	2.05	0.56
1:C:150:ARG:O	1:C:154:ILE:HG13	2.06	0.55
1:D:316:ALA:HB1	1:D:318:GLU:OE2	2.05	0.55
1:A:302:SER:HB2	1:A:303:PRO:HD3	1.87	0.55
1:B:318:GLU:CG	1:D:293:GLU:HB2	2.37	0.55
1:C:319:ARG:NH2	1:C:323:GLN:HE21	1.96	0.55
1:A:358:TYR:CE2	1:B:191:PRO:HD3	2.40	0.55
1:D:148:GLN:HB2	1:D:152:GLU:OE2	2.06	0.55
1:A:293:GLU:HB2	1:C:318:GLU:HG2	1.84	0.55
1:C:122:GLN:HE21	1:C:143:ARG:NH1	2.02	0.55
1:D:80:TYR:CD2	1:D:81:GLU:HG3	2.42	0.55
1:C:179:LEU:O	1:C:272:THR:HG23	2.07	0.54
1:A:98:HIS:CD2	1:A:101:ARG:NH1	2.73	0.54
1:D:214:GLU:OE1	1:D:249:HIS:HE1	1.90	0.54
1:A:66:VAL:HG21	1:A:236:ALA:HA	1.90	0.54
1:A:372:ASP:HB2	1:A:373:GLN:HE21	1.70	0.54
1:B:118:LYS:H	1:B:118:LYS:HD2	1.72	0.54
1:C:343:LYS:HD2	1:D:343:LYS:CD	2.37	0.54
1:D:185:GLY:O	1:D:188:LEU:HB2	2.07	0.54
1:A:331:ARG:HB3	1:A:331:ARG:NH1	2.22	0.54
1:A:86:LEU:O	1:A:90:ILE:HG13	2.07	0.54
1:A:319:ARG:HH21	1:A:323:GLN:NE2	2.06	0.54
1:A:27:GLU:HG3	1:A:54:SER:HB3	1.88	0.54
1:B:249:HIS:HD2	3:B:1427:HOH:O	1.89	0.53
1:B:379:PHE:HB2	1:C:382:ILE:HG13	1.90	0.53
1:C:70:VAL:O	1:C:74:MET:HG3	2.08	0.53
1:C:343:LYS:HD2	1:D:343:LYS:HD3	1.90	0.53
1:C:364:SER:O	1:D:118:LYS:NZ	2.35	0.53
1:D:262:VAL:O	1:D:262:VAL:CG1	2.55	0.53
1:A:120:ASN:HD21	1:A:261:PHE:H	1.57	0.53
1:D:392:LEU:O	1:D:395:ARG:HA	2.08	0.53
1:B:393:VAL:C	1:B:395:ARG:N	2.61	0.53
1:B:2:LYS:HB2	1:B:108:ALA:HA	1.90	0.53
1:B:34:ASP:HA	1:B:37:GLN:HE22	1.73	0.53
1:C:176:ALA:CB	1:C:181:ILE:HG12	2.39	0.52
1:B:37:GLN:HE21	1:B:37:GLN:N	2.07	0.52
1:B:390:ARG:O	1:B:394:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:GLN:H	1:C:373:GLN:NE2	2.07	0.52
1:B:98:HIS:HD2	1:B:101:ARG:NH1	2.07	0.52
1:B:124:ARG:O	1:B:128:THR:HG23	2.10	0.52
1:C:394:GLU:O	1:C:395:ARG:HB2	2.10	0.52
1:C:34:ASP:HB2	1:C:41:VAL:HG21	1.90	0.52
1:C:104:GLU:OE2	1:C:133:LYS:HD3	2.10	0.52
1:A:137:LYS:N	1:A:137:LYS:HD3	2.24	0.52
1:B:80:TYR:HB3	1:B:84:TYR:HB3	1.91	0.52
1:D:150:ARG:HG3	1:D:154:ILE:HD11	1.92	0.52
1:D:87:GLY:HA2	1:D:179:LEU:HD13	1.91	0.51
1:D:148:GLN:H	1:D:152:GLU:CD	2.12	0.51
1:C:37:GLN:HB2	1:C:39:GLU:HG2	1.92	0.51
1:B:86:LEU:O	1:B:90:ILE:HG13	2.11	0.51
1:B:319:ARG:HH21	1:B:323:GLN:HE21	1.56	0.51
1:C:2:LYS:HB2	1:C:108:ALA:HA	1.92	0.51
1:C:109:GLU:O	1:C:137:LYS:HE2	2.11	0.51
1:D:393:VAL:O	1:D:395:ARG:N	2.44	0.51
1:C:18:LYS:HG2	1:C:162:ILE:HD11	1.92	0.51
1:A:40:GLU:HG3	1:A:43:GLU:HG3	1.93	0.51
1:D:93:PRO:HA	1:D:128:THR:HG21	1.93	0.51
1:A:21:LYS:HD2	1:A:26:ALA:O	2.11	0.50
1:A:97:LYS:HD2	1:A:315:TYR:OH	2.11	0.50
1:B:179:LEU:HD22	1:B:272:THR:HG23	1.93	0.50
1:C:373:GLN:HG2	1:C:374:LYS:N	2.27	0.50
1:A:293:GLU:CB	1:C:318:GLU:CG	2.86	0.50
1:B:123:VAL:HG12	1:B:127:LEU:HD12	1.94	0.50
1:A:373:GLN:H	1:A:373:GLN:HE21	1.57	0.50
1:D:260:ARG:HD2	1:D:264:MET:SD	2.52	0.50
1:D:360:GLN:O	1:D:364:SER:HB2	2.11	0.50
1:B:359:ARG:C	1:B:361:ASP:H	2.15	0.50
1:D:84:TYR:CE2	1:D:86:LEU:HA	2.46	0.50
1:D:252:GLY:O	1:D:271:GLU:HA	2.11	0.50
1:C:378:GLY:O	1:C:382:ILE:HG12	2.11	0.49
1:D:351:ARG:HD2	1:D:351:ARG:H	1.74	0.49
1:A:319:ARG:HH21	1:A:323:GLN:HE21	1.60	0.49
1:C:27:GLU:HG3	1:C:54:SER:OG	2.12	0.49
1:C:390:ARG:O	1:C:394:GLU:HG2	2.13	0.49
1:B:98:HIS:CD2	1:B:101:ARG:NH1	2.80	0.49
1:C:176:ALA:HB2	1:C:181:ILE:HG12	1.94	0.49
1:C:241:ARG:NH1	3:C:1267:HOH:O	2.43	0.49
1:C:51:THR:HG22	1:C:51:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:C	1:A:395:ARG:N	2.66	0.49
1:B:338:ARG:HD3	3:B:1416:HOH:O	2.12	0.49
1:B:122:GLN:HE22	1:B:143:ARG:HD3	1.78	0.49
1:B:318:GLU:CG	1:D:293:GLU:CB	2.91	0.49
1:A:24:TYR:OH	1:A:144:GLU:OE2	2.28	0.48
1:D:66:VAL:HG21	1:D:236:ALA:HA	1.95	0.48
1:D:101:ARG:HG2	1:D:105:GLU:OE2	2.14	0.48
1:D:328:HIS:CE1	1:D:331:ARG:HH22	2.31	0.48
1:D:384:ALA:O	1:D:388:ARG:HG3	2.13	0.48
1:A:84:TYR:CE2	1:A:86:LEU:HA	2.49	0.48
1:A:339:LEU:HD12	1:A:339:LEU:N	2.29	0.48
1:B:36:GLY:N	1:B:37:GLN:HE21	2.12	0.48
1:C:178:LEU:HB3	1:C:239:LEU:HD13	1.96	0.48
1:C:180:HIS:ND1	1:C:180:HIS:C	2.67	0.48
1:D:395:ARG:CB	1:D:395:ARG:HH11	2.26	0.48
1:D:16:ILE:HG23	1:D:141:PRO:HG2	1.95	0.48
1:A:146:SER:O	1:A:147:PHE:C	2.53	0.47
1:B:180:HIS:ND1	1:B:180:HIS:C	2.68	0.47
1:C:174:MET:HA	1:C:182:SER:O	2.14	0.47
1:A:179:LEU:HD22	1:A:272:THR:HG23	1.97	0.47
1:D:314:TRP:CE3	1:D:319:ARG:HD2	2.49	0.47
1:A:98:HIS:CD2	1:A:101:ARG:HH11	2.33	0.47
1:A:120:ASN:ND2	1:A:261:PHE:H	2.12	0.47
1:B:179:LEU:O	1:B:272:THR:HG23	2.14	0.47
1:C:180:HIS:HB2	1:C:271:GLU:O	2.14	0.47
1:C:395:ARG:CG	1:C:395:ARG:NH1	2.68	0.47
1:A:316:ALA:HB1	1:A:318:GLU:OE2	2.15	0.47
1:C:252:GLY:O	1:C:271:GLU:HA	2.14	0.47
1:B:185:GLY:O	1:B:188:LEU:HB2	2.15	0.47
1:D:80:TYR:CE2	1:D:81:GLU:HG3	2.49	0.47
1:A:3:ILE:HD13	1:A:139:ILE:HD12	1.97	0.47
1:D:22:GLU:HA	1:D:25:ARG:NH1	2.30	0.47
1:C:75:ARG:NH2	3:C:1156:HOH:O	2.48	0.46
1:C:389:VAL:O	1:C:393:VAL:HG23	2.15	0.46
1:A:154:ILE:HG22	1:A:155:ALA:N	2.31	0.46
1:C:101:ARG:NH2	3:C:1140:HOH:O	2.34	0.46
1:A:121:ASP:HA	1:A:124:ARG:HD2	1.96	0.46
1:B:355:LYS:HE3	1:C:393:VAL:HG12	1.96	0.46
1:A:21:LYS:O	1:A:25:ARG:HA	2.16	0.46
1:B:359:ARG:C	1:B:361:ASP:N	2.68	0.46
1:B:328:HIS:CD2	1:D:321:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:TRP:O	1:C:319:ARG:HD3	2.15	0.46
1:D:84:TYR:CZ	1:D:86:LEU:HA	2.50	0.46
1:D:146:SER:O	1:D:147:PHE:C	2.53	0.46
1:C:35:ILE:H	1:C:37:GLN:HE22	1.64	0.46
1:C:98:HIS:HD2	1:C:101:ARG:NH1	2.13	0.46
1:B:318:GLU:HG3	1:D:293:GLU:HB2	1.97	0.46
1:C:126:GLU:HG2	1:C:138:VAL:HG11	1.97	0.46
1:D:203:THR:HB	1:D:250:GLY:HA2	1.98	0.46
3:A:1265:HOH:O	1:B:191:PRO:HG2	2.16	0.45
1:A:189:GLU:OE2	1:B:360:GLN:OE1	2.34	0.45
1:B:34:ASP:HB2	1:B:41:VAL:CG2	2.39	0.45
1:B:293:GLU:HB2	1:D:318:GLU:HG2	1.92	0.45
1:B:182:SER:HB2	1:B:270:TYR:CE2	2.52	0.45
1:C:35:ILE:N	1:C:37:GLN:HE22	2.15	0.45
1:C:92:ARG:HE	1:C:121:ASP:CG	2.19	0.45
1:D:29:ILE:HD12	1:D:29:ILE:N	2.31	0.45
1:C:374:LYS:HE2	1:C:377:GLU:OE2	2.17	0.45
1:A:11:LEU:O	1:A:15:ILE:HG13	2.17	0.45
1:A:373:GLN:H	1:A:373:GLN:CD	2.16	0.45
1:D:150:ARG:HG3	1:D:154:ILE:CD1	2.46	0.45
1:B:110:ALA:HB2	1:B:137:LYS:HB3	1.98	0.45
1:A:80:TYR:HB3	1:A:84:TYR:HB3	1.98	0.44
1:A:151:LYS:HE3	1:A:151:LYS:N	2.25	0.44
1:A:331:ARG:CB	1:A:331:ARG:NH1	2.79	0.44
1:A:11:LEU:HD21	1:A:154:ILE:HD12	1.98	0.44
1:D:302:SER:HB2	1:D:303:PRO:HD3	1.99	0.44
1:B:174:MET:HG2	1:B:183:TYR:CD2	2.53	0.44
1:C:34:ASP:HA	1:C:37:GLN:HE22	1.82	0.44
1:D:128:THR:HB	1:D:315:TYR:HD1	1.83	0.44
1:A:100:VAL:O	1:A:104:GLU:HG3	2.16	0.44
1:A:191:PRO:HD3	1:B:358:TYR:CE2	2.52	0.44
1:D:204:GLN:HG2	1:D:205:ASP:N	2.32	0.44
1:A:194:GLU:HB2	1:B:349:VAL:HB	1.99	0.44
1:A:50:ARG:NH1	3:A:1289:HOH:O	2.50	0.44
1:A:252:GLY:O	1:A:271:GLU:HA	2.18	0.44
1:A:328:HIS:CD2	1:C:321:ALA:HA	2.53	0.44
1:B:126:GLU:CG	1:B:138:VAL:HG11	2.42	0.44
1:A:257:VAL:HG11	1:B:288:LEU:HD23	2.00	0.44
1:B:321:ALA:HA	1:D:328:HIS:CD2	2.53	0.44
1:C:66:VAL:HA	1:C:70:VAL:HB	2.00	0.44
1:D:133:LYS:HE2	1:D:135:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:HG3	1:A:54:SER:OG	2.17	0.43
1:B:172:TYR:CZ	1:B:199:MET:HG3	2.53	0.43
1:C:360:GLN:OE1	1:D:189:GLU:OE2	2.36	0.43
1:B:92:ARG:HB2	1:B:93:PRO:HD3	2.00	0.43
1:B:123:VAL:HG12	1:B:127:LEU:CD1	2.49	0.43
1:A:197:LYS:H	1:A:197:LYS:HG2	1.57	0.43
1:C:117:GLY:HA3	1:D:373:GLN:OE1	2.18	0.43
1:C:312:GLY:HA2	3:C:1083:HOH:O	2.19	0.43
1:D:7:TYR:CD2	1:D:48:ALA:HB2	2.53	0.43
1:D:64:GLU:OE1	1:D:98:HIS:HE1	2.01	0.43
1:D:154:ILE:O	1:D:157:ALA:HB3	2.19	0.43
1:D:316:ALA:O	1:D:320:GLU:HG3	2.19	0.43
1:D:341:LEU:HD22	1:D:346:VAL:HG22	2.00	0.43
1:B:122:GLN:NE2	1:B:143:ARG:HD3	2.33	0.43
1:A:122:GLN:OE1	1:A:143:ARG:HD3	2.19	0.43
1:C:109:GLU:HG2	1:C:137:LYS:CE	2.49	0.43
1:C:37:GLN:NE2	1:C:37:GLN:N	2.33	0.43
1:A:185:GLY:HA2	1:A:189:GLU:HG3	2.01	0.43
1:D:73:MET:CE	1:D:90:ILE:HG12	2.48	0.43
1:A:4:VAL:O	1:A:111:ILE:HA	2.19	0.43
1:A:179:LEU:O	1:A:272:THR:HG23	2.18	0.43
1:B:37:GLN:NE2	1:B:37:GLN:N	2.58	0.42
1:D:353:ALA:HA	1:D:354:PRO:HD3	1.90	0.42
1:A:90:ILE:CD1	1:A:179:LEU:HD12	2.49	0.42
1:B:101:ARG:O	1:B:105:GLU:HG3	2.19	0.42
1:D:92:ARG:HB2	1:D:93:PRO:HD3	2.01	0.42
1:A:174:MET:HA	1:A:182:SER:O	2.19	0.42
1:A:321:ALA:HA	1:C:328:HIS:CD2	2.55	0.42
1:B:136:ILE:HG13	1:B:137:LYS:N	2.34	0.42
1:C:172:TYR:CZ	1:C:199:MET:HG3	2.54	0.42
1:A:124:ARG:O	1:A:128:THR:HG23	2.19	0.42
1:A:331:ARG:HH11	1:A:331:ARG:HB2	1.84	0.42
1:C:360:GLN:O	1:C:363:VAL:HG22	2.20	0.42
1:B:238:LEU:HD23	1:B:238:LEU:O	2.19	0.42
1:A:7:TYR:CE2	1:A:9:GLY:HA2	2.54	0.42
1:A:15:ILE:HG23	1:A:156:TYR:CD2	2.55	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.83	0.42
1:D:205:ASP:OD2	1:D:207:GLU:HB2	2.20	0.42
1:A:350:GLY:C	1:A:351:ARG:HD2	2.38	0.42
1:A:117:GLY:HA3	1:B:373:GLN:NE2	2.35	0.42
1:D:71:PHE:HB2	1:D:72:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:GLY:C	1:C:351:ARG:HD2	2.40	0.42
1:B:238:LEU:HD23	1:B:238:LEU:C	2.40	0.41
1:D:34:ASP:HB2	1:D:41:VAL:HG11	2.02	0.41
1:D:171:PRO:HG2	1:D:172:TYR:H	1.84	0.41
1:A:181:ILE:HD12	1:A:202:MET:HB2	2.02	0.41
1:B:351:ARG:N	1:B:351:ARG:CD	2.80	0.41
1:C:80:TYR:HB3	1:C:84:TYR:HB3	2.02	0.41
1:C:343:LYS:HD2	1:D:343:LYS:HD2	2.02	0.41
1:D:359:ARG:NH2	1:D:361:ASP:OD1	2.52	0.41
1:C:224:ASP:HA	1:C:225:PRO:HD3	1.91	0.41
1:B:353:ALA:HA	1:B:354:PRO:HD3	1.91	0.41
1:A:345:ASN:HB3	1:A:347:TYR:CE1	2.56	0.41
1:C:40:GLU:O	1:C:43:GLU:N	2.50	0.41
1:D:360:GLN:O	1:D:364:SER:N	2.53	0.41
1:A:282:ARG:O	1:A:286:GLU:HG3	2.21	0.41
1:B:68:ASP:O	1:B:72:PRO:HG2	2.21	0.41
1:B:298:ARG:HD2	1:B:298:ARG:C	2.41	0.41
1:A:383:GLN:NE2	1:B:261:PHE:CZ	2.89	0.41
1:A:383:GLN:NE2	1:B:261:PHE:HZ	2.19	0.41
1:A:386:ARG:HA	1:C:264:MET:SD	2.61	0.41
1:B:350:GLY:C	1:B:351:ARG:HD2	2.41	0.41
1:B:392:LEU:O	1:B:395:ARG:HA	2.21	0.41
1:A:80:TYR:CD2	1:A:81:GLU:HG3	2.56	0.41
1:A:73:MET:CE	1:A:90:ILE:HG12	2.51	0.40
1:A:154:ILE:HG13	1:A:164:VAL:HG11	2.02	0.40
1:A:185:GLY:O	1:A:188:LEU:HB2	2.21	0.40
1:C:314:TRP:O	1:C:319:ARG:CD	2.69	0.40
1:C:359:ARG:NE	1:C:361:ASP:OD1	2.54	0.40
1:C:71:PHE:HB2	1:C:72:PRO:HD3	2.03	0.40
1:C:207:GLU:OE1	1:D:213:PRO:HG2	2.21	0.40
1:D:238:LEU:HD23	1:D:238:LEU:C	2.41	0.40
1:A:118:LYS:H	1:A:118:LYS:HD2	1.87	0.40
1:A:180:HIS:HB2	1:A:271:GLU:O	2.22	0.40
1:A:298:ARG:C	1:A:298:ARG:HD2	2.41	0.40
1:B:179:LEU:HD22	1:B:272:THR:CG2	2.50	0.40
1:D:195:PRO:HB3	1:D:199:MET:CE	2.51	0.40
1:D:359:ARG:NH2	3:D:1096:HOH:O	2.53	0.40
1:A:75:ARG:NH2	3:A:1346:HOH:O	2.54	0.40
1:A:154:ILE:CG2	1:A:155:ALA:N	2.84	0.40
1:B:196:PRO:HG2	1:B:199:MET:HB2	2.04	0.40
1:C:151:LYS:CD	1:C:151:LYS:N	2.58	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	374/400 (94%)	360 (96%)	13 (4%)	1 (0%)	41	50
1	B	376/400 (94%)	362 (96%)	13 (4%)	1 (0%)	41	50
1	C	380/400 (95%)	365 (96%)	14 (4%)	1 (0%)	41	50
1	D	379/400 (95%)	365 (96%)	14 (4%)	0	100	100
All	All	1509/1600 (94%)	1452 (96%)	54 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	GLN
1	A	147	PHE
1	C	159	ALA

### 5.3.2 Protein sidechains [i](#)

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	304/319 (95%)	289 (95%)	15 (5%)	25	35
1	B	306/319 (96%)	285 (93%)	21 (7%)	15	20
1	C	310/319 (97%)	292 (94%)	18 (6%)	20	27
1	D	309/319 (97%)	286 (93%)	23 (7%)	13	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1229/1276 (96%)	1152 (94%)	77 (6%)	18 24

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ILE
1	A	101	ARG
1	A	118	LYS
1	A	128	THR
1	A	145	TRP
1	A	151	LYS
1	A	154	ILE
1	A	172	TYR
1	A	179	LEU
1	A	180	HIS
1	A	239	LEU
1	A	267	ARG
1	A	319	ARG
1	A	351	ARG
1	A	373	GLN
1	B	37	GLN
1	B	62	LYS
1	B	90	ILE
1	B	94	LEU
1	B	118	LYS
1	B	121	ASP
1	B	128	THR
1	B	145	TRP
1	B	151	LYS
1	B	165	PRO
1	B	179	LEU
1	B	180	HIS
1	B	184	GLU
1	B	216	VAL
1	B	239	LEU
1	B	267	ARG
1	B	291	ASP
1	B	319	ARG
1	B	351	ARG
1	B	355	LYS
1	B	361	ASP
1	C	22	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	37	GLN
1	C	62	LYS
1	C	101	ARG
1	C	145	TRP
1	C	150	ARG
1	C	151	LYS
1	C	158	GLU
1	C	179	LEU
1	C	180	HIS
1	C	188	LEU
1	C	197	LYS
1	C	239	LEU
1	C	267	ARG
1	C	319	ARG
1	C	351	ARG
1	C	361	ASP
1	C	373	GLN
1	D	25	ARG
1	D	37	GLN
1	D	39	GLU
1	D	62	LYS
1	D	90	ILE
1	D	94	LEU
1	D	128	THR
1	D	137	LYS
1	D	145	TRP
1	D	179	LEU
1	D	180	HIS
1	D	188	LEU
1	D	239	LEU
1	D	264	MET
1	D	267	ARG
1	D	291	ASP
1	D	319	ARG
1	D	351	ARG
1	D	360	GLN
1	D	361	ASP
1	D	364	SER
1	D	371	TYR
1	D	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	249	HIS
1	A	323	GLN
1	A	373	GLN
1	B	37	GLN
1	B	98	HIS
1	B	122	GLN
1	B	249	HIS
1	B	323	GLN
1	B	360	GLN
1	C	37	GLN
1	C	98	HIS
1	C	122	GLN
1	C	323	GLN
1	C	360	GLN
1	C	373	GLN
1	D	37	GLN
1	D	98	HIS
1	D	122	GLN
1	D	148	GLN
1	D	249	HIS
1	D	297	GLN
1	D	323	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	510	-	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	C	2510	-	4,4,4	0.47	0	6,6,6	0.07	0
2	SO4	B	1510	-	4,4,4	0.36	0	6,6,6	0.21	0
2	SO4	D	3510	-	4,4,4	0.43	0	6,6,6	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	380/400 (95%)	-0.03	8 (2%) 63 70	20, 31, 54, 70	0
1	B	382/400 (95%)	-0.14	5 (1%) 77 81	22, 31, 48, 83	0
1	C	386/400 (96%)	0.12	17 (4%) 34 41	23, 34, 60, 82	0
1	D	385/400 (96%)	0.14	21 (5%) 25 31	20, 34, 59, 82	0
All	All	1533/1600 (95%)	0.02	51 (3%) 46 53	20, 32, 56, 83	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	365	PHE	4.4
1	C	165	PRO	4.2
1	D	165	PRO	4.1
1	B	360	GLN	3.9
1	D	163	PRO	3.8
1	D	164	VAL	3.7
1	D	40	GLU	3.2
1	D	362	LEU	3.2
1	D	371	TYR	3.1
1	D	361	ASP	3.1
1	A	154	ILE	3.0
1	B	361	ASP	3.0
1	A	157	ALA	3.0
1	D	41	VAL	2.9
1	C	50	ARG	2.8
1	B	165	PRO	2.8
1	C	157	ALA	2.8
1	C	43	GLU	2.7
1	D	154	ILE	2.7
1	A	162	ILE	2.7
1	D	161	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	163	PRO	2.6
1	D	300	MET	2.6
1	D	44	ALA	2.5
1	D	364	SER	2.4
1	A	41	VAL	2.4
1	A	165	PRO	2.4
1	C	361	ASP	2.4
1	C	161	GLY	2.4
1	C	40	GLU	2.4
1	C	41	VAL	2.4
1	D	159	ALA	2.3
1	A	395	ARG	2.3
1	C	395	ARG	2.3
1	D	363	VAL	2.3
1	D	50	ARG	2.3
1	C	162	ILE	2.3
1	C	364	SER	2.2
1	B	40	GLU	2.2
1	C	232	ARG	2.1
1	C	46	GLU	2.1
1	D	49	LEU	2.1
1	D	395	ARG	2.1
1	C	163	PRO	2.1
1	A	161	GLY	2.1
1	B	300	MET	2.0
1	D	51	THR	2.0
1	C	48	ALA	2.0
1	D	162	ILE	2.0
1	C	18	LYS	2.0
1	D	58	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	510	5/5	0.98	0.15	43,44,46,46	0
2	SO4	C	2510	5/5	0.98	0.11	50,51,53,55	0
2	SO4	B	1510	5/5	0.99	0.12	41,44,47,49	0
2	SO4	D	3510	5/5	0.99	0.11	45,49,51,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.