



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:28 AM EDT

PDB ID : 2R6A / pdb_00002r6a
Title : Crystal Form BH1
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on : 2007-09-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

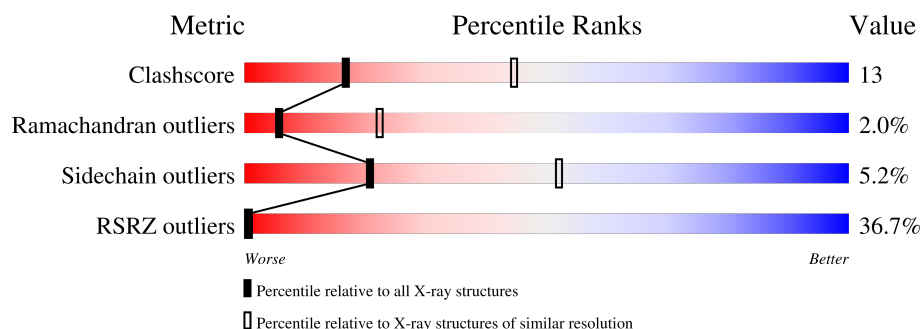
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	454	30% 67% 22% 7%
1	B	454	32% 57% 21% 18%
2	C	143	42% 80% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7352 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 Replicative helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3268	2045	574	635	14			
1	B	374	Total	C	N	O	S	0	0	0
			2889	1826	494	558	11			

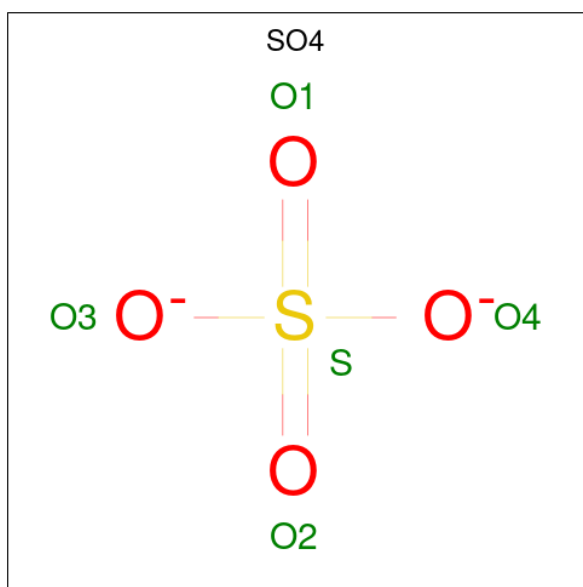
- Molecule 2 is a protein called DnaG Primase, Helicase Binding Domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	141	Total	C	N	O	Se	0	0	0
			1145	727	203	209	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	GLU	ASP	conflict	UNP Q9X4D0
C	531	LEU	VAL	conflict	UNP Q9X4D0

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



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

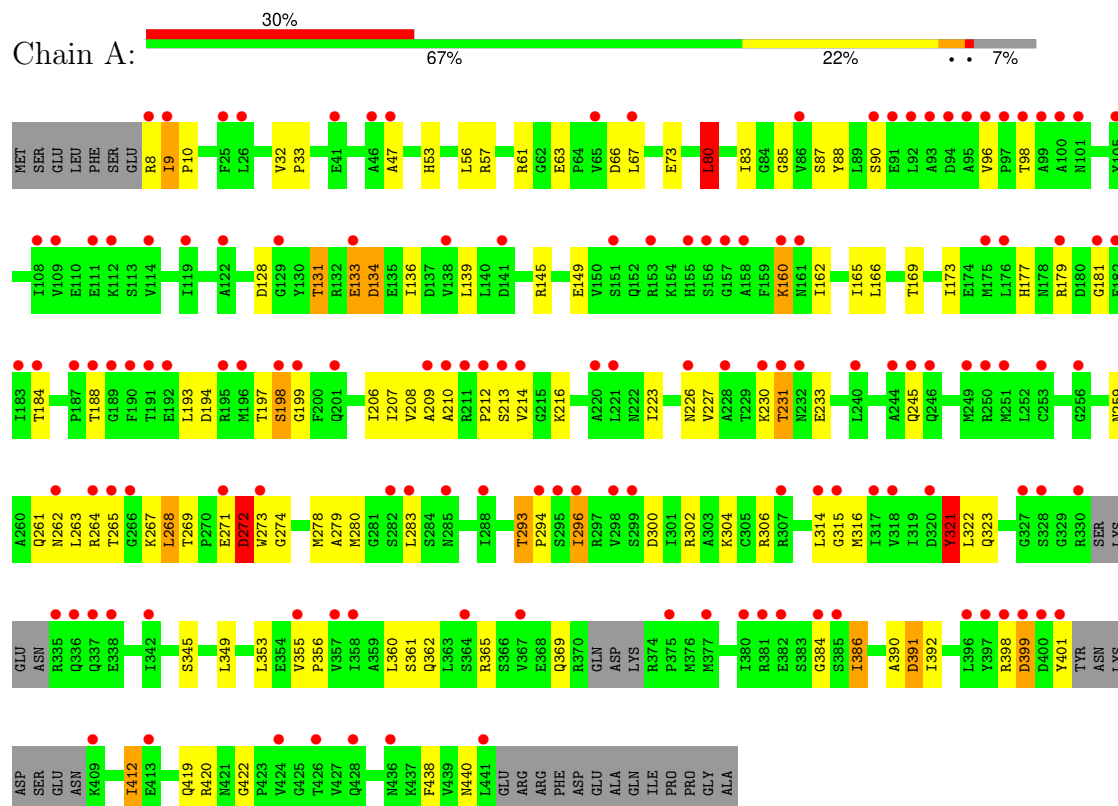
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	10	Total	O	0	0
			10	10		
4	C	5	Total	O	0	0
			5	5		

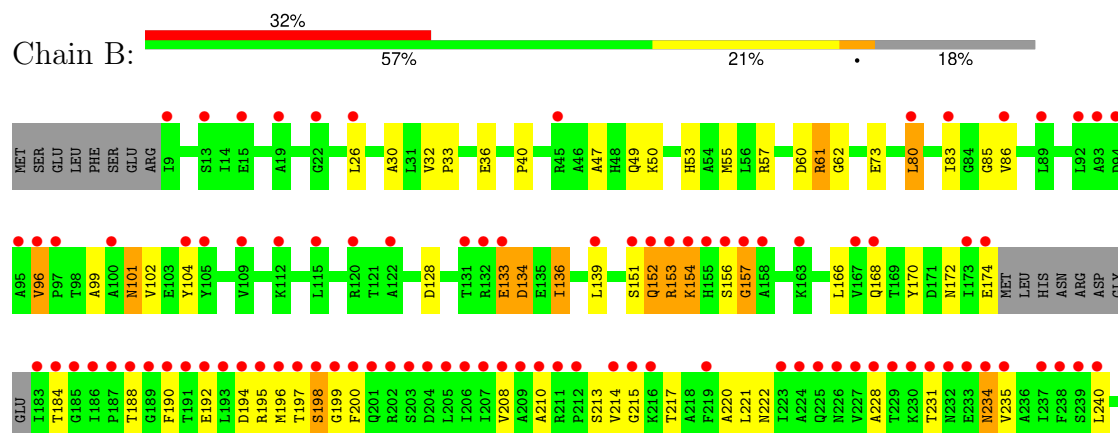
3 Residue-property plots

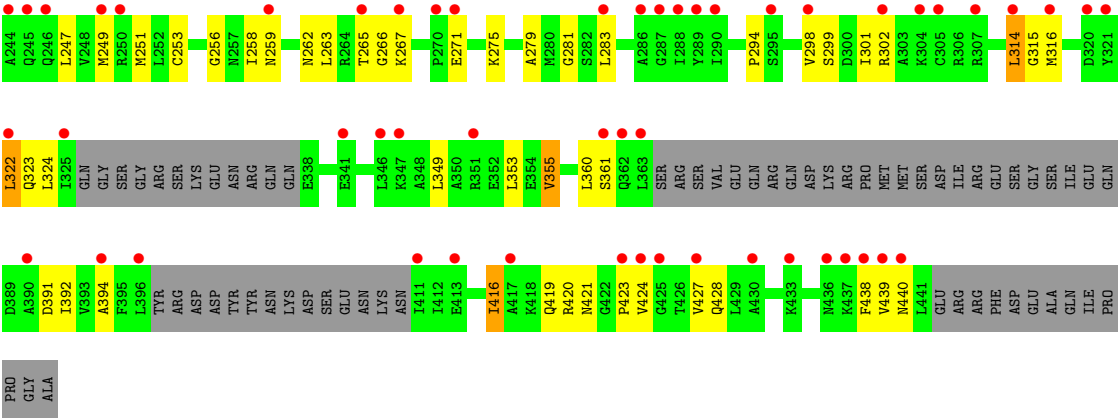
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Replicative helicase

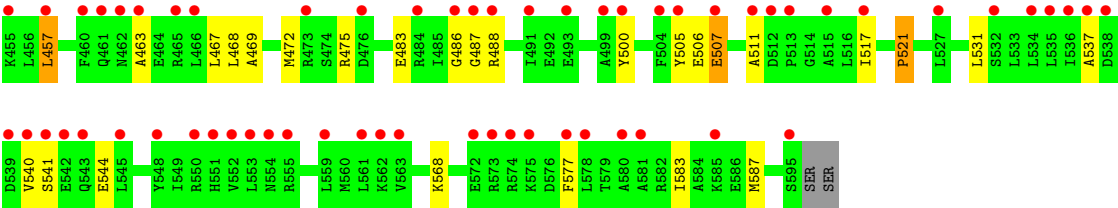
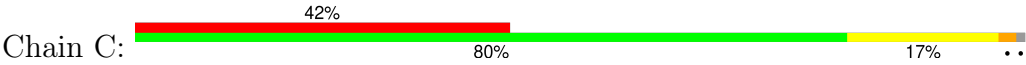


• Molecule 1: Replicative helicase





● Molecule 2: DnaG Primase, Helicase Binding Domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.75Å 226.75Å 75.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.88 – 2.90 49.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.88-2.90) 99.7 (49.88-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.259 , 0.297 0.268 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7352	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	2/3306 (0.1%)	1.00	10/4464 (0.2%)
1	B	0.54	0/2922	1.01	10/3953 (0.3%)
2	C	0.57	2/1157 (0.2%)	0.95	1/1544 (0.1%)
All	All	0.57	4/7385 (0.1%)	1.00	21/9961 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	507	GLU	CD-OE2	7.10	1.38	1.25
2	C	507	GLU	CD-OE1	6.86	1.38	1.25
1	A	88	TYR	CA-CB	6.66	1.64	1.53
1	A	133	GLU	CA-C	5.26	1.57	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	GLU	N-CA-C	10.80	128.24	114.31
2	C	577	PHE	N-CA-C	8.10	120.11	111.28
1	B	61	ARG	N-CA-C	7.18	122.14	113.23
1	A	293	THR	CA-C-N	6.98	128.56	119.84
1	A	293	THR	C-N-CA	6.98	128.56	119.84
1	B	133	GLU	CA-C-N	6.79	133.93	121.70
1	B	133	GLU	C-N-CA	6.79	133.93	121.70
1	A	133	GLU	CA-C-N	6.50	133.40	121.70
1	A	133	GLU	C-N-CA	6.50	133.40	121.70
1	A	133	GLU	N-CA-C	6.36	122.11	113.21
1	B	281	GLY	N-CA-C	-6.33	104.83	112.49
1	A	422	GLY	CA-C-N	5.95	125.93	120.21
1	A	422	GLY	C-N-CA	5.95	125.93	120.21
1	A	272	ASP	N-CA-C	-5.72	105.56	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	SER	N-CA-C	5.72	118.05	108.73
1	B	152	GLN	N-CA-C	-5.50	100.05	109.24
1	B	198	SER	N-CA-C	5.43	119.12	111.52
1	A	321	TYR	N-CA-C	5.36	122.21	110.80
1	B	136	ILE	CB-CA-C	-5.28	105.12	111.88
1	B	228	ALA	N-CA-C	5.13	117.77	111.82
1	A	80	LEU	N-CA-C	5.05	117.19	111.02

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	3268	0	3309	98	0
1	B	2889	0	2956	82	0
2	C	1145	0	1173	15	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0
All	All	7352	0	7438	189	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 13.

All (189) 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:A:133:GLU:N	1:A:134:ASP:HB2	1.53	1.22
1:B:153:ARG:HA	1:B:154:LYS:CB	1.76	1.15
1:A:398:ARG:HD2	1:A:401:TYR:CE1	1.84	1.12
1:B:314:LEU:HB2	1:B:315:GLY:HA3	1.34	1.05
1:B:153:ARG:HA	1:B:154:LYS:HB2	1.34	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HG2	1:A:412:ILE:HG12	1.40	1.02
1:B:314:LEU:HB2	1:B:315:GLY:CA	1.88	1.02
1:A:133:GLU:N	1:A:134:ASP:CB	2.24	1.00
1:A:133:GLU:H	1:A:134:ASP:HB2	0.85	0.99
1:A:133:GLU:H	1:A:134:ASP:CB	1.77	0.98
1:B:133:GLU:H	1:B:134:ASP:HB3	1.29	0.97
1:A:8:ARG:HB3	1:A:9:ILE:HA	1.47	0.97
1:A:398:ARG:HD2	1:A:401:TYR:CZ	2.02	0.93
1:A:207:ILE:HD12	1:A:390:ALA:HB2	1.52	0.91
1:B:133:GLU:N	1:B:134:ASP:HB3	1.85	0.90
1:A:412:ILE:HG21	1:A:438:PHE:HE2	1.41	0.85
1:B:153:ARG:HA	1:B:154:LYS:HB3	1.57	0.82
1:A:398:ARG:CG	1:A:412:ILE:HG12	2.09	0.81
1:A:207:ILE:HD13	1:A:386:ILE:HG22	1.61	0.81
1:B:153:ARG:CA	1:B:154:LYS:HB2	2.10	0.80
1:B:133:GLU:H	1:B:134:ASP:CB	1.96	0.79
1:B:153:ARG:CA	1:B:154:LYS:CB	2.59	0.76
1:A:296:ILE:HG22	1:A:300:ASP:HB2	1.66	0.76
1:B:271:GLU:O	1:B:275:LYS:HB2	1.87	0.75
1:A:8:ARG:CB	1:A:9:ILE:HA	2.13	0.74
1:A:412:ILE:HG21	1:A:438:PHE:CE2	2.24	0.73
1:A:398:ARG:CD	1:A:401:TYR:CZ	2.71	0.73
1:B:168:GLN:O	1:B:172:ASN:HB2	1.89	0.72
1:A:188:THR:HG21	1:A:193:LEU:HD23	1.70	0.72
1:B:214:VAL:H	1:B:215:GLY:HA2	1.55	0.70
1:A:398:ARG:HG2	1:A:412:ILE:CG1	2.18	0.70
2:C:487:GLY:HA2	2:C:488:ARG:HB2	1.74	0.70
1:A:302:ARG:HG2	1:A:349:LEU:HD13	1.73	0.69
1:A:198:SER:N	1:A:199:GLY:HA2	2.06	0.68
1:A:207:ILE:CD1	1:A:386:ILE:HG22	2.24	0.67
1:B:188:THR:HG23	1:B:190:PHE:H	1.59	0.67
1:A:227:VAL:O	1:A:231:THR:HG22	1.95	0.67
1:B:104:TYR:CE2	2:C:537:ALA:HB2	2.30	0.67
1:A:8:ARG:HB3	1:A:9:ILE:CA	2.24	0.65
1:B:99:ALA:O	1:B:102:VAL:HG23	1.96	0.65
1:A:269:THR:OG1	1:A:272:ASP:HB2	1.97	0.65
1:B:152:GLN:HA	1:B:153:ARG:HB3	1.78	0.64
1:A:304:LYS:HE2	1:B:157:GLY:HA2	1.79	0.64
1:B:314:LEU:CB	1:B:315:GLY:HA3	2.22	0.63
1:A:398:ARG:CD	1:A:401:TYR:OH	2.46	0.62
1:B:152:GLN:HA	1:B:153:ARG:CB	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:486:GLY:H	2:C:488:ARG:HB2	1.64	0.62
1:B:61:ARG:NH2	1:B:73:GLU:OE1	2.27	0.62
1:A:61:ARG:NH1	1:A:63:GLU:OE1	2.32	0.62
2:C:583:ILE:O	2:C:587:MSE:HG3	2.01	0.61
1:A:267:LYS:O	1:A:268:LEU:HD23	2.01	0.61
1:B:314:LEU:HB2	1:B:315:GLY:HA2	1.77	0.61
1:B:128:ASP:HB3	1:B:139:LEU:HD21	1.84	0.60
1:B:234:ASN:N	1:B:234:ASN:HD22	2.00	0.60
1:A:188:THR:HG23	1:A:223:ILE:HG12	1.83	0.60
1:B:214:VAL:H	1:B:215:GLY:CA	2.14	0.60
1:A:274:GLY:O	1:A:278:MET:HG3	2.02	0.59
1:A:391:ASP:HB3	1:A:420:ARG:HH11	1.68	0.59
1:B:217:THR:O	1:B:221:LEU:HG	2.03	0.59
2:C:541:SER:HB3	2:C:544:GLU:HG3	1.85	0.59
1:A:207:ILE:HD13	1:A:386:ILE:CG2	2.32	0.58
1:A:32:VAL:HB	1:A:33:PRO:HD3	1.85	0.58
2:C:517:ILE:HG22	2:C:517:ILE:O	2.04	0.58
1:A:177:HIS:C	1:A:179:ARG:H	2.12	0.58
1:B:133:GLU:N	1:B:134:ASP:CB	2.59	0.57
1:B:235:VAL:HG12	1:B:316:MET:HB3	1.87	0.57
1:A:398:ARG:HD2	1:A:401:TYR:OH	2.03	0.57
1:A:8:ARG:HG2	1:A:10:PRO:HD3	1.86	0.57
1:A:133:GLU:N	1:A:134:ASP:HB3	2.19	0.56
1:B:80:LEU:HD22	1:B:85:GLY:HA2	1.88	0.56
1:B:30:ALA:O	1:B:33:PRO:HD2	2.05	0.56
2:C:505:TYR:C	2:C:507:GLU:H	2.13	0.56
1:B:30:ALA:HB1	1:B:102:VAL:HG21	1.87	0.56
1:B:61:ARG:N	1:B:62:GLY:HA2	2.20	0.56
1:A:208:VAL:HB	1:A:360:LEU:HD23	1.89	0.55
1:A:206:ILE:HG12	1:A:392:ILE:CG2	2.37	0.55
1:B:26:LEU:HD22	1:B:96:VAL:HG12	1.88	0.54
1:A:233:GLU:CG	1:A:315:GLY:HA3	2.37	0.54
1:A:321:TYR:H	1:A:360:LEU:HB2	1.71	0.54
1:A:316:MET:HG2	1:A:356:PRO:HG2	1.88	0.54
1:A:323:GLN:HE21	1:A:362:GLN:H	1.54	0.54
1:A:233:GLU:HG3	1:A:315:GLY:HA3	1.90	0.53
1:A:384:GLY:HA2	1:A:386:ILE:H	1.73	0.53
1:B:258:ILE:HG21	1:B:263:LEU:HD11	1.88	0.53
1:B:210:ALA:HB1	1:B:214:VAL:HG11	1.91	0.53
1:A:398:ARG:HD2	1:A:401:TYR:HE1	1.61	0.53
1:A:61:ARG:NH2	1:A:73:GLU:OE1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:CG	1:A:412:ILE:CG1	2.82	0.52
1:B:198:SER:N	1:B:199:GLY:HA2	2.23	0.52
2:C:486:GLY:N	2:C:488:ARG:HB2	2.24	0.52
2:C:500:TYR:CZ	2:C:521:PRO:HD3	2.44	0.52
1:A:214:VAL:O	1:A:398:ARG:NH2	2.42	0.52
1:B:40:PRO:O	1:B:49:GLN:HG3	2.10	0.51
1:A:214:VAL:O	1:A:398:ARG:CZ	2.59	0.51
1:B:314:LEU:HD13	1:B:355:VAL:HG21	1.94	0.50
1:A:184:THR:N	1:A:198:SER:O	2.45	0.50
1:A:398:ARG:CD	1:A:401:TYR:CE1	2.76	0.50
1:A:80:LEU:HD22	1:A:85:GLY:HA2	1.94	0.50
1:A:198:SER:H	1:A:199:GLY:HA2	1.75	0.50
1:A:206:ILE:HG12	1:A:392:ILE:HG21	1.94	0.50
1:A:209:ALA:HA	1:A:361:SER:O	2.12	0.49
1:B:279:ALA:O	1:B:283:LEU:HB2	2.12	0.49
1:B:299:SER:HA	1:B:302:ARG:HG3	1.94	0.49
1:B:214:VAL:N	1:B:215:GLY:HA2	2.22	0.49
1:A:279:ALA:O	1:A:283:LEU:HB2	2.12	0.49
1:B:192:GLU:HG3	1:B:195:ARG:NH2	2.26	0.49
1:A:197:THR:O	1:A:198:SER:HB2	2.12	0.49
1:B:30:ALA:C	1:B:33:PRO:HD2	2.38	0.49
1:B:208:VAL:HB	1:B:360:LEU:HD23	1.95	0.49
1:B:222:ASN:ND2	1:B:438:PHE:H	2.11	0.48
1:B:259:ASN:HB3	1:B:262:ASN:OD1	2.13	0.48
1:A:212:PRO:O	1:A:213:SER:HB2	2.14	0.48
1:B:256:GLY:O	1:B:275:LYS:HD3	2.14	0.48
1:A:57:ARG:HH21	1:A:73:GLU:HG3	1.78	0.47
1:A:261:GLN:HA	1:A:264:ARG:HD2	1.96	0.47
1:A:188:THR:HB	1:A:194:ASP:OD1	2.13	0.47
1:A:365:ARG:O	1:A:369:GLN:HG2	2.14	0.47
1:A:293:THR:HA	1:A:294:PRO:HD2	1.70	0.47
1:A:160:LYS:HG3	1:A:165:ILE:HD11	1.96	0.47
1:B:47:ALA:HA	1:B:83:ILE:HG22	1.97	0.47
1:B:83:ILE:C	1:B:83:ILE:HD12	2.40	0.47
1:A:259:ASN:HD22	1:A:262:ASN:HB2	1.79	0.46
1:B:391:ASP:CG	1:B:420:ARG:HD3	2.40	0.46
1:A:259:ASN:O	1:A:262:ASN:HB3	2.15	0.46
1:B:200:PHE:HD2	1:B:316:MET:HE3	1.80	0.46
1:B:256:GLY:O	1:B:275:LYS:HG2	2.16	0.46
1:B:349:LEU:HD12	1:B:353:LEU:HD13	1.97	0.46
1:B:322:LEU:HD22	1:B:361:SER:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:457:LEU:HB2	4:C:599:HOH:O	2.15	0.46
2:C:463:ALA:O	2:C:467:LEU:HB2	2.16	0.46
1:A:169:THR:O	1:A:173:ILE:HG12	2.15	0.46
1:A:90:SER:OG	2:C:568:LYS:HE3	2.16	0.46
1:A:128:ASP:HB3	1:A:139:LEU:HD21	1.98	0.46
1:B:240:LEU:HD12	1:B:324:LEU:HB2	1.98	0.45
1:B:188:THR:HG22	1:B:194:ASP:OD1	2.16	0.45
1:B:196:MET:O	1:B:423:PRO:HD2	2.17	0.45
1:B:53:HIS:HE1	1:B:57:ARG:HH11	1.65	0.44
1:B:416:ILE:HD11	1:B:424:VAL:HA	1.97	0.44
1:B:184:THR:N	1:B:198:SER:O	2.50	0.44
1:B:214:VAL:CG1	1:B:215:GLY:HA2	2.47	0.44
1:B:222:ASN:HD22	1:B:438:PHE:HD1	1.65	0.44
1:A:66:ASP:OD1	1:A:66:ASP:C	2.61	0.44
1:A:207:ILE:HD12	1:A:390:ALA:CB	2.37	0.44
1:A:399:ASP:OD1	1:A:399:ASP:N	2.51	0.44
1:B:32:VAL:HB	1:B:33:PRO:HD3	2.00	0.44
1:B:298:VAL:O	1:B:301:ILE:HB	2.17	0.44
1:A:384:GLY:HA2	1:A:386:ILE:HG13	1.99	0.44
1:B:208:VAL:HA	1:B:394:ALA:O	2.19	0.43
1:A:61:ARG:HH11	1:A:63:GLU:CD	2.25	0.43
1:A:263:LEU:HD23	1:A:268:LEU:HD21	1.99	0.43
1:A:296:ILE:CG2	1:A:300:ASP:HB2	2.44	0.43
1:A:345:SER:OG	1:B:36:GLU:OE2	2.33	0.43
2:C:469:ALA:HA	2:C:472:MSE:HE2	2.00	0.43
1:A:280:MET:HE3	1:B:166:LEU:HB3	2.00	0.43
1:A:197:THR:HA	1:A:419:GLN:OE1	2.19	0.43
1:B:101:ASN:ND2	1:B:101:ASN:H	2.17	0.43
1:A:268:LEU:HD12	1:A:273:TRP:CE3	2.53	0.43
1:B:392:ILE:HG12	1:B:419:GLN:HG3	2.01	0.43
1:B:234:ASN:O	1:B:315:GLY:HA2	2.19	0.43
1:B:249:MET:HE3	1:B:249:MET:HB3	1.96	0.43
1:A:47:ALA:HA	1:A:83:ILE:HG22	2.00	0.42
1:B:101:ASN:H	1:B:101:ASN:HD22	1.68	0.42
1:A:131:THR:O	1:A:133:GLU:HB2	2.19	0.42
1:A:162:ILE:O	1:A:166:LEU:HG	2.19	0.42
1:B:265:THR:O	1:B:267:LYS:N	2.53	0.42
1:B:439:VAL:HG12	1:B:440:ASN:N	2.35	0.42
1:A:233:GLU:HG2	1:A:315:GLY:HA3	2.01	0.42
1:A:177:HIS:C	1:A:179:ARG:N	2.78	0.42
1:A:314:LEU:HD13	1:A:353:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD23	1:B:251:MET:HE2	2.02	0.41
1:B:196:MET:HE2	1:B:196:MET:HA	2.01	0.41
1:A:321:TYR:HA	1:A:360:LEU:O	2.21	0.41
1:B:170:TYR:C	1:B:172:ASN:H	2.28	0.41
2:C:472:MSE:HE1	2:C:531:LEU:HB2	2.01	0.41
1:B:197:THR:HB	1:B:199:GLY:O	2.21	0.41
1:A:296:ILE:HG22	1:A:300:ASP:CB	2.44	0.41
1:B:220:ALA:HB2	1:B:360:LEU:HD11	2.03	0.41
1:A:83:ILE:C	1:A:83:ILE:HD12	2.46	0.41
1:A:133:GLU:CA	1:A:134:ASP:CB	2.97	0.41
1:A:145:ARG:NH1	1:A:149:GLU:OE2	2.54	0.41
1:A:53:HIS:CD2	1:A:57:ARG:NH1	2.89	0.41
1:A:226:ASN:O	1:A:230:LYS:HB2	2.20	0.41
1:B:249:MET:O	1:B:253:CYS:HB2	2.20	0.41
1:A:133:GLU:CA	1:A:134:ASP:HB2	2.43	0.40
1:A:179:ARG:HD2	1:A:179:ARG:HA	1.69	0.40
1:A:245:GLN:HE22	1:B:421:ASN:HA	1.85	0.40
1:B:427:VAL:HG12	1:B:428:GLN:N	2.36	0.40
2:C:475:ARG:CZ	2:C:505:TYR:HB2	2.52	0.40
1:A:210:ALA:HB3	1:A:216:LYS:HB3	2.03	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	412/454 (91%)	380 (92%)	26 (6%)	6 (2%)	8	28
1	B	364/454 (80%)	341 (94%)	14 (4%)	9 (2%)	4	17
2	C	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	5	20
All	All	915/1051 (87%)	846 (92%)	51 (6%)	18 (2%)	6	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	A	321	TYR
1	B	134	ASP
1	B	154	LYS
1	B	156	SER
1	B	266	GLY
1	B	294	PRO
1	A	198	SER
1	B	157	GLY
1	A	131	THR
1	A	181	GLY
1	B	153	ARG
1	B	213	SER
2	C	511	ALA
1	B	314	LEU
2	C	506	GLU
1	A	440	ASN
2	C	521	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	354/386 (92%)	332 (94%)	22 (6%)	16	46
1	B	313/386 (81%)	298 (95%)	15 (5%)	23	55
2	C	120/116 (103%)	116 (97%)	4 (3%)	33	67
All	All	787/888 (89%)	746 (95%)	41 (5%)	21	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	56	LEU
1	A	67	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	LEU
1	A	87	SER
1	A	96	VAL
1	A	98	THR
1	A	136	ILE
1	A	160	LYS
1	A	231	THR
1	A	265	THR
1	A	268	LEU
1	A	271	GLU
1	A	272	ASP
1	A	296	ILE
1	A	306	ARG
1	A	322	LEU
1	A	355	VAL
1	A	386	ILE
1	A	391	ASP
1	A	399	ASP
1	A	412	ILE
1	B	50	LYS
1	B	55	MET
1	B	60	ASP
1	B	80	LEU
1	B	86	VAL
1	B	96	VAL
1	B	101	ASN
1	B	136	ILE
1	B	174	GLU
1	B	231	THR
1	B	234	ASN
1	B	322	LEU
1	B	323	GLN
1	B	355	VAL
1	B	416	ILE
2	C	457	LEU
2	C	468	LEU
2	C	483	GLU
2	C	540	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	225	GLN
1	A	226	ASN
1	A	245	GLN
1	A	259	ASN
1	A	261	GLN
1	A	262	ASN
1	A	323	GLN
1	A	369	GLN
1	A	388	GLN
1	B	18	GLN
1	B	53	HIS
1	B	101	ASN
1	B	222	ASN
1	B	234	ASN
1	B	245	GLN
1	B	257	ASN
1	B	436	ASN
2	C	551	HIS

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 oligosaccharides 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	$\# Z > 2$
3	SO4	A	500	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	B	1002	-	4,4,4	0.28	0	6,6,6	0.22	0
3	SO4	A	1001	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	B	500	-	4,4,4	0.26	0	6,6,6	0.16	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	420/454 (92%)	1.72	136 (32%)  	28, 98, 121, 134	0
1	B	374/454 (82%)	1.94	145 (38%)  	29, 98, 106, 135	0
2	C	135/143 (94%)	1.96	60 (44%)  	77, 99, 109, 121	0
All	All	929/1051 (88%)	1.84	341 (36%)  	28, 98, 112, 135	0

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ARG	7.3
1	B	440	ASN	6.1
1	B	193	LEU	5.4
1	A	409	LYS	5.4
1	B	439	VAL	5.3
1	B	417	ALA	5.3
1	A	133	GLU	5.3
1	A	441	LEU	5.3
1	B	210	ALA	5.2
1	B	239	SER	5.2
1	A	95	ALA	5.2
1	A	399	ASP	5.1
1	B	396	LEU	5.1
1	A	401	TYR	5.1
1	B	267	LYS	5.0
1	B	363	LEU	5.0
1	B	202	ARG	4.8
1	B	207	ILE	4.7
1	A	158	ALA	4.7
2	C	463	ALA	4.6
1	A	367	VAL	4.6
1	A	192	GLU	4.5
1	B	191	THR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	4.4
2	C	461	GLN	4.4
2	C	535	LEU	4.4
1	B	9	ILE	4.3
1	B	155	HIS	4.3
1	A	400	ASP	4.3
1	A	92	LEU	4.3
1	B	185	GLY	4.3
1	B	183	ILE	4.2
1	B	190	PHE	4.2
1	B	304	LYS	4.2
1	A	330	ARG	4.2
1	B	200	PHE	4.2
2	C	537	ALA	4.2
1	B	188	THR	4.1
1	B	153	ARG	4.1
1	A	271	GLU	4.1
1	B	187	PRO	4.1
1	A	99	ALA	4.1
1	B	195	ARG	4.1
1	A	94	ASP	4.0
1	A	93	ALA	4.0
1	B	225	GLN	4.0
2	C	555	ARG	4.0
2	C	554	ASN	4.0
1	A	96	VAL	4.0
1	B	289	TYR	3.9
1	B	209	ALA	3.9
1	B	199	GLY	3.9
1	A	295	SER	3.9
1	B	249	MET	3.8
1	A	428	GLN	3.8
1	B	122	ALA	3.8
1	B	204	ASP	3.8
1	B	216	LYS	3.8
1	B	219	PHE	3.8
1	B	214	VAL	3.8
1	B	194	ASP	3.8
1	B	205	LEU	3.8
1	B	186	ILE	3.7
1	B	230	LYS	3.7
2	C	580	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	197	THR	3.7
1	B	231	THR	3.7
2	C	578	LEU	3.7
1	A	228	ALA	3.7
2	C	511	ALA	3.7
2	C	577	PHE	3.7
1	B	154	LYS	3.7
1	B	184	THR	3.7
1	A	86	VAL	3.7
1	B	325	ILE	3.7
1	A	189	GLY	3.7
1	B	211	ARG	3.7
1	B	307	ARG	3.6
1	B	411	ILE	3.6
1	A	100	ALA	3.6
1	A	327	GLY	3.6
1	A	97	PRO	3.6
1	A	328	SER	3.5
1	A	105	TYR	3.5
1	B	295	SER	3.5
2	C	462	ASN	3.5
1	A	266	GLY	3.5
2	C	513	PRO	3.5
1	A	161	ASN	3.5
1	B	157	GLY	3.4
1	B	198	SER	3.4
2	C	512	ASP	3.4
2	C	575	LYS	3.4
1	B	438	PHE	3.4
2	C	553	LEU	3.4
1	B	173	ILE	3.4
1	A	336	GLN	3.4
2	C	538	ASP	3.4
1	A	9	ILE	3.3
1	B	229	THR	3.3
2	C	499	ALA	3.3
1	B	96	VAL	3.3
1	A	213	SER	3.2
1	A	210	ALA	3.2
1	B	26	LEU	3.2
2	C	550	ARG	3.2
1	B	298	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	168	GLN	3.2
1	A	273	TRP	3.2
1	A	220	ALA	3.2
1	B	192	GLU	3.2
1	B	423	PRO	3.2
2	C	545	LEU	3.2
1	B	132	ARG	3.1
1	A	364	SER	3.1
1	A	176	LEU	3.1
1	B	131	THR	3.1
1	B	86	VAL	3.1
1	B	436	ASN	3.1
1	A	211	ARG	3.1
1	B	430	ALA	3.0
2	C	548	TYR	3.0
1	A	91	GLU	3.0
1	B	15	GLU	3.0
1	B	115	LEU	3.0
1	B	321	TYR	3.0
1	B	189	GLY	3.0
1	A	314	LEU	3.0
2	C	561	LEU	3.0
1	A	184	THR	3.0
1	B	93	ALA	3.0
1	A	195	ARG	3.0
2	C	491	ILE	3.0
1	B	314	LEU	3.0
1	A	191	THR	3.0
1	B	158	ALA	3.0
2	C	473	ARG	3.0
1	A	181	GLY	3.0
1	A	232	ASN	3.0
1	A	212	PRO	3.0
1	B	320	ASP	2.9
1	A	253	CYS	2.9
1	B	212	PRO	2.9
1	A	230	LYS	2.9
1	B	206	ILE	2.9
2	C	559	LEU	2.9
1	B	232	ASN	2.9
1	A	65	VAL	2.9
1	A	221	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	322	LEU	2.9
2	C	486	GLY	2.8
1	A	413	GLU	2.8
1	A	335	ARG	2.8
1	B	89	LEU	2.8
1	B	240	LEU	2.8
1	B	290	ILE	2.8
2	C	488	ARG	2.8
1	A	190	PHE	2.8
1	B	238	PHE	2.8
2	C	460	PHE	2.8
1	A	296	ILE	2.8
1	A	358	ILE	2.8
1	A	157	GLY	2.8
1	A	337	GLN	2.8
1	A	298	VAL	2.8
2	C	551	HIS	2.8
1	B	215	GLY	2.8
2	C	542	GLU	2.7
1	A	183	ILE	2.7
1	B	163	LYS	2.7
2	C	455	LYS	2.7
1	B	287	GLY	2.7
1	B	227	VAL	2.7
1	B	196	MET	2.7
1	B	151	SER	2.7
1	A	182	GLU	2.7
1	A	382	GLU	2.7
1	B	224	ALA	2.7
1	A	384	GLY	2.7
1	B	413	GLU	2.7
1	B	424	VAL	2.7
2	C	552	VAL	2.7
1	B	80	LEU	2.7
2	C	466	LEU	2.7
1	A	285	ASN	2.7
1	B	152	GLN	2.7
1	B	361	SER	2.7
2	C	517	ILE	2.6
1	A	122	ALA	2.6
1	B	100	ALA	2.6
1	A	196	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	265	THR	2.6
1	A	201	GLN	2.6
1	A	245	GLN	2.6
1	B	109	VAL	2.6
1	A	299	SER	2.6
1	A	385	SER	2.6
2	C	541	SER	2.6
1	A	397	TYR	2.6
2	C	500	TYR	2.6
1	A	187	PRO	2.6
1	B	425	GLY	2.6
2	C	540	VAL	2.6
1	B	316	MET	2.6
1	B	394	ALA	2.6
1	B	104	TYR	2.6
1	B	201	GLN	2.6
2	C	543	GLN	2.6
1	A	90	SER	2.6
1	A	375	PRO	2.6
1	B	208	VAL	2.6
1	B	286	ALA	2.6
1	A	26	LEU	2.5
1	A	8	ARG	2.5
1	A	141	ASP	2.5
1	B	92	LEU	2.5
1	A	214	VAL	2.5
2	C	505	TYR	2.5
1	B	341	GLU	2.5
1	B	250	ARG	2.5
1	B	234	ASN	2.5
1	B	305	CYS	2.5
1	B	433	LYS	2.5
1	A	249	MET	2.5
2	C	507	GLU	2.5
1	A	282	SER	2.4
2	C	532	SER	2.4
2	C	563	VAL	2.4
2	C	484	ARG	2.4
1	B	105	TYR	2.4
1	B	228	ALA	2.4
1	B	203	SER	2.4
1	B	390	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	265	THR	2.4
1	A	119	ILE	2.4
2	C	465	ARG	2.4
1	B	13	SER	2.4
2	C	504	PHE	2.4
1	B	246	GLN	2.4
1	A	342	ILE	2.4
1	B	223	ILE	2.4
1	A	355	VAL	2.4
1	B	233	GLU	2.4
1	A	156	SER	2.4
1	B	156	SER	2.4
1	B	288	ILE	2.4
1	A	109	VAL	2.3
1	A	436	ASN	2.3
1	A	47	ALA	2.3
2	C	595	SER	2.3
1	A	231	THR	2.3
2	C	527	LEU	2.3
1	A	112	LYS	2.3
1	A	264	ARG	2.3
1	A	424	VAL	2.3
1	A	226	ASN	2.3
1	A	262	ASN	2.3
1	A	111	GLU	2.3
1	B	94	ASP	2.3
1	B	133	GLU	2.3
1	A	396	LEU	2.3
1	A	381	ARG	2.3
1	B	270	PRO	2.3
2	C	573	ARG	2.3
2	C	574	ARG	2.3
1	A	46	ALA	2.3
1	B	244	ALA	2.3
2	C	581	ALA	2.3
1	A	246	GLN	2.3
1	B	347	LYS	2.3
1	A	98	THR	2.3
1	B	283	LEU	2.3
1	A	317	ILE	2.3
1	A	380	ILE	2.3
1	A	198	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	426	THR	2.3
1	A	357	VAL	2.3
1	B	167	VAL	2.3
2	C	585	LYS	2.2
1	A	188	THR	2.2
1	A	138	VAL	2.2
1	A	256	GLY	2.2
1	B	22	GLY	2.2
2	C	487	GLY	2.2
1	A	338	GLU	2.2
1	B	174	GLU	2.2
1	A	101	ASN	2.2
1	B	83	ILE	2.2
1	B	245	GLN	2.2
2	C	539	ASP	2.2
1	A	151	SER	2.2
1	A	129	GLY	2.2
1	A	283	LEU	2.2
2	C	515	ALA	2.2
2	C	562	LYS	2.2
1	A	114	VAL	2.2
1	A	25	PHE	2.2
1	A	153	ARG	2.2
1	A	307	ARG	2.2
1	A	155	HIS	2.2
2	C	476	ASP	2.2
1	A	251	MET	2.2
1	A	377	MET	2.2
1	B	346	LEU	2.2
1	A	108	ILE	2.1
1	A	320	ASP	2.1
1	A	67	LEU	2.1
1	B	139	LEU	2.1
1	A	179	ARG	2.1
1	B	120	ARG	2.1
1	A	288	ILE	2.1
1	A	318	VAL	2.1
1	B	97	PRO	2.1
1	A	41	GLU	2.1
2	C	572	GLU	2.1
1	B	362	GLN	2.1
1	B	226	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	427	VAL	2.1
1	A	315	GLY	2.1
1	A	250	ARG	2.1
1	B	95	ALA	2.1
1	B	271	GLU	2.1
2	C	536	ILE	2.1
1	A	160	LYS	2.1
1	B	112	LYS	2.1
2	C	457	LEU	2.1
1	A	244	ALA	2.1
1	A	175	MET	2.0
1	B	437	LYS	2.0
1	A	199	GLY	2.0
1	B	302	ARG	2.0
1	B	19	ALA	2.0
2	C	493	GLU	2.0
1	B	235	VAL	2.0
1	A	294	PRO	2.0
2	C	534	LEU	2.0
1	B	45	ARG	2.0
1	B	259	ASN	2.0
1	B	351	ARG	2.0
1	B	237	ILE	2.0
1	A	209	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	500	5/5	0.82	0.15	138,138,139,140	0
3	SO4	A	1001	5/5	0.83	0.28	112,113,114,115	0
3	SO4	B	1002	5/5	0.88	0.20	107,108,109,110	0
3	SO4	A	500	5/5	0.89	0.15	105,107,108,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.