Full wwPDB X-ray Structure Validation Report (i)

Nov 25, 2024 – 05:12 PM EST

PDB ID	:	2R6A
Title	:	Crystal Form BH1
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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 (i) 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 (1)) were used in the production of this report:

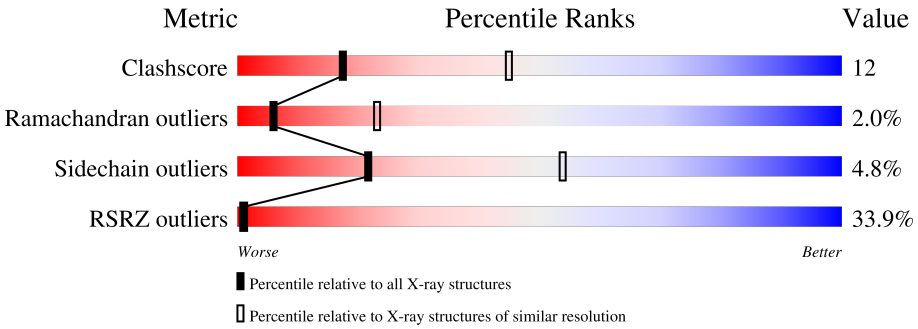
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	454	28% 68% 22% • 7%
1	B	454	29% 59% 21% • 18%
2	C	143	39% 80% 16% • •

2 Entry composition (i)

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			

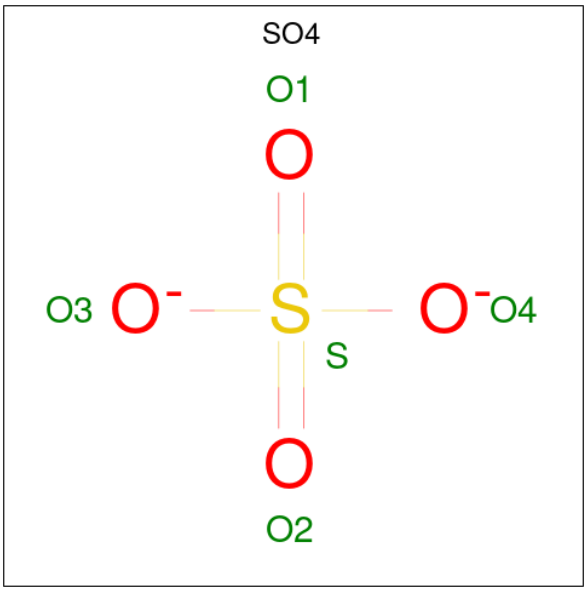
- Molecule 2 is a protein called DnaG Primase, Helicase Binding Domain.

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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

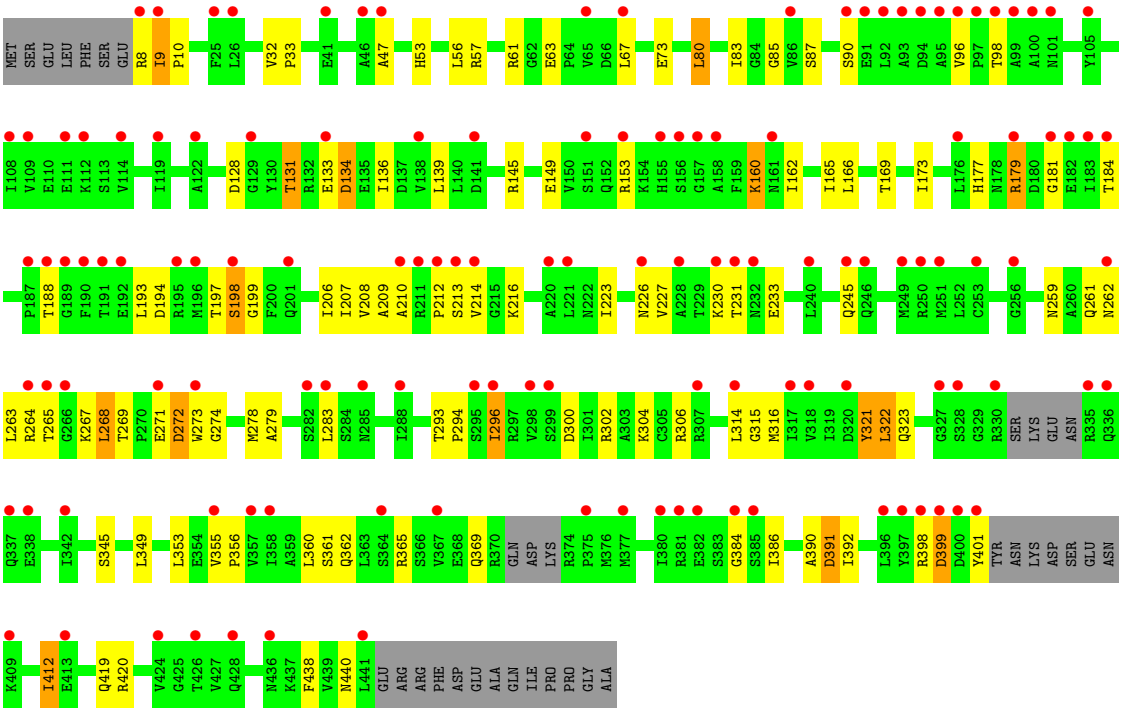
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	15	Total O 15 15	0	0
4	B	10	Total O 10 10	0	0
4	C	5	Total O 5 5	0	0

3 Residue-property plots (i)

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. 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. 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.

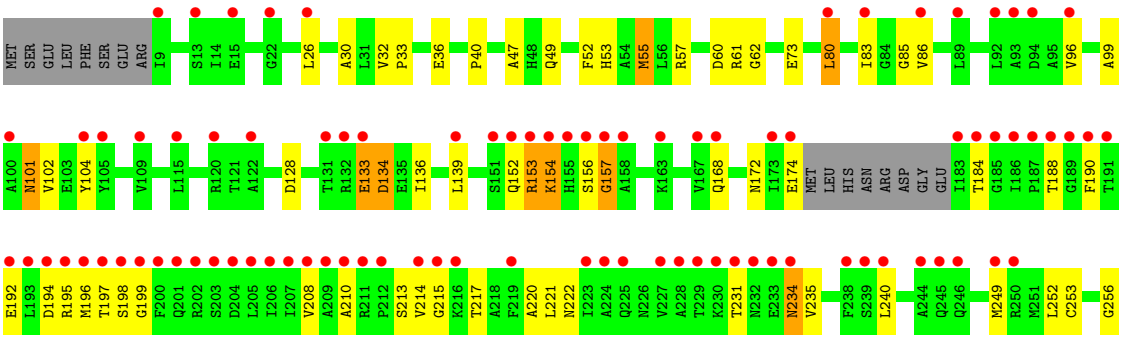
- Molecule 1: Replicative helicase

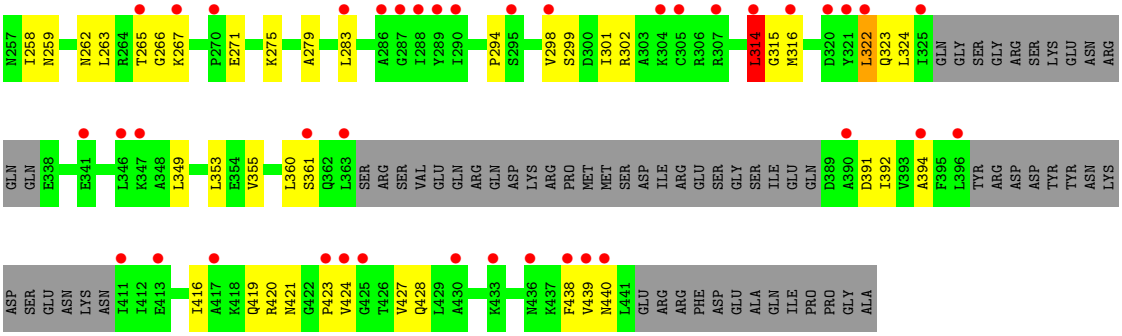
Chain A:



- Molecule 1: Replicative helicase

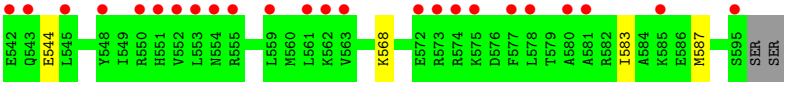
Chain B:





• Molecule 2: DnaG Primase, Helicase Binding Domain

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.45	0/3306	0.68	1/4464 (0.0%)
1	B	0.41	0/2922	0.69	2/3953 (0.1%)
2	C	0.63	2/1157 (0.2%)	0.63	0/1544
All	All	0.47	2/7385 (0.0%)	0.68	3/9961 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	507	GLU	CD-OE2	11.98	1.38	1.25
2	C	507	GLU	CD-OE1	11.58	1.38	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	GLU	N-CA-C	6.39	128.24	111.00
1	B	314	LEU	CA-CB-CG	6.25	129.66	115.30
1	A	322	LEU	CA-CB-CG	5.52	128.00	115.30

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	93	0
1	B	2889	0	2956	78	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	181	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 12.

All (181) 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
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	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:177:HIS:C	1:A:179:ARG:H	2.12	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
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
2:C:505:TYR:C	2:C:507:GLU:H	2.13	0.51
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:208:VAL:HB	1:B:360:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:259:ASN:HD22	1:A:262:ASN:HB2	1.79	0.46
1:A:259:ASN:O	1:A:262:ASN:HB3	2.15	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
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:196:MET:HE2	1:B:196:MET:HA	1.99	0.44
1:B:416:ILE:HD11	1:B:424:VAL:HA	1.97	0.44
1:B:30:ALA:C	1:B:33:PRO:HD2	2.38	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:207:ILE:HD12	1:A:390:ALA:CB	2.37	0.44
1:A:399:ASP:N	1:A:399:ASP:OD1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:83:ILE:C	1:B:83:ILE:HD12	2.40	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:B:391:ASP:CG	1:B:420:ARG:HD3	2.40	0.42
1:A:314:LEU:HD13	1:A:353:LEU:HD23	2.02	0.41
1:A:321:TYR:HA	1:A:360:LEU:O	2.21	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: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
1:B:52:PHE:HD1	1:B:55:MET:HE1	1.87	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 29
1	B	364/454 (80%)	341 (94%)	14 (4%)	9 (2%)	4 18
2	C	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	5 21
All	All	915/1051 (87%)	846 (92%)	51 (6%)	18 (2%)	6 23

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 (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	354/386 (92%)	332 (94%)	22 (6%)	15 43
1	B	313/386 (81%)	301 (96%)	12 (4%)	28 63
2	C	120/116 (103%)	116 (97%)	4 (3%)	33 68
All	All	787/888 (89%)	749 (95%)	38 (5%)	21 54

All (38) 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
1	A	80	LEU
1	A	87	SER
1	A	96	VAL
1	A	98	THR
1	A	136	ILE
1	A	153	ARG
1	A	160	LYS
1	A	179	ARG
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	391	ASP
1	A	399	ASP
1	A	412	ILE
1	B	55	MET
1	B	60	ASP
1	B	80	LEU
1	B	86	VAL
1	B	101	ASN
1	B	136	ILE
1	B	174	GLU
1	B	231	THR
1	B	234	ASN
1	B	252	LEU
1	B	322	LEU
1	B	323	GLN

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Mol	Chain	Res	Type
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	53	HIS
1	A	225	GLN
1	A	245	GLN
1	A	259	ASN
1	A	323	GLN
1	A	436	ASN
1	B	12	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	259	ASN
2	C	551	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 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	B	500	-	4,4,4	0.26	0	6,6,6	0.16	0
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

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

Warning: The R factor obtained from EDS is 0.3313, which does not match the depositor's R factor of 0.25894. Please interpret the results in this section carefully.

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	420/454 (92%)	1.60	129 (30%)	1	1	28, 98, 121, 134	0
1	B	374/454 (82%)	1.83	130 (34%)	1	1	29, 98, 106, 135	0
2	C	135/143 (94%)	1.85	56 (41%)	1	1	77, 99, 109, 121	0
All	All	929/1051 (88%)	1.73	315 (33%)	1	1	28, 98, 112, 135	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ARG	7.4
1	B	440	ASN	6.1
1	A	409	LYS	5.4
1	A	133	GLU	5.3
1	B	193	LEU	5.3
1	B	439	VAL	5.3
1	B	417	ALA	5.3
1	B	239	SER	5.2
1	A	441	LEU	5.2
1	B	210	ALA	5.2
1	A	95	ALA	5.2
1	A	399	ASP	5.1
1	B	267	LYS	5.0
1	B	396	LEU	5.0
1	A	401	TYR	4.9
1	B	363	LEU	4.8
1	B	202	ARG	4.8
1	B	207	ILE	4.6
1	A	158	ALA	4.6
1	A	192	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
2	C	463	ALA	4.5
1	A	367	VAL	4.5
2	C	461	GLN	4.3
1	B	191	THR	4.3
1	A	240	LEU	4.3
1	B	9	ILE	4.3
2	C	535	LEU	4.3
1	A	400	ASP	4.2
1	B	155	HIS	4.2
1	A	330	ARG	4.2
1	B	304	LYS	4.2
1	B	183	ILE	4.2
1	B	185	GLY	4.1
1	A	92	LEU	4.1
1	B	153	ARG	4.1
1	A	271	GLU	4.1
1	B	190	PHE	4.1
1	B	195	ARG	4.1
2	C	537	ALA	4.1
1	B	188	THR	4.1
1	B	200	PHE	4.0
1	A	99	ALA	4.0
1	B	187	PRO	4.0
1	A	94	ASP	4.0
2	C	555	ARG	4.0
1	A	93	ALA	3.9
1	B	225	GLN	3.9
2	C	554	ASN	3.9
1	A	96	VAL	3.9
1	B	209	ALA	3.8
1	B	289	TYR	3.8
1	A	428	GLN	3.8
1	A	295	SER	3.8
1	B	216	LYS	3.8
1	B	199	GLY	3.8
1	B	122	ALA	3.7
1	B	204	ASP	3.7
1	B	249	MET	3.7
1	B	230	LYS	3.7
1	B	194	ASP	3.7
1	B	214	VAL	3.7
1	B	186	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	580	ALA	3.7
1	B	219	PHE	3.6
1	B	197	THR	3.6
1	B	231	THR	3.6
1	B	205	LEU	3.6
1	B	154	LYS	3.6
1	B	211	ARG	3.6
1	A	228	ALA	3.6
2	C	511	ALA	3.6
2	C	578	LEU	3.6
1	B	184	THR	3.6
1	A	86	VAL	3.6
1	B	307	ARG	3.6
1	B	325	ILE	3.6
1	A	189	GLY	3.5
2	C	577	PHE	3.5
1	B	411	ILE	3.5
1	A	100	ALA	3.5
1	A	328	SER	3.5
1	A	327	GLY	3.4
1	A	97	PRO	3.4
1	B	295	SER	3.4
2	C	462	ASN	3.4
1	A	105	TYR	3.4
1	A	161	ASN	3.4
1	A	266	GLY	3.4
2	C	513	PRO	3.3
2	C	575	LYS	3.3
1	B	157	GLY	3.3
1	B	198	SER	3.3
2	C	512	ASP	3.3
1	A	336	GLN	3.3
2	C	538	ASP	3.3
1	B	173	ILE	3.3
2	C	553	LEU	3.3
1	A	9	ILE	3.2
1	B	229	THR	3.2
1	B	438	PHE	3.2
2	C	499	ALA	3.2
1	B	96	VAL	3.2
2	C	550	ARG	3.2
1	A	213	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	168	GLN	3.1
1	B	192	GLU	3.1
1	A	210	ALA	3.1
1	B	298	VAL	3.1
1	B	132	ARG	3.1
1	A	220	ALA	3.1
1	B	26	LEU	3.1
1	B	423	PRO	3.1
1	A	273	TRP	3.1
2	C	545	LEU	3.0
1	A	364	SER	3.0
1	A	211	ARG	3.0
1	B	131	THR	3.0
1	B	436	ASN	3.0
1	A	176	LEU	3.0
1	A	91	GLU	3.0
1	B	15	GLU	3.0
1	B	86	VAL	3.0
1	B	430	ALA	3.0
1	A	195	ARG	2.9
2	C	473	ARG	2.9
1	B	115	LEU	2.9
2	C	548	TYR	2.9
1	A	184	THR	2.9
1	B	93	ALA	2.9
1	B	189	GLY	2.9
1	A	314	LEU	2.9
2	C	491	ILE	2.9
2	C	561	LEU	2.9
1	B	321	TYR	2.9
1	B	158	ALA	2.9
1	A	191	THR	2.9
1	A	232	ASN	2.9
1	B	314	LEU	2.9
1	A	181	GLY	2.8
1	A	212	PRO	2.8
1	B	320	ASP	2.8
1	A	230	LYS	2.8
1	B	212	PRO	2.8
1	A	335	ARG	2.8
1	A	253	CYS	2.8
1	A	413	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	2.8
1	B	232	ASN	2.8
1	A	65	VAL	2.8
2	C	488	ARG	2.8
2	C	559	LEU	2.8
1	A	221	LEU	2.7
1	B	322	LEU	2.7
1	B	290	ILE	2.7
2	C	486	GLY	2.7
1	A	337	GLN	2.7
1	B	89	LEU	2.7
1	B	240	LEU	2.7
1	A	296	ILE	2.7
1	A	358	ILE	2.7
1	A	298	VAL	2.7
2	C	542	GLU	2.7
1	A	157	GLY	2.7
1	B	163	LYS	2.7
2	C	455	LYS	2.7
1	A	190	PHE	2.7
1	B	238	PHE	2.7
2	C	460	PHE	2.7
2	C	551	HIS	2.7
1	A	183	ILE	2.6
1	A	182	GLU	2.6
1	A	382	GLU	2.6
1	B	215	GLY	2.6
1	B	227	VAL	2.6
1	B	413	GLU	2.6
1	B	151	SER	2.6
1	B	287	GLY	2.6
1	B	224	ALA	2.6
1	B	196	MET	2.6
1	B	424	VAL	2.6
2	C	552	VAL	2.6
1	B	152	GLN	2.6
1	A	285	ASN	2.6
1	A	384	GLY	2.6
1	B	361	SER	2.6
1	A	122	ALA	2.5
1	B	80	LEU	2.6
1	B	100	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	466	LEU	2.6
2	C	517	ILE	2.5
1	A	201	GLN	2.5
1	A	245	GLN	2.5
1	A	265	THR	2.5
1	B	109	VAL	2.5
1	A	299	SER	2.5
1	A	385	SER	2.5
2	C	541	SER	2.5
1	A	196	MET	2.5
2	C	540	VAL	2.5
1	B	394	ALA	2.5
1	B	201	GLN	2.5
2	C	543	GLN	2.5
1	A	187	PRO	2.5
1	B	425	GLY	2.5
1	A	397	TYR	2.5
1	B	316	MET	2.5
2	C	500	TYR	2.5
1	A	90	SER	2.5
1	A	8	ARG	2.5
1	B	208	VAL	2.5
1	B	286	ALA	2.5
1	B	104	TYR	2.5
1	A	375	PRO	2.4
1	B	250	ARG	2.4
1	A	141	ASP	2.4
1	A	26	LEU	2.4
1	B	341	GLU	2.4
1	B	433	LYS	2.4
1	B	92	LEU	2.4
1	A	214	VAL	2.4
2	C	507	GLU	2.4
1	B	234	ASN	2.4
2	C	484	ARG	2.4
2	C	505	TYR	2.3
1	A	249	MET	2.3
1	A	282	SER	2.3
2	C	532	SER	2.3
2	C	563	VAL	2.3
1	B	228	ALA	2.3
2	C	465	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	305	CYS	2.3
1	B	203	SER	2.3
1	B	390	ALA	2.3
1	B	265	THR	2.3
1	B	105	TYR	2.3
1	B	246	GLN	2.3
1	A	119	ILE	2.3
1	B	233	GLU	2.3
1	B	13	SER	2.3
1	A	342	ILE	2.3
1	A	355	VAL	2.3
1	B	223	ILE	2.3
1	A	264	ARG	2.3
1	A	156	SER	2.3
1	B	156	SER	2.3
1	A	112	LYS	2.3
1	A	436	ASN	2.2
1	A	109	VAL	2.2
1	B	288	ILE	2.2
2	C	504	PHE	2.2
1	A	47	ALA	2.2
1	A	111	GLU	2.2
1	A	381	ARG	2.2
1	B	133	GLU	2.2
2	C	573	ARG	2.2
2	C	574	ARG	2.2
2	C	595	SER	2.2
1	A	231	THR	2.2
1	A	226	ASN	2.2
1	A	262	ASN	2.2
1	A	424	VAL	2.2
2	C	527	LEU	2.2
1	B	94	ASP	2.2
1	B	347	LYS	2.2
1	A	246	GLN	2.2
1	A	46	ALA	2.2
1	B	244	ALA	2.2
2	C	581	ALA	2.2
1	A	396	LEU	2.2
1	B	270	PRO	2.2
1	A	98	THR	2.2
2	C	585	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	SER	2.2
1	A	317	ILE	2.2
1	A	380	ILE	2.2
1	A	357	VAL	2.2
1	B	167	VAL	2.2
1	A	426	THR	2.1
1	B	283	LEU	2.1
1	A	338	GLU	2.1
1	B	174	GLU	2.1
1	A	138	VAL	2.1
1	A	188	THR	2.1
1	B	245	GLN	2.1
2	C	562	LYS	2.1
1	A	101	ASN	2.1
1	B	83	ILE	2.1
1	A	153	ARG	2.1
1	A	256	GLY	2.1
1	A	307	ARG	2.1
1	B	22	GLY	2.1
2	C	487	GLY	2.1
2	C	539	ASP	2.1
1	A	151	SER	2.1
2	C	515	ALA	2.1
1	A	114	VAL	2.1
1	A	129	GLY	2.1
1	A	283	LEU	2.1
1	A	179	ARG	2.1
1	B	120	ARG	2.1
1	A	155	HIS	2.1
2	C	476	ASP	2.0
1	A	108	ILE	2.0
1	A	251	MET	2.0
1	A	377	MET	2.0
1	A	25	PHE	2.0
1	B	346	LEU	2.0
1	A	320	ASP	2.0
1	A	41	GLU	2.0
1	A	288	ILE	2.0
2	C	572	GLU	2.0
1	A	250	ARG	2.0
1	A	318	VAL	2.0
1	A	67	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	139	LEU	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^{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	B-factors(Å^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.