



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:57 AM GMT

PDB ID : 2R6A  
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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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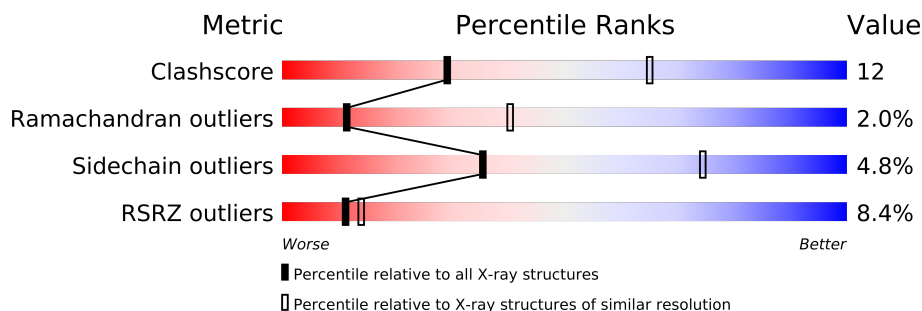
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	
2	C	143	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7352 atoms, of which 0 are hydrogen and 0 are deuterium.

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<sub>4</sub>S).



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.

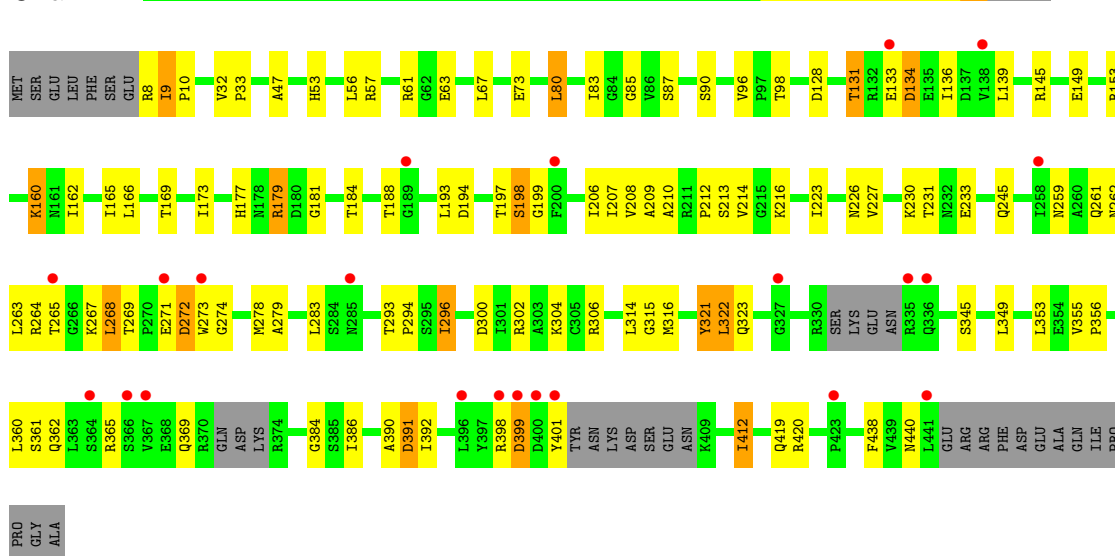
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	10	Total	O	0	0
			10	10		
4	C	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

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

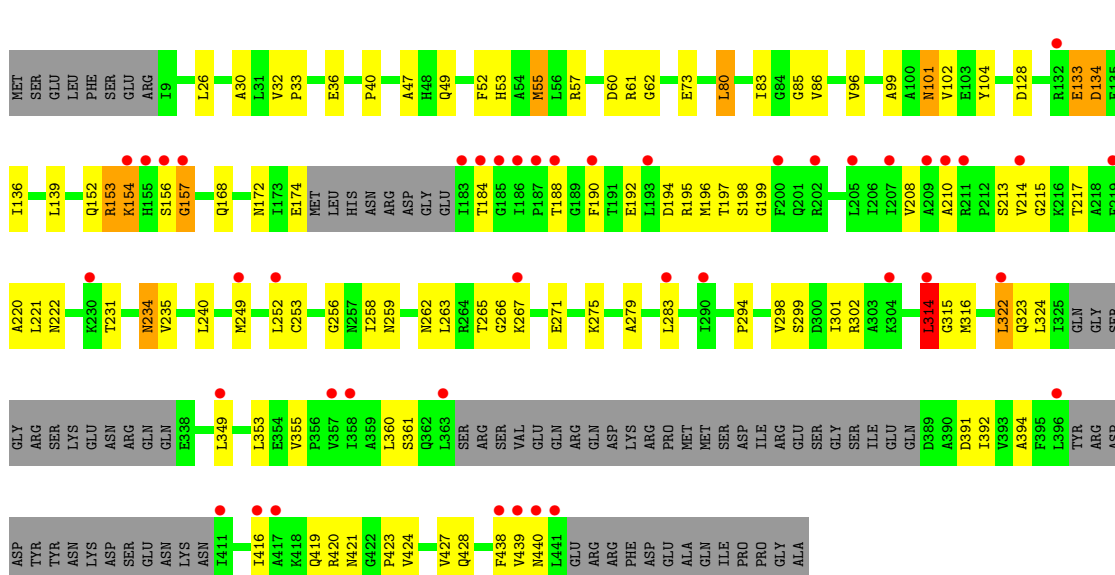
#### • Molecule 1: Replicative helicase

Chain A:



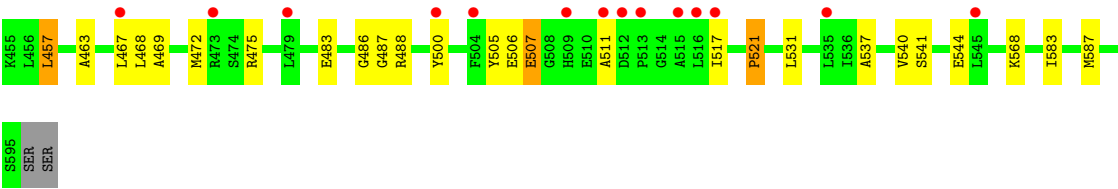
#### • Molecule 1: Replicative helicase

Chain B:



● Molecule 2: DnaG Primase, Helicase Binding Domain

Chain C: 



SER  
SER  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.75Å 226.75Å 75.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.88 – 2.90 45.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.88-2.90) 99.8 (45.42-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.259 , 0.297 0.272 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.2	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49634 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (181) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:152:GLN:HA	1:B:153:ARG:CB	2.29	0.62
1:A:398:ARG:CD	1:A:401:TYR:OH	2.46	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:B:314:LEU:HB2	1:B:315:GLY:HA2	1.77	0.61
1:A:267:LYS:O	1:A:268:LEU:HD23	2.01	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:O	2:C:517:ILE:HG22	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:321:TYR:H	1:A:360:LEU:HB2	1.71	0.54
1:A:233:GLU:CG	1:A:315:GLY:HA3	2.37	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:398:ARG:CG	1:A:412:ILE:CG1	2.82	0.52
1:A:61:ARG:NH2	1:A:73:GLU:OE1	2.42	0.52
2:C:486:GLY:N	2:C:488:ARG:HB2	2.24	0.52
1:B:198:SER:N	1:B:199:GLY:HA2	2.23	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:398:ARG:CD	1:A:401:TYR:CE1	2.76	0.50
1:A:184:THR:N	1:A:198:SER:O	2.45	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:B:299:SER:HA	1:B:302:ARG:HG3	1.94	0.49
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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:256:GLY:O	1:B:275:LYS:HG2	2.16	0.46
1:A:259:ASN:O	1:A:262:ASN:HB3	2.15	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:463:ALA:O	2:C:467:LEU:HB2	2.16	0.46
2:C:457:LEU:HB2	4:C:599:HOH:O	2.15	0.46
1:A:169:THR:O	1:A:173:ILE:HG12	2.15	0.46
1:A:128:ASP:HB3	1:A:139:LEU:HD21	1.98	0.46
1:A:90:SER:OG	2:C:568:LYS:HE3	2.16	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:196:MET:HA	1:B:196:MET:HE2	1.99	0.44
1:B:416:ILE:HD11	1:B:424:VAL:HA	1.97	0.44
1:B:53:HIS:HE1	1:B:57:ARG:HH11	1.65	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: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:399:ASP:OD1	1:A:399:ASP:N	2.51	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:296:ILE:CG2	1:A:300:ASP:HB2	2.44	0.43
1:A:263:LEU:HD23	1:A:268:LEU:HD21	1.99	0.43
2:C:469:ALA:HA	2:C:472:MSE:HE2	2.00	0.43
1:A:345:SER:OG	1:B:36:GLU:OE2	2.33	0.43
1:A:197:THR:HA	1:A:419:GLN:OE1	2.19	0.43
1:B:101:ASN:H	1:B:101:ASN:ND2	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HD12	1:B:83:ILE:C	2.40	0.42
1:A:162:ILE:O	1:A:166:LEU:HG	2.19	0.42
1:B:439:VAL:HG12	1:B:440:ASN:N	2.35	0.42
1:B:265:THR:O	1:B:267:LYS:N	2.53	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

### 5.3.1 Protein backbone ⓘ

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%)	15	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	364/454 (80%)	341 (94%)	14 (4%)	9 (2%)	9	32
2	C	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	10	37
All	All	915/1051 (87%)	846 (92%)	51 (6%)	18 (2%)	11	40

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%)	26	61
1	B	313/386 (81%)	301 (96%)	12 (4%)	44	83
2	C	120/116 (103%)	116 (97%)	4 (3%)	50	87
All	All	787/888 (89%)	749 (95%)	38 (5%)	35	74

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
2	C	457	LEU
2	C	468	LEU
2	C	483	GLU
2	C	540	VAL

Some 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 chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	1001	-	4,4,4	0.18	0	6,6,6	0.12	0
3	SO4	A	500	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	1002	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	B	500	-	4,4,4	0.14	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	500	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	B	500	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	420/454 (92%)	0.37	22 (5%) 26 32	28, 98, 121, 134	0
1	B	374/454 (82%)	0.63	43 (11%) 5 7	29, 98, 106, 135	0
2	C	141/143 (98%)	0.47	14 (9%) 8 10	77, 99, 109, 121	0
All	All	935/1051 (88%)	0.49	79 (8%) 11 14	28, 98, 112, 135	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	LEU	9.6
1	B	396	LEU	7.5
1	A	401	TYR	5.6
1	B	417	ALA	5.4
1	A	133	GLU	4.9
1	B	193	LEU	4.9
1	A	400	ASP	4.9
1	B	440	ASN	4.8
2	C	513	PRO	4.7
2	C	473	ARG	4.6
1	B	209	ALA	4.4
1	B	187	PRO	4.3
1	B	200	PHE	4.1
1	B	411	ILE	4.1
2	C	517	ILE	4.0
1	B	157	GLY	4.0
1	A	367	VAL	3.8
1	A	398	ARG	3.8
1	B	438	PHE	3.8
1	B	210	ALA	3.8
1	B	441	LEU	3.7
1	B	416	ILE	3.7
1	B	156	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	211	ARG	3.6
1	A	396	LEU	3.6
1	A	399	ASP	3.5
1	B	439	VAL	3.4
1	B	155	HIS	3.4
1	B	249	MET	3.4
1	B	214	VAL	3.3
1	A	335	ARG	3.3
1	B	322	LEU	3.2
1	B	154	LYS	3.2
2	C	479	LEU	3.1
2	C	535	LEU	3.1
1	B	183	ILE	3.1
1	A	271	GLU	3.0
1	A	138	VAL	3.0
1	B	185	GLY	2.8
1	B	186	ILE	2.8
1	A	441	LEU	2.7
1	B	190	PHE	2.7
1	B	349	LEU	2.7
1	B	357	VAL	2.7
1	B	304	LYS	2.6
2	C	504	PHE	2.6
2	C	511	ALA	2.6
1	A	265	THR	2.5
1	B	358	ILE	2.5
2	C	467	LEU	2.5
1	B	252	LEU	2.4
2	C	516	LEU	2.4
1	B	230	LYS	2.4
1	A	336	GLN	2.4
2	C	500	TYR	2.4
1	B	188	THR	2.3
1	A	273	TRP	2.3
1	A	258	ILE	2.3
1	A	366	SER	2.3
1	B	205	LEU	2.3
1	A	189	GLY	2.3
1	B	202	ARG	2.2
2	C	515	ALA	2.2
1	A	364	SER	2.2
1	B	184	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	290	ILE	2.2
2	C	509	HIS	2.2
2	C	512	ASP	2.2
1	B	283	LEU	2.2
1	A	423	PRO	2.1
1	B	267	LYS	2.1
2	C	545	LEU	2.0
1	B	207	ILE	2.0
1	A	285	ASN	2.0
1	B	132	ARG	2.0
1	A	200	PHE	2.0
1	B	219	PHE	2.0
1	A	327	GLY	2.0
1	B	314	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	500	5/5	0.18	-0.21	105,107,108,110	0
3	SO4	B	1002	5/5	0.17	-0.63	107,108,109,110	0
3	SO4	A	1001	5/5	0.17	-0.72	112,113,114,115	0
3	SO4	B	500	5/5	0.18	-1.15	138,138,139,140	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.