



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 03:34 pm 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 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : (not set)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

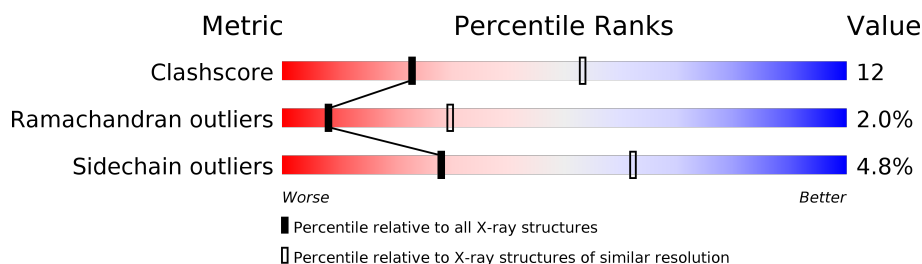
# 1 Overall quality at a glance

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	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (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. 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  $\leq 5\%$ .

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 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<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		

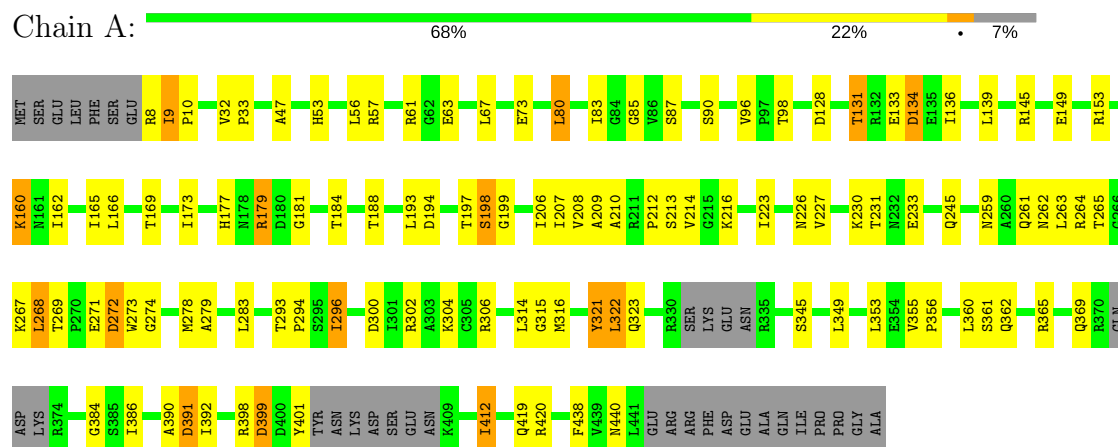
- Molecule 4 is water.

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		

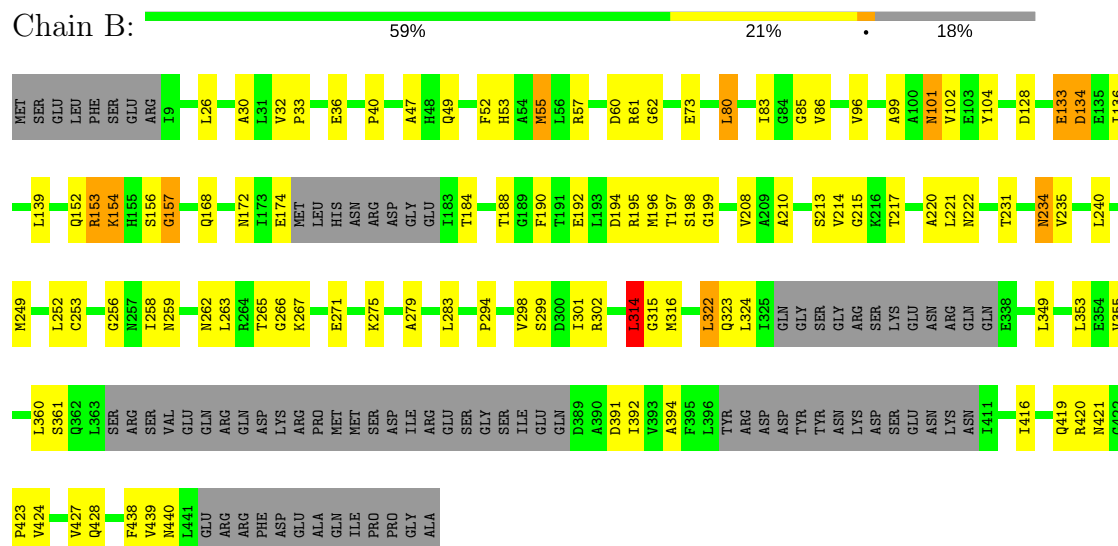
### 3 Residue-property plots

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

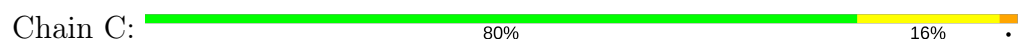
#### • Molecule 1: Replicative helicase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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 0.269 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
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 , 82.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <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.

<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	0.45	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 Too-close contacts [i](#)

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: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

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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:323:GLN:HE21	1:A:362:GLN:H	1.54	0.54
1:A:316:MET:HG2	1:A:356:PRO:HG2	1.88	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
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: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:184:THR:N	1:B:198:SER:O	2.50	0.44
1:B:30:ALA:C	1:B:33:PRO:HD2	2.38	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:OD1	1:A:399:ASP:N	2.51	0.44
1:B:298:VAL:O	1:B:301:ILE:HB	2.17	0.44
1:B:32:VAL:HB	1:B:33:PRO:HD3	2.00	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: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
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: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 ⓘ

### 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%)	11	37
1	B	364/454 (80%)	341 (94%)	14 (4%)	9 (2%)	6	23
2	C	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	7	27
All	All	915/1051 (87%)	846 (92%)	51 (6%)	18 (2%)	8	30

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%)	20	51
1	B	313/386 (81%)	301 (96%)	12 (4%)	36	71
2	C	120/116 (103%)	116 (97%)	4 (3%)	41	75
All	All	787/888 (89%)	749 (95%)	38 (5%)	28	62

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

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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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	0.21	0	6,6,6	0.16	0
3	SO4	A	500	-	4,4,4	0.16	0	6,6,6	0.15	0
3	SO4	B	1002	-	4,4,4	0.22	0	6,6,6	0.20	0
3	SO4	B	500	-	4,4,4	0.19	0	6,6,6	0.17	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.

No monomer is involved in short contacts.

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.