



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:52 am GMT

PDB ID : 2Q6T  
Title : Crystal structure of the Thermus aquaticus DnaB monomer  
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.  
Deposited on : 2007-06-05  
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

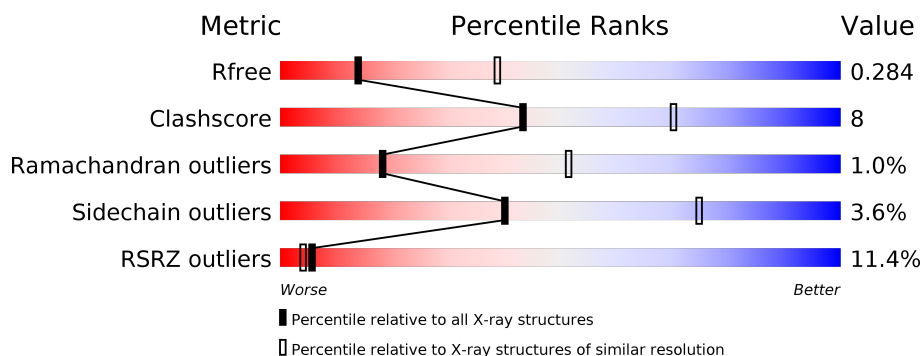
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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  $\leq 5\%$ . 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	444	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	B	444	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	C	444	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 9%</div> </div> </div>
1	D	444	<div> <div>14%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12746 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 DnaB replication fork helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3247	2032	578	623	14			
1	B	414	Total	C	N	O	S	0	0	0
			3207	2010	571	612	14			
1	C	406	Total	C	N	O	S	0	0	0
			3138	1968	552	604	14			
1	D	402	Total	C	N	O	S	0	0	0
			3109	1955	547	594	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

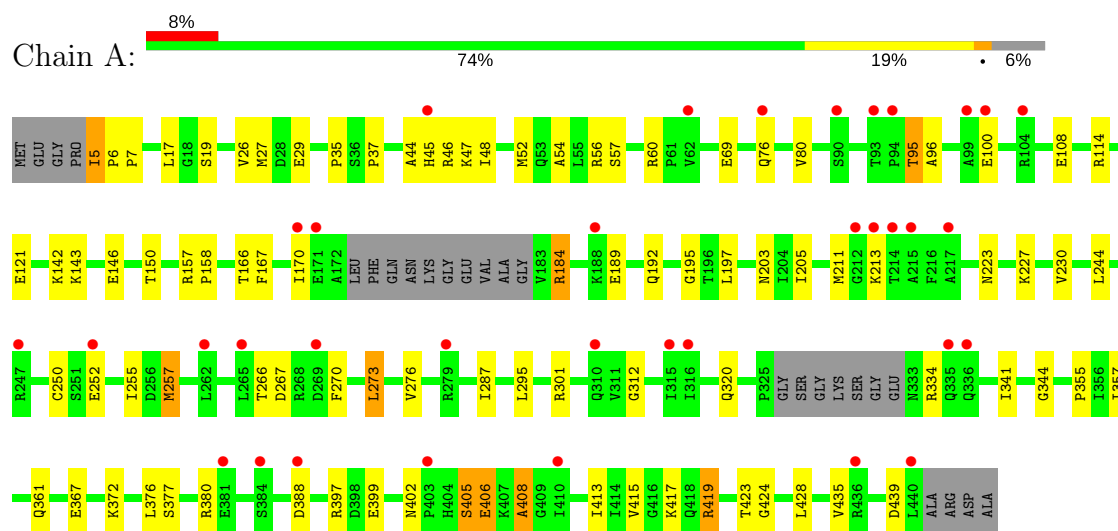
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	5	Total	O	0	0
			5	5		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		

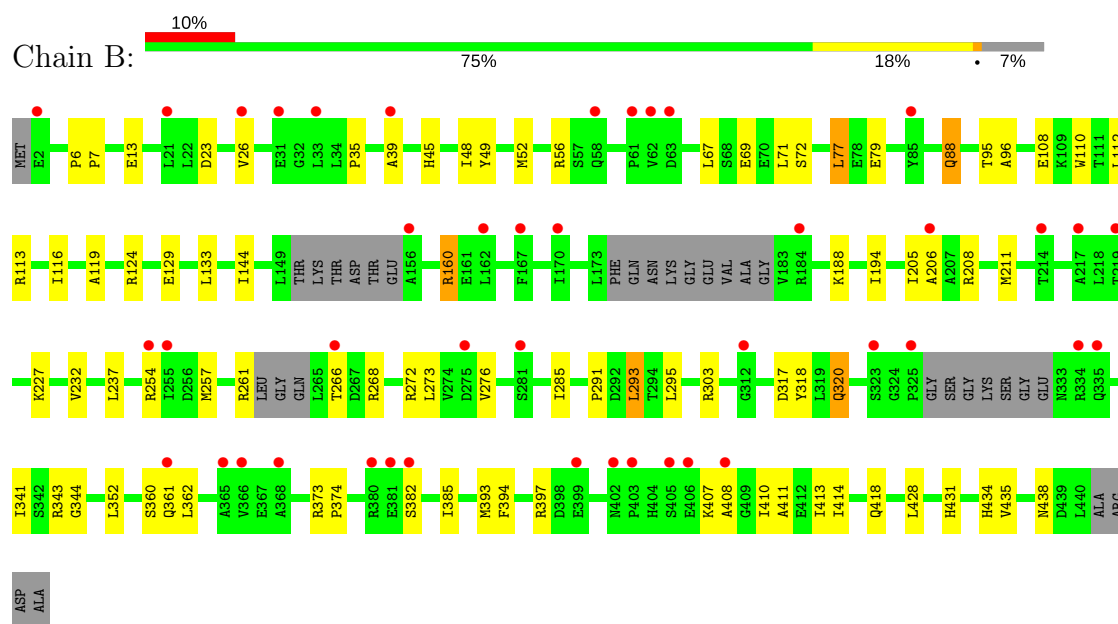
### 3 Residue-property plots [i](#)

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 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.

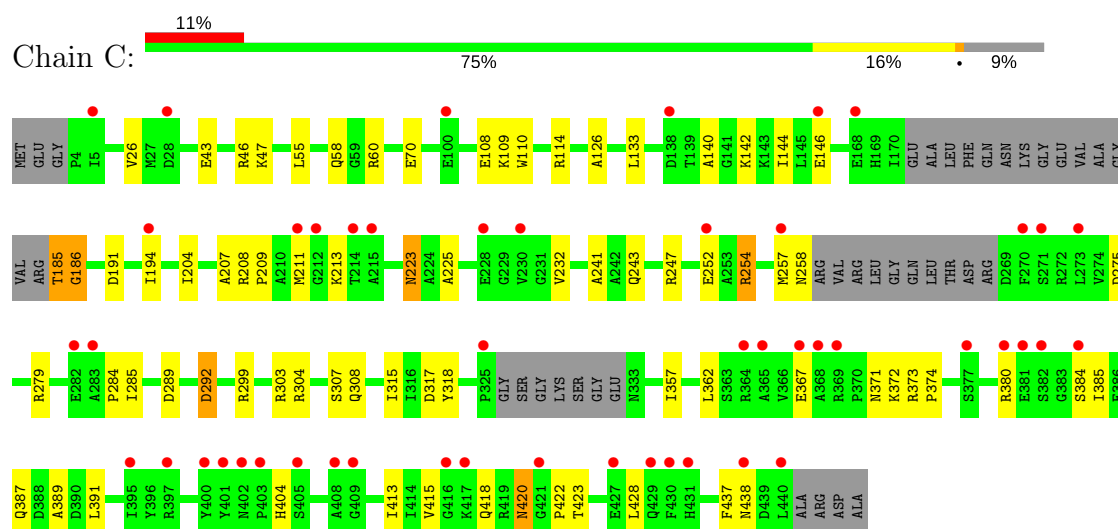
- Molecule 1: DnaB replication fork helicase



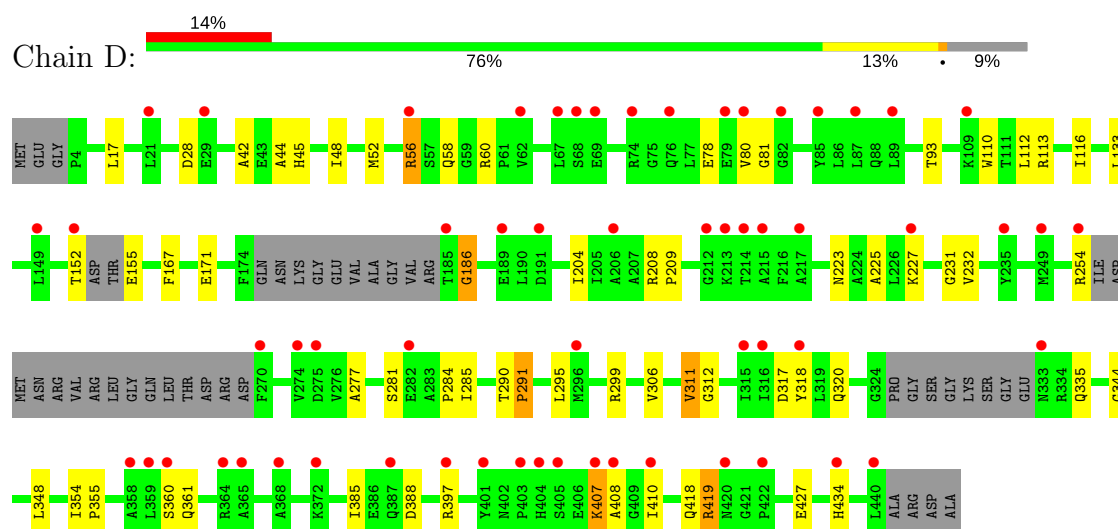
- Molecule 1: DnaB replication fork helicase



- Molecule 1: DnaB replication fork helicase



• Molecule 1: DnaB replication fork helicase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.71Å 104.71Å 363.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 29.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.90) 99.1 (29.85-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.241 , 0.285 0.238 , 0.284	Depositor DCC
$R_{free}$ test set	2646 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 106.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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	0.35	0/3292	0.61	0/4450
1	B	0.33	0/3251	0.60	0/4392
1	C	0.35	0/3183	0.56	0/4303
1	D	0.34	0/3153	0.56	0/4259
All	All	0.34	0/12879	0.58	0/17404

There are no bond length outliers.

There are no bond angle outliers.

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	3247	0	3290	61	0
1	B	3207	0	3249	54	0
1	C	3138	0	3172	52	0
1	D	3109	0	3150	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
All	All	12746	0	12861	197	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 8.

All (197) 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:D:56:ARG:HH21	1:D:56:ARG:HG2	1.24	1.01
1:A:419:ARG:HG3	1:A:419:ARG:HH11	1.26	0.99
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.32	0.91
1:B:237:LEU:HD21	1:B:293:LEU:HD12	1.51	0.89
1:A:29:GLU:HG2	1:A:100:GLU:HG3	1.55	0.89
1:A:184:ARG:CG	1:A:184:ARG:HH11	1.90	0.85
1:D:254:ARG:C	1:D:434:HIS:CE1	2.50	0.83
1:B:160:ARG:CG	1:B:160:ARG:HH11	1.93	0.82
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.45	0.80
1:A:48:ILE:HD11	1:A:80:VAL:HB	1.64	0.79
1:D:225:ALA:HB1	1:D:284:PRO:HD2	1.66	0.78
1:B:295:LEU:HD21	1:B:344:GLY:HA3	1.65	0.77
1:C:371:ASN:HD21	1:C:373:ARG:HD2	1.54	0.73
1:A:419:ARG:CG	1:A:419:ARG:HH11	2.03	0.72
1:D:320:GLN:HE21	1:D:361:GLN:H	1.39	0.70
1:A:184:ARG:NH1	1:A:184:ARG:HG3	2.04	0.69
1:D:44:ALA:O	1:D:48:ILE:HG22	1.93	0.69
1:B:407:LYS:HB3	1:B:410:ILE:HB	1.76	0.68
1:A:197:LEU:HD13	1:A:357:ILE:HD11	1.77	0.67
1:A:377:SER:O	1:A:380:ARG:HG2	1.95	0.67
1:C:418:GLN:NE2	1:C:422:PRO:O	2.29	0.66
1:D:208:ARG:CD	1:D:209:PRO:HD2	2.26	0.66
1:B:254:ARG:HG3	1:B:434:HIS:CE1	2.32	0.64
1:A:5:ILE:N	1:A:6:PRO:CD	2.60	0.64
1:C:225:ALA:HB1	1:C:284:PRO:HD2	1.79	0.64
1:A:320:GLN:HE21	1:A:361:GLN:H	1.47	0.63
1:C:43:GLU:HG3	1:C:47:LYS:HE2	1.80	0.63
1:C:304:ARG:O	1:C:308:GLN:HG2	1.99	0.63
1:D:56:ARG:HH21	1:D:56:ARG:CG	2.06	0.62
1:A:320:GLN:NE2	1:A:361:GLN:H	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ARG:HD2	1:D:209:PRO:HD2	1.83	0.61
1:A:211:MET:HE1	1:A:397:ARG:N	2.17	0.60
1:C:204:ILE:HD13	1:C:385:ILE:HG22	1.84	0.60
1:C:420:ASN:H	1:C:420:ASN:HD22	1.50	0.59
1:D:56:ARG:NH2	1:D:56:ARG:HG2	2.03	0.59
1:A:27:MET:HG2	1:A:56:ARG:HD2	1.86	0.58
1:D:312:GLY:O	1:D:355:PRO:HD2	2.04	0.58
1:A:195:GLY:CA	1:B:261:ARG:HB2	2.34	0.58
1:C:110:TRP:CE2	1:C:114:ARG:HD3	2.39	0.58
1:B:116:ILE:HD11	1:C:126:ALA:HB3	1.85	0.58
1:A:54:ALA:HA	1:A:57:SER:HB3	1.86	0.57
1:A:44:ALA:O	1:A:48:ILE:HD12	2.04	0.57
1:B:320:GLN:NE2	1:B:360:SER:HA	2.18	0.57
1:B:194:ILE:HA	1:B:418:GLN:NE2	2.20	0.57
1:A:415:VAL:O	1:A:423:THR:HG23	2.04	0.57
1:B:23:ASP:O	1:B:26:VAL:HG22	2.05	0.56
1:C:207:ALA:HB3	1:C:213:LYS:HG3	1.86	0.56
1:C:275:ASP:O	1:C:279:ARG:HB2	2.05	0.56
1:C:241:ALA:N	1:C:289:ASP:OD1	2.38	0.56
1:A:367:GLU:HA	1:A:372:LYS:HG2	1.87	0.55
1:C:185:THR:OG1	1:C:186:GLY:N	2.39	0.55
1:C:367:GLU:HA	1:C:372:LYS:HG2	1.89	0.55
1:D:418:GLN:HG2	1:D:419:ARG:H	1.71	0.55
1:C:58:GLN:HE21	1:C:60:ARG:HE	1.53	0.55
1:B:129:GLU:OE1	1:C:109:LYS:NZ	2.35	0.54
1:D:204:ILE:HD13	1:D:385:ILE:CG2	2.38	0.54
1:A:295:LEU:HD21	1:A:344:GLY:HA3	1.89	0.54
1:C:420:ASN:ND2	1:C:420:ASN:H	2.04	0.54
1:A:244:LEU:HD23	1:A:287:ILE:HD13	1.88	0.54
1:A:402:ASN:HB3	1:A:405:SER:HB2	1.90	0.53
1:D:277:ALA:O	1:D:281:SER:HB2	2.08	0.53
1:A:192:GLN:O	1:B:261:ARG:NH1	2.40	0.53
1:A:48:ILE:O	1:A:52:MET:HG3	2.08	0.53
1:C:415:VAL:O	1:C:423:THR:HG23	2.08	0.53
1:D:295:LEU:HD21	1:D:344:GLY:HA3	1.91	0.53
1:D:299:ARG:HG3	1:D:348:LEU:HD13	1.91	0.53
1:A:203:ASN:HB2	1:A:357:ILE:HD13	1.91	0.52
1:D:42:ALA:HB3	1:D:45:HIS:HD2	1.74	0.52
1:D:306:VAL:HA	1:D:311:VAL:HG22	1.92	0.52
1:B:13:GLU:HB3	1:B:45:HIS:HD2	1.75	0.52
1:C:299:ARG:HB3	1:C:303:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASP:HA	1:D:56:ARG:HH12	1.75	0.51
1:C:232:VAL:HG22	1:C:285:ILE:HG12	1.92	0.51
1:B:49:TYR:HA	1:B:52:MET:HE2	1.92	0.51
1:C:208:ARG:HD2	1:C:209:PRO:HD2	1.93	0.51
1:D:48:ILE:O	1:D:52:MET:HG3	2.11	0.51
1:C:207:ALA:O	1:C:213:LYS:HE3	2.11	0.51
1:A:419:ARG:NH1	1:A:419:ARG:HG3	2.06	0.51
1:B:160:ARG:CG	1:B:160:ARG:NH1	2.62	0.51
1:B:303:ARG:HG2	1:B:352:LEU:HD21	1.93	0.50
1:B:257:MET:O	1:B:261:ARG:HG2	2.11	0.50
1:B:7:PRO:O	1:B:113:ARG:HD3	2.11	0.50
1:C:204:ILE:HD12	1:C:389:ALA:HB2	1.93	0.50
1:B:72:SER:HB2	1:B:77:LEU:HD12	1.93	0.50
1:A:195:GLY:HA3	1:B:261:ARG:HB2	1.94	0.49
1:A:270:PHE:O	1:A:273:LEU:HD23	2.12	0.49
1:B:133:LEU:HD22	1:C:108:GLU:HG2	1.96	0.48
1:C:371:ASN:HD21	1:C:373:ARG:CD	2.24	0.48
1:A:211:MET:HE1	1:A:397:ARG:HG3	1.96	0.48
1:D:223:ASN:O	1:D:227:LYS:CB	2.62	0.48
1:D:290:THR:HA	1:D:291:PRO:HD3	1.73	0.48
1:C:315:ILE:HG13	1:C:357:ILE:HB	1.94	0.48
1:A:252:GLU:HB3	1:A:276:VAL:HG11	1.94	0.48
1:D:419:ARG:HA	1:D:419:ARG:NE	2.29	0.48
1:C:55:LEU:HG	1:C:70:GLU:HG3	1.96	0.48
1:C:208:ARG:CD	1:C:209:PRO:HD2	2.44	0.48
1:C:43:GLU:OE1	1:C:46:ARG:NH1	2.44	0.48
1:A:27:MET:HG2	1:A:56:ARG:CD	2.44	0.47
1:A:376:LEU:HD11	1:A:417:LYS:HB2	1.96	0.47
1:A:95:THR:HG22	1:A:96:ALA:H	1.78	0.47
1:A:29:GLU:CG	1:A:100:GLU:HG3	2.36	0.47
1:C:185:THR:HG23	1:C:191:ASP:CG	2.35	0.47
1:C:384:SER:HB3	1:C:387:GLN:HB2	1.96	0.47
1:A:47:LYS:HD3	1:A:76:GLN:HG2	1.97	0.47
1:B:95:THR:O	1:B:96:ALA:HB3	2.15	0.47
1:B:317:ASP:HA	1:B:318:TYR:HA	1.63	0.47
1:B:39:ALA:HA	1:B:110:TRP:CG	2.50	0.46
1:D:186:GLY:HA3	1:D:223:ASN:ND2	2.30	0.46
1:B:119:ALA:HA	1:B:144:ILE:HD11	1.98	0.46
1:A:19:SER:HB2	1:A:96:ALA:HA	1.97	0.46
1:A:35:PRO:HD2	3:A:452:HOH:O	2.14	0.46
1:B:431:HIS:CE1	1:B:438:ASN:HD21	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:CD1	1:C:126:ALA:HB3	2.44	0.46
1:C:243:GLN:O	1:C:247:ARG:HB2	2.15	0.46
1:A:413:ILE:HD11	1:A:428:LEU:HD12	1.98	0.46
1:B:208:ARG:NH1	1:B:362:LEU:O	2.49	0.46
1:C:194:ILE:HD12	1:C:391:LEU:HD11	1.97	0.46
1:C:213:LYS:NZ	2:C:445:SO4:O2	2.47	0.46
1:A:423:THR:HG22	1:A:424:GLY:N	2.31	0.45
1:B:394:PHE:HB2	1:B:414:ILE:HB	1.98	0.45
1:C:204:ILE:HD13	1:C:385:ILE:CG2	2.46	0.45
1:D:42:ALA:HB3	1:D:45:HIS:CD2	2.51	0.45
1:D:17:LEU:HD13	1:D:48:ILE:HD13	1.98	0.45
1:A:167:PHE:HA	1:A:170:ILE:HG12	1.97	0.45
1:B:272:ARG:O	1:B:276:VAL:HG23	2.16	0.45
1:D:167:PHE:O	1:D:171:GLU:HG2	2.17	0.45
1:D:231:GLY:HA2	1:D:284:PRO:HB2	1.99	0.45
1:A:312:GLY:O	1:A:355:PRO:HD2	2.17	0.45
1:B:52:MET:HG2	1:B:67:LEU:HD13	1.97	0.45
1:B:108:GLU:HG2	1:C:133:LEU:HD12	1.99	0.45
1:C:194:ILE:HD11	1:C:415:VAL:HG21	1.98	0.45
1:A:250:CYS:HB3	1:A:255:ILE:O	2.17	0.45
1:C:428:LEU:HD23	1:C:437:PHE:HD2	1.82	0.45
1:C:142:LYS:O	1:C:146:GLU:HG3	2.17	0.45
1:A:295:LEU:HD22	1:A:341:ILE:HA	1.99	0.44
1:B:160:ARG:HG3	1:B:160:ARG:NH1	2.24	0.44
1:C:304:ARG:HA	1:C:307:SER:HB3	1.98	0.44
1:A:108:GLU:HG2	1:D:133:LEU:HD22	1.99	0.44
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.17	0.44
1:B:343:ARG:NH1	1:C:289:ASP:O	2.50	0.44
1:A:301:ARG:NH1	1:D:155:GLU:HG3	2.32	0.44
1:B:320:GLN:NE2	1:B:361:GLN:H	2.16	0.44
1:B:266:THR:HG22	1:B:268:ARG:H	1.83	0.44
1:C:428:LEU:HG	1:C:438:ASN:O	2.18	0.44
1:D:407:LYS:HB2	1:D:410:ILE:HD12	2.00	0.44
1:B:382:SER:HB3	1:B:385:ILE:HD12	1.99	0.44
1:B:413:ILE:HD11	1:B:428:LEU:CD1	2.48	0.44
1:D:223:ASN:O	1:D:227:LYS:HB3	2.18	0.44
1:C:373:ARG:HA	1:C:374:PRO:HD3	1.88	0.44
1:D:419:ARG:HE	1:D:419:ARG:HA	1.80	0.44
1:A:213:LYS:NZ	1:A:361:GLN:OE1	2.46	0.43
1:B:232:VAL:HG22	1:B:285:ILE:HG12	2.00	0.43
1:D:110:TRP:HD1	1:D:113:ARG:NH2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ARG:NH2	1:D:56:ARG:CG	2.72	0.43
1:C:252:GLU:O	1:C:254:ARG:NE	2.48	0.43
1:C:140:ALA:O	1:C:144:ILE:HG12	2.19	0.43
1:D:232:VAL:HG22	1:D:285:ILE:HG12	2.00	0.43
1:A:197:LEU:CD1	1:A:357:ILE:HD11	2.46	0.43
1:C:110:TRP:O	1:C:114:ARG:HG3	2.19	0.43
1:A:170:ILE:HD12	1:B:273:LEU:HD21	2.00	0.43
1:C:223:ASN:HD22	1:C:223:ASN:C	2.22	0.43
1:B:144:ILE:HG21	1:C:144:ILE:HG13	2.02	0.42
1:C:208:ARG:NH1	1:C:362:LEU:O	2.52	0.42
1:A:6:PRO:HA	1:A:7:PRO:HD3	1.79	0.42
1:B:295:LEU:HD22	1:B:341:ILE:HA	2.00	0.42
1:B:48:ILE:O	1:B:52:MET:HG3	2.19	0.42
1:B:211:MET:HA	1:B:211:MET:CE	2.50	0.42
1:D:317:ASP:HA	1:D:318:TYR:HA	1.63	0.42
1:D:44:ALA:HB1	1:D:80:VAL:HG13	2.02	0.42
1:A:17:LEU:HD12	1:A:45:HIS:CD2	2.55	0.42
1:A:223:ASN:O	1:A:227:LYS:HB2	2.20	0.42
1:B:6:PRO:HA	1:B:7:PRO:HD3	1.90	0.42
1:D:58:GLN:HG3	1:D:60:ARG:HG2	2.02	0.42
1:A:26:VAL:HG11	1:A:96:ALA:HB1	2.02	0.41
1:B:320:GLN:HE22	1:B:360:SER:HA	1.81	0.41
1:A:114:ARG:NH2	1:A:150:THR:O	2.49	0.41
1:B:112:LEU:O	1:B:116:ILE:HG12	2.20	0.41
1:A:37:PRO:O	1:A:46:ARG:HG3	2.20	0.41
1:B:206:ALA:O	1:B:394:PHE:HA	2.20	0.41
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.70	0.41
1:C:317:ASP:HA	1:C:318:TYR:HA	1.80	0.41
1:D:311:VAL:HG23	1:D:312:GLY:H	1.85	0.41
1:D:112:LEU:O	1:D:116:ILE:HG12	2.21	0.41
1:D:320:GLN:HE21	1:D:361:GLN:N	2.11	0.41
1:A:257:MET:CE	1:A:257:MET:H	2.34	0.41
1:B:205:ILE:HG12	1:B:393:MET:HE2	2.03	0.41
1:C:413:ILE:HD11	1:C:428:LEU:HD22	2.03	0.41
1:B:397:ARG:HB3	1:B:411:ALA:HA	2.02	0.41
1:D:418:GLN:HG2	1:D:419:ARG:N	2.36	0.41
1:A:399:GLU:HG3	1:A:408:ALA:HA	2.03	0.40
1:D:320:GLN:NE2	1:D:360:SER:OG	2.54	0.40
1:A:157:ARG:HA	1:A:158:PRO:HD3	1.91	0.40
1:A:189:GLU:HA	1:A:192:GLN:HE21	1.86	0.40
1:A:121:GLU:HG2	1:A:143:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HB3	1:B:188:LYS:HE2	1.51	0.40
1:A:205:ILE:HG22	1:A:213:LYS:HG2	2.02	0.40
1:B:373:ARG:HA	1:B:374:PRO:HD3	1.85	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	413/444 (93%)	396 (96%)	13 (3%)	4 (1%)	18	51
1	B	404/444 (91%)	385 (95%)	15 (4%)	4 (1%)	18	51
1	C	398/444 (90%)	376 (94%)	19 (5%)	3 (1%)	22	57
1	D	392/444 (88%)	370 (94%)	17 (4%)	5 (1%)	14	43
All	All	1607/1776 (90%)	1527 (95%)	64 (4%)	16 (1%)	18	51

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	A	408	ALA
1	D	291	PRO
1	D	408	ALA
1	A	405	SER
1	B	35	PRO
1	B	408	ALA
1	C	257	MET
1	C	292	ASP
1	D	186	GLY
1	B	291	PRO
1	D	81	GLY

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Mol	Chain	Res	Type
1	B	435	VAL
1	A	435	VAL
1	D	311	VAL
1	C	186	GLY

### 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	343/359 (96%)	327 (95%)	16 (5%)	30	65
1	B	338/359 (94%)	327 (97%)	11 (3%)	43	77
1	C	332/359 (92%)	322 (97%)	10 (3%)	46	80
1	D	327/359 (91%)	316 (97%)	11 (3%)	42	76
All	All	1340/1436 (93%)	1292 (96%)	48 (4%)	40	75

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	60	ARG
1	A	69	GLU
1	A	95	THR
1	A	166	THR
1	A	184	ARG
1	A	230	VAL
1	A	257	MET
1	A	266	THR
1	A	267	ASP
1	A	273	LEU
1	A	334	ARG
1	A	388	ASP
1	A	406	GLU
1	A	419	ARG
1	A	439	ASP
1	B	56	ARG

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Mol	Chain	Res	Type
1	B	69	GLU
1	B	71	LEU
1	B	77	LEU
1	B	79	GLU
1	B	88	GLN
1	B	124	ARG
1	B	160	ARG
1	B	227	LYS
1	B	293	LEU
1	B	320	GLN
1	C	26	VAL
1	C	185	THR
1	C	211	MET
1	C	223	ASN
1	C	254	ARG
1	C	258	ASN
1	C	292	ASP
1	C	380	ARG
1	C	404	HIS
1	C	420	ASN
1	D	56	ARG
1	D	78	GLU
1	D	93	THR
1	D	152	THR
1	D	335	GLN
1	D	354	ILE
1	D	388	ASP
1	D	397	ARG
1	D	407	LYS
1	D	419	ARG
1	D	427	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	192	GLN
1	A	222	GLN
1	A	320	GLN
1	B	45	HIS
1	B	88	GLN
1	B	320	GLN

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Mol	Chain	Res	Type
1	B	336	GLN
1	B	361	GLN
1	B	418	GLN
1	B	429	GLN
1	B	438	ASN
1	C	58	GLN
1	C	223	ASN
1	C	308	GLN
1	C	320	GLN
1	C	371	ASN
1	C	420	ASN
1	D	45	HIS
1	D	320	GLN
1	D	336	GLN
1	D	371	ASN
1	D	418	GLN
1	D	434	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	445	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	B	445	-	4,4,4	0.13	0	6,6,6	0.20	0
2	SO4	C	445	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	D	445	-	4,4,4	0.11	0	6,6,6	0.26	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
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	C	445	-	-	0/0/0/0	0/0/0/0
2	SO4	D	445	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	445	SO4	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	419/444 (94%)	0.56	35 (8%) 12 8	91, 103, 118, 128	0
1	B	414/444 (93%)	0.63	43 (10%) 7 5	91, 104, 115, 130	0
1	C	406/444 (91%)	0.73	49 (12%) 5 3	91, 104, 115, 124	0
1	D	402/444 (90%)	0.87	60 (14%) 3 2	93, 105, 116, 118	0
All	All	1641/1776 (92%)	0.69	187 (11%) 6 4	91, 104, 116, 130	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	PHE	8.3
1	B	62	VAL	7.5
1	C	283	ALA	7.3
1	D	85	TYR	6.9
1	D	387	GLN	6.9
1	C	368	ALA	6.6
1	C	381	GLU	6.5
1	C	365	ALA	6.3
1	C	400	TYR	5.9
1	B	61	PRO	5.8
1	D	87	LEU	5.3
1	D	420	ASN	5.3
1	C	403	PRO	5.2
1	B	366	VAL	5.2
1	C	401	TYR	5.2
1	D	407	LYS	5.1
1	B	325	PRO	5.0
1	B	2	GLU	5.0
1	D	29	GLU	4.9
1	A	384	SER	4.9
1	D	404	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	408	ALA	4.8
1	C	438	ASN	4.6
1	C	367	GLU	4.6
1	D	69	GLU	4.5
1	B	58	GLN	4.5
1	D	359	LEU	4.5
1	D	189	GLU	4.3
1	C	380	ARG	4.3
1	B	402	ASN	4.3
1	A	336	GLN	4.2
1	C	440	LEU	4.2
1	C	252	GLU	4.2
1	D	152	THR	4.1
1	B	85	TYR	4.1
1	A	100	GLU	4.0
1	C	405	SER	4.0
1	B	266	THR	4.0
1	D	358	ALA	3.9
1	B	33	LEU	3.9
1	C	408	ALA	3.9
1	A	212	GLY	3.8
1	C	273	LEU	3.8
1	C	325	PRO	3.8
1	B	167	PHE	3.8
1	C	5	ILE	3.7
1	A	252	GLU	3.6
1	C	168	GLU	3.6
1	B	368	ALA	3.6
1	D	360	SER	3.6
1	C	270	PHE	3.6
1	B	408	ALA	3.6
1	C	214	THR	3.6
1	D	215	ALA	3.6
1	D	191	ASP	3.5
1	D	56	ARG	3.5
1	C	384	SER	3.5
1	D	282	GLU	3.5
1	D	405	SER	3.4
1	C	369	ARG	3.4
1	D	76	GLN	3.4
1	D	368	ALA	3.4
1	D	275	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLN	3.3
1	C	430	PHE	3.3
1	D	401	TYR	3.3
1	B	365	ALA	3.3
1	D	67	LEU	3.2
1	D	440	LEU	3.2
1	B	26	VAL	3.2
1	B	381	GLU	3.2
1	D	89	LEU	3.2
1	A	99	ALA	3.2
1	A	171	GLU	3.2
1	D	109	LYS	3.2
1	A	93	THR	3.2
1	A	76	GLN	3.2
1	A	262	LEU	3.2
1	A	170	ILE	3.1
1	D	315	ILE	3.1
1	B	312	GLY	3.1
1	B	405	SER	3.1
1	D	212	GLY	3.1
1	D	74	ARG	3.1
1	B	214	THR	3.0
1	A	381	GLU	3.0
1	B	382	SER	3.0
1	C	211	MET	3.0
1	C	257	MET	3.0
1	B	254	ARG	2.9
1	C	397	ARG	2.9
1	A	215	ALA	2.9
1	A	403	PRO	2.9
1	D	274	VAL	2.9
1	B	21	LEU	2.9
1	D	316	ILE	2.9
1	C	28	ASP	2.9
1	D	397	ARG	2.9
1	C	431	HIS	2.9
1	A	90	SER	2.8
1	A	310	GLN	2.8
1	D	214	THR	2.8
1	D	82	GLY	2.8
1	A	214	THR	2.8
1	A	217	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	146	GLU	2.8
1	D	372	LYS	2.8
1	D	410	ILE	2.8
1	B	63	ASP	2.7
1	B	184	ARG	2.7
1	C	212	GLY	2.7
1	D	365	ALA	2.7
1	C	395	ILE	2.7
1	D	333	ASN	2.7
1	D	422	PRO	2.6
1	A	213	LYS	2.6
1	A	410	ILE	2.6
1	A	440	LEU	2.6
1	C	421	GLY	2.6
1	D	364	ARG	2.6
1	A	388	ASP	2.6
1	A	265	LEU	2.6
1	C	427	GLU	2.6
1	B	170	ILE	2.5
1	A	315	ILE	2.5
1	A	279	ARG	2.5
1	D	296	MET	2.5
1	B	255	ILE	2.5
1	B	217	ALA	2.5
1	A	269	ASP	2.5
1	A	94	PRO	2.4
1	A	62	VAL	2.4
1	B	39	ALA	2.4
1	C	230	VAL	2.4
1	D	213	LYS	2.4
1	D	62	VAL	2.4
1	D	79	GLU	2.4
1	B	361	GLN	2.4
1	D	403	PRO	2.3
1	B	380	ARG	2.3
1	D	434	HIS	2.3
1	C	100	GLU	2.3
1	A	316	ILE	2.3
1	C	271	SER	2.3
1	B	206	ALA	2.3
1	A	436	ARG	2.3
1	B	403	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	206	ALA	2.3
1	B	323	SER	2.3
1	B	162	LEU	2.3
1	A	188	LYS	2.3
1	B	275	ASP	2.2
1	D	318	TYR	2.2
1	B	219	THR	2.2
1	C	409	GLY	2.2
1	D	249	MET	2.2
1	D	227	LYS	2.2
1	A	247	ARG	2.2
1	B	281	SER	2.2
1	D	217	ALA	2.2
1	A	104	ARG	2.2
1	B	31	GLU	2.2
1	C	138	ASP	2.2
1	C	416	GLY	2.2
1	B	156	ALA	2.2
1	A	45	HIS	2.2
1	C	215	ALA	2.1
1	B	335	GLN	2.1
1	C	194	ILE	2.1
1	B	399	GLU	2.1
1	C	377	SER	2.1
1	C	382	SER	2.1
1	D	68	SER	2.1
1	D	149	LEU	2.1
1	C	402	ASN	2.1
1	C	364	ARG	2.1
1	D	21	LEU	2.1
1	C	429	GLN	2.0
1	D	185	THR	2.0
1	D	235	TYR	2.0
1	D	80	VAL	2.0
1	D	254	ARG	2.0
1	B	406	GLU	2.0
1	C	282	GLU	2.0
1	C	417	LYS	2.0
1	C	228	GLU	2.0
1	B	334	ARG	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	445	5/5	0.91	0.23	-0.59	106,108,109,110	0
2	SO4	A	445	5/5	0.95	0.19	-1.20	77,77,78,80	0
2	SO4	C	445	5/5	0.92	0.16	-2.16	107,108,109,110	0
2	SO4	B	445	5/5	0.97	0.14	-2.38	86,87,90,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.