Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:43 am BST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

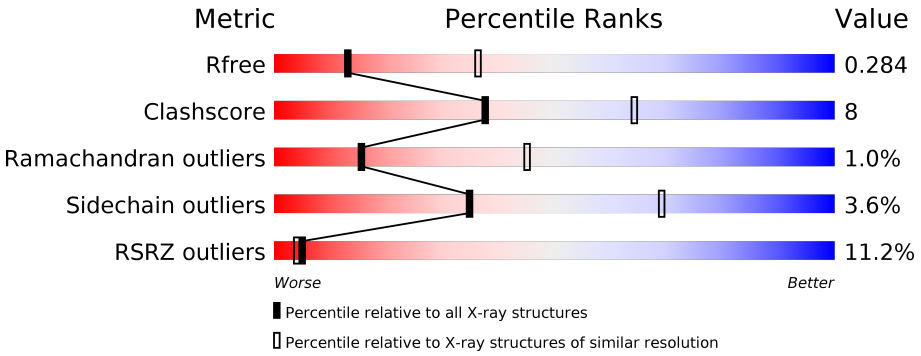
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 >=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% 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	8% 74% 19% • 6%
1	B	444	9% 75% 18% • 7%
1	C	444	11% 75% 16% • 9%
1	D	444	13% 76% 13% • 9%

2 Entry composition

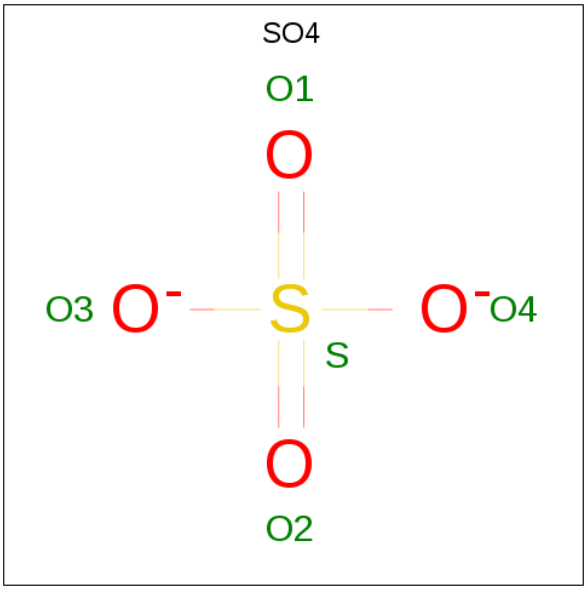
There are 3 unique types of molecules in this entry. The entry contains 12746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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_4S).



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 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

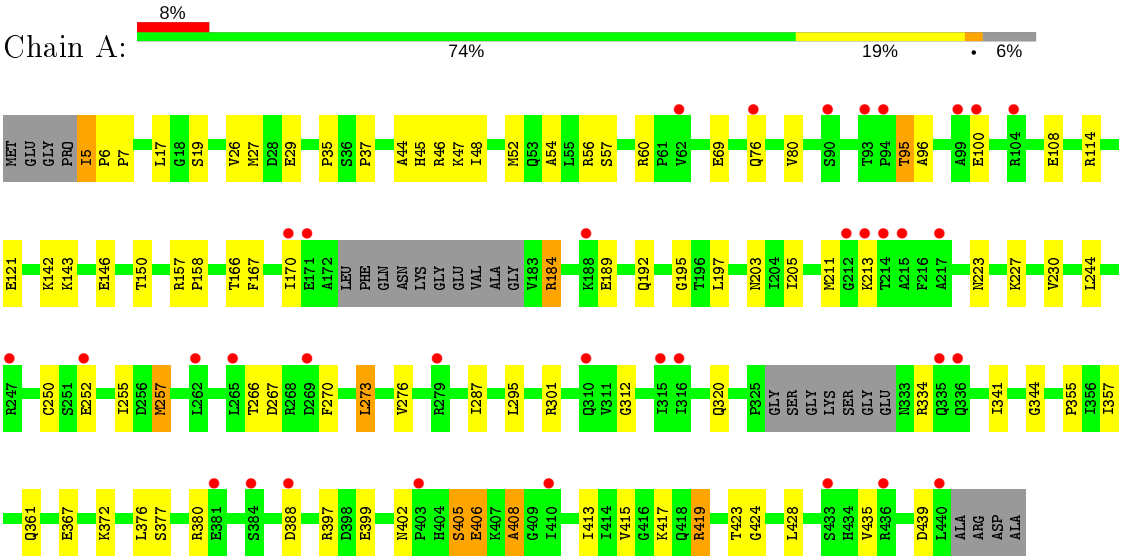
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	5	Total O 5 5	0	0
3	C	6	Total O 6 6	0	0
3	D	3	Total O 3 3	0	0

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.

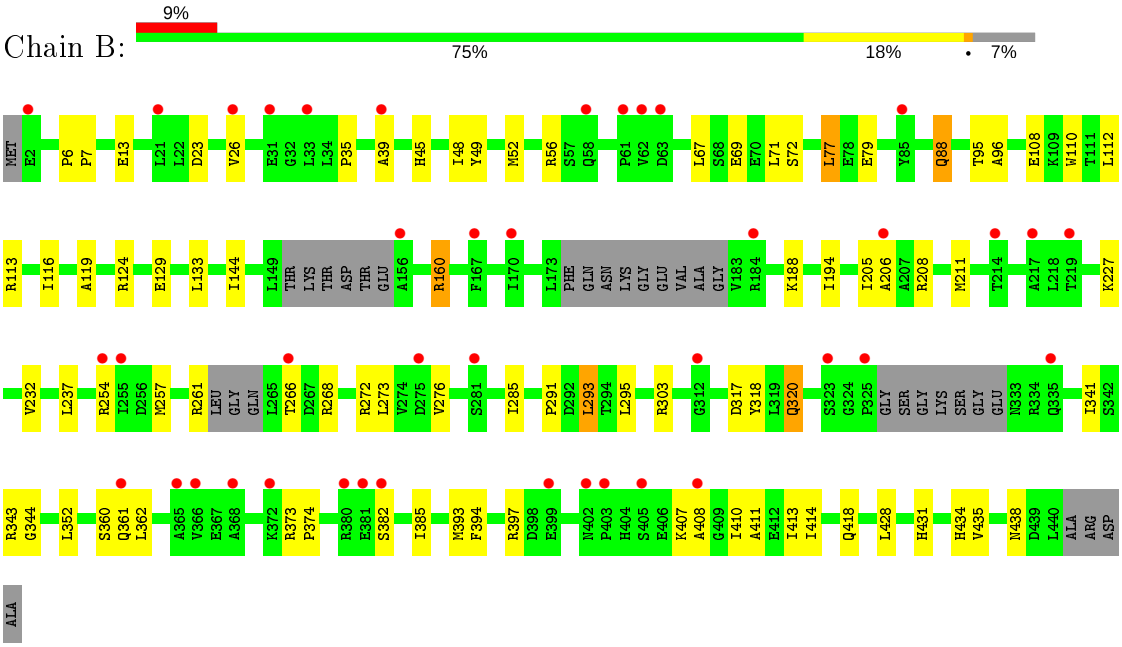
- Molecule 1: DnaB replication fork helicase

Chain A:



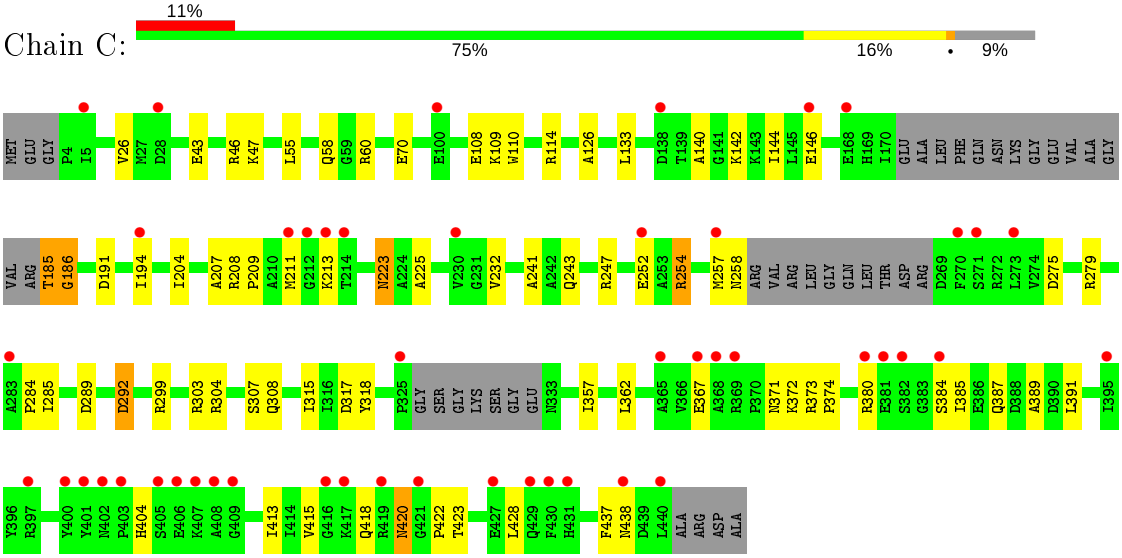
- Molecule 1: DnaB replication fork helicase

Chain B:



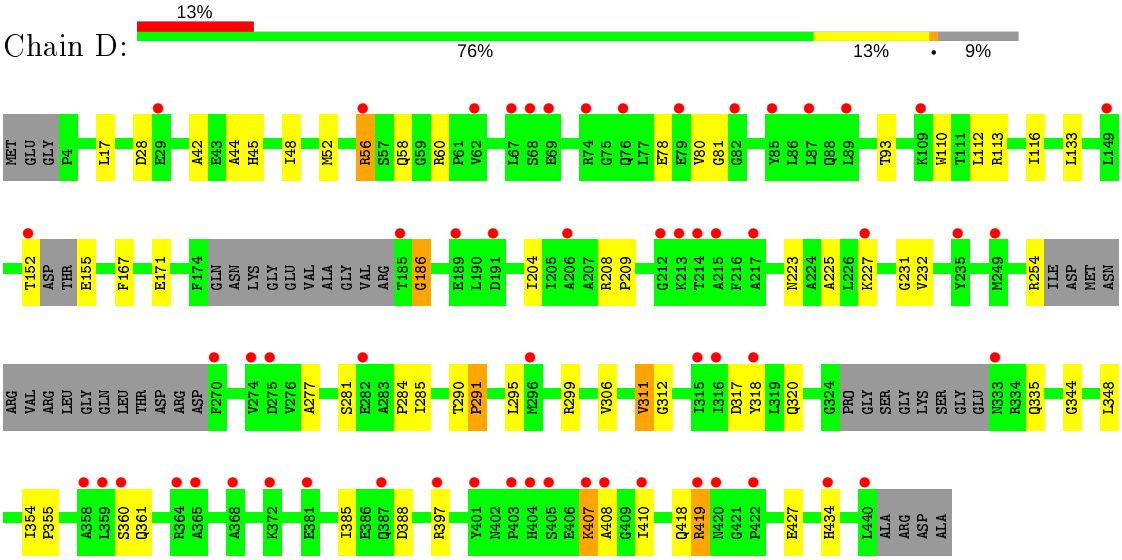
• Molecule 1: DnaB replication fork helicase

Chain C:



• Molecule 1: DnaB replication fork helicase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 106.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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^2)	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.*

[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	0.35	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

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%)	15	45
1	B	404/444 (91%)	385 (95%)	15 (4%)	4 (1%)	15	45
1	C	398/444 (90%)	376 (94%)	19 (5%)	3 (1%)	19	51
1	D	392/444 (88%)	370 (94%)	17 (4%)	5 (1%)	12	37
All	All	1607/1776 (90%)	1527 (95%)	64 (4%)	16 (1%)	15	45

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 (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	343/359 (96%)	327 (95%)	16 (5%)	26	59
1	B	338/359 (94%)	327 (97%)	11 (3%)	38	72
1	C	332/359 (92%)	322 (97%)	10 (3%)	41	75
1	D	327/359 (91%)	316 (97%)	11 (3%)	37	71
All	All	1340/1436 (93%)	1292 (96%)	48 (4%)	35	69

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

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	$\#\|Z\|>2$
2	SO4	C	445	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	D	445	-	4,4,4	0.11	0	6,6,6	0.27	0
2	SO4	A	445	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	B	445	-	4,4,4	0.14	0	6,6,6	0.21	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

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^{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	419/444 (94%)	0.54	35 (8%) 11 8	91, 103, 118, 128	0
1	B	414/444 (93%)	0.63	41 (9%) 7 5	91, 104, 115, 130	0
1	C	406/444 (91%)	0.73	48 (11%) 4 3	91, 104, 115, 124	0
1	D	402/444 (90%)	0.86	59 (14%) 2 1	93, 105, 116, 118	0
All	All	1641/1776 (92%)	0.69	183 (11%) 5 4	91, 104, 116, 130	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	PHE	8.4
1	C	283	ALA	7.2
1	B	62	VAL	7.1
1	D	85	TYR	6.7
1	C	381	GLU	6.7
1	C	368	ALA	6.5
1	D	387	GLN	6.5
1	C	365	ALA	6.2
1	B	61	PRO	5.7
1	C	401	TYR	5.6
1	C	400	TYR	5.4
1	B	325	PRO	5.4
1	C	403	PRO	5.3
1	D	87	LEU	5.2
1	D	29	GLU	5.2
1	B	2	GLU	5.1
1	D	420	ASN	5.1
1	B	366	VAL	5.1
1	D	407	LYS	5.0
1	D	408	ALA	5.0
1	A	384	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	404	HIS	4.7
1	D	359	LEU	4.5
1	D	69	GLU	4.4
1	B	58	GLN	4.4
1	C	438	ASN	4.4
1	C	367	GLU	4.4
1	B	402	ASN	4.3
1	D	189	GLU	4.3
1	C	440	LEU	4.2
1	A	100	GLU	4.2
1	A	336	GLN	4.1
1	C	325	PRO	4.1
1	C	380	ARG	4.0
1	D	152	THR	4.0
1	B	266	THR	4.0
1	C	252	GLU	3.9
1	C	270	PHE	3.9
1	D	358	ALA	3.9
1	B	85	TYR	3.8
1	C	273	LEU	3.8
1	A	252	GLU	3.8
1	C	408	ALA	3.7
1	B	381	GLU	3.7
1	D	215	ALA	3.7
1	C	168	GLU	3.7
1	D	191	ASP	3.7
1	C	384	SER	3.7
1	B	408	ALA	3.6
1	A	212	GLY	3.6
1	C	214	THR	3.6
1	D	401	TYR	3.5
1	C	405	SER	3.5
1	D	360	SER	3.5
1	B	167	PHE	3.5
1	C	369	ARG	3.5
1	D	89	LEU	3.5
1	C	5	ILE	3.5
1	B	368	ALA	3.4
1	B	33	LEU	3.4
1	B	26	VAL	3.4
1	D	405	SER	3.4
1	D	275	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	430	PHE	3.3
1	D	282	GLU	3.3
1	D	56	ARG	3.3
1	D	82	GLY	3.2
1	B	365	ALA	3.2
1	D	76	GLN	3.2
1	A	335	GLN	3.2
1	A	171	GLU	3.2
1	D	315	ILE	3.2
1	A	381	GLU	3.2
1	D	74	ARG	3.2
1	D	109	LYS	3.1
1	B	312	GLY	3.1
1	D	440	LEU	3.1
1	C	397	ARG	3.1
1	B	21	LEU	3.1
1	B	382	SER	3.1
1	B	405	SER	3.1
1	A	93	THR	3.1
1	A	214	THR	3.0
1	D	212	GLY	3.0
1	B	214	THR	3.0
1	D	274	VAL	3.0
1	A	215	ALA	3.0
1	D	368	ALA	3.0
1	A	170	ILE	3.0
1	D	316	ILE	3.0
1	A	403	PRO	3.0
1	A	262	LEU	3.0
1	D	67	LEU	3.0
1	C	28	ASP	3.0
1	C	257	MET	3.0
1	A	76	GLN	2.9
1	C	211	MET	2.9
1	A	99	ALA	2.9
1	C	431	HIS	2.8
1	D	62	VAL	2.8
1	D	422	PRO	2.8
1	A	217	ALA	2.8
1	B	184	ARG	2.8
1	C	427	GLU	2.8
1	C	212	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	254	ARG	2.7
1	A	310	GLN	2.7
1	D	397	ARG	2.7
1	B	170	ILE	2.7
1	D	372	LYS	2.7
1	A	440	LEU	2.7
1	D	365	ALA	2.7
1	D	364	ARG	2.7
1	A	213	LYS	2.6
1	C	146	GLU	2.6
1	C	230	VAL	2.6
1	D	214	THR	2.6
1	C	421	GLY	2.6
1	D	79	GLU	2.5
1	D	296	MET	2.5
1	A	265	LEU	2.5
1	A	279	ARG	2.5
1	C	382	SER	2.5
1	D	333	ASN	2.5
1	D	434	HIS	2.5
1	C	395	ILE	2.5
1	A	269	ASP	2.5
1	A	388	ASP	2.5
1	B	63	ASP	2.5
1	A	315	ILE	2.5
1	A	410	ILE	2.4
1	B	217	ALA	2.4
1	D	213	LYS	2.4
1	B	403	PRO	2.4
1	A	436	ARG	2.4
1	D	206	ALA	2.4
1	A	62	VAL	2.4
1	B	380	ARG	2.4
1	A	94	PRO	2.3
1	D	410	ILE	2.3
1	B	335	GLN	2.3
1	A	90	SER	2.3
1	B	39	ALA	2.3
1	D	249	MET	2.3
1	D	318	TYR	2.3
1	A	104	ARG	2.3
1	D	217	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	361	GLN	2.3
1	B	219	THR	2.2
1	C	271	SER	2.2
1	D	68	SER	2.2
1	A	316	ILE	2.2
1	B	206	ALA	2.2
1	B	156	ALA	2.2
1	B	275	ASP	2.2
1	C	409	GLY	2.2
1	C	100	GLU	2.2
1	D	149	LEU	2.2
1	B	255	ILE	2.2
1	B	323	SER	2.2
1	C	416	GLY	2.2
1	D	185	THR	2.2
1	D	381	GLU	2.2
1	A	433	SER	2.1
1	C	213	LYS	2.1
1	D	227	LYS	2.1
1	B	281	SER	2.1
1	B	31	GLU	2.1
1	C	194	ILE	2.1
1	C	138	ASP	2.1
1	A	188	LYS	2.1
1	C	419	ARG	2.1
1	C	402	ASN	2.1
1	D	403	PRO	2.1
1	D	235	TYR	2.0
1	C	406	GLU	2.0
1	C	407	LYS	2.0
1	D	419	ARG	2.0
1	C	417	LYS	2.0
1	C	429	GLN	2.0
1	B	372	LYS	2.0
1	B	399	GLU	2.0
1	A	247	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. 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
2	SO4	D	445	5/5	0.91	0.23	106,108,109,110	0
2	SO4	C	445	5/5	0.92	0.16	107,108,109,110	0
2	SO4	A	445	5/5	0.95	0.19	77,77,78,80	0
2	SO4	B	445	5/5	0.97	0.14	86,87,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.