



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 2Q6T / pdb_00002q6t
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

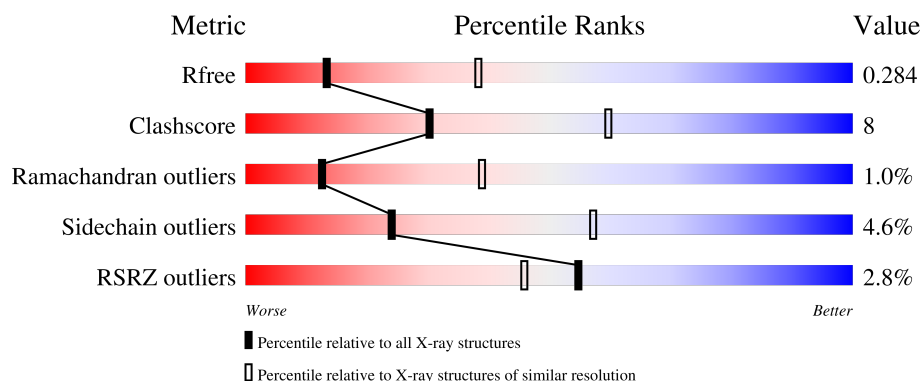
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	72% 20% 6%
1	B	444	73% 19% 7%
1	C	444	73% 17% 9%
1	D	444	75% 14% 9%

2 Entry composition [i](#)

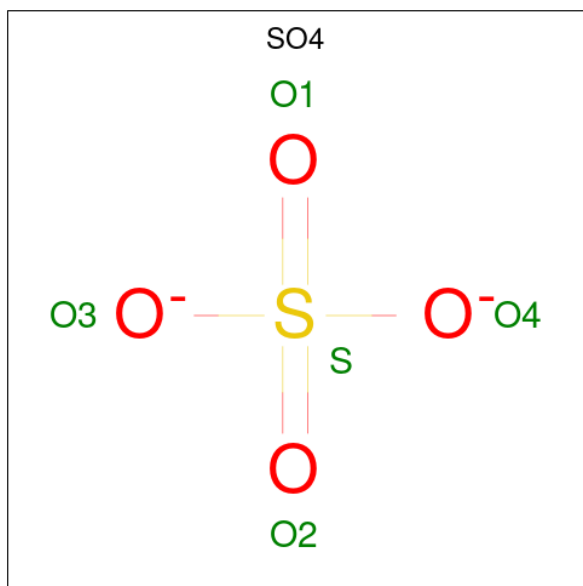
There are 3 unique types of molecules in this entry. The entry contains 12746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



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		

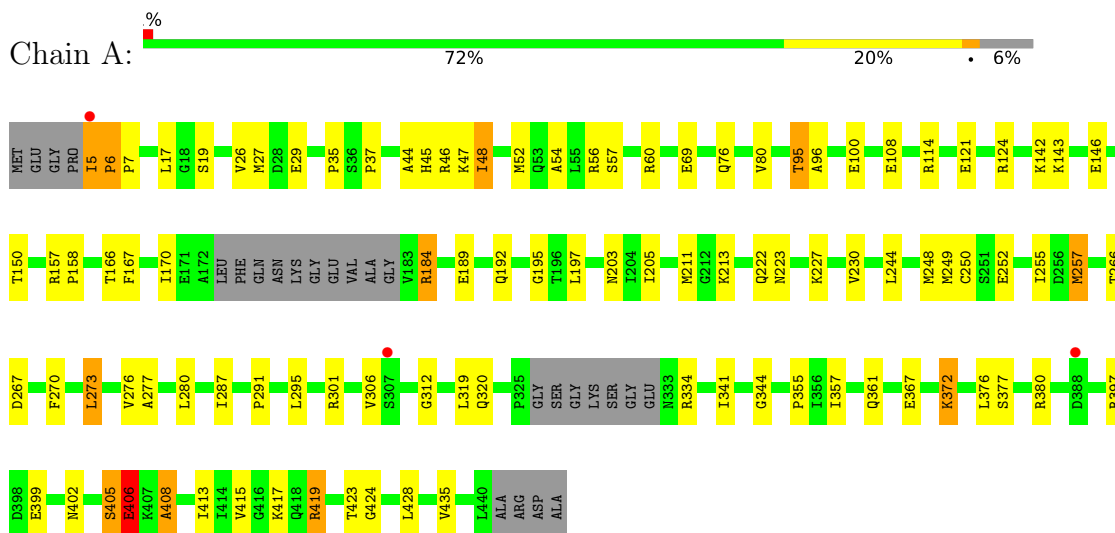
- Molecule 3 is water.

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		

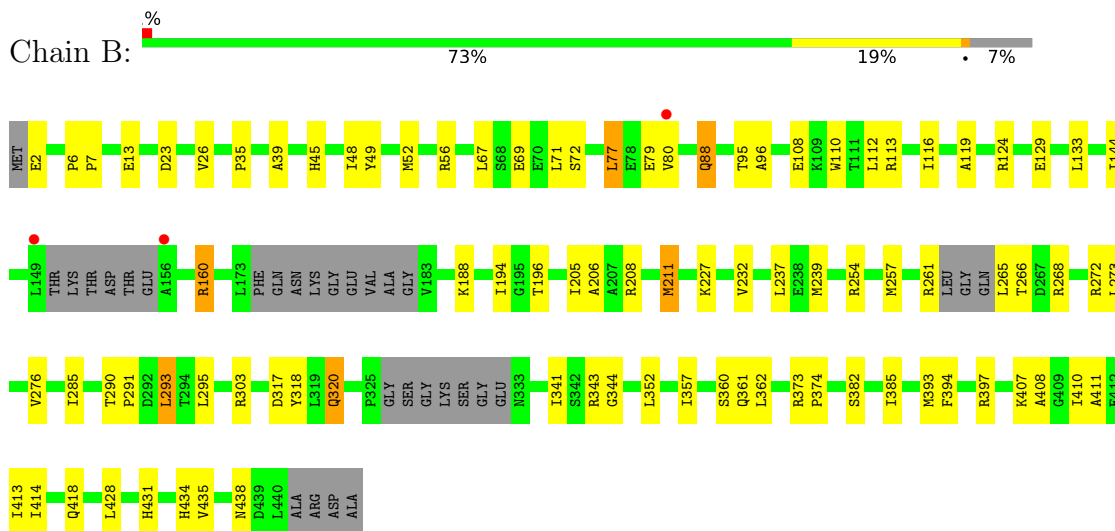
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

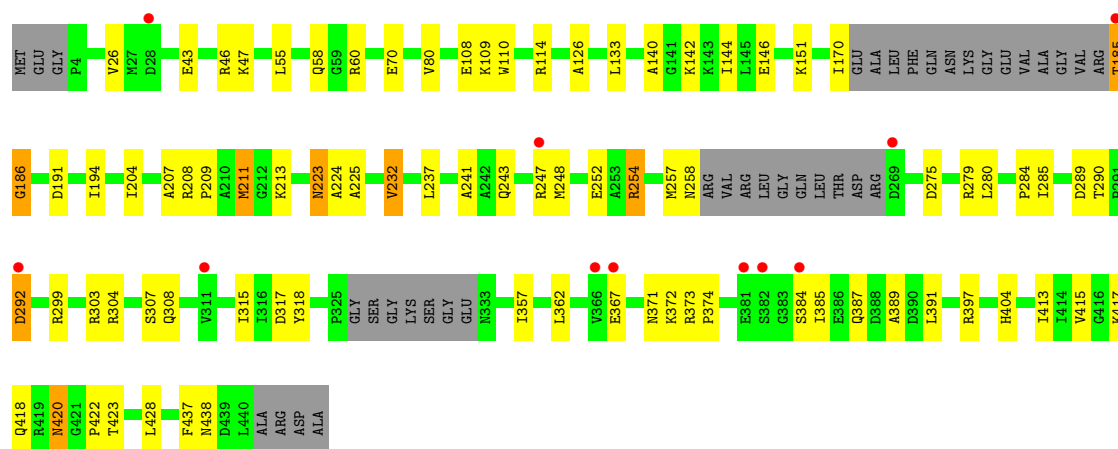


- Molecule 1: DnaB replication fork helicase

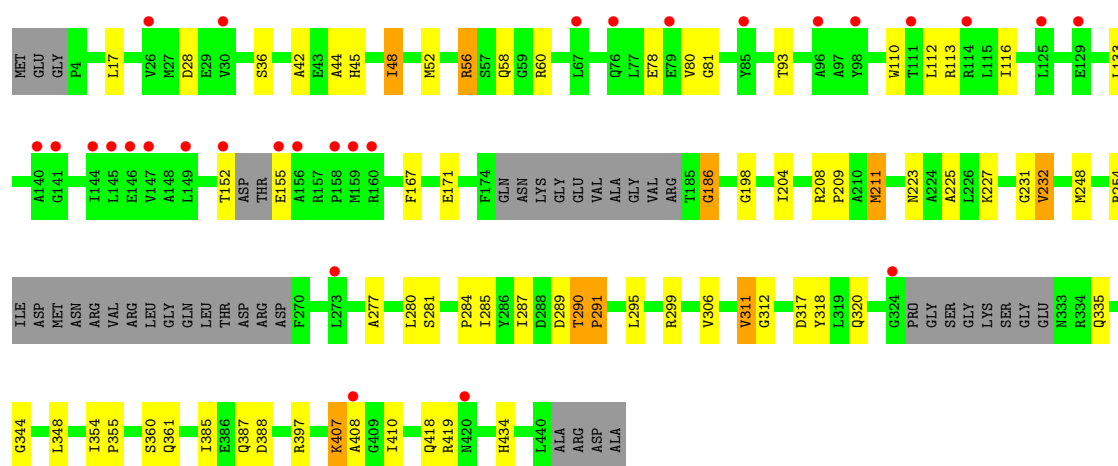
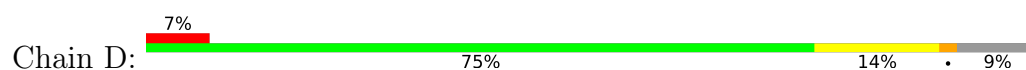


- Molecule 1: DnaB replication fork helicase





• 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, α , β , γ	104.71Å 104.71Å 363.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.90) 98.8 (20.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.06%)	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)	0.29 , 96.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.47	0/3292	0.94	4/4450 (0.1%)
1	B	0.44	0/3251	0.92	2/4392 (0.0%)
1	C	0.46	0/3183	0.89	1/4303 (0.0%)
1	D	0.45	0/3153	0.92	7/4259 (0.2%)
All	All	0.46	0/12879	0.91	14/17404 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	PRO	N-CA-C	7.14	122.79	113.86
1	B	290	THR	CA-C-N	7.08	128.69	119.84
1	B	290	THR	C-N-CA	7.08	128.69	119.84
1	D	290	THR	CA-C-N	6.96	128.54	119.84
1	D	290	THR	C-N-CA	6.96	128.54	119.84
1	A	406	GLU	N-CA-C	5.73	123.00	110.80
1	D	36	SER	CA-C-N	5.60	125.27	119.56
1	D	36	SER	C-N-CA	5.60	125.27	119.56
1	A	6	PRO	N-CA-C	5.38	117.26	110.70
1	D	387	GLN	N-CA-C	5.31	117.07	111.28
1	A	319	LEU	N-CA-C	5.25	117.41	111.11
1	C	224	ALA	N-CA-C	-5.04	107.68	113.88
1	D	198	GLY	CA-C-N	5.03	126.12	119.84
1	D	198	GLY	C-N-CA	5.03	126.12	119.84

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	69	0
1	B	3207	0	3249	57	0
1	C	3138	0	3172	57	0
1	D	3109	0	3150	46	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
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	214	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 (214) 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:HG2	1:D:56:ARG:HH21	1.24	1.01
1:A:419:ARG:HG3	1:A:419:ARG:HH11	1.26	0.99
1:A:184:ARG:HG3	1:A:184:ARG:HH11	1.32	0.91
1:B:237:LEU:HD21	1:B:293:LEU:HD12	1.51	0.89
1:D:254:ARG:C	1:D:434:HIS:CE1	2.50	0.89
1:A:29:GLU:HG2	1:A:100:GLU:HG3	1.55	0.89
1:A:184:ARG:HH11	1:A:184:ARG:CG	1.90	0.85
1:B:160:ARG:HH11	1:B:160:ARG:CG	1.93	0.82
1:B:160:ARG:HH11	1:B:160:ARG:HG3	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:A:257:MET:HE2	1:A:257:MET:H	1.49	0.77
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:HH11	1:A:419:ARG:CG	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLN:HE21	1:D:361:GLN:H	1.39	0.70
1:A:248:MET:HE2	1:A:280:LEU:HD11	1.73	0.69
1:A:184:ARG:HG3	1:A:184:ARG:NH1	2.04	0.69
1:A:257:MET:HE2	1:A:257:MET:N	2.07	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:211:MET:HA	1:B:211:MET:HE2	1.78	0.66
1:D:248:MET:HE3	1:D:280:LEU:HD21	1.78	0.65
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
1:D:208:ARG:HD2	1:D:209:PRO:HD2	1.83	0.61
1:C:204:ILE:HD13	1:C:385:ILE:HG22	1.84	0.60
1:C:420:ASN:HD22	1:C:420:ASN:H	1.50	0.59
1:D:56:ARG:HG2	1:D:56:ARG:NH2	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:A:211:MET:HE1	1:A:397:ARG:HG3	1.86	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:D:211:MET:HA	1:D:211:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:222:GLN:HE21	1:A:248:MET:HE3	1.72	0.54
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:H	1:C:420:ASN:ND2	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:48:ILE:O	1:A:52:MET:HG3	2.08	0.53
1:A:192:GLN:O	1:B:261:ARG:NH1	2.40	0.53
1:B:49:TYR:HA	1:B:52:MET:HE2	1.89	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
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:C:185:THR:HG23	1:C:191:ASP:CG	2.35	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:HG3	1:A:419:ARG:NH1	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:7:PRO:O	1:B:113:ARG:HD3	2.11	0.50
1:B:257:MET:O	1:B:261:ARG:HG2	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:C:248:MET:HE3	1:C:280:LEU:HD21	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:223:ASN:C	1:C:223:ASN:HD22	2.22	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:A:211:MET:HE1	1:A:397:ARG:N	2.29	0.48
1:C:43:GLU:OE1	1:C:46:ARG:NH1	2.44	0.48
1:C:208:ARG:CD	1:C:209:PRO:HD2	2.44	0.48
1:A:27:MET:HG2	1:A:56:ARG:CD	2.44	0.47
1:A:95:THR:HG22	1:A:96:ALA:H	1.78	0.47
1:A:222:GLN:NE2	1:A:248:MET:HE3	2.29	0.47
1:A:376:LEU:HD11	1:A:417:LYS:HB2	1.96	0.47
1:A:29:GLU:CG	1:A:100:GLU:HG3	2.36	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:C:211:MET:HE1	1:C:397:ARG:HB2	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:116:ILE:CD1	1:C:126:ALA:HB3	2.44	0.46
1:B:431:HIS:CE1	1:B:438:ASN:HD21	2.33	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:17:LEU:HD13	1:D:48:ILE:HD13	1.98	0.45
1:D:42:ALA:HB3	1:D:45:HIS:CD2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:GLU:CD	1:A:124:ARG:HH12	2.24	0.44
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:A:301:ARG:NH1	1:D:155:GLU:HG3	2.32	0.44
1:B:343:ARG:NH1	1:C:289:ASP:O	2.50	0.44
1:B:320:GLN:NE2	1:B:361:GLN:H	2.16	0.44
1:A:249:MET:HE3	1:A:277:ALA:HB2	1.97	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:205:ILE:HG12	1:B:393:MET:HE2	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:HA	1:D:419:ARG:HE	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
1:A:419:ARG:HE	1:B:239:MET:HE2	1.83	0.43
1:D:56:ARG:CG	1:D:56:ARG:NH2	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:211:MET:HE2	1:C:211:MET:HA	2.01	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:O	1:B:52:MET:HG3	2.19	0.42
1:B:295:LEU:HD22	1:B:341:ILE:HA	2.00	0.42
1:D:44:ALA:HB1	1:D:80:VAL:HG13	2.02	0.42
1:D:317:ASP:HA	1:D:318:TYR:HA	1.63	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:D:289:ASP:O	1:D:290:THR:C	2.63	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:88:GLN:HE21	1:B:88:GLN:HB3	1.70	0.41
1:B:206:ALA:O	1:B:394:PHE:HA	2.20	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:B:343:ARG:HH22	1:C:237:LEU:C	2.28	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:B:343:ARG:O	1:B:344:GLY:C	2.63	0.41
1:C:413:ILE:HD11	1:C:428:LEU:HD22	2.03	0.41
1:A:213:LYS:NZ	1:A:361:GLN:CD	2.79	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
1:C:289:ASP:O	1:C:290:THR:C	2.63	0.40
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%)	12	39
1	B	404/444 (91%)	385 (95%)	15 (4%)	4 (1%)	12	39
1	C	398/444 (90%)	376 (94%)	19 (5%)	3 (1%)	16	44
1	D	392/444 (88%)	370 (94%)	17 (4%)	5 (1%)	9	32
All	All	1607/1776 (90%)	1527 (95%)	64 (4%)	16 (1%)	12	39

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
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%)	326 (95%)	17 (5%)	22	53
1	B	338/359 (94%)	321 (95%)	17 (5%)	22	53
1	C	332/359 (92%)	318 (96%)	14 (4%)	26	60
1	D	327/359 (91%)	314 (96%)	13 (4%)	28	62
All	All	1340/1436 (93%)	1279 (95%)	61 (5%)	24	57

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	48	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	306	VAL
1	A	334	ARG
1	A	372	LYS
1	A	406	GLU
1	A	419	ARG
1	B	2	GLU
1	B	56	ARG
1	B	69	GLU
1	B	71	LEU
1	B	77	LEU
1	B	79	GLU
1	B	80	VAL
1	B	88	GLN
1	B	124	ARG
1	B	160	ARG
1	B	196	THR
1	B	211	MET
1	B	227	LYS

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Mol	Chain	Res	Type
1	B	265	LEU
1	B	293	LEU
1	B	320	GLN
1	B	357	ILE
1	C	26	VAL
1	C	80	VAL
1	C	151	LYS
1	C	170	ILE
1	C	185	THR
1	C	211	MET
1	C	223	ASN
1	C	232	VAL
1	C	254	ARG
1	C	258	ASN
1	C	292	ASP
1	C	404	HIS
1	C	417	LYS
1	C	420	ASN
1	D	48	ILE
1	D	56	ARG
1	D	78	GLU
1	D	93	THR
1	D	152	THR
1	D	211	MET
1	D	232	VAL
1	D	287	ILE
1	D	335	GLN
1	D	354	ILE
1	D	388	ASP
1	D	397	ARG
1	D	407	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	169	HIS
1	A	192	GLN
1	A	222	GLN
1	A	320	GLN
1	B	88	GLN
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
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	402	ASN
1	C	404	HIS
1	C	420	ASN
1	D	45	HIS
1	D	320	GLN
1	D	336	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	445	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	B	445	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	A	445	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	D	445	-	4,4,4	0.20	0	6,6,6	0.28	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, 95th 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%)	0.33	3 (0%) 84 79	91, 103, 118, 128	0
1	B	414/444 (93%)	0.12	3 (0%) 84 79	91, 104, 115, 130	0
1	C	406/444 (91%)	0.33	11 (2%) 56 47	91, 104, 115, 124	0
1	D	402/444 (90%)	0.56	29 (7%) 21 17	93, 105, 116, 118	0
All	All	1641/1776 (92%)	0.33	46 (2%) 55 46	91, 104, 116, 130	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	420	ASN	4.3
1	D	149	LEU	3.9
1	D	145	LEU	3.8
1	A	388	ASP	3.5
1	D	324	GLY	3.3
1	D	408	ALA	3.0
1	B	156	ALA	2.9
1	B	149	LEU	2.8
1	D	147	VAL	2.8
1	C	28	ASP	2.8
1	C	269	ASP	2.8
1	D	156	ALA	2.7
1	A	5	ILE	2.7
1	C	292	ASP	2.7
1	D	146	GLU	2.6
1	D	273	LEU	2.6
1	D	155	GLU	2.6
1	D	159	MET	2.6
1	C	367	GLU	2.5
1	C	311	VAL	2.5
1	D	67	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	152	THR	2.4
1	D	160	ARG	2.3
1	D	30	VAL	2.3
1	D	125	LEU	2.3
1	D	76	GLN	2.3
1	D	26	VAL	2.3
1	C	366	VAL	2.3
1	D	158	PRO	2.2
1	D	114	ARG	2.2
1	D	144	ILE	2.2
1	D	79	GLU	2.2
1	B	80	VAL	2.2
1	C	185	THR	2.2
1	D	111	THR	2.2
1	C	247	ARG	2.1
1	D	141	GLY	2.1
1	D	96	ALA	2.1
1	D	85	TYR	2.1
1	A	307	SER	2.1
1	D	140	ALA	2.1
1	C	381	GLU	2.0
1	D	129	GLU	2.0
1	D	98	TYR	2.0
1	C	382	SER	2.0
1	C	384	SER	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	Q<0.9
2	SO4	C	445	5/5	0.86	0.14	107,108,109,110	0
2	SO4	D	445	5/5	0.89	0.20	106,108,109,110	0
2	SO4	A	445	5/5	0.95	0.16	77,77,78,80	0
2	SO4	B	445	5/5	0.95	0.18	86,87,90,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.