



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:56 PM UTC

PDB ID : 2BE7 / pdb_00002be7
Title : Crystal structure of the unliganded (T-state) aspartate transcarbamoylase of the psychrophilic bacterium *Moritella profunda*
Authors : De Vos, D.; Savvides, S.N.; Van Beeumen, J.
Deposited on : 2005-10-23
Resolution : 2.85 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

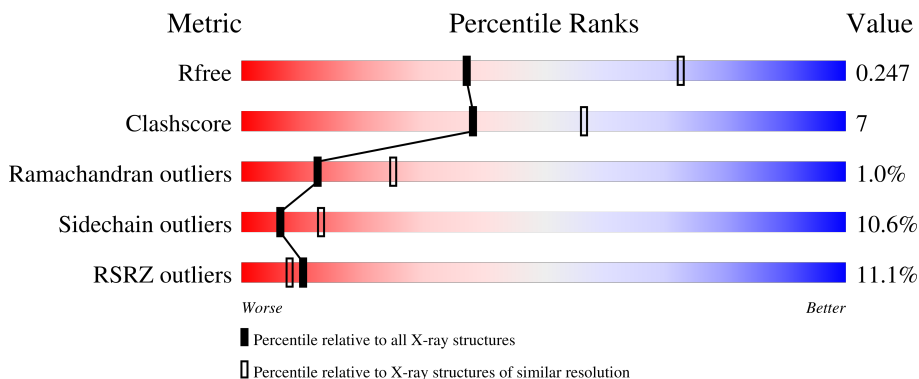
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	326	
1	B	326	
1	C	326	
2	D	153	
2	E	153	

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Mol	Chain	Length	Quality of chain
2	F	153	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '30%', a green segment labeled '69%', a yellow segment labeled '11%', and a grey segment on the right labeled '18%'. A small black dot is located on the yellow segment.</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9959 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 Aspartate Carbamoyltransferase Catalytic Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	Total 2385	C 1519	N 397	O 463	S 6	0	0	0
1	B	309	Total 2374	C 1512	N 397	O 459	S 6	0	0	0
1	C	309	Total 2390	C 1521	N 401	O 462	S 6	0	0	0

- Molecule 2 is a protein called Aspartate Carbamoyltransferase Regulatory Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	133	Total 945	C 597	N 155	O 188	S 5	0	0	0
2	E	130	Total 944	C 597	N 157	O 185	S 5	0	0	0
2	F	125	Total 867	C 552	N 142	O 169	S 4	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	B	10	Total O 10 10	0	0
5	C	9	Total O 9 9	0	0

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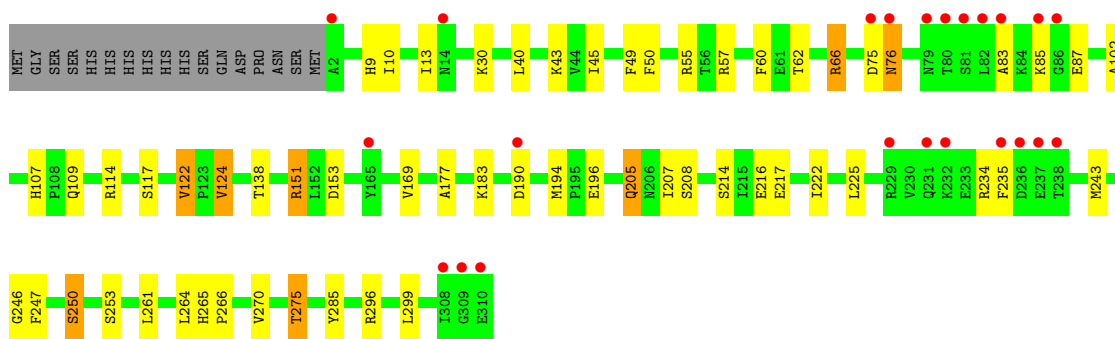
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)


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.

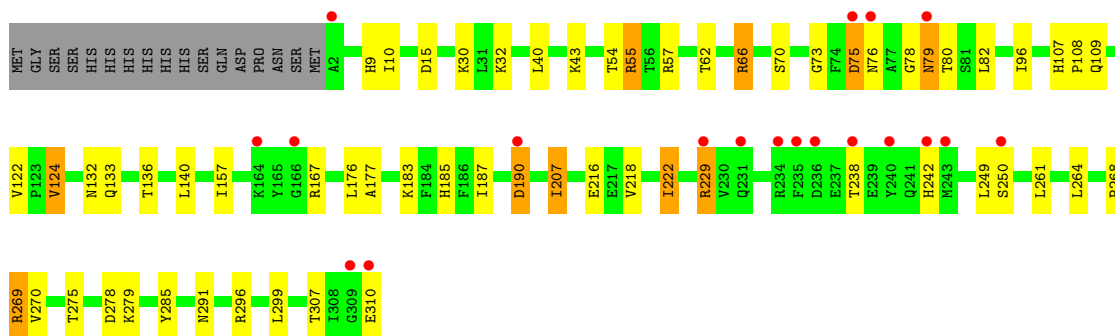
- Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain

Chain A: 



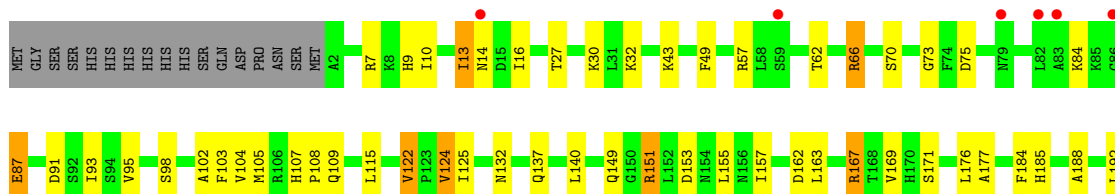
- Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain

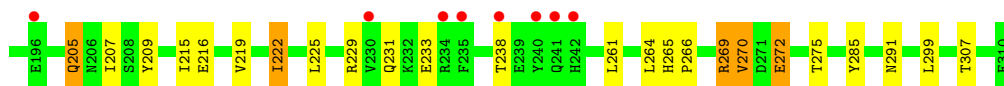
Chain B: 



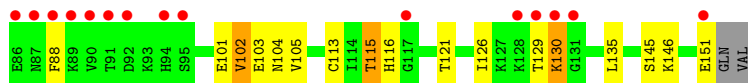
- Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain

Chain C: 

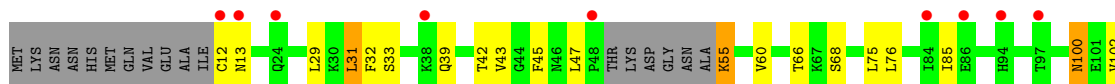




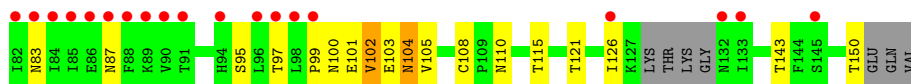
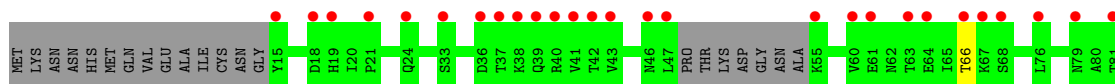
- Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain



- Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain



- Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.24Å 129.24Å 207.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.85) 95.8 (20.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.257 0.260 , 0.247	Depositor DCC
R_{free} test set	2970 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9959	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.73	0/2432	0.89	1/3303 (0.0%)
1	B	0.69	0/2421	0.90	0/3291
1	C	0.72	0/2437	0.95	0/3309
2	D	0.65	0/958	0.86	1/1314 (0.1%)
2	E	0.70	1/958 (0.1%)	0.88	0/1311
2	F	0.68	0/878	0.87	0/1204
All	All	0.70	1/10084 (0.0%)	0.90	2/13732 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	55	LYS	N-CA	7.44	1.60	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	116	HIS	N-CA-C	6.76	118.54	111.03
1	A	50	PHE	N-CA-C	-5.14	105.37	111.69

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	2385	0	2332	25	0
1	B	2374	0	2308	40	0
1	C	2390	0	2340	40	0
2	D	945	0	865	13	0
2	E	944	0	878	15	0
2	F	867	0	771	6	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	14	0	0	0	0
5	B	10	0	0	1	0
5	C	9	0	0	0	0
5	D	3	0	0	0	0
All	All	9959	0	9494	133	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 7.

All (133) 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:B:32:LYS:NZ	1:B:291:ASN:HD21	1.68	0.90
2:E:75:LEU:HD11	2:E:102:VAL:HG21	1.63	0.80
1:B:9:HIS:HD2	1:B:124:VAL:H	1.37	0.73
1:A:9:HIS:HD2	1:A:124:VAL:H	1.37	0.73
1:B:32:LYS:HZ3	1:B:291:ASN:HD21	1.34	0.72
2:E:102:VAL:HG23	2:E:126:ILE:HD11	1.72	0.71
1:C:151:ARG:HD2	1:C:153:ASP:O	1.93	0.69
2:D:12:CYS:SG	2:D:13:ASN:N	2.65	0.68
1:B:157:ILE:HD13	1:B:176:LEU:HD13	1.78	0.66
1:B:32:LYS:HZ2	1:B:291:ASN:HD21	1.42	0.64
1:C:9:HIS:HD2	1:C:124:VAL:H	1.46	0.64
2:F:102:VAL:HG22	2:F:126:ILE:HD11	1.81	0.63
1:C:10:ILE:HG21	1:C:299:LEU:HD21	1.79	0.63
1:B:177:ALA:HA	1:B:207:ILE:CD1	2.29	0.62
1:A:83:ALA:HA	1:A:87:GLU:HB3	1.82	0.61
2:D:12:CYS:SG	2:D:88:PHE:N	2.73	0.61
1:A:177:ALA:HA	1:A:207:ILE:CD1	2.31	0.60
1:A:107:HIS:HD2	1:A:109:GLN:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ALA:HA	1:C:122:VAL:HG13	1.85	0.59
1:B:269:ARG:NH1	1:B:278:ASP:OD2	2.34	0.58
1:C:177:ALA:HA	1:C:207:ILE:CD1	2.35	0.57
1:A:10:ILE:HG13	1:A:299:LEU:HD11	1.86	0.57
2:E:100:ASN:H	2:E:100:ASN:HD22	1.51	0.56
1:B:229:ARG:H	1:B:229:ARG:HD2	1.70	0.56
1:C:177:ALA:HA	1:C:207:ILE:HD13	1.90	0.54
1:C:157:ILE:HD13	1:C:176:LEU:HD13	1.91	0.53
1:B:177:ALA:HA	1:B:207:ILE:HD13	1.89	0.53
1:B:229:ARG:H	1:B:229:ARG:CD	2.21	0.53
2:D:129:THR:O	2:D:130:LYS:C	2.52	0.53
1:B:132:ASN:O	1:B:167:ARG:NH2	2.42	0.52
2:E:102:VAL:CG2	2:E:126:ILE:HD11	2.39	0.52
2:D:113:CYS:SG	2:D:115:THR:HB	2.50	0.51
1:B:66:ARG:HG2	5:B:315:HOH:O	2.09	0.51
1:B:132:ASN:OD1	1:B:133:GLN:HG2	2.10	0.50
2:E:113:CYS:SG	2:E:115:THR:HB	2.51	0.50
1:C:10:ILE:HG13	1:C:299:LEU:HD11	1.93	0.50
1:C:9:HIS:CD2	1:C:124:VAL:H	2.29	0.49
1:A:107:HIS:CD2	1:A:109:GLN:H	2.28	0.49
1:A:177:ALA:O	1:A:205:GLN:HG2	2.12	0.49
1:A:114:ARG:O	1:A:117:SER:HB2	2.13	0.49
1:B:187:ILE:HD11	1:B:218:VAL:HG21	1.94	0.49
1:A:151:ARG:HD2	1:A:153:ASP:O	2.12	0.49
2:E:104:ASN:CG	2:E:104:ASN:O	2.56	0.49
2:E:47:LEU:HD12	2:E:55:LYS:O	2.11	0.48
2:D:126:ILE:HG12	2:D:135:LEU:CD2	2.43	0.48
2:D:43:VAL:HG22	2:D:58:ILE:HG23	1.94	0.48
1:C:107:HIS:HD2	1:C:109:GLN:H	1.61	0.48
1:B:136:THR:OG1	1:B:296:ARG:NH2	2.45	0.48
1:B:190:ASP:N	1:B:190:ASP:OD1	2.45	0.48
1:B:55:ARG:CG	1:C:95:VAL:HG11	2.44	0.47
1:B:55:ARG:HG2	1:C:95:VAL:HG11	1.97	0.47
1:B:82:LEU:HD11	1:B:96:ILE:HD11	1.97	0.47
2:D:29:LEU:HD12	2:D:35:THR:HG23	1.97	0.47
1:A:57:ARG:NH1	1:B:73:GLY:O	2.47	0.47
2:F:103:GLU:O	2:F:105:VAL:HG23	2.15	0.47
1:A:49:PHE:CE1	1:A:57:ARG:HG3	2.49	0.47
1:A:62:THR:O	1:A:66:ARG:HB2	2.14	0.47
1:B:107:HIS:CD2	1:B:108:PRO:HD2	2.50	0.47
1:B:185:HIS:CG	1:B:222:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ASP:OD2	1:C:192:LEU:HD22	2.15	0.47
1:A:102:ALA:HA	1:A:122:VAL:HG13	1.97	0.46
2:D:145:SER:O	2:D:146:LYS:C	2.59	0.46
2:E:103:GLU:O	2:E:105:VAL:HG23	2.15	0.46
1:B:40:LEU:O	1:B:43:LYS:HB2	2.15	0.46
1:B:10:ILE:HG21	1:B:299:LEU:HD21	1.97	0.46
1:C:215:ILE:O	1:C:219:VAL:HG23	2.16	0.46
1:A:243:MET:O	1:A:247:PHE:HD1	1.99	0.45
1:B:57:ARG:CD	1:B:75:ASP:HB3	2.45	0.45
1:C:62:THR:O	1:C:66:ARG:HB2	2.17	0.45
1:A:9:HIS:CD2	1:A:124:VAL:HG13	2.52	0.45
1:B:9:HIS:CD2	1:B:124:VAL:HG13	2.52	0.45
1:C:137:GLN:O	1:C:140:LEU:HG	2.17	0.45
1:A:250:SER:O	1:A:253:SER:HB2	2.17	0.45
1:B:76:ASN:HD22	1:B:78:GLY:N	2.15	0.45
1:C:205:GLN:HE21	1:C:205:GLN:HB2	1.58	0.44
1:A:76:ASN:HD22	1:A:76:ASN:N	2.16	0.44
1:B:57:ARG:NH1	1:C:73:GLY:O	2.50	0.44
1:C:132:ASN:O	1:C:167:ARG:NH2	2.50	0.44
1:C:32:LYS:NZ	1:C:291:ASN:HD21	2.15	0.44
1:C:49:PHE:CE1	1:C:57:ARG:HG3	2.53	0.44
2:E:32:PHE:O	2:E:33:SER:C	2.60	0.44
2:D:72:GLN:HE21	2:D:72:GLN:HA	1.82	0.44
2:D:102:VAL:CG2	2:D:126:ILE:HD11	2.48	0.44
1:C:184:PHE:O	1:C:209:TYR:HA	2.18	0.43
1:C:107:HIS:CD2	1:C:108:PRO:HD2	2.54	0.43
1:B:107:HIS:HD2	1:B:109:GLN:H	1.65	0.43
1:C:13:ILE:HD13	1:C:16:ILE:HD12	1.99	0.43
2:D:102:VAL:HG22	2:D:126:ILE:HD11	2.01	0.43
1:C:104:VAL:HG22	1:C:125:ILE:HB	2.00	0.43
1:C:163:LEU:HG	1:C:188:ALA:HB2	2.00	0.43
1:C:185:HIS:CG	1:C:222:ILE:HD11	2.54	0.43
1:B:30:LYS:CD	1:B:310:GLU:CB	2.96	0.42
1:C:231:GLN:HB3	1:C:233:GLU:HG2	2.01	0.42
1:C:265:HIS:NE2	1:C:272:GLU:OE2	2.50	0.42
2:E:85:ILE:HD12	2:E:85:ILE:N	2.34	0.42
1:C:27:THR:O	1:C:30:LYS:HG3	2.20	0.42
2:D:41:VAL:HG13	2:D:60:VAL:HG12	2.01	0.42
1:B:32:LYS:HZ3	1:B:291:ASN:ND2	2.09	0.42
1:C:185:HIS:CD2	1:C:222:ILE:HD11	2.54	0.42
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:PRO:CB	1:C:87:GLU:HG3	2.50	0.42
2:D:103:GLU:O	2:D:105:VAL:HG23	2.19	0.42
2:E:126:ILE:HG12	2:E:135:LEU:HD22	2.02	0.42
1:C:103:PHE:O	1:C:124:VAL:HA	2.20	0.42
1:A:214:SER:OG	1:A:217:GLU:HB2	2.20	0.42
1:A:40:LEU:O	1:A:43:LYS:HB2	2.20	0.41
1:A:60:PHE:CZ	1:A:296:ARG:HD3	2.55	0.41
1:B:62:THR:O	1:B:66:ARG:HB2	2.19	0.41
1:B:185:HIS:CD2	1:B:222:ILE:HD11	2.55	0.41
1:B:79:ASN:C	1:B:79:ASN:HD22	2.28	0.41
2:E:110:ASN:O	2:E:116:HIS:HE1	2.04	0.41
2:F:99:PRO:O	2:F:126:ILE:HD12	2.19	0.41
2:F:104:ASN:O	2:F:104:ASN:CG	2.63	0.41
1:A:13:ILE:HG13	1:A:138:THR:HG21	2.02	0.41
1:A:265:HIS:ND1	1:A:266:PRO:HD2	2.36	0.41
1:B:79:ASN:HD22	1:B:80:THR:N	2.19	0.41
1:B:269:ARG:HD3	1:C:91:ASP:OD1	2.20	0.41
1:C:149:GLN:HB3	1:C:155:LEU:HD21	2.02	0.41
1:A:169:VAL:CG1	1:A:194:MET:HE1	2.51	0.41
1:B:229:ARG:HD2	1:B:229:ARG:N	2.35	0.41
1:B:9:HIS:CD2	1:B:124:VAL:H	2.27	0.41
2:E:12:CYS:O	2:E:13:ASN:ND2	2.54	0.41
2:E:43:VAL:HG11	2:E:45:PHE:CZ	2.55	0.41
1:A:246:GLY:C	1:A:247:PHE:CG	2.99	0.41
1:C:93:ILE:HD12	1:C:103:PHE:CE1	2.56	0.41
2:E:31:LEU:HD23	2:E:76:LEU:HD11	2.03	0.41
2:F:100:ASN:N	2:F:100:ASN:HD22	2.19	0.41
1:B:238:THR:O	1:B:242:HIS:ND1	2.32	0.40
1:C:115:LEU:HD23	1:C:115:LEU:C	2.47	0.40
1:A:55:ARG:NH2	3:A:311:SO4:O3	2.53	0.40
1:C:269:ARG:HA	1:C:272:GLU:OE2	2.20	0.40
1:C:14:ASN:N	1:C:14:ASN:HD22	2.19	0.40
2:F:108:CYS:SG	2:F:110:ASN:HB3	2.62	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	307/326 (94%)	289 (94%)	14 (5%)	4 (1%)	9	21
1	B	307/326 (94%)	286 (93%)	21 (7%)	0	100	100
1	C	307/326 (94%)	296 (96%)	9 (3%)	2 (1%)	18	35
2	D	129/153 (84%)	114 (88%)	12 (9%)	3 (2%)	5	11
2	E	124/153 (81%)	109 (88%)	13 (10%)	2 (2%)	7	17
2	F	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	7	16
All	All	1293/1437 (90%)	1199 (93%)	81 (6%)	13 (1%)	12	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
2	D	130	LYS
2	E	104	ASN
2	F	104	ASN
2	D	104	ASN
2	F	87	ASN
1	A	275	THR
2	D	13	ASN
1	A	234	ARG
1	C	84	LYS
2	E	68	SER
1	A	270	VAL
1	C	270	VAL

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	252/277 (91%)	230 (91%)	22 (9%)	9	21
1	B	248/277 (90%)	222 (90%)	26 (10%)	6	13
1	C	252/277 (91%)	223 (88%)	29 (12%)	5	10
2	D	96/139 (69%)	84 (88%)	12 (12%)	4	8
2	E	99/139 (71%)	89 (90%)	10 (10%)	7	15
2	F	81/139 (58%)	71 (88%)	10 (12%)	4	8
All	All	1028/1248 (82%)	919 (89%)	109 (11%)	6	13

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	45	ILE
1	A	66	ARG
1	A	75	ASP
1	A	76	ASN
1	A	122	VAL
1	A	124	VAL
1	A	151	ARG
1	A	183	LYS
1	A	190	ASP
1	A	196	GLU
1	A	205	GLN
1	A	208	SER
1	A	216	GLU
1	A	222	ILE
1	A	225	LEU
1	A	235	PHE
1	A	250	SER
1	A	261	LEU
1	A	264	LEU
1	A	275	THR
1	A	285	TYR
1	B	15	ASP
1	B	54	THR
1	B	55	ARG
1	B	66	ARG
1	B	70	SER

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Mol	Chain	Res	Type
1	B	75	ASP
1	B	79	ASN
1	B	122	VAL
1	B	124	VAL
1	B	140	LEU
1	B	183	LYS
1	B	190	ASP
1	B	207	ILE
1	B	216	GLU
1	B	222	ILE
1	B	229	ARG
1	B	249	LEU
1	B	250	SER
1	B	261	LEU
1	B	264	LEU
1	B	269	ARG
1	B	270	VAL
1	B	275	THR
1	B	279	LYS
1	B	285	TYR
1	B	307	THR
1	C	7	ARG
1	C	13	ILE
1	C	43	LYS
1	C	66	ARG
1	C	70	SER
1	C	75	ASP
1	C	87	GLU
1	C	98	SER
1	C	105	MET
1	C	122	VAL
1	C	124	VAL
1	C	151	ARG
1	C	167	ARG
1	C	169	VAL
1	C	171	SER
1	C	205	GLN
1	C	216	GLU
1	C	222	ILE
1	C	225	LEU
1	C	229	ARG
1	C	238	THR

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Mol	Chain	Res	Type
1	C	261	LEU
1	C	264	LEU
1	C	269	ARG
1	C	270	VAL
1	C	272	GLU
1	C	275	THR
1	C	285	TYR
1	C	307	THR
2	D	29	LEU
2	D	31	LEU
2	D	37	THR
2	D	42	THR
2	D	60	VAL
2	D	65	ILE
2	D	66	THR
2	D	101	GLU
2	D	102	VAL
2	D	115	THR
2	D	121	THR
2	D	151	GLU
2	E	29	LEU
2	E	31	LEU
2	E	39	GLN
2	E	42	THR
2	E	60	VAL
2	E	66	THR
2	E	100	ASN
2	E	104	ASN
2	E	115	THR
2	E	121	THR
2	F	66	THR
2	F	83	ASN
2	F	95	SER
2	F	97	THR
2	F	101	GLU
2	F	102	VAL
2	F	115	THR
2	F	121	THR
2	F	143	THR
2	F	150	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	65	GLN
1	A	76	ASN
1	A	79	ASN
1	A	107	HIS
1	A	185	HIS
1	A	256	HIS
1	B	9	HIS
1	B	36	GLN
1	B	76	ASN
1	B	79	ASN
1	B	107	HIS
1	B	291	ASN
1	C	9	HIS
1	C	14	ASN
1	C	65	GLN
1	C	107	HIS
1	C	149	GLN
1	C	174	GLN
1	C	185	HIS
1	C	205	GLN
1	C	256	HIS
1	C	260	ASN
1	C	291	ASN
2	D	71	ASN
2	D	72	GLN
2	D	112	ASN
2	D	116	HIS
2	E	13	ASN
2	E	19	HIS
2	E	39	GLN
2	E	46	ASN
2	E	62	ASN
2	E	100	ASN
2	E	116	HIS
2	F	100	ASN
2	F	112	ASN

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	311	-	4,4,4	0.39	0	6,6,6	0.49	0
3	SO4	C	311	-	4,4,4	0.34	0	6,6,6	0.44	0
3	SO4	B	311	-	4,4,4	0.24	0	6,6,6	0.17	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
3	A	311	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	309/326 (94%)	0.61	23 (7%) 20 14	41, 52, 73, 79	0
1	B	309/326 (94%)	0.47	19 (6%) 27 20	44, 52, 71, 79	0
1	C	309/326 (94%)	0.51	14 (4%) 38 29	45, 52, 69, 75	0
2	D	133/153 (86%)	1.32	33 (24%) 2 1	47, 54, 61, 75	0
2	E	130/153 (84%)	0.94	11 (8%) 16 12	43, 53, 60, 66	0
2	F	125/153 (81%)	1.67	46 (36%) 1 1	46, 63, 72, 83	0
All	All	1315/1437 (91%)	0.76	146 (11%) 10 8	41, 53, 71, 83	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	86	GLU	6.3
2	F	132	ASN	5.0
1	A	309	GLY	4.7
2	F	94	HIS	4.5
1	B	238	THR	4.5
1	A	231	GLN	4.4
1	B	309	GLY	4.3
1	B	235	PHE	4.2
1	A	232	LYS	4.1
2	F	85	ILE	4.1
1	A	310	GLU	4.0
1	A	79	ASN	3.9
2	F	68	SER	3.6
2	D	41	VAL	3.5
2	F	84	ILE	3.5
2	E	94	HIS	3.5
1	A	237	GLU	3.5
2	D	84	ILE	3.4
2	F	89	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	33	SER	3.4
2	D	89	LYS	3.4
2	F	42	THR	3.3
2	D	94	HIS	3.3
2	F	90	VAL	3.3
2	F	37	THR	3.3
2	F	61	GLU	3.3
1	A	85	LYS	3.3
1	C	83	ALA	3.3
2	D	129	THR	3.3
2	F	24	GLN	3.2
2	F	46	ASN	3.2
1	B	229	ARG	3.2
2	D	86	GLU	3.2
1	A	2	ALA	3.2
1	A	236	ASP	3.2
1	A	235	PHE	3.1
1	B	79	ASN	3.1
2	E	86	GLU	3.1
2	D	88	PHE	3.1
1	A	14	ASN	3.1
1	B	2	ALA	3.0
2	D	14	GLY	3.0
2	D	24	GLN	3.0
1	A	86	GLY	3.0
2	D	85	ILE	3.0
2	F	87	ASN	3.0
2	D	13	ASN	3.0
1	B	243	MET	2.9
2	F	55	LYS	2.9
2	F	15	TYR	2.9
2	D	130	LYS	2.9
2	F	97	THR	2.9
2	F	96	LEU	2.8
2	E	38	LYS	2.8
2	F	39	GLN	2.8
1	B	310	GLU	2.8
1	B	234	ARG	2.7
2	F	60	VAL	2.7
1	A	83	ALA	2.7
1	A	308	ILE	2.7
2	F	67	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	231	GLN	2.7
2	E	132	ASN	2.7
2	F	47	LEU	2.7
1	A	81	SER	2.7
1	B	242	HIS	2.6
1	C	79	ASN	2.6
2	F	21	PRO	2.6
2	F	91	THR	2.6
2	D	57	LEU	2.6
2	D	91	THR	2.6
2	F	63	THR	2.6
1	A	75	ASP	2.6
1	B	250	SER	2.6
2	D	90	VAL	2.5
1	C	240	TYR	2.5
2	D	39	GLN	2.5
1	A	76	ASN	2.5
1	A	238	THR	2.5
2	F	82	ILE	2.4
2	E	151	GLU	2.4
2	F	64	GLU	2.4
1	A	80	THR	2.4
1	A	190	ASP	2.4
2	F	18	ASP	2.4
2	D	12	CYS	2.4
2	D	36	ASP	2.4
2	D	38	LYS	2.4
2	F	38	LYS	2.4
1	B	240	TYR	2.4
1	C	230	VAL	2.3
2	E	13	ASN	2.3
1	C	59	SER	2.3
1	A	229	ARG	2.3
2	E	24	GLN	2.3
2	F	98	LEU	2.3
2	F	145	SER	2.3
2	F	36	ASP	2.3
1	C	238	THR	2.3
2	F	99	PRO	2.3
2	F	126	ILE	2.3
2	D	95	SER	2.3
2	F	40	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	236	ASP	2.2
2	D	92	ASP	2.2
1	C	82	LEU	2.2
1	B	190	ASP	2.2
1	C	234	ARG	2.2
2	D	131	GLY	2.2
2	F	83	ASN	2.2
1	C	241	GLN	2.2
2	E	12	CYS	2.2
1	B	76	ASN	2.2
2	D	16	VAL	2.2
2	D	81	THR	2.2
1	B	164	LYS	2.2
1	C	235	PHE	2.2
2	D	15	TYR	2.2
1	C	242	HIS	2.1
2	F	41	VAL	2.1
2	F	43	VAL	2.1
1	B	75	ASP	2.1
2	E	97	THR	2.1
2	F	19	HIS	2.1
2	D	87	ASN	2.1
1	C	86	GLY	2.1
2	F	76	LEU	2.1
2	D	62	ASN	2.1
1	B	166	GLY	2.1
2	D	117	GLY	2.1
2	F	133	ILE	2.1
2	D	128	LYS	2.1
2	F	79	ASN	2.1
2	D	47	LEU	2.1
2	D	151	GLU	2.1
1	A	165	TYR	2.1
2	E	48	PRO	2.0
2	F	88	PHE	2.0
2	F	66	THR	2.0
2	F	81	THR	2.0
1	C	196	GLU	2.0
2	D	60	VAL	2.0
1	A	82	LEU	2.0
1	C	14	ASN	2.0
2	D	46	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	84	ILE	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 oligosaccharides 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, 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(\AA^2)	Q<0.9
3	SO4	A	311	5/5	0.90	0.16	85,85,86,86	0
3	SO4	C	311	5/5	0.93	0.14	85,85,86,86	0
3	SO4	B	311	5/5	0.96	0.09	91,91,91,92	0
4	ZN	D	1108	1/1	0.99	0.05	49,49,49,49	0
4	ZN	E	1108	1/1	0.99	0.02	44,44,44,44	0
4	ZN	F	1108	1/1	0.99	0.03	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.