



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 AM GMT

PDB ID : 2BE7  
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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

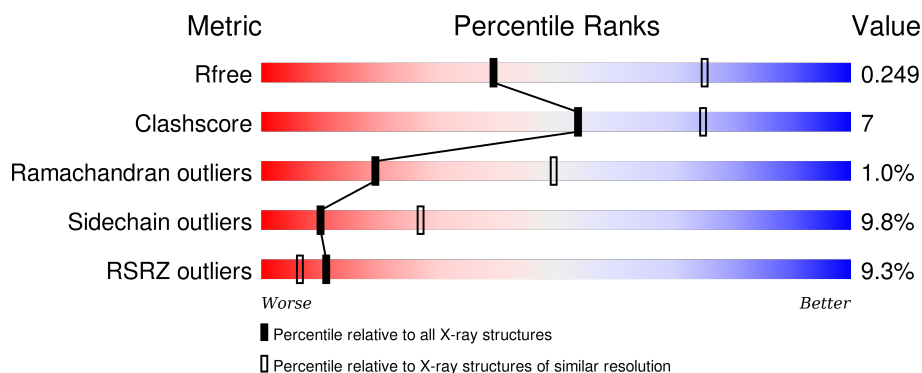
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	326	<div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	B	326	<div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div>
1	C	326	<div> <div>72%</div> <div>20%</div> <div>• 5%</div> </div>
2	D	153	<div> <div>25%</div> <div>67%</div> <div>18%</div> <div>• 13%</div> </div>
2	E	153	<div> <div>14%</div> <div>67%</div> <div>15%</div> <div>• • 15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	153	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (38%), green (70%), yellow (11%), and grey (18%). The segments are stacked horizontally, with the red segment starting from the left and ending at 38%, the green segment starting at 38% and ending at 70%, the yellow segment starting at 70% and ending at 81%, and the grey segment starting at 81% and ending at 99%. The percentages are labeled above or below the segments.

## 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
1	A	309	Total	C	N	O	S	0	0	0
			2385	1519	397	463	6			
1	B	309	Total	C	N	O	S	0	0	0
			2374	1512	397	459	6			
1	C	309	Total	C	N	O	S	0	0	0
			2390	1521	401	462	6			

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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



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

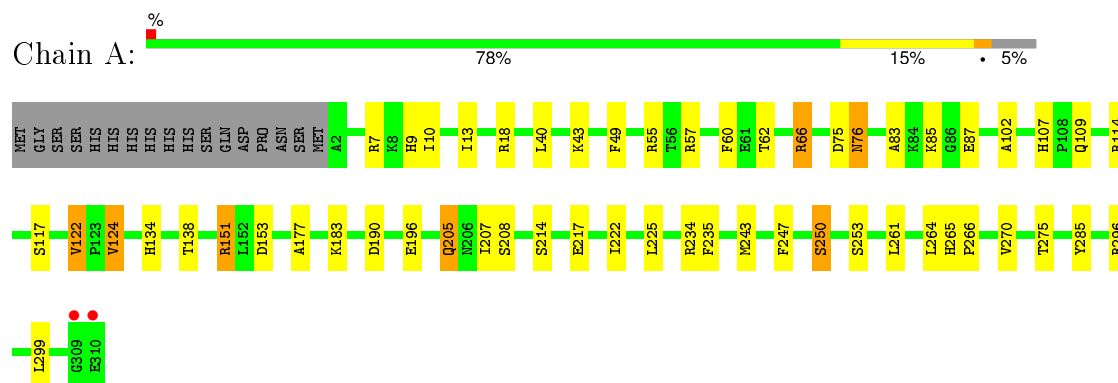
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	10	Total	O	0	0
			10	10		
5	C	9	Total	O	0	0
			9	9		
5	D	3	Total	O	0	0
			3	3		

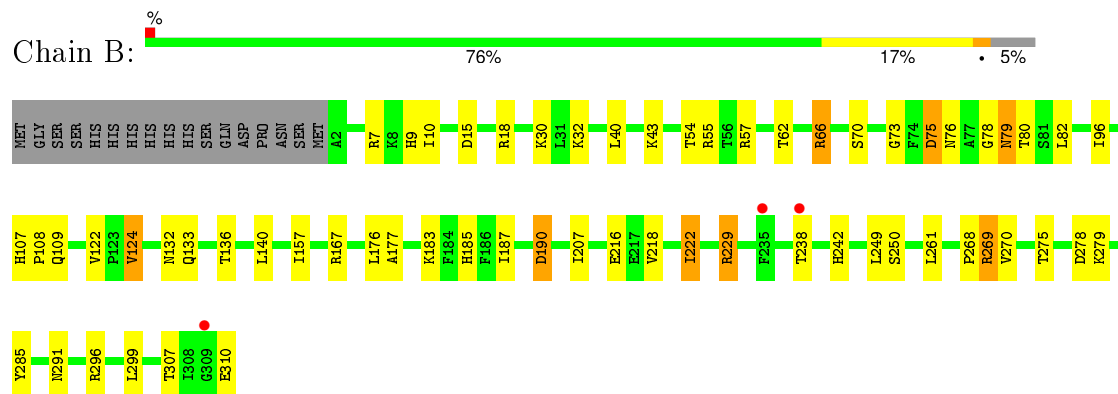
### 3 Residue-property plots [i](#)

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

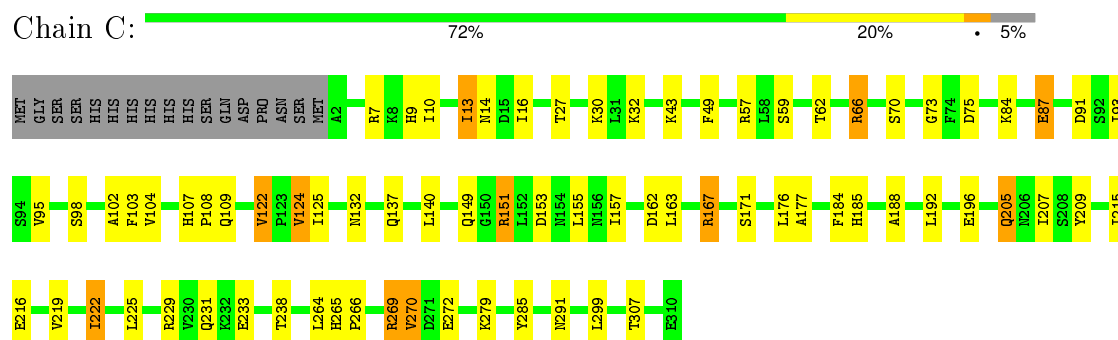
#### • Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain



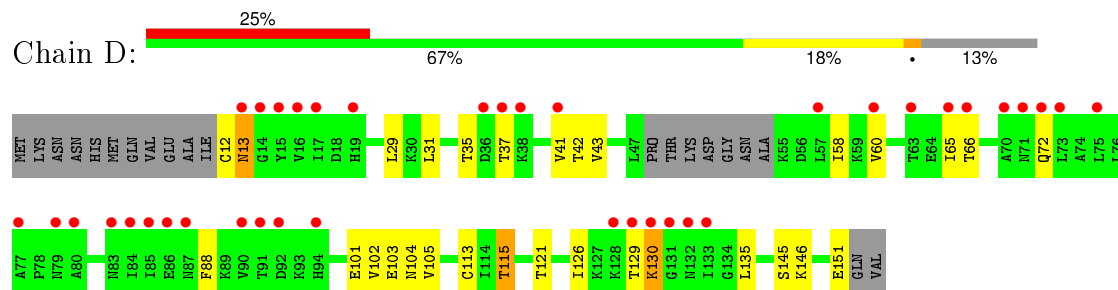
#### • Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain



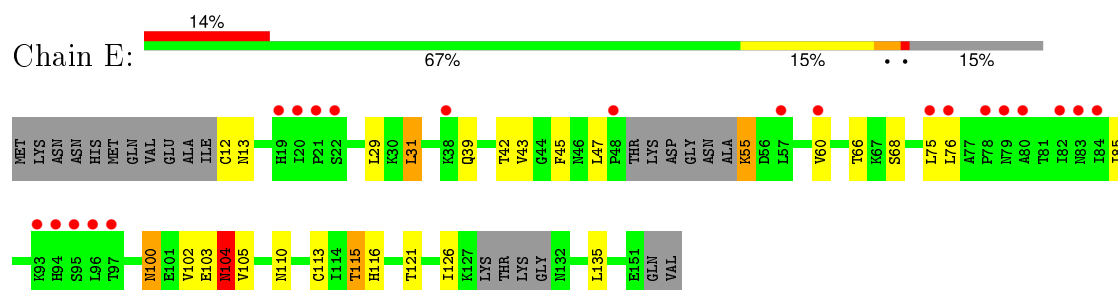
#### • Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain



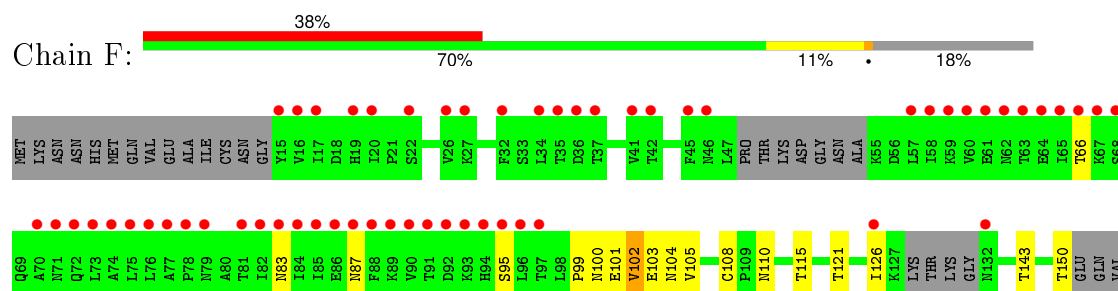
- Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain



- 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, $\alpha$ , $\beta$ , $\gamma$	129.24Å 129.24Å 207.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.85 49.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.85) 95.8 (49.24-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212 , 0.257 0.253 , 0.249	Depositor DCC
$R_{free}$ test set	2241 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 59604 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage'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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.56	0/2432	0.66	0/3303
1	B	0.54	0/2421	0.68	0/3291
1	C	0.56	0/2437	0.70	0/3309
2	D	0.51	0/958	0.61	0/1314
2	E	0.55	1/958 (0.1%)	0.64	0/1311
2	F	0.47	0/878	0.58	0/1204
All	All	0.54	1/10084 (0.0%)	0.66	0/13732

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	55	LYS	N-CA	7.01	1.60	1.46

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	2385	0	2332	23	0
1	B	2374	0	2308	39	0
1	C	2390	0	2340	39	0
2	D	945	0	865	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	944	0	878	14	0
2	F	867	0	771	5	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	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	127	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 (127) 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
2:E:102:VAL:HG23	2:E:126:ILE:HD11	1.72	0.71
1:B:32:LYS:HZ2	1:B:291:ASN:HD21	1.37	0.71
1:C:151:ARG:HD2	1:C:153:ASP:O	1.93	0.69
1:B:32:LYS:HZ3	1:B:291:ASN:HD21	1.39	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG13	1:A:299:LEU:HD11	1.86	0.57
2:E:100:ASN:HD22	2:E:100:ASN:H	1.51	0.56
1:B:229:ARG:HD2	1:B:229:ARG:H	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:CD	1:B:229:ARG:H	2.21	0.53
2:E:102:VAL:CG2	2:E:126:ILE:HD11	2.39	0.52
1:B:132:ASN:O	1:B:167:ARG:NH2	2.42	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:B:187:ILE:HD11	1:B:218:VAL:HG21	1.94	0.49
1:A:114:ARG:O	1:A:117:SER:HB2	2.13	0.49
1:A:151:ARG:HD2	1:A:153:ASP:O	2.12	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:OD1	1:B:190:ASP:N	2.45	0.48
2:D:129:THR:O	2:D:130:LYS:C	2.52	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: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
1:C:162:ASP:OD2	1:C:192:LEU:HD22	2.15	0.47
1:A:62:THR:O	1:A:66:ARG:HB2	2.14	0.47
1:A:102:ALA:HA	1:A:122:VAL:HG13	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:76:ASN:HD22	1:B:78:GLY:N	2.15	0.45
1:A:250:SER:O	1:A:253:SER:HB2	2.17	0.45
1:C:205:GLN:HB2	1:C:205:GLN:HE21	1.58	0.44
1:B:57:ARG:NH1	1:C:73:GLY:O	2.50	0.44
1:A:76:ASN:HD22	1:A:76:ASN:N	2.16	0.44
1:C:132:ASN:O	1:C:167:ARG:NH2	2.50	0.44
1:C:49:PHE:CE1	1:C:57:ARG:HG3	2.53	0.44
1:C:32:LYS:NZ	1:C:291:ASN:HD21	2.15	0.44
2:E:104:ASN:CG	2:E:104:ASN:O	2.56	0.44
2:D:102:VAL:CG2	2:D:126:ILE:HD11	2.48	0.44
2:D:72:GLN:HA	2:D:72:GLN:HE21	1.82	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:B:32:LYS:HZ2	1:B:291:ASN:ND2	2.11	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:N	2:E:85:ILE:HD12	2.34	0.42
2:D:41:VAL:HG13	2:D:60:VAL:HG12	2.01	0.42
1:C:27:THR:O	1:C:30:LYS:HG3	2.20	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
2:D:103:GLU:O	2:D:105:VAL:HG23	2.19	0.42
1:B:268:PRO:CB	1:C:87:GLU:HG3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:O	1:A:43:LYS:HB2	2.20	0.41
2:D:145:SER:O	2:D:146:LYS:C	2.59	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
2:F:99:PRO:O	2:F:126:ILE:HD12	2.19	0.41
2:E:110:ASN:O	2:E:116:HIS:HE1	2.04	0.41
1:B:269:ARG:HD3	1:C:91:ASP:OD1	2.20	0.41
1:A:13:ILE:HG13	1:A:138:THR:HG21	2.02	0.41
1:B:79:ASN:HD22	1:B:80:THR:N	2.19	0.41
1:A:265:HIS:ND1	1:A:266:PRO:HD2	2.36	0.41
1:C:149:GLN:HB3	1:C:155:LEU:HD21	2.02	0.41
1:B:229:ARG:N	1:B:229:ARG:HD2	2.35	0.41
1:B:9:HIS:CD2	1:B:124:VAL:H	2.27	0.41
2:E:43:VAL:HG11	2:E:45:PHE:CZ	2.55	0.41
2:E:12:CYS:O	2:E:13:ASN:ND2	2.54	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:269:ARG:HA	1:C:272:GLU:OE2	2.20	0.40
1:A:55:ARG:NH2	4:A:311:SO4:O3	2.53	0.40
1:C:14:ASN:HD22	1:C:14:ASN:N	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%)	15 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/326 (94%)	286 (93%)	21 (7%)	0	100	100
1	C	307/326 (94%)	296 (96%)	9 (3%)	2 (1%)	26	59
2	D	129/153 (84%)	114 (88%)	12 (9%)	3 (2%)	8	26
2	E	124/153 (81%)	109 (88%)	13 (10%)	2 (2%)	12	36
2	F	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	11	35
All	All	1293/1437 (90%)	1199 (93%)	81 (6%)	13 (1%)	19	49

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 ⓘ

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%)	231 (92%)	21 (8%)	14	36
1	B	248/277 (90%)	223 (90%)	25 (10%)	9	25
1	C	252/277 (91%)	225 (89%)	27 (11%)	8	22
2	D	96/139 (69%)	87 (91%)	9 (9%)	11	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	99/139 (71%)	89 (90%)	10 (10%)	9	25
2	F	81/139 (58%)	72 (89%)	9 (11%)	8	20
All	All	1028/1248 (82%)	927 (90%)	101 (10%)	10	27

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	18	ARG
1	A	66	ARG
1	A	75	ASP
1	A	76	ASN
1	A	122	VAL
1	A	124	VAL
1	A	134	HIS
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	222	ILE
1	A	225	LEU
1	A	235	PHE
1	A	250	SER
1	A	261	LEU
1	A	264	LEU
1	A	285	TYR
1	B	7	ARG
1	B	15	ASP
1	B	18	ARG
1	B	54	THR
1	B	66	ARG
1	B	70	SER
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

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Mol	Chain	Res	Type
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	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	59	SER
1	C	66	ARG
1	C	70	SER
1	C	75	ASP
1	C	87	GLU
1	C	98	SER
1	C	122	VAL
1	C	124	VAL
1	C	151	ARG
1	C	167	ARG
1	C	171	SER
1	C	196	GLU
1	C	205	GLN
1	C	216	GLU
1	C	222	ILE
1	C	225	LEU
1	C	229	ARG
1	C	238	THR
1	C	264	LEU
1	C	269	ARG
1	C	270	VAL
1	C	279	LYS
1	C	285	TYR
1	C	307	THR
2	D	31	LEU
2	D	37	THR
2	D	42	THR

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Mol	Chain	Res	Type
2	D	65	ILE
2	D	66	THR
2	D	101	GLU
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	101	GLU
2	F	102	VAL
2	F	115	THR
2	F	121	THR
2	F	143	THR
2	F	150	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	76	ASN
1	A	107	HIS
1	A	109	GLN
1	A	185	HIS
1	B	9	HIS
1	B	36	GLN
1	B	76	ASN
1	B	79	ASN
1	B	107	HIS
1	B	109	GLN
1	B	156	ASN
1	B	291	ASN

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Mol	Chain	Res	Type
1	C	9	HIS
1	C	14	ASN
1	C	65	GLN
1	C	107	HIS
1	C	149	GLN
1	C	185	HIS
1	C	205	GLN
1	C	260	ASN
1	C	291	ASN
2	D	46	ASN
2	D	112	ASN
2	D	116	HIS
2	E	13	ASN
2	E	39	GLN
2	E	62	ASN
2	E	100	ASN
2	E	116	HIS
2	F	100	ASN
2	F	112	ASN

### 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 ⓘ

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	$\# Z  > 2$
4	SO4	A	311	-	4,4,4	0.24	0	6,6,6	0.30	0
4	SO4	B	311	-	4,4,4	0.18	0	6,6,6	0.13	0
4	SO4	C	311	-	4,4,4	0.17	0	6,6,6	0.59	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
4	SO4	A	311	-	-	0/0/0/0	0/0/0/0
4	SO4	B	311	-	-	0/0/0/0	0/0/0/0
4	SO4	C	311	-	-	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
4	A	311	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<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	309/326 (94%)	0.08	2 (0%) 90 89	41, 52, 73, 79	0
1	B	309/326 (94%)	-0.11	3 (0%) 84 81	44, 52, 71, 79	0
1	C	309/326 (94%)	-0.07	0 100 100	45, 52, 69, 75	0
2	D	133/153 (86%)	1.21	38 (28%) 1 0	47, 54, 61, 75	0
2	E	130/153 (84%)	0.76	21 (16%) 3 1	43, 53, 60, 66	0
2	F	125/153 (81%)	1.72	58 (46%) 0 0	46, 63, 72, 83	0
All	All	1315/1437 (91%)	0.34	122 (9%) 11 6	41, 53, 71, 83	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	85	ILE	5.8
2	F	87	ASN	5.7
2	F	66	THR	5.1
2	F	83	ASN	5.1
2	E	95	SER	5.0
2	F	68	SER	4.8
2	F	86	GLU	4.7
2	F	65	ILE	4.4
2	F	46	ASN	4.4
2	F	62	ASN	4.3
2	F	96	LEU	4.3
2	F	15	TYR	4.3
1	A	309	GLY	4.2
2	D	14	GLY	4.2
2	D	90	VAL	4.2
2	F	84	ILE	4.2
2	F	57	LEU	4.1
2	F	91	THR	4.1
2	F	34	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	94	HIS	4.0
2	D	130	LYS	4.0
2	F	94	HIS	4.0
2	F	17	ILE	3.9
1	A	310	GLU	3.8
2	D	91	THR	3.7
2	E	97	THR	3.7
2	F	126	ILE	3.7
2	F	63	THR	3.6
2	D	41	VAL	3.6
2	D	94	HIS	3.6
2	E	96	LEU	3.6
2	F	32	PHE	3.6
2	F	71	ASN	3.6
2	D	63	THR	3.6
2	D	73	LEU	3.5
2	F	92	ASP	3.5
2	D	85	ILE	3.5
2	D	71	ASN	3.4
2	F	58	ILE	3.4
2	D	84	ILE	3.4
2	D	132	ASN	3.3
2	D	13	ASN	3.3
2	D	87	ASN	3.3
2	D	65	ILE	3.2
2	F	79	ASN	3.1
2	F	36	ASP	3.1
2	D	57	LEU	3.1
2	D	15	TYR	3.0
2	F	37	THR	3.0
2	D	38	LYS	3.0
2	E	21	PRO	3.0
2	F	82	ILE	3.0
2	F	73	LEU	3.0
2	E	82	ILE	2.9
2	F	45	PHE	2.9
2	E	93	LYS	2.9
2	D	75	LEU	2.9
2	D	70	ALA	2.9
2	F	95	SER	2.9
2	F	60	VAL	2.9
2	F	61	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	86	GLU	2.8
2	F	19	HIS	2.8
2	F	81	THR	2.7
2	E	79	ASN	2.7
2	F	97	THR	2.7
2	E	38	LYS	2.7
2	D	83	ASN	2.7
2	F	64	GLU	2.7
2	F	132	ASN	2.7
2	F	72	GLN	2.6
2	E	83	ASN	2.6
2	E	20	ILE	2.6
2	D	129	THR	2.6
2	F	90	VAL	2.6
2	D	60	VAL	2.6
2	D	66	THR	2.6
2	D	131	GLY	2.6
2	D	19	HIS	2.6
2	E	22	SER	2.6
2	F	78	PRO	2.6
2	F	20	ILE	2.5
2	E	60	VAL	2.5
2	D	92	ASP	2.5
2	F	70	ALA	2.4
2	F	42	THR	2.4
2	F	76	LEU	2.4
2	E	75	LEU	2.4
1	B	235	PHE	2.4
2	F	41	VAL	2.4
2	F	22	SER	2.4
2	F	26	VAL	2.4
2	F	77	ALA	2.3
2	D	79	ASN	2.3
2	F	74	ALA	2.3
2	E	48	PRO	2.3
2	E	78	PRO	2.3
1	B	309	GLY	2.3
2	D	80	ALA	2.3
2	D	128	LYS	2.3
2	E	19	HIS	2.3
2	F	75	LEU	2.3
2	D	77	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	35	THR	2.2
2	F	67	LYS	2.2
2	E	57	LEU	2.2
2	F	93	LYS	2.2
2	D	17	ILE	2.2
2	D	72	GLN	2.2
2	E	80	ALA	2.2
2	F	88	PHE	2.2
2	D	133	ILE	2.2
2	F	16	VAL	2.2
2	F	27	LYS	2.2
2	D	16	VAL	2.1
2	E	76	LEU	2.1
2	D	36	ASP	2.1
2	F	89	LYS	2.1
2	F	59	LYS	2.1
2	D	37	THR	2.1
2	E	84	ILE	2.0
1	B	238	THR	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(Å <sup>2</sup> )	Q<0.9
3	ZN	D	1108	1/1	0.99	0.18	0.62	49,49,49,49	0
4	SO4	A	311	5/5	0.88	0.19	0.02	85,85,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	F	1108	1/1	0.99	0.15	-0.16	50,50,50,50	0
3	ZN	E	1108	1/1	0.99	0.14	-0.59	44,44,44,44	0
4	SO4	B	311	5/5	0.93	0.16	-1.38	91,91,91,92	0
4	SO4	C	311	5/5	0.95	0.14	-3.52	85,85,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.