Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 08:32 PM EDT

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*
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:

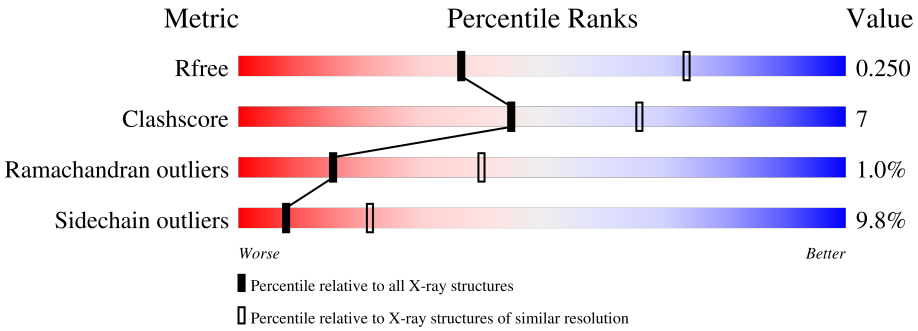
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	326	78% 15% • 5%
1	B	326	76% 17% • 5%
1	C	326	72% 20% • 5%
2	D	153	67% 18% • 13%
2	E	153	67% 15% • • 15%
2	F	153	70% 11% • 18%

2 Entry composition (i)

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.

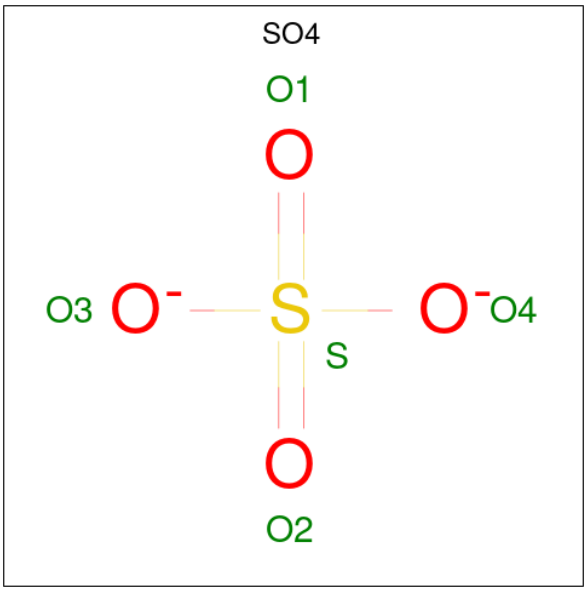
- Molecule 1 is a protein called Aspartate Carbamoyltransferase Catalytic Chain.

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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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 (three-letter code: 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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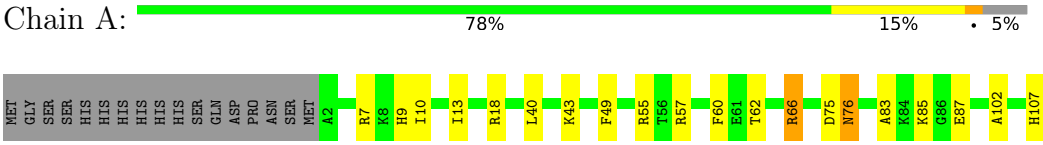
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total O 3 3	0	0

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. 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. 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:

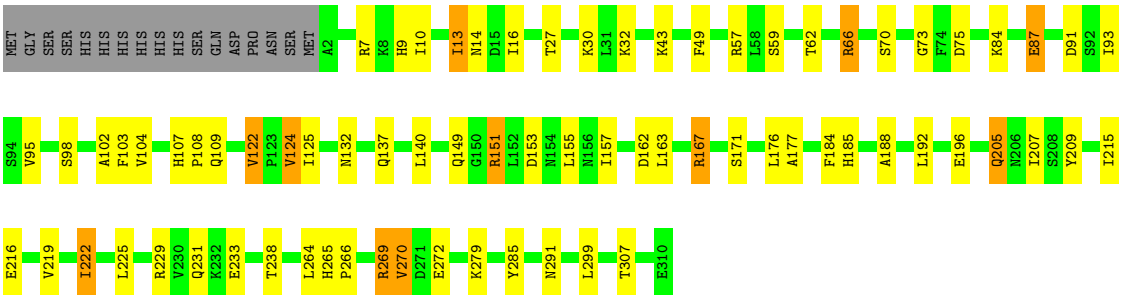


• Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain

Chain B:

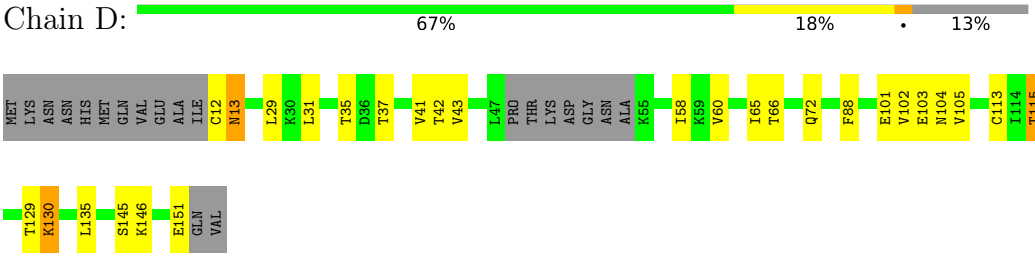
• Molecule 1: Aspartate Carbamoyltransferase Catalytic Chain

Chain C:



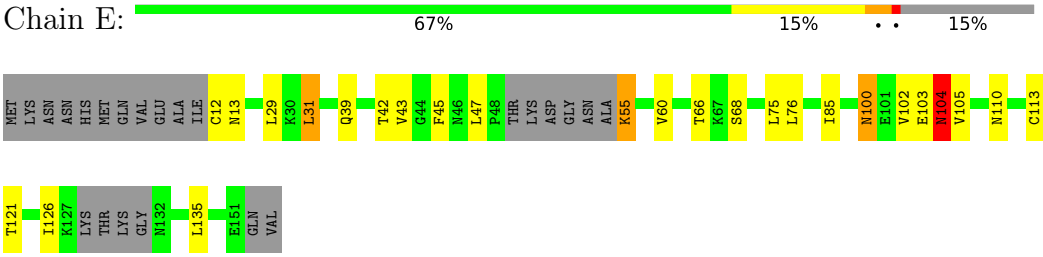
• Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain

Chain D:



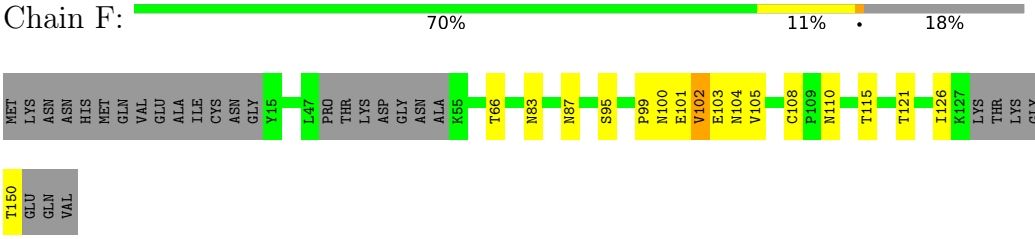
• Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain

Chain E:



• Molecule 2: Aspartate Carbamoyltransferase Regulatory Chain

Chain F:



4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [1]	1.64 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.257 0.257 , 0.250	Depositor DCC
R_{free} test set	2970 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9959	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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, ZN

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

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	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	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: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
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: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
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: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
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: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: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:104:ASN:CG	2:E:104:ASN:O	2.56	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: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: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: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
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

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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
1:A:60:PHE:CZ	1:A:296:ARG:HD3	2.55	0.41
2:D:145:SER:O	2:D:146:LYS:C	2.59	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: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
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: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: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: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%)	12 33

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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%)	22 50
2	D	129/153 (84%)	114 (88%)	12 (9%)	3 (2%)	6 20
2	E	124/153 (81%)	109 (88%)	13 (10%)	2 (2%)	9 28
2	F	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	9 27
All	All	1293/1437 (90%)	1199 (93%)	81 (6%)	13 (1%)	15 40

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%)	231 (92%)	21 (8%)	11 29
1	B	248/277 (90%)	223 (90%)	25 (10%)	7 20
1	C	252/277 (91%)	225 (89%)	27 (11%)	6 18
2	D	96/139 (69%)	87 (91%)	9 (9%)	8 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	99/139 (71%)	89 (90%)	10 (10%)	7 20
2	F	81/139 (58%)	72 (89%)	9 (11%)	6 16
All	All	1028/1248 (82%)	927 (90%)	101 (10%)	8 21

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

Sometimes 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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	C	311	-	4,4,4	0.23	0	6,6,6	0.41	0
3	SO4	A	311	-	4,4,4	0.28	0	6,6,6	0.51	0
3	SO4	B	311	-	4,4,4	0.13	0	6,6,6	0.15	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.