



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:30 am BST

PDB ID : 1ZNN
Title : Structure of the synthase subunit of PLP synthase
Authors : Zhu, J.; Burgner, J.W.; Harms, E.; Belitsky, B.R.; Smith, J.L.
Deposited on : 2005-05-11
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

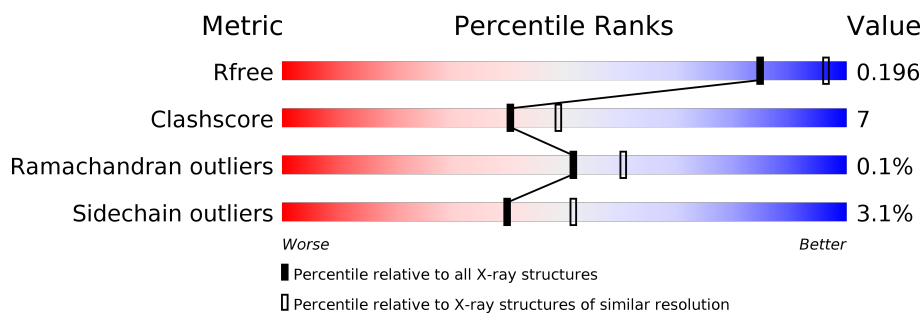
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	325	64% (green), 10% (yellow), 25% (grey)
1	B	325	65% (green), 8% (yellow), 25% (grey)
1	C	325	65% (green), 10% (yellow), 25% (grey)
1	D	325	64% (green), 10% (yellow), 25% (grey)
1	E	325	66% (green), 8% (yellow), 25% (grey)
1	F	325	66% (green), 10% (yellow), 25% (grey)

2 Entry composition [i](#)

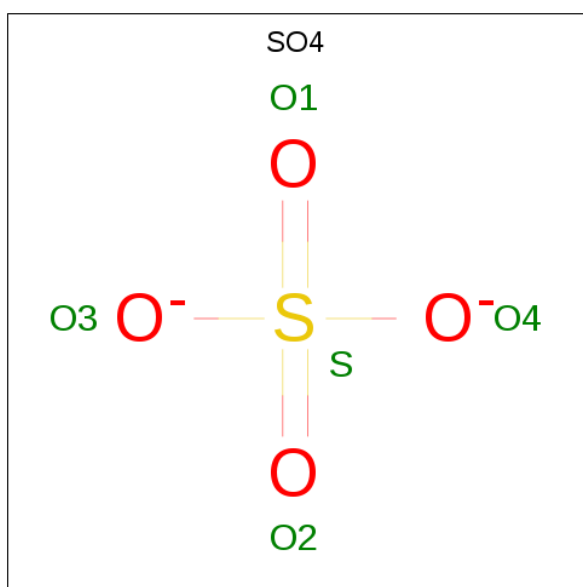
There are 4 unique types of molecules in this entry. The entry contains 12649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLP SYNTHASE.

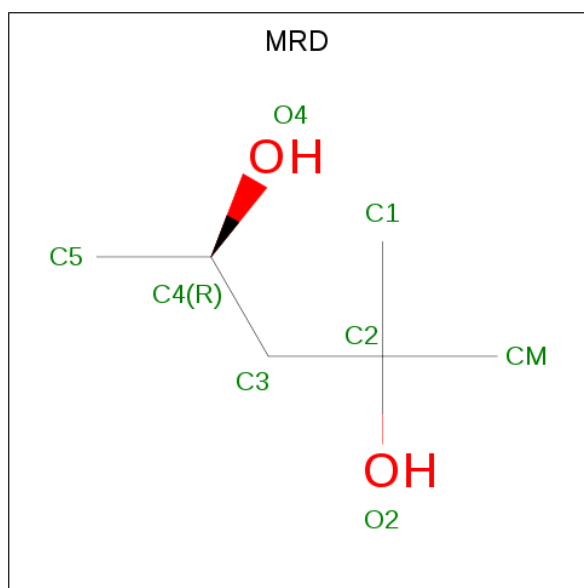
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0
1	B	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0
1	C	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0
1	D	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0
1	E	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0
1	F	245	Total 1839	C 1153	N 325	O 349	S 12	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

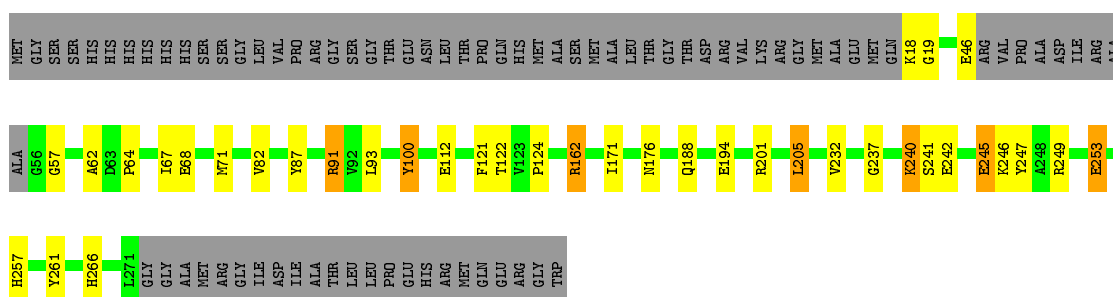
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	349	Total	O	0	0
			349	349		
4	B	396	Total	O	0	0
			396	396		
4	C	243	Total	O	0	0
			243	243		
4	D	152	Total	O	0	0
			152	152		
4	E	162	Total	O	0	0
			162	162		
4	F	205	Total	O	0	0
			205	205		

3 Residue-property plots [i](#)

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

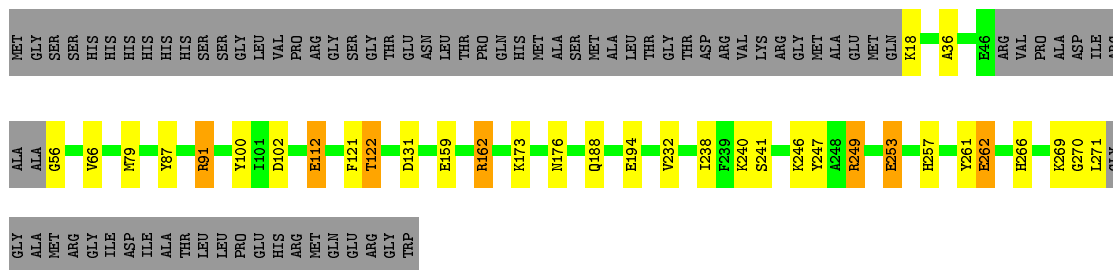
- Molecule 1: PLP SYNTHASE

Chain A: 



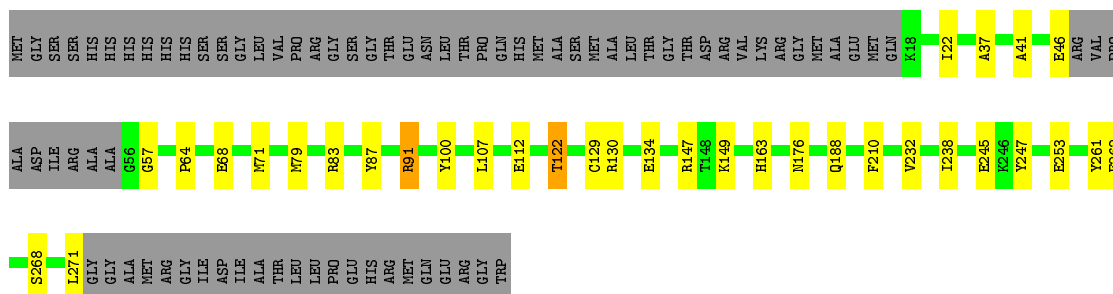
- Molecule 1: PLP SYNTHASE

Chain B: 

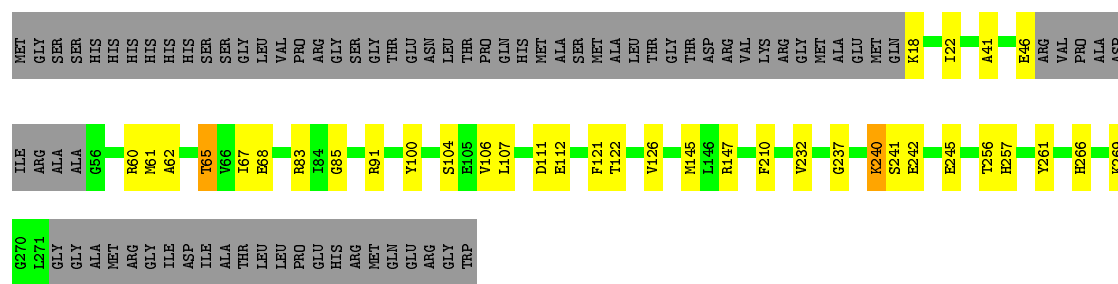


- Molecule 1: PLP SYNTHASE

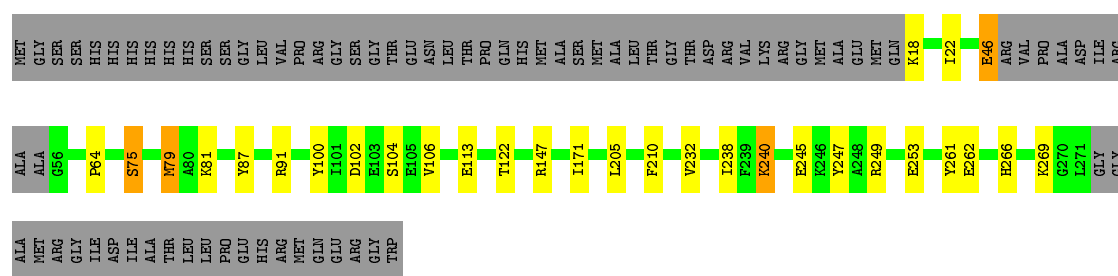
Chain C: 



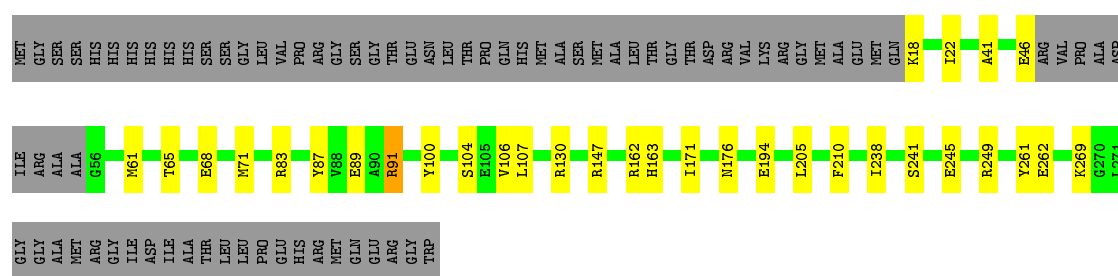
- Molecule 1: PLP SYNTHASE



Molecule 1: PLP SYNTHASE



Molecule 1: PLP SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.53Å 163.92Å 186.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 2.20 49.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.94-2.20) 99.9 (49.91-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.159 , 0.198 0.159 , 0.196	Depositor DCC
R_{free} test set	6320 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12649	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: MRD, 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	0.98	4/1863 (0.2%)	0.86	5/2516 (0.2%)
1	B	1.21	8/1863 (0.4%)	1.08	10/2516 (0.4%)
1	C	0.82	4/1863 (0.2%)	0.75	1/2516 (0.0%)
1	D	0.59	0/1863	0.65	0/2516
1	E	0.65	1/1863 (0.1%)	0.67	0/2516
1	F	0.67	0/1863	0.72	0/2516
All	All	0.85	17/11178 (0.2%)	0.80	16/15096 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	GLU	CB-CG	16.29	1.83	1.52
1	B	253	GLU	CG-CD	15.50	1.75	1.51
1	A	253	GLU	CG-CD	12.68	1.71	1.51
1	A	253	GLU	CB-CG	12.67	1.76	1.52
1	B	253	GLU	CD-OE1	-11.49	1.13	1.25
1	B	194	GLU	CG-CD	7.93	1.63	1.51
1	C	262	GLU	C-N	6.78	1.49	1.34
1	A	253	GLU	CD-OE2	6.40	1.32	1.25
1	C	268	SER	CB-OG	6.37	1.50	1.42
1	B	194	GLU	CD-OE1	6.34	1.32	1.25
1	C	262	GLU	C-O	6.12	1.34	1.23
1	B	262	GLU	CB-CG	-6.09	1.40	1.52
1	B	194	GLU	CD-OE2	5.96	1.32	1.25
1	B	112	GLU	CD-OE1	5.76	1.31	1.25
1	C	37	ALA	C-N	5.37	1.42	1.33
1	A	194	GLU	CG-CD	5.12	1.59	1.51
1	E	245	GLU	CG-CD	5.11	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	OE1-CD-OE2	-22.16	96.70	123.30
1	B	91	ARG	NE-CZ-NH1	14.26	127.43	120.30
1	B	253	GLU	CG-CD-OE1	9.31	136.92	118.30
1	B	91	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	B	249	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	253	GLU	OE1-CD-OE2	-6.56	115.43	123.30
1	B	249	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	79	MET	CG-SD-CE	5.93	109.69	100.20
1	C	91	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	162	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	162	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	131	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	253	GLU	CG-CD-OE2	5.22	128.73	118.30
1	A	91	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	102	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	205	LEU	CB-CG-CD1	-5.08	102.36	111.00

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	1839	0	1864	37	1
1	B	1839	0	1864	40	7
1	C	1839	0	1864	23	0
1	D	1839	0	1864	26	0
1	E	1839	0	1864	22	1
1	F	1839	0	1864	21	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	14	2	0
3	D	8	0	14	0	0
3	E	8	0	14	0	0
3	F	8	0	14	0	0
4	A	349	0	0	20	4
4	B	396	0	0	24	1
4	C	243	0	0	12	0
4	D	152	0	0	12	0
4	E	162	0	0	7	1
4	F	205	0	0	7	0
All	All	12649	0	11268	161	14

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 (161) 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:A:253:GLU:CG	1:A:253:GLU:CB	1.76	1.64
1:B:253:GLU:CB	1:B:253:GLU:CG	1.83	1.56
1:B:253:GLU:CG	1:B:253:GLU:CD	1.75	1.52
1:A:266:HIS:HE1	4:A:2889:HOH:O	1.28	1.16
1:B:18:LYS:HG3	4:B:3130:HOH:O	1.53	1.06
1:B:112:GLU:HG2	4:B:3163:HOH:O	1.58	1.02
1:F:65:THR:HB	4:F:3005:HOH:O	1.59	1.02
1:B:249:ARG:HD3	4:B:3275:HOH:O	1.63	0.99
1:C:176:ASN:HB2	4:C:2946:HOH:O	1.63	0.98
1:C:71:MET:SD	4:C:3087:HOH:O	2.24	0.94
1:B:253:GLU:CD	1:B:257:HIS:HE2	1.70	0.93
1:A:176:ASN:HB2	4:A:2961:HOH:O	1.65	0.93
1:A:266:HIS:CE1	4:A:2937:HOH:O	2.21	0.93
1:A:246:LYS:NZ	4:A:3225:HOH:O	2.09	0.86
1:A:266:HIS:HE1	4:A:2937:HOH:O	1.57	0.84
1:D:256:THR:HG22	1:D:257:HIS:CD2	2.14	0.82
1:B:249:ARG:HD2	4:B:3278:HOH:O	1.82	0.80
1:A:253:GLU:CD	1:A:257:HIS:HE2	1.86	0.79
1:D:266:HIS:CE1	4:D:2979:HOH:O	2.37	0.76
1:B:176:ASN:HB2	4:B:2944:HOH:O	1.86	0.76
1:D:18:LYS:HG3	4:D:2932:HOH:O	1.88	0.74
1:F:18:LYS:HD2	4:F:3026:HOH:O	1.87	0.74
1:B:253:GLU:CD	1:B:257:HIS:NE2	2.40	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:CB	4:B:2944:HOH:O	2.36	0.73
1:D:112:GLU:HG2	4:D:2974:HOH:O	1.89	0.73
1:A:266:HIS:CE1	4:A:2889:HOH:O	2.15	0.73
1:B:56:GLY:HA2	4:B:3256:HOH:O	1.91	0.71
1:C:176:ASN:CB	4:C:2946:HOH:O	2.27	0.71
1:B:253:GLU:OE1	1:B:257:HIS:NE2	2.23	0.70
1:F:238:ILE:O	1:F:241:SER:HB3	1.91	0.70
1:E:261:TYR:CE2	1:F:91:ARG:HD3	2.27	0.68
1:B:240:LYS:HD2	4:B:3182:HOH:O	1.94	0.67
1:A:261:TYR:CE2	1:B:91:ARG:HD3	2.29	0.67
1:A:237:GLY:HA2	1:A:240:LYS:HE3	1.77	0.67
1:A:176:ASN:CB	4:A:2961:HOH:O	2.31	0.66
1:E:238:ILE:HD13	1:E:247:TYR:CD1	2.31	0.66
1:C:245:GLU:HG3	4:C:3052:HOH:O	1.94	0.66
1:A:249:ARG:NH1	4:A:3176:HOH:O	2.30	0.65
1:A:91:ARG:HD3	1:F:261:TYR:CE2	2.32	0.64
1:C:112:GLU:HG2	4:C:3001:HOH:O	1.96	0.64
1:A:68:GLU:HA	1:A:71:MET:HE2	1.79	0.64
1:C:46:GLU:C	4:C:2934:HOH:O	2.36	0.64
1:D:266:HIS:NE2	4:D:2979:HOH:O	2.30	0.63
1:A:18:LYS:HA	4:A:2952:HOH:O	2.00	0.62
1:B:266:HIS:HD2	4:B:2997:HOH:O	1.83	0.61
1:A:46:GLU:C	4:A:3007:HOH:O	2.39	0.61
1:B:238:ILE:O	1:B:241:SER:HB3	2.00	0.61
1:D:245:GLU:HG2	4:D:2916:HOH:O	2.02	0.60
1:B:238:ILE:HG12	4:B:3285:HOH:O	2.00	0.60
1:A:253:GLU:CA	1:A:253:GLU:CG	2.77	0.60
1:A:122:THR:HG21	4:A:3168:HOH:O	2.01	0.59
1:B:188:GLN:HG2	4:B:3088:HOH:O	2.03	0.59
1:D:122:THR:HG22	4:D:2994:HOH:O	2.03	0.59
1:B:159:GLU:OE1	1:B:162:ARG:NH2	2.36	0.58
1:D:65:THR:HB	4:D:3023:HOH:O	2.03	0.58
1:F:162:ARG:NH2	4:F:3024:HOH:O	2.28	0.58
1:D:62:ALA:HB3	1:D:67:ILE:HD11	1.85	0.58
1:D:91:ARG:HG2	1:D:121:PHE:CE1	2.39	0.58
1:E:22:ILE:HD13	1:E:79:MET:CE	2.34	0.57
1:F:194:GLU:HG2	4:F:3051:HOH:O	2.03	0.57
1:B:87:TYR:CZ	1:B:91:ARG:HD2	2.40	0.56
1:E:75:SER:HB2	4:E:2972:HOH:O	2.06	0.56
1:A:240:LYS:HE2	4:A:3120:HOH:O	2.04	0.56
1:A:82:VAL:HG13	1:A:93:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:SER:OG	1:D:106:VAL:HG22	2.05	0.56
1:B:246:LYS:HE2	4:B:3216:HOH:O	2.07	0.55
1:F:87:TYR:CZ	1:F:91:ARG:HD2	2.40	0.55
1:B:249:ARG:HG3	4:B:3008:HOH:O	2.06	0.55
1:B:270:GLY:O	1:B:271:LEU:HB2	2.06	0.55
1:A:188:GLN:HB2	4:A:3187:HOH:O	2.07	0.55
1:A:171:ILE:HD11	1:A:205:LEU:HG	1.90	0.54
1:D:22:ILE:HG12	1:D:41:ALA:HB3	1.88	0.54
1:D:257:HIS:NE2	4:D:2913:HOH:O	2.34	0.54
1:B:66:VAL:HG13	4:B:3277:HOH:O	2.07	0.53
1:C:122:THR:HG22	4:C:2923:HOH:O	2.07	0.53
1:D:261:TYR:CE2	1:E:91:ARG:HD3	2.44	0.53
1:B:271:LEU:HD11	4:B:3120:HOH:O	2.08	0.53
1:C:83:ARG:HG2	1:C:107:LEU:HB3	1.91	0.53
1:A:201:ARG:HB2	4:A:3228:HOH:O	2.09	0.53
1:B:173:LYS:HE2	4:B:3272:HOH:O	2.08	0.52
1:A:253:GLU:CD	1:A:257:HIS:NE2	2.61	0.52
1:D:46:GLU:HB3	4:D:2986:HOH:O	2.10	0.52
1:B:271:LEU:C	4:B:3084:HOH:O	2.48	0.52
1:E:238:ILE:HD13	1:E:247:TYR:HD1	1.73	0.52
1:A:122:THR:HG23	4:A:2973:HOH:O	2.09	0.52
1:C:46:GLU:HG2	4:C:3091:HOH:O	2.10	0.51
1:C:87:TYR:CZ	1:C:91:ARG:HD2	2.44	0.51
1:A:112:GLU:HG2	4:A:3113:HOH:O	2.11	0.51
1:F:176:ASN:HB3	4:F:3096:HOH:O	2.11	0.51
1:B:240:LYS:HG3	4:B:3072:HOH:O	2.11	0.51
1:B:249:ARG:CD	4:B:3278:HOH:O	2.49	0.51
1:B:249:ARG:HB2	4:B:3275:HOH:O	2.10	0.51
1:B:261:TYR:CE2	1:C:91:ARG:HD3	2.46	0.51
1:F:68:GLU:HA	1:F:71:MET:HE2	1.93	0.51
1:E:46:GLU:HA	4:E:2903:HOH:O	2.12	0.50
1:A:19:GLY:HA3	4:A:3231:HOH:O	2.10	0.50
1:D:46:GLU:C	4:D:3025:HOH:O	2.50	0.49
1:B:269:LYS:HG2	1:C:64:PRO:HB2	1.93	0.49
1:D:83:ARG:HG2	1:D:107:LEU:HB3	1.95	0.49
1:B:176:ASN:CG	4:B:2944:HOH:O	2.48	0.48
1:C:238:ILE:HA	1:C:247:TYR:CE2	2.48	0.48
1:E:113:GLU:HB3	4:E:2942:HOH:O	2.14	0.48
1:E:22:ILE:HD13	1:E:79:MET:HE1	1.95	0.48
1:B:253:GLU:OE2	1:B:257:HIS:NE2	2.32	0.48
1:A:87:TYR:CZ	1:A:91:ARG:HD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:HA	1:E:210:PHE:O	2.14	0.48
1:B:188:GLN:HB2	4:B:3153:HOH:O	2.13	0.48
1:F:249:ARG:HG2	1:F:249:ARG:HH11	1.79	0.48
1:C:261:TYR:CE2	1:D:91:ARG:HD3	2.49	0.47
1:E:104:SER:OG	1:E:106:VAL:HG22	2.14	0.47
1:F:245:GLU:HG3	4:F:3041:HOH:O	2.14	0.47
1:A:18:LYS:N	4:A:3060:HOH:O	2.47	0.47
1:A:245:GLU:HG3	4:A:3020:HOH:O	2.14	0.47
1:F:46:GLU:C	4:F:2938:HOH:O	2.52	0.47
1:B:91:ARG:HG2	1:B:121:PHE:CE1	2.50	0.46
1:C:130:ARG:HG3	1:C:149:LYS:HD2	1.97	0.46
1:C:64:PRO:O	1:C:68:GLU:HG3	2.16	0.46
1:E:81:LYS:HG2	1:E:102:ASP:HB3	1.97	0.46
1:B:253:GLU:CD	1:B:257:HIS:CD2	2.90	0.46
1:C:130:ARG:N	1:C:134:GLU:OE1	2.49	0.45
1:A:242:GLU:OE2	1:A:242:GLU:HA	2.16	0.45
1:A:64:PRO:HB2	1:F:269:LYS:HG2	1.98	0.45
1:E:87:TYR:CZ	1:E:91:ARG:HD2	2.52	0.44
1:F:83:ARG:HG2	1:F:107:LEU:HB3	1.99	0.44
1:E:22:ILE:HD13	1:E:79:MET:HE3	1.99	0.44
1:C:147:ARG:HA	1:C:210:PHE:O	2.18	0.43
1:A:188:GLN:HG3	4:A:3139:HOH:O	2.18	0.43
1:A:62:ALA:HB3	1:A:67:ILE:HD11	2.01	0.43
1:E:171:ILE:HD11	1:E:205:LEU:HG	2.01	0.43
1:E:249:ARG:HG2	4:E:3036:HOH:O	2.18	0.43
1:D:68:GLU:HB2	4:D:2964:HOH:O	2.18	0.43
1:E:262:GLU:HG2	4:E:3043:HOH:O	2.19	0.43
1:A:162:ARG:NH2	1:B:112:GLU:OE2	2.51	0.43
1:C:253:GLU:HG2	4:C:3027:HOH:O	2.18	0.43
1:D:60:ARG:HG2	1:D:83:ARG:CZ	2.49	0.42
1:F:61:MET:HB2	1:F:89:GLU:CD	2.40	0.42
1:D:269:LYS:HG2	1:E:64:PRO:HB2	2.01	0.42
1:C:130:ARG:HG2	1:C:163:HIS:CE1	2.54	0.42
1:E:238:ILE:HD13	1:E:247:TYR:CE1	2.54	0.42
1:A:100:TYR:CZ	1:A:124:PRO:HB2	2.54	0.42
3:C:2890:MRD:H1C3	4:C:3133:HOH:O	2.18	0.42
1:F:104:SER:OG	1:F:106:VAL:HG22	2.20	0.42
1:B:18:LYS:N	4:B:2991:HOH:O	2.52	0.42
1:F:22:ILE:HG12	1:F:41:ALA:HB3	2.01	0.42
1:D:237:GLY:HA2	1:D:240:LYS:HE3	2.02	0.42
1:D:85:GLY:HA3	1:D:111:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ILE:HG12	1:C:41:ALA:HB3	2.01	0.41
1:E:240:LYS:HD3	4:E:2957:HOH:O	2.20	0.41
1:D:18:LYS:HD3	4:D:3010:HOH:O	2.21	0.41
1:F:147:ARG:HA	1:F:210:PHE:O	2.20	0.41
3:C:2890:MRD:HMC3	4:C:3133:HOH:O	2.21	0.41
1:C:64:PRO:HD3	4:C:3057:HOH:O	2.19	0.41
1:F:130:ARG:HG2	1:F:163:HIS:CE1	2.56	0.41
1:D:147:ARG:HA	1:D:210:PHE:O	2.20	0.41
1:E:266:HIS:HD2	4:E:2973:HOH:O	2.03	0.41
1:C:129:CYS:HA	1:C:134:GLU:OE1	2.20	0.41
1:F:171:ILE:HD11	1:F:205:LEU:HG	2.02	0.41
1:A:91:ARG:HG2	1:A:121:PHE:CE1	2.56	0.40
1:B:122:THR:HG22	4:B:2939:HOH:O	2.20	0.40
1:D:126:VAL:HA	1:D:145:MET:O	2.21	0.40
1:E:266:HIS:HA	1:E:269:LYS:HE3	2.03	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLU:OE1	1:B:253:GLU:OE2[4_565]	1.02	1.18
1:B:253:GLU:CD	1:B:253:GLU:OE2[4_565]	1.20	1.00
1:B:253:GLU:OE1	1:B:253:GLU:OE1[4_565]	1.44	0.76
1:B:253:GLU:CD	1:B:253:GLU:OE1[4_565]	1.65	0.55
4:A:2937:HOH:O	4:A:2937:HOH:O[3_555]	1.65	0.55
1:B:253:GLU:CD	1:B:253:GLU:CD[4_565]	1.66	0.54
4:E:2893:HOH:O	4:E:2893:HOH:O[6_555]	1.69	0.51
1:A:253:GLU:OE1	1:A:253:GLU:OE1[3_555]	1.94	0.26
4:A:2945:HOH:O	4:A:3224:HOH:O[3_555]	1.95	0.25
4:A:3217:HOH:O	4:A:3224:HOH:O[3_555]	1.99	0.21
1:B:253:GLU:OE1	1:B:257:HIS:NE2[4_565]	1.99	0.21
1:B:36:ALA:O	4:B:3275:HOH:O[4_565]	2.01	0.19
4:A:2937:HOH:O	4:A:3217:HOH:O[3_555]	2.05	0.15
1:E:253:GLU:OE1	1:E:253:GLU:OE1[3_556]	2.10	0.10

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	241/325 (74%)	237 (98%)	3 (1%)	1 (0%)	34	37
1	B	241/325 (74%)	240 (100%)	1 (0%)	0	100	100
1	C	241/325 (74%)	238 (99%)	2 (1%)	1 (0%)	34	37
1	D	241/325 (74%)	238 (99%)	3 (1%)	0	100	100
1	E	241/325 (74%)	233 (97%)	8 (3%)	0	100	100
1	F	241/325 (74%)	237 (98%)	4 (2%)	0	100	100
All	All	1446/1950 (74%)	1423 (98%)	21 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	57	GLY
1	A	57	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	189/251 (75%)	183 (97%)	6 (3%)	39	50
1	B	189/251 (75%)	184 (97%)	5 (3%)	46	58
1	C	189/251 (75%)	183 (97%)	6 (3%)	39	50
1	D	189/251 (75%)	182 (96%)	7 (4%)	34	43
1	E	189/251 (75%)	181 (96%)	8 (4%)	30	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	189/251 (75%)	186 (98%)	3 (2%)	62 76
All	All	1134/1506 (75%)	1099 (97%)	35 (3%)	40 51

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	TYR
1	A	232	VAL
1	A	240	LYS
1	A	241	SER
1	A	245	GLU
1	A	247	TYR
1	B	100	TYR
1	B	122	THR
1	B	232	VAL
1	B	247	TYR
1	B	262	GLU
1	C	79	MET
1	C	100	TYR
1	C	122	THR
1	C	188	GLN
1	C	232	VAL
1	C	271	LEU
1	D	61	MET
1	D	65	THR
1	D	100	TYR
1	D	232	VAL
1	D	240	LYS
1	D	241	SER
1	D	242	GLU
1	E	18	LYS
1	E	46	GLU
1	E	75	SER
1	E	79	MET
1	E	100	TYR
1	E	122	THR
1	E	232	VAL
1	E	240	LYS
1	F	91	ARG
1	F	100	TYR
1	F	262	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	188	GLN
1	A	266	HIS
1	B	115	HIS
1	B	188	GLN
1	C	115	HIS
1	D	188	GLN
1	D	257	HIS
1	E	188	GLN
1	F	188	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
3	MRD	D	2891	-	7,7,7	0.25	0	9,10,10	0.55	0
2	SO4	E	2410	-	4,4,4	0.22	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	2411	-	4,4,4	0.27	0	6,6,6	0.58	0
2	SO4	E	2409	-	4,4,4	0.15	0	6,6,6	0.72	0
3	MRD	C	2890	-	7,7,7	0.41	0	9,10,10	0.29	0
2	SO4	B	2404	-	4,4,4	0.17	0	6,6,6	0.63	0
2	SO4	D	2407	-	4,4,4	0.37	0	6,6,6	1.15	0
2	SO4	D	2408	-	4,4,4	0.18	0	6,6,6	0.55	0
3	MRD	F	2893	-	7,7,7	0.39	0	9,10,10	0.42	0
3	MRD	A	2888	-	7,7,7	0.28	0	9,10,10	0.47	0
2	SO4	C	2405	-	4,4,4	0.50	0	6,6,6	0.86	0
2	SO4	A	2402	-	4,4,4	0.23	0	6,6,6	0.96	0
3	MRD	B	2889	-	7,7,7	0.42	0	9,10,10	0.65	0
2	SO4	B	2403	-	4,4,4	0.78	0	6,6,6	0.86	0
3	MRD	E	2892	-	7,7,7	0.26	0	9,10,10	0.42	0
2	SO4	A	2401	-	4,4,4	0.55	0	6,6,6	0.50	0
2	SO4	C	2406	-	4,4,4	0.17	0	6,6,6	0.39	0
2	SO4	F	2412	-	4,4,4	0.13	0	6,6,6	0.36	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
3	MRD	D	2891	-	-	0/5/5/5	-
3	MRD	A	2888	-	-	0/5/5/5	-
3	MRD	F	2893	-	-	0/5/5/5	-
3	MRD	B	2889	-	-	0/5/5/5	-
3	MRD	E	2892	-	-	0/5/5/5	-
3	MRD	C	2890	-	-	0/5/5/5	-

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2890	MRD	2	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.