



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:02 AM UTC

PDB ID : 1ZNN / pdb_00001znn
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 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

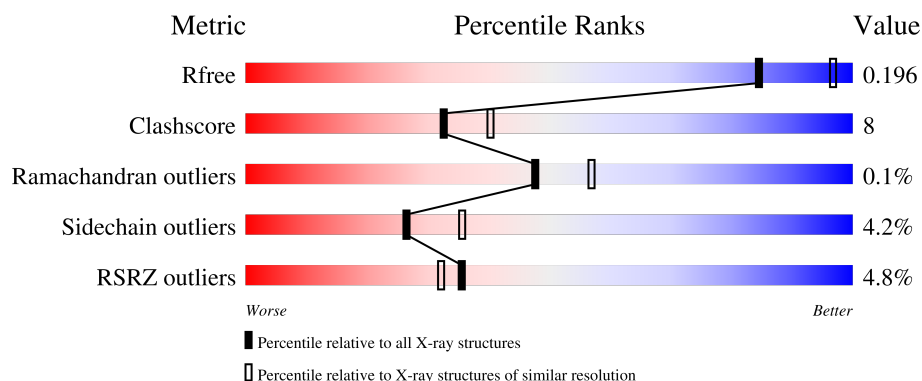
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	325	3% 64% 9% • 25%
1	B	325	4% 64% 10% • 25%
1	C	325	8% 63% 11% • 25%
1	D	325	2% 63% 11% • 25%
1	E	325	2% 64% 10% • 25%

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Mol	Chain	Length	Quality of chain
1	F	325	2% 64% 11% 25%

2 Entry composition [i](#)

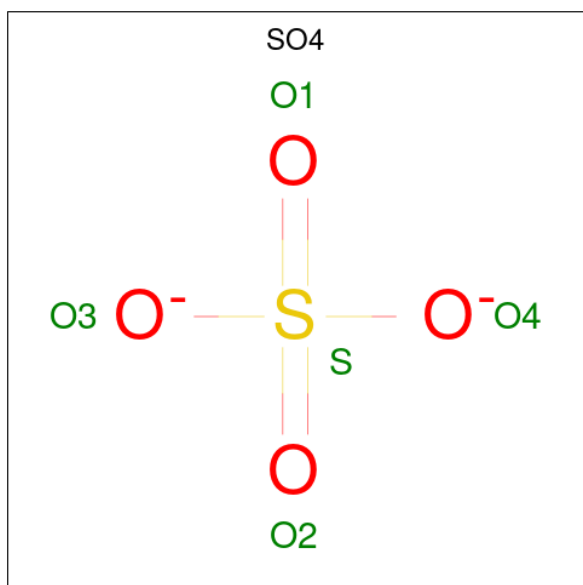
There are 4 unique types of molecules in this entry. The entry contains 12649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

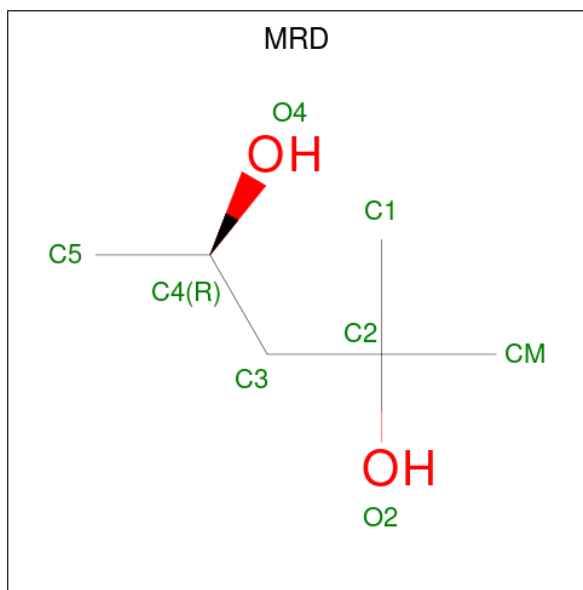
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1839	1153	325	349	12			
1	B	245	Total	C	N	O	S	0	0	0
			1839	1153	325	349	12			
1	C	245	Total	C	N	O	S	0	0	0
			1839	1153	325	349	12			
1	D	245	Total	C	N	O	S	0	0	0
			1839	1153	325	349	12			
1	E	245	Total	C	N	O	S	0	0	0
	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

- Molecule 2 is SULFATE ION (CCD ID: 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 (CCD ID: MRD) (formula: C₆H₁₄O₂).



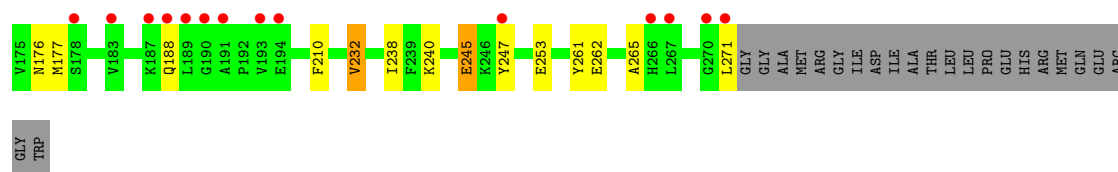
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

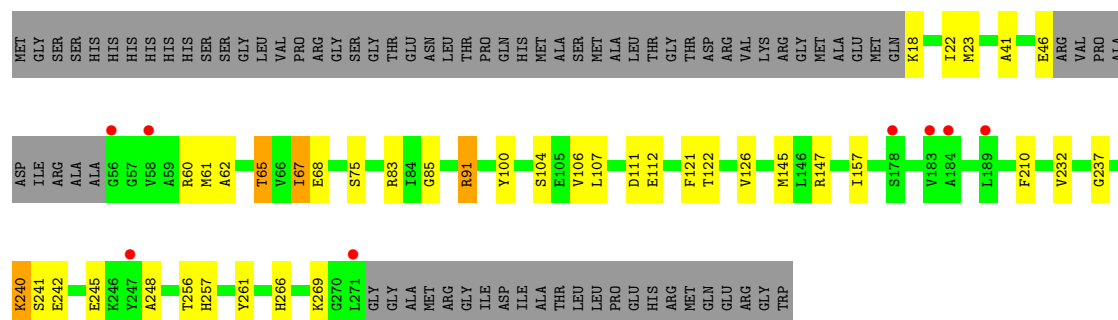
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	349	Total O 349 349	0	0
4	B	396	Total O 396 396	0	0
4	C	243	Total O 243 243	0	0
4	D	152	Total O 152 152	0	0
4	E	162	Total O 162 162	0	0
4	F	205	Total O 205 205	0	0

- Molecule 1: PLP SYNTHASE

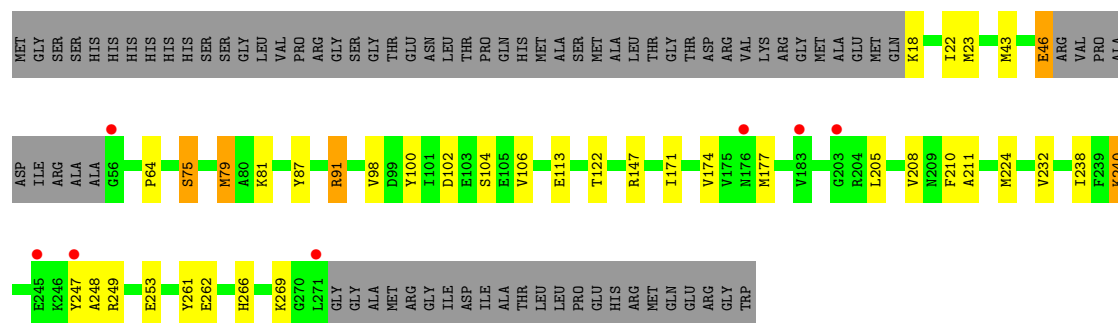




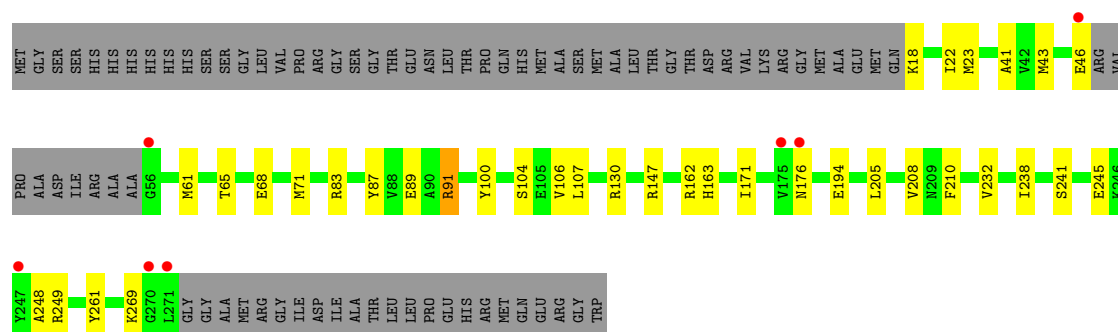
• Molecule 1: PLP SYNTHASE



• 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 49.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.94-2.20) 99.9 (49.94-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.20Å)	Xtriage
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	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12649	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage'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	1.06	2/1863 (0.1%)	1.01	1/2516 (0.0%)
1	B	1.25	6/1863 (0.3%)	1.14	9/2516 (0.4%)
1	C	1.01	5/1863 (0.3%)	0.99	3/2516 (0.1%)
1	D	0.73	0/1863	0.91	0/2516
1	E	0.82	1/1863 (0.1%)	0.93	0/2516
1	F	0.79	0/1863	0.93	0/2516
All	All	0.96	14/11178 (0.1%)	0.99	13/15096 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	GLU	C-N	11.99	1.49	1.33
1	B	253	GLU	CB-CG	10.22	1.83	1.52
1	C	262	GLU	C-O	9.36	1.34	1.24
1	B	253	GLU	CG-CD	9.26	1.75	1.52
1	A	253	GLU	CB-CG	7.92	1.76	1.52
1	A	253	GLU	CG-CD	7.57	1.71	1.52
1	C	37	ALA	C-N	6.88	1.42	1.33
1	B	253	GLU	CA-CB	6.50	1.64	1.53
1	B	253	GLU	CD-OE1	-6.50	1.13	1.25
1	C	265	ALA	C-N	6.22	1.42	1.33
1	B	208	VAL	CA-CB	5.64	1.60	1.54
1	E	98	VAL	CA-CB	5.42	1.59	1.54
1	C	232	VAL	CA-CB	5.20	1.61	1.54
1	B	192	PRO	CA-C	5.08	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	OE1-CD-OE2	-10.91	96.70	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	CG-CD-OE1	8.05	136.92	118.40
1	B	253	GLU	CB-CG-CD	7.12	124.70	112.60
1	B	63	ASP	CA-C-N	5.94	126.36	119.47
1	B	63	ASP	C-N-CA	5.94	126.36	119.47
1	B	91	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	B	232	VAL	N-CA-CB	-5.90	101.77	111.45
1	B	91	ARG	CB-CG-CD	5.69	124.40	111.30
1	C	262	GLU	CA-C-N	-5.66	112.70	120.28
1	C	262	GLU	C-N-CA	-5.66	112.70	120.28
1	A	253	GLU	CB-CG-CD	5.57	122.06	112.60
1	B	107	LEU	N-CA-C	-5.36	103.62	110.53
1	C	262	GLU	O-C-N	5.10	127.59	122.09

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	1839	0	1864	37	1
1	B	1839	0	1864	43	7
1	C	1839	0	1864	26	0
1	D	1839	0	1864	28	0
1	E	1839	0	1864	27	1
1	F	1839	0	1864	23	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
3	C	8	0	14	2	0
3	D	8	0	14	0	0
3	E	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8	0	14	1	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	13	0
4	E	162	0	0	7	1
4	F	205	0	0	7	0
All	All	12649	0	11268	176	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 8.

All (176) 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:CB	1:A:253:GLU:CG	1.76	1.64
1:B:253:GLU:CD	1:B:253:GLU:CG	1.75	1.56
1:B:253:GLU:CG	1:B:253:GLU:CB	1.83	1.56
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:B:253:GLU:CD	1:B:257:HIS:HE2	1.70	0.98
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: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:A:253:GLU:CD	1:A:257:HIS:HE2	1.86	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:B:253:GLU:CD	1:B:257:HIS:NE2	2.40	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:266:HIS:NE2	4:D:3043:HOH:O	2.17	0.75
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:238:ILE:O	1:F:241:SER:HB3	1.91	0.70
1:B:253:GLU:OE1	1:B:257:HIS:NE2	2.23	0.70
1:E:261:TYR:CE2	1:F:91:ARG:HD3	2.27	0.68
1:C:46:GLU:C	4:C:2934:HOH:O	2.36	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:A:46:GLU:C	4:A:3007:HOH:O	2.39	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: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:174:VAL:HA	1:B:177:MET:HE3	1.80	0.62
1:B:266:HIS:HD2	4:B:2997:HOH:O	1.83	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:CG	1:A:253:GLU:CA	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:E:22:ILE:HD13	1:E:79:MET:HE3	1.87	0.57
1:B:176:ASN:CG	4:B:2944:HOH:O	2.48	0.57
1:F:194:GLU:HG2	4:F:3051:HOH:O	2.03	0.57
1:A:253:GLU:CD	1:A:257:HIS:NE2	2.61	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG13	1:A:93:LEU:HD12	1.86	0.56
1:D:104:SER:OG	1:D:106:VAL:HG22	2.05	0.56
1:B:271:LEU:C	4:B:3084:HOH:O	2.48	0.55
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:E:211:ALA:HB1	1:E:224:MET:HE2	1.90	0.54
1:D:257:HIS:NE2	4:D:2913:HOH:O	2.34	0.54
1:D:46:GLU:C	4:D:3025:HOH:O	2.50	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:D:46:GLU:HB3	4:D:2986:HOH:O	2.10	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:B:211:ALA:HB1	1:B:224:MET:HE2	1.93	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:46:GLU:C	4:F:2938:HOH:O	2.52	0.51
1:B:253:GLU:CD	1:B:257:HIS:CD2	2.90	0.50
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:A:68:GLU:HA	1:A:71:MET:HE2	1.92	0.50
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:E:174:VAL:HA	1:E:177:MET:HE3	1.94	0.48
1:C:238:ILE:HA	1:C:247:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:GLU:HB3	4:E:2942:HOH:O	2.14	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
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:23:MET:HE1	1:F:248:ALA:HB1	1.96	0.47
1:B:91:ARG:HG2	1:B:121:PHE:CE1	2.50	0.46
1:C:64:PRO:O	1:C:68:GLU:HG3	2.16	0.46
1:C:130:ARG:HG3	1:C:149:LYS:HD2	1.97	0.46
1:E:43:MET:HE3	3:E:2892:MRD:H5C1	1.97	0.46
1:F:68:GLU:HA	1:F:71:MET:HE2	1.98	0.46
1:F:61:MET:HB2	1:F:89:GLU:CD	2.40	0.46
1:E:81:LYS:HG2	1:E:102:ASP:HB3	1.97	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:B:211:ALA:CB	1:B:224:MET:HE2	2.46	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:C:173:LYS:HG2	1:C:177:MET:HE2	1.98	0.44
1:D:23:MET:HE1	1:D:248:ALA:HB1	1.99	0.44
1:F:43:MET:HE3	3:F:2893:MRD:H5C1	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:174:VAL:HA	1:C:177:MET:HE3	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:43:MET:HE1	1:E:102:ASP:HB2	2.02	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
1:C:22:ILE:HG12	1:C:41:ALA:HB3	2.01	0.41
1:E:211:ALA:CB	1:E:224:MET:HE2	2.50	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
1:C:64:PRO:HD3	4:C:3057:HOH:O	2.19	0.41
3:C:2890:MRD:HMC3	4:C:3133:HOH:O	2.21	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:C:23:MET:HE3	1:C:39:ALA:HB2	2.03	0.40
1:D:126:VAL:HA	1:D:145:MET:O	2.21	0.40
1:E:23:MET:HE1	1:E:248:ALA:HB1	2.03	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
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:OE1[4_565]	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	34
1	B	241/325 (74%)	240 (100%)	1 (0%)	0	100	100
1	C	241/325 (74%)	238 (99%)	2 (1%)	1 (0%)	30	34
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%)	48	57

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%)	182 (96%)	7 (4%)	30	41
1	B	189/251 (75%)	183 (97%)	6 (3%)	34	47
1	C	189/251 (75%)	179 (95%)	10 (5%)	20	26
1	D	189/251 (75%)	178 (94%)	11 (6%)	18	22
1	E	189/251 (75%)	179 (95%)	10 (5%)	20	26
1	F	189/251 (75%)	185 (98%)	4 (2%)	47	63
All	All	1134/1506 (75%)	1086 (96%)	48 (4%)	26	36

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	91	ARG
1	A	100	TYR
1	A	232	VAL
1	A	240	LYS
1	A	241	SER
1	A	245	GLU
1	B	91	ARG
1	B	100	TYR
1	B	122	THR
1	B	232	VAL
1	B	245	GLU
1	B	262	GLU
1	C	46	GLU
1	C	79	MET
1	C	91	ARG
1	C	100	TYR
1	C	122	THR
1	C	188	GLN
1	C	232	VAL
1	C	240	LYS
1	C	245	GLU
1	C	271	LEU
1	D	61	MET
1	D	65	THR
1	D	67	ILE
1	D	75	SER

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Mol	Chain	Res	Type
1	D	91	ARG
1	D	100	TYR
1	D	157	ILE
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	91	ARG
1	E	100	TYR
1	E	122	THR
1	E	208	VAL
1	E	232	VAL
1	E	240	LYS
1	F	91	ARG
1	F	100	TYR
1	F	208	VAL
1	F	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	209	ASN
1	D	115	HIS
1	D	188	GLN
1	D	209	ASN
1	D	257	HIS
1	E	188	GLN
1	E	209	ASN
1	F	115	HIS
1	F	188	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.56	0
2	SO4	F	2411	-	4,4,4	0.23	0	6,6,6	0.59	0
2	SO4	C	2405	-	4,4,4	0.47	0	6,6,6	0.82	0
3	MRD	B	2889	-	7,7,7	0.41	0	9,10,10	0.68	0
2	SO4	B	2403	-	4,4,4	0.66	0	6,6,6	0.85	0
2	SO4	B	2404	-	4,4,4	0.26	0	6,6,6	0.54	0
3	MRD	E	2892	-	7,7,7	0.28	0	9,10,10	0.46	0
2	SO4	D	2407	-	4,4,4	0.33	0	6,6,6	1.06	0
2	SO4	E	2409	-	4,4,4	0.20	0	6,6,6	0.69	0
3	MRD	F	2893	-	7,7,7	0.39	0	9,10,10	0.45	0
2	SO4	D	2408	-	4,4,4	0.28	0	6,6,6	0.44	0
2	SO4	E	2410	-	4,4,4	0.32	0	6,6,6	0.55	0
2	SO4	F	2412	-	4,4,4	0.24	0	6,6,6	0.33	0
3	MRD	A	2888	-	7,7,7	0.30	0	9,10,10	0.45	0
2	SO4	A	2401	-	4,4,4	0.48	0	6,6,6	0.47	0
3	MRD	C	2890	-	7,7,7	0.40	0	9,10,10	0.34	0
2	SO4	C	2406	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	A	2402	-	4,4,4	0.34	0	6,6,6	0.87	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	E	2892	-	-	0/5/5/5	-
3	MRD	B	2889	-	-	0/5/5/5	-
3	MRD	F	2893	-	-	0/5/5/5	-
3	MRD	A	2888	-	-	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2892	MRD	1	0
3	F	2893	MRD	1	0
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

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	245/325 (75%)	0.71	10 (4%) 41 38	31, 39, 51, 65	0
1	B	245/325 (75%)	0.63	12 (4%) 35 31	30, 40, 50, 65	0
1	C	245/325 (75%)	1.06	27 (11%) 10 8	32, 40, 52, 62	0
1	D	245/325 (75%)	0.83	8 (3%) 49 46	25, 35, 47, 60	0
1	E	245/325 (75%)	0.69	7 (2%) 53 50	25, 34, 45, 62	0
1	F	245/325 (75%)	0.56	7 (2%) 53 50	27, 37, 50, 64	0
All	All	1470/1950 (75%)	0.75	71 (4%) 35 32	25, 38, 50, 65	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	271	LEU	5.9
1	E	271	LEU	5.3
1	C	271	LEU	4.7
1	C	114	PHE	4.3
1	F	271	LEU	4.2
1	B	56	GLY	3.9
1	C	247	TYR	3.9
1	B	271	LEU	3.8
1	A	271	LEU	3.6
1	C	56	GLY	3.5
1	E	56	GLY	3.5
1	C	270	GLY	3.4
1	A	63	ASP	3.3
1	A	19	GLY	3.2
1	C	193	VAL	3.2
1	D	56	GLY	3.0
1	B	194	GLU	3.0
1	F	176	ASN	2.9
1	B	188	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	56	GLY	2.8
1	E	183	VAL	2.8
1	B	240	LYS	2.8
1	C	88	VAL	2.7
1	F	270	GLY	2.7
1	B	112	GLU	2.7
1	C	266	HIS	2.7
1	C	188	GLN	2.7
1	D	183	VAL	2.7
1	C	112	GLU	2.7
1	A	62	ALA	2.6
1	E	247	TYR	2.6
1	C	110	ALA	2.6
1	C	117	ASP	2.6
1	F	247	TYR	2.6
1	C	187	LYS	2.6
1	B	262	GLU	2.6
1	A	270	GLY	2.5
1	C	111	ASP	2.5
1	C	108	THR	2.5
1	A	57	GLY	2.4
1	B	46	GLU	2.4
1	C	113	GLU	2.4
1	C	190	GLY	2.4
1	E	203	GLY	2.4
1	E	245	GLU	2.4
1	C	183	VAL	2.4
1	C	140	ALA	2.4
1	D	178	SER	2.3
1	C	191	ALA	2.3
1	D	189	LEU	2.3
1	A	56	GLY	2.3
1	C	189	LEU	2.2
1	F	175	VAL	2.3
1	C	85	GLY	2.2
1	B	176	ASN	2.2
1	E	176	ASN	2.2
1	C	92	VAL	2.1
1	F	46	GLU	2.1
1	B	57	GLY	2.1
1	C	87	TYR	2.1
1	B	18	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	267	LEU	2.1
1	A	194	GLU	2.1
1	D	58	VAL	2.1
1	D	247	TYR	2.1
1	A	176	ASN	2.1
1	C	178	SER	2.0
1	B	247	TYR	2.0
1	C	194	GLU	2.0
1	D	184	ALA	2.0
1	A	188	GLN	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($\text{\AA}^2$)	Q<0.9
2	SO4	D	2408	5/5	0.86	0.16	75,75,76,77	0
3	MRD	C	2890	8/8	0.89	0.16	41,45,46,47	0
3	MRD	E	2892	8/8	0.89	0.18	42,46,50,51	0
3	MRD	F	2893	8/8	0.89	0.17	44,45,45,46	0
3	MRD	D	2891	8/8	0.90	0.15	46,47,47,49	0
2	SO4	E	2409	5/5	0.92	0.23	48,51,55,56	0
2	SO4	F	2412	5/5	0.92	0.18	60,60,61,63	0
2	SO4	E	2410	5/5	0.93	0.19	58,60,60,63	0
2	SO4	D	2407	5/5	0.94	0.17	47,50,53,53	0
2	SO4	F	2411	5/5	0.95	0.18	50,50,53,55	0
2	SO4	A	2402	5/5	0.95	0.19	36,38,38,43	0
3	MRD	A	2888	8/8	0.96	0.17	26,28,29,29	0
3	MRD	B	2889	8/8	0.96	0.16	20,22,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	2406	5/5	0.96	0.18	58,58,60,61	0
2	SO4	C	2405	5/5	0.97	0.16	35,37,40,40	0
2	SO4	B	2404	5/5	0.97	0.19	32,35,37,38	0
2	SO4	B	2403	5/5	0.98	0.15	26,32,32,34	0
2	SO4	A	2401	5/5	0.98	0.17	33,36,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.