



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 4Z7Y / pdb_00004z7y
Title : diphosphomevalonate decarboxylase from the *Sulfolobus solfataricus*, space group P21
Authors : Hattori, A.; Unno, H.; Hemmi, H.
Deposited on : 2015-04-08
Resolution : 2.70 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

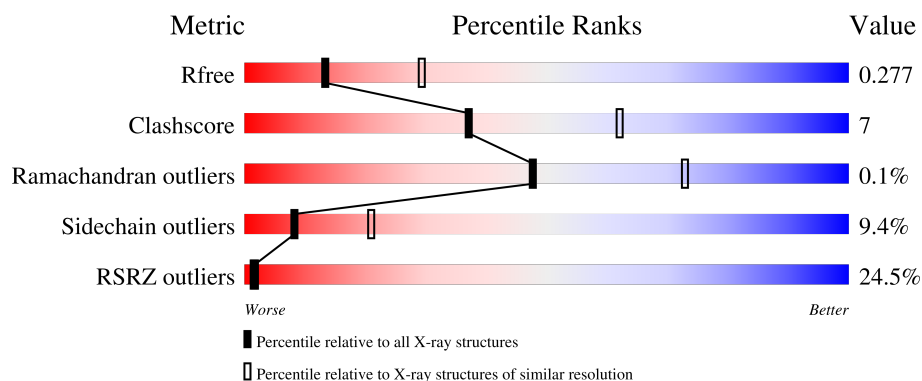
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	324	
1	B	324	
1	C	324	
1	D	324	
1	E	324	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	324	48% 80% 17%

2 Entry composition [i](#)

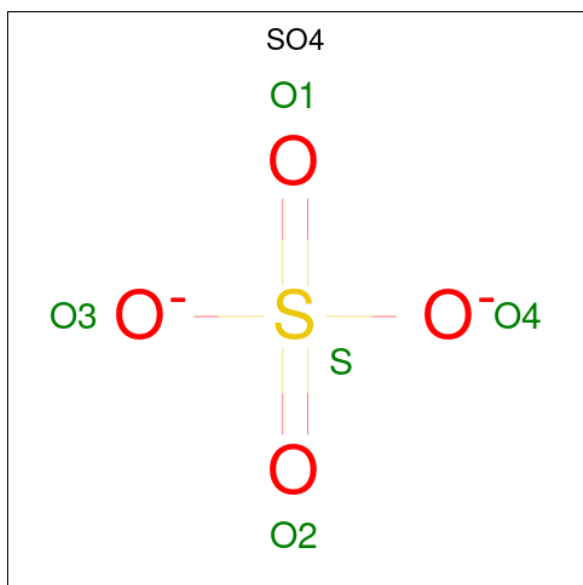
There are 3 unique types of molecules in this entry. The entry contains 15693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diphosphomevalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			
1	B	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			
1	C	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			
1	D	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			
1	E	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			
1	F	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			

- 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	B	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	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

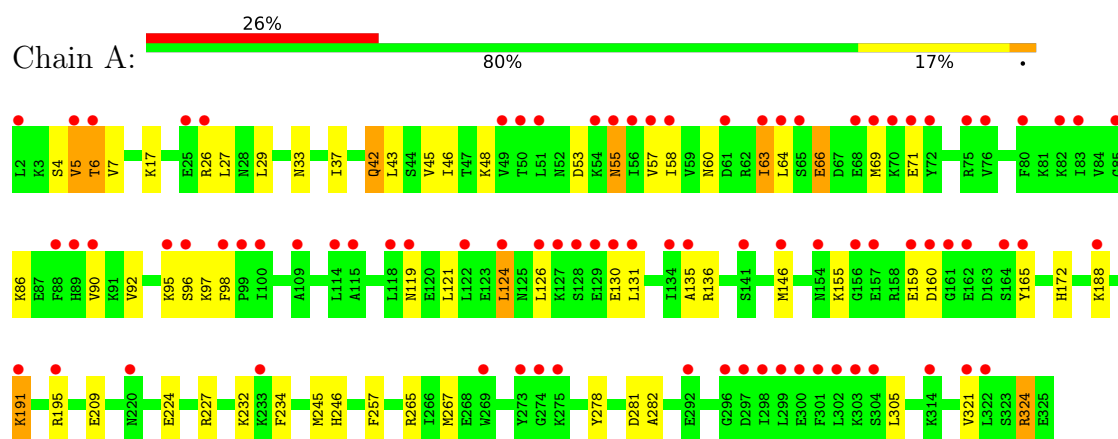
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	22	Total O 22 22	0	0
3	C	21	Total O 21 21	0	0
3	D	14	Total O 14 14	0	0
3	E	3	Total O 3 3	0	0
3	F	10	Total O 10 10	0	0

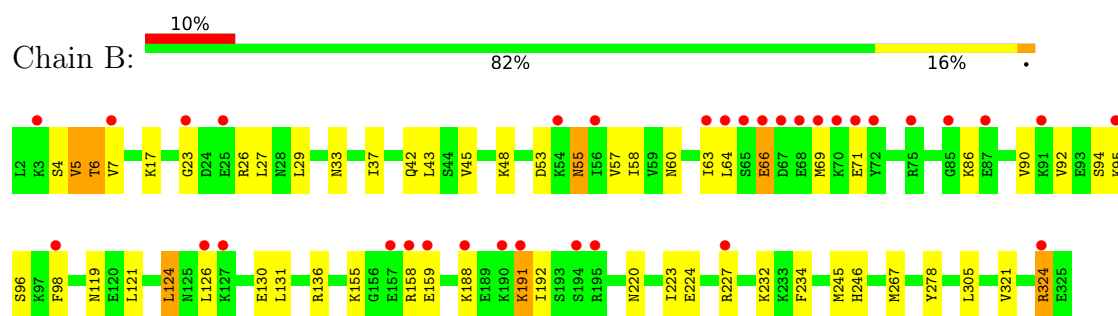
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

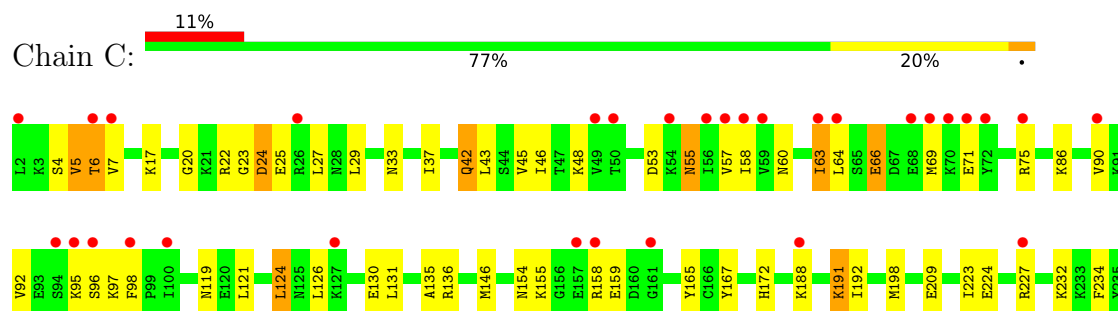
• Molecule 1: Diphosphomevalonate decarboxylase



• Molecule 1: Diphosphomevalonate decarboxylase

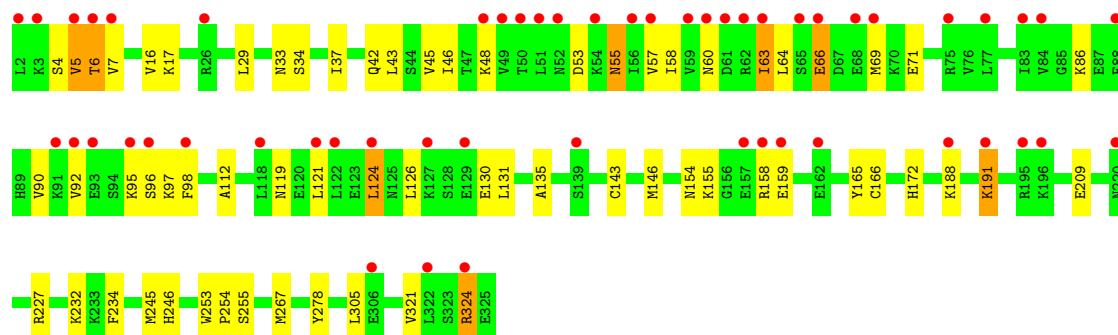
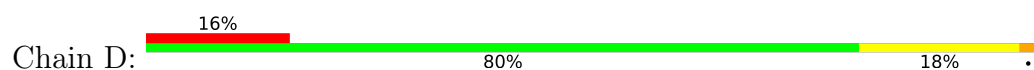


• Molecule 1: Diphosphomevalonate decarboxylase

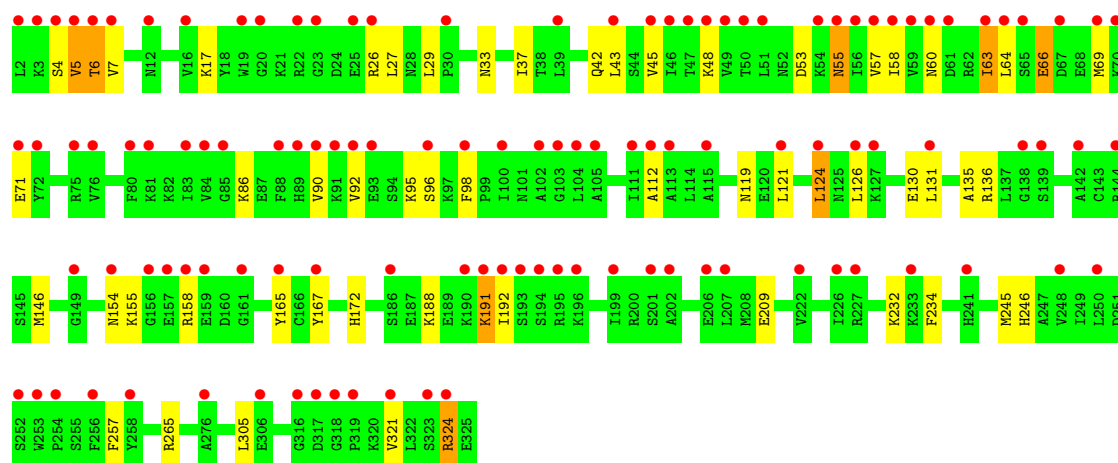
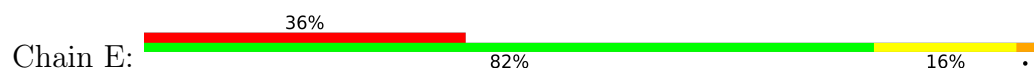




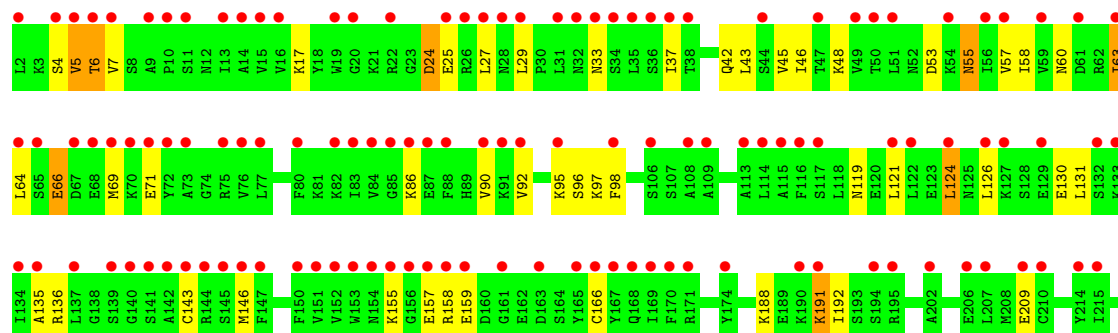
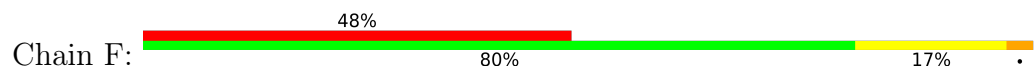
• Molecule 1: Diphosphomevalonate decarboxylase

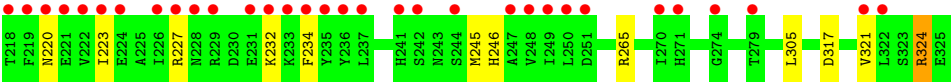


• Molecule 1: Diphosphomevalonate decarboxylase



• Molecule 1: Diphosphomevalonate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 154.39Å 109.97Å 90.00° 114.41° 90.00°	Depositor
Resolution (Å)	47.63 – 2.70 47.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.63-2.70) 98.9 (47.63-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.254 , 0.277 0.254 , 0.277	Depositor DCC
R_{free} test set	3879 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15693	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4226e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.64	0/2645	1.02	0/3558
1	B	0.68	0/2645	1.04	0/3558
1	C	0.70	0/2645	1.04	0/3558
1	D	0.65	0/2645	1.02	0/3558
1	E	0.67	0/2645	1.02	0/3558
1	F	0.67	0/2645	1.02	0/3558
All	All	0.67	0/15870	1.03	0/21348

There are no bond length outliers.

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	2597	0	2622	33	0
1	B	2597	0	2622	61	0
1	C	2597	0	2622	76	0
1	D	2597	0	2622	38	0
1	E	2597	0	2622	31	0
1	F	2597	0	2622	49	0
2	A	5	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	11	0	0	0	0
3	B	22	0	0	1	0
3	C	21	0	0	2	0
3	D	14	0	0	0	0
3	E	3	0	0	0	0
3	F	10	0	0	1	0
All	All	15693	0	15732	223	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 (223) 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:227:ARG:CZ	1:C:24:ASP:HA	1.42	1.47
1:C:227:ARG:CZ	1:F:24:ASP:HA	1.58	1.30
1:C:227:ARG:NH2	1:F:24:ASP:HA	1.57	1.19
1:B:227:ARG:NH2	1:C:24:ASP:HA	1.63	1.14
1:B:227:ARG:NH2	1:C:24:ASP:CA	2.12	1.11
1:B:227:ARG:CZ	1:C:24:ASP:CA	2.29	1.09
1:C:227:ARG:NH2	1:F:24:ASP:CA	2.17	1.07
1:B:227:ARG:NH1	1:C:24:ASP:HA	1.68	1.07
1:B:227:ARG:NH2	1:C:24:ASP:CB	2.27	0.97
1:A:165:TYR:OH	1:E:158:ARG:NH1	2.05	0.90
1:B:227:ARG:HE	1:C:24:ASP:CG	1.81	0.88
1:C:227:ARG:CZ	1:F:24:ASP:CA	2.49	0.87
1:B:227:ARG:NE	1:C:24:ASP:CG	2.33	0.87
1:B:159:GLU:HG3	1:F:223:ILE:HD12	1.58	0.86
1:B:227:ARG:NE	1:C:24:ASP:OD1	2.08	0.86
1:C:33:ASN:ND2	1:C:155:LYS:H	1.75	0.85
1:A:33:ASN:ND2	1:A:155:LYS:H	1.76	0.83
1:F:33:ASN:HD22	1:F:155:LYS:H	1.27	0.83
1:B:33:ASN:HD22	1:B:155:LYS:H	1.25	0.82
1:C:33:ASN:HD22	1:C:155:LYS:H	1.25	0.82
1:C:75:ARG:NH1	3:C:502:HOH:O	2.07	0.81
1:B:33:ASN:ND2	1:B:155:LYS:H	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:HD22	1:A:155:LYS:H	1.24	0.81
1:F:33:ASN:ND2	1:F:155:LYS:H	1.78	0.81
1:F:227:ARG:NH2	3:F:501:HOH:O	2.14	0.81
1:E:33:ASN:HD22	1:E:155:LYS:H	1.26	0.81
1:E:33:ASN:ND2	1:E:155:LYS:H	1.80	0.79
1:D:33:ASN:HD22	1:D:155:LYS:H	1.30	0.78
1:C:227:ARG:NH2	1:F:24:ASP:CB	2.47	0.77
1:D:33:ASN:ND2	1:D:155:LYS:H	1.82	0.77
1:D:159:GLU:HB2	1:E:167:TYR:OH	1.86	0.74
1:C:227:ARG:NH1	1:F:24:ASP:HA	2.02	0.73
1:D:158:ARG:HD3	1:E:165:TYR:OH	1.89	0.72
1:B:223:ILE:HG22	1:B:227:ARG:HH22	1.52	0.72
1:A:26:ARG:NH2	1:D:227:ARG:HH21	1.90	0.70
1:B:26:ARG:HH22	1:F:227:ARG:HD3	1.56	0.69
1:B:227:ARG:HH21	1:C:24:ASP:CB	2.05	0.68
1:C:227:ARG:HE	1:F:24:ASP:CG	2.03	0.66
1:A:159:GLU:H	1:D:154:ASN:HD21	1.43	0.66
1:D:17:LYS:HG2	1:D:245:MET:SD	2.37	0.65
1:B:227:ARG:NH2	1:C:24:ASP:HB2	2.09	0.64
1:B:223:ILE:HG22	1:B:227:ARG:NH2	2.12	0.64
1:B:224:GLU:CD	1:C:25:GLU:HG3	2.23	0.64
1:C:154:ASN:ND2	1:F:157:GLU:OE1	2.31	0.64
1:A:17:LYS:HG2	1:A:245:MET:SD	2.38	0.63
1:B:227:ARG:CZ	1:C:24:ASP:CG	2.72	0.63
1:C:223:ILE:HG22	1:C:227:ARG:HH22	1.62	0.63
1:B:224:GLU:OE2	1:B:227:ARG:NH1	2.34	0.60
1:B:224:GLU:OE2	1:C:25:GLU:HG3	2.02	0.59
1:B:227:ARG:NH2	1:C:24:ASP:CG	2.60	0.59
1:B:23:GLY:HA2	1:F:220:ASN:HD22	1.68	0.59
1:C:223:ILE:HG22	1:C:227:ARG:NH2	2.18	0.59
1:C:227:ARG:HH21	1:F:24:ASP:CB	2.14	0.59
1:C:227:ARG:NE	1:F:24:ASP:CG	2.61	0.58
1:E:42:GLN:HA	1:E:98:PHE:CD1	2.39	0.58
1:C:165:TYR:OH	1:F:158:ARG:NE	2.37	0.58
1:C:268:GLU:OE2	1:D:191:LYS:NZ	2.37	0.57
1:D:57:VAL:HG12	1:D:69:MET:HG3	1.87	0.56
1:F:42:GLN:HA	1:F:98:PHE:CD1	2.40	0.55
1:A:165:TYR:CZ	1:E:158:ARG:NH1	2.75	0.55
1:B:42:GLN:HA	1:B:98:PHE:CD1	2.42	0.55
1:B:159:GLU:HG3	1:F:223:ILE:CD1	2.33	0.55
1:E:57:VAL:HG12	1:E:69:MET:HG3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ASN:HB2	1:F:131:LEU:HD21	1.89	0.54
1:F:143:CYS:HG	1:F:166:CYS:HG	1.54	0.54
1:B:159:GLU:OE1	1:F:220:ASN:CB	2.55	0.54
1:C:245:MET:HE2	1:C:246:HIS:CE1	2.43	0.54
1:A:6:THR:HG22	1:A:48:LYS:HG3	1.89	0.54
1:D:42:GLN:HA	1:D:98:PHE:CD1	2.43	0.54
1:B:227:ARG:CZ	1:B:227:ARG:CB	2.86	0.53
1:D:158:ARG:HD3	1:E:165:TYR:HH	1.73	0.53
1:C:227:ARG:NE	1:F:24:ASP:OD1	2.41	0.53
1:C:158:ARG:NH1	3:C:501:HOH:O	1.97	0.53
1:B:158:ARG:HD3	3:B:501:HOH:O	2.07	0.53
1:C:42:GLN:HA	1:C:98:PHE:CD1	2.44	0.53
1:B:60:ASN:HD21	1:B:96:SER:H	1.58	0.52
1:F:57:VAL:HG12	1:F:69:MET:HG3	1.92	0.52
1:D:55:ASN:ND2	1:D:90:VAL:H	2.07	0.52
1:B:227:ARG:HH21	1:C:24:ASP:HB2	1.70	0.52
1:C:57:VAL:HG12	1:C:69:MET:HG3	1.91	0.52
1:D:60:ASN:HD21	1:D:96:SER:H	1.58	0.52
1:D:6:THR:HG22	1:D:48:LYS:HG3	1.92	0.51
1:F:6:THR:HG22	1:F:48:LYS:HG3	1.90	0.51
1:A:57:VAL:HG12	1:A:69:MET:HG3	1.91	0.51
1:B:223:ILE:HD11	1:C:159:GLU:HG3	1.92	0.51
1:C:66:GLU:O	1:C:66:GLU:HG2	2.11	0.51
1:C:17:LYS:HG2	1:C:245:MET:SD	2.50	0.51
1:D:66:GLU:O	1:D:66:GLU:HG2	2.08	0.51
1:E:6:THR:HG22	1:E:48:LYS:HG3	1.91	0.51
1:A:165:TYR:CE2	1:E:158:ARG:NH1	2.79	0.51
1:B:66:GLU:O	1:B:66:GLU:HG2	2.11	0.51
1:B:159:GLU:CD	1:F:220:ASN:HB3	2.34	0.51
1:B:55:ASN:ND2	1:B:90:VAL:H	2.09	0.50
1:B:57:VAL:HG12	1:B:69:MET:HG3	1.92	0.50
1:C:55:ASN:ND2	1:C:90:VAL:H	2.08	0.50
1:B:159:GLU:CG	1:F:223:ILE:HD12	2.38	0.50
1:B:227:ARG:HH21	1:C:24:ASP:CG	2.18	0.50
1:C:20:GLY:H	1:C:198:MET:HG2	1.77	0.50
1:A:42:GLN:HA	1:A:98:PHE:CD1	2.46	0.50
1:A:55:ASN:ND2	1:A:90:VAL:H	2.09	0.50
1:C:224:GLU:OE2	1:C:227:ARG:NH1	2.44	0.50
1:C:224:GLU:OE2	1:F:25:GLU:HG3	2.10	0.50
1:B:227:ARG:CZ	1:B:227:ARG:HB2	2.40	0.50
1:F:55:ASN:ND2	1:F:90:VAL:H	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:HG2	1:B:245:MET:SD	2.52	0.49
1:C:172:HIS:HB3	2:C:401:SO4:O3	2.12	0.49
1:F:66:GLU:O	1:F:66:GLU:HG2	2.12	0.49
1:E:27:LEU:O	1:E:136:ARG:NH1	2.44	0.49
1:E:37:ILE:HD11	1:E:234:PHE:HZ	1.76	0.49
1:E:66:GLU:O	1:E:66:GLU:HG2	2.11	0.49
1:E:17:LYS:HG2	1:E:245:MET:SD	2.52	0.49
1:C:243:ASN:ND2	1:D:255:SER:HB2	2.27	0.49
1:A:66:GLU:O	1:A:66:GLU:HG2	2.11	0.49
1:F:60:ASN:HD21	1:F:96:SER:H	1.60	0.49
1:B:224:GLU:HA	1:B:227:ARG:NH1	2.28	0.49
1:E:60:ASN:HD21	1:E:96:SER:H	1.61	0.49
1:E:55:ASN:ND2	1:E:90:VAL:H	2.11	0.48
1:A:245:MET:HE2	1:A:246:HIS:CE1	2.48	0.48
1:F:37:ILE:HD11	1:F:234:PHE:HZ	1.79	0.48
1:B:159:GLU:OE1	1:F:220:ASN:HB3	2.13	0.48
1:B:191:LYS:HD2	1:B:192:ILE:N	2.29	0.48
1:C:33:ASN:HD22	1:C:155:LYS:N	2.04	0.47
1:D:57:VAL:HG23	1:D:92:VAL:HB	1.96	0.47
1:A:5:VAL:HG12	1:A:324:ARG:HB3	1.96	0.47
1:B:6:THR:HG22	1:B:48:LYS:HG3	1.95	0.47
1:F:124:LEU:HB3	1:F:126:LEU:HG	1.96	0.47
1:C:60:ASN:HD21	1:C:96:SER:H	1.62	0.47
1:A:60:ASN:HD21	1:A:96:SER:H	1.61	0.47
1:A:159:GLU:HG2	1:D:154:ASN:ND2	2.29	0.47
1:B:245:MET:HE2	1:B:246:HIS:CE1	2.49	0.47
1:A:119:ASN:HB2	1:A:131:LEU:HD21	1.95	0.47
1:C:46:ILE:HD11	1:C:97:LYS:HG3	1.96	0.47
1:F:17:LYS:HG2	1:F:245:MET:SD	2.55	0.47
1:A:172:HIS:ND1	2:A:401:SO4:O2	2.44	0.47
1:D:172:HIS:HB3	2:D:401:SO4:O1	2.14	0.47
1:E:63:ILE:H	1:E:63:ILE:HG13	1.58	0.47
1:B:37:ILE:HD11	1:B:234:PHE:HZ	1.79	0.46
1:B:227:ARG:CZ	1:C:24:ASP:CB	2.82	0.46
1:C:267:MET:HG2	1:C:278:TYR:CE1	2.50	0.46
1:D:37:ILE:HD11	1:D:234:PHE:HZ	1.81	0.46
1:A:267:MET:HG2	1:A:278:TYR:CE1	2.51	0.46
1:B:223:ILE:CD1	1:C:159:GLU:HG3	2.46	0.46
1:C:227:ARG:CZ	1:C:227:ARG:CB	2.92	0.46
1:C:227:ARG:NH2	1:F:24:ASP:HB2	2.30	0.46
1:C:57:VAL:HG23	1:C:92:VAL:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:HB3	1:A:126:LEU:HG	1.98	0.46
1:B:220:ASN:HB2	1:C:23:GLY:H	1.80	0.46
1:A:227:ARG:NH2	1:E:26:ARG:HH22	2.14	0.46
1:B:119:ASN:HB2	1:B:131:LEU:HD21	1.96	0.46
1:C:119:ASN:HB2	1:C:131:LEU:HD21	1.98	0.46
1:C:124:LEU:HB3	1:C:126:LEU:HG	1.97	0.46
1:F:317:ASP:HA	2:F:401:SO4:O4	2.16	0.46
1:B:224:GLU:HG2	1:C:23:GLY:O	2.16	0.46
1:C:27:LEU:O	1:C:136:ARG:NH1	2.43	0.45
1:F:57:VAL:HG23	1:F:92:VAL:HB	1.97	0.45
1:C:6:THR:HG22	1:C:48:LYS:HG3	1.98	0.45
1:D:46:ILE:HD11	1:D:97:LYS:HG3	1.98	0.45
1:A:27:LEU:O	1:A:136:ARG:NH1	2.45	0.45
1:F:5:VAL:HG12	1:F:324:ARG:HB3	1.97	0.45
1:D:119:ASN:HB2	1:D:131:LEU:HD21	1.97	0.45
1:F:191:LYS:HD2	1:F:192:ILE:N	2.32	0.45
1:A:159:GLU:H	1:D:154:ASN:ND2	2.10	0.45
1:B:57:VAL:HG23	1:B:92:VAL:HB	1.99	0.45
1:C:227:ARG:HH21	1:F:24:ASP:HB2	1.79	0.45
1:B:159:GLU:OE1	1:F:220:ASN:HB2	2.15	0.45
1:B:159:GLU:CD	1:F:220:ASN:CB	2.90	0.45
1:E:5:VAL:HG12	1:E:324:ARG:HB3	1.98	0.45
1:B:124:LEU:HB3	1:B:126:LEU:HG	1.99	0.45
1:F:63:ILE:H	1:F:63:ILE:HG13	1.58	0.45
1:C:5:VAL:HG12	1:C:324:ARG:HB3	1.99	0.44
1:C:191:LYS:HD2	1:C:192:ILE:N	2.31	0.44
1:A:37:ILE:HD11	1:A:234:PHE:HZ	1.83	0.44
1:A:57:VAL:HG23	1:A:92:VAL:HB	1.99	0.44
1:D:5:VAL:HG12	1:D:324:ARG:HB3	1.99	0.44
1:E:57:VAL:HG23	1:E:92:VAL:HB	2.00	0.44
1:C:37:ILE:HD11	1:C:234:PHE:HZ	1.83	0.44
1:D:112:ALA:HA	1:D:146:MET:HE1	2.00	0.44
1:E:124:LEU:HB3	1:E:126:LEU:HG	1.98	0.44
1:C:167:TYR:OH	1:F:159:GLU:HG2	2.18	0.44
1:D:63:ILE:H	1:D:63:ILE:HG13	1.58	0.44
1:E:191:LYS:NZ	1:E:257:PHE:H	2.16	0.44
1:D:267:MET:HG2	1:D:278:TYR:CE1	2.53	0.44
1:E:119:ASN:HB2	1:E:131:LEU:HD21	2.00	0.43
1:E:172:HIS:HB3	2:E:401:SO4:O2	2.18	0.43
1:C:236:TYR:HE1	1:D:253:TRP:CD1	2.36	0.43
1:E:245:MET:HE2	1:E:246:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:HD22	1:B:155:LYS:N	2.05	0.43
1:D:135:ALA:HB2	1:D:146:MET:HE3	2.01	0.43
1:B:55:ASN:HD22	1:B:55:ASN:HA	1.67	0.43
1:A:135:ALA:HB2	1:A:146:MET:HE3	2.01	0.43
1:D:124:LEU:HB3	1:D:126:LEU:HG	2.01	0.43
1:C:63:ILE:H	1:C:63:ILE:HG13	1.59	0.42
1:A:160:ASP:CG	1:D:165:TYR:HH	2.26	0.42
1:B:5:VAL:HG12	1:B:324:ARG:HB3	2.01	0.42
1:D:55:ASN:HD22	1:D:55:ASN:HA	1.66	0.42
1:D:159:GLU:HG2	1:E:154:ASN:HD22	1.84	0.42
1:A:46:ILE:HD11	1:A:97:LYS:HG3	2.02	0.42
1:A:281:ASP:HB3	1:A:282:ALA:H	1.70	0.42
1:B:227:ARG:NH2	1:C:24:ASP:N	2.65	0.42
1:C:97:LYS:HD3	1:C:98:PHE:CE1	2.55	0.42
1:C:227:ARG:CZ	1:C:227:ARG:HB2	2.48	0.42
1:F:245:MET:HE2	1:F:246:HIS:CE1	2.55	0.42
1:D:253:TRP:CD2	1:D:254:PRO:HA	2.54	0.42
1:E:135:ALA:HB2	1:E:146:MET:HE3	2.02	0.42
1:F:27:LEU:O	1:F:136:ARG:NH1	2.45	0.42
1:A:63:ILE:H	1:A:63:ILE:HG13	1.56	0.42
1:C:135:ALA:HB2	1:C:146:MET:HE3	2.02	0.42
1:D:245:MET:HE2	1:D:246:HIS:CE1	2.54	0.42
1:B:267:MET:HG2	1:B:278:TYR:CE1	2.55	0.42
1:E:33:ASN:HD22	1:E:155:LYS:N	2.06	0.42
1:B:191:LYS:HD2	1:B:192:ILE:H	1.85	0.41
1:E:191:LYS:HD2	1:E:192:ILE:N	2.36	0.41
1:B:27:LEU:O	1:B:136:ARG:NH1	2.48	0.41
1:F:46:ILE:HD11	1:F:97:LYS:HG3	2.02	0.41
1:A:191:LYS:NZ	1:A:257:PHE:H	2.18	0.41
1:C:267:MET:HG2	1:C:278:TYR:CZ	2.56	0.41
1:E:112:ALA:HA	1:E:146:MET:HE1	2.02	0.41
1:A:224:GLU:OE2	1:A:227:ARG:NH1	2.54	0.41
1:C:22:ARG:NH2	1:C:155:LYS:O	2.53	0.40
1:D:143:CYS:HG	1:D:166:CYS:HG	1.62	0.40
1:F:135:ALA:HB2	1:F:146:MET:HE3	2.03	0.40
1:D:16:VAL:O	1:D:34:SER:HB2	2.22	0.40
1:D:97:LYS:HD3	1:D:98:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	322/324 (99%)	314 (98%)	8 (2%)	0	100	100
1	B	322/324 (99%)	315 (98%)	7 (2%)	0	100	100
1	C	322/324 (99%)	314 (98%)	7 (2%)	1 (0%)	36	60
1	D	322/324 (99%)	315 (98%)	7 (2%)	0	100	100
1	E	322/324 (99%)	314 (98%)	8 (2%)	0	100	100
1	F	322/324 (99%)	314 (98%)	7 (2%)	1 (0%)	36	60
All	All	1932/1944 (99%)	1886 (98%)	44 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24	ASP
1	F	24	ASP

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	288/288 (100%)	259 (90%)	29 (10%)	7	18
1	B	288/288 (100%)	262 (91%)	26 (9%)	9	23
1	C	288/288 (100%)	260 (90%)	28 (10%)	8	20
1	D	288/288 (100%)	262 (91%)	26 (9%)	9	23
1	E	288/288 (100%)	261 (91%)	27 (9%)	8	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	288/288 (100%)	261 (91%)	27 (9%)	8	21
All	All	1728/1728 (100%)	1565 (91%)	163 (9%)	8	21

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	5	VAL
1	A	6	THR
1	A	7	VAL
1	A	29	LEU
1	A	42	GLN
1	A	43	LEU
1	A	45	VAL
1	A	53	ASP
1	A	55	ASN
1	A	58	ILE
1	A	63	ILE
1	A	64	LEU
1	A	66	GLU
1	A	71	GLU
1	A	86	LYS
1	A	95	LYS
1	A	121	LEU
1	A	124	LEU
1	A	130	GLU
1	A	188	LYS
1	A	191	LYS
1	A	195	ARG
1	A	209	GLU
1	A	232	LYS
1	A	265	ARG
1	A	305	LEU
1	A	321	VAL
1	A	324	ARG
1	B	4	SER
1	B	5	VAL
1	B	6	THR
1	B	7	VAL
1	B	29	LEU
1	B	43	LEU
1	B	45	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	53	ASP
1	B	55	ASN
1	B	58	ILE
1	B	63	ILE
1	B	64	LEU
1	B	66	GLU
1	B	71	GLU
1	B	86	LYS
1	B	94	SER
1	B	95	LYS
1	B	121	LEU
1	B	124	LEU
1	B	130	GLU
1	B	188	LYS
1	B	191	LYS
1	B	232	LYS
1	B	305	LEU
1	B	321	VAL
1	B	324	ARG
1	C	4	SER
1	C	5	VAL
1	C	6	THR
1	C	7	VAL
1	C	29	LEU
1	C	42	GLN
1	C	43	LEU
1	C	45	VAL
1	C	53	ASP
1	C	55	ASN
1	C	58	ILE
1	C	63	ILE
1	C	64	LEU
1	C	66	GLU
1	C	71	GLU
1	C	86	LYS
1	C	95	LYS
1	C	121	LEU
1	C	124	LEU
1	C	130	GLU
1	C	188	LYS
1	C	191	LYS
1	C	209	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	232	LYS
1	C	265	ARG
1	C	305	LEU
1	C	321	VAL
1	C	324	ARG
1	D	4	SER
1	D	5	VAL
1	D	6	THR
1	D	7	VAL
1	D	29	LEU
1	D	43	LEU
1	D	45	VAL
1	D	53	ASP
1	D	55	ASN
1	D	58	ILE
1	D	63	ILE
1	D	64	LEU
1	D	66	GLU
1	D	71	GLU
1	D	86	LYS
1	D	95	LYS
1	D	121	LEU
1	D	124	LEU
1	D	130	GLU
1	D	188	LYS
1	D	191	LYS
1	D	209	GLU
1	D	232	LYS
1	D	305	LEU
1	D	321	VAL
1	D	324	ARG
1	E	4	SER
1	E	5	VAL
1	E	6	THR
1	E	7	VAL
1	E	29	LEU
1	E	43	LEU
1	E	45	VAL
1	E	53	ASP
1	E	55	ASN
1	E	58	ILE
1	E	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	64	LEU
1	E	66	GLU
1	E	71	GLU
1	E	86	LYS
1	E	95	LYS
1	E	121	LEU
1	E	124	LEU
1	E	130	GLU
1	E	188	LYS
1	E	191	LYS
1	E	209	GLU
1	E	232	LYS
1	E	265	ARG
1	E	305	LEU
1	E	321	VAL
1	E	324	ARG
1	F	4	SER
1	F	5	VAL
1	F	6	THR
1	F	7	VAL
1	F	29	LEU
1	F	43	LEU
1	F	45	VAL
1	F	53	ASP
1	F	55	ASN
1	F	58	ILE
1	F	63	ILE
1	F	64	LEU
1	F	66	GLU
1	F	71	GLU
1	F	86	LYS
1	F	95	LYS
1	F	121	LEU
1	F	124	LEU
1	F	130	GLU
1	F	188	LYS
1	F	191	LYS
1	F	209	GLU
1	F	232	LYS
1	F	265	ARG
1	F	305	LEU
1	F	321	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	324	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	ASN
1	A	55	ASN
1	A	60	ASN
1	A	89	HIS
1	A	154	ASN
1	A	246	HIS
1	B	28	ASN
1	B	33	ASN
1	B	55	ASN
1	B	60	ASN
1	B	89	HIS
1	B	154	ASN
1	B	246	HIS
1	C	28	ASN
1	C	33	ASN
1	C	55	ASN
1	C	60	ASN
1	C	89	HIS
1	C	220	ASN
1	C	246	HIS
1	C	271	HIS
1	D	28	ASN
1	D	33	ASN
1	D	55	ASN
1	D	60	ASN
1	D	89	HIS
1	D	154	ASN
1	D	246	HIS
1	D	271	HIS
1	E	28	ASN
1	E	33	ASN
1	E	55	ASN
1	E	60	ASN
1	E	89	HIS
1	E	154	ASN
1	E	220	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	246	HIS
1	F	28	ASN
1	F	33	ASN
1	F	55	ASN
1	F	60	ASN
1	F	89	HIS
1	F	154	ASN
1	F	220	ASN
1	F	246	HIS
1	F	271	HIS

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 ⓘ

6 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	$\# Z > 2$
2	SO4	E	401	-	4,4,4	0.49	0	6,6,6	0.30	0
2	SO4	A	401	-	4,4,4	0.47	0	6,6,6	0.83	0
2	SO4	D	401	-	4,4,4	0.36	0	6,6,6	0.54	0
2	SO4	B	401	-	4,4,4	0.59	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	401	-	4,4,4	0.49	0	6,6,6	0.13	0
2	SO4	F	401	-	4,4,4	0.51	0	6,6,6	0.32	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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	SO4	1	0
2	A	401	SO4	1	0
2	D	401	SO4	1	0
2	C	401	SO4	1	0
2	F	401	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, 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	324/324 (100%)	1.35	84 (25%) 1 1	20, 59, 134, 162	0
1	B	324/324 (100%)	0.59	34 (10%) 11 9	21, 44, 98, 151	0
1	C	324/324 (100%)	0.85	35 (10%) 11 9	20, 46, 102, 148	0
1	D	324/324 (100%)	0.86	53 (16%) 4 4	22, 50, 109, 137	0
1	E	324/324 (100%)	1.78	116 (35%) 1 0	33, 61, 133, 167	0
1	F	324/324 (100%)	2.06	155 (47%) 0 0	29, 64, 124, 177	0
All	All	1944/1944 (100%)	1.25	477 (24%) 2 1	20, 54, 120, 177	0

All (477) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	8.5
1	E	56	ILE	7.4
1	F	135	ALA	6.6
1	F	141	SER	6.4
1	E	72	TYR	6.4
1	F	139	SER	6.0
1	F	72	TYR	5.8
1	F	220	ASN	5.8
1	F	233	LYS	5.6
1	F	222	VAL	5.3
1	A	71	GLU	5.3
1	A	303	LYS	5.2
1	F	227	ARG	5.2
1	A	297	ASP	5.2
1	E	92	VAL	5.2
1	A	165	TYR	5.0
1	E	207	LEU	4.9
1	A	273	TYR	4.9
1	A	299	LEU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	142	ALA	4.8
1	A	68	GLU	4.8
1	F	92	VAL	4.7
1	F	165	TYR	4.7
1	C	71	GLU	4.7
1	E	63	ILE	4.6
1	E	98	PHE	4.6
1	B	63	ILE	4.6
1	A	296	GLY	4.6
1	A	70	LYS	4.6
1	A	80	PHE	4.6
1	F	143	CYS	4.5
1	B	190	LYS	4.5
1	F	64	LEU	4.5
1	E	47	THR	4.5
1	E	64	LEU	4.5
1	E	96	SER	4.4
1	F	35	LEU	4.4
1	F	56	ILE	4.4
1	E	2	LEU	4.4
1	E	111	ILE	4.4
1	F	63	ILE	4.3
1	E	58	ILE	4.2
1	F	215	ILE	4.2
1	A	72	TYR	4.2
1	D	68	GLU	4.2
1	C	56	ILE	4.2
1	E	75	ARG	4.2
1	F	157	GLU	4.1
1	D	127	LYS	4.1
1	A	98	PHE	4.1
1	C	72	TYR	4.1
1	A	159	GLU	4.1
1	F	154	ASN	4.1
1	E	319	PRO	4.1
1	A	162	GLU	4.1
1	F	221	GLU	4.1
1	E	316	GLY	4.1
1	C	100	ILE	4.0
1	A	154	ASN	4.0
1	F	5	VAL	4.0
1	D	191	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	190	LYS	4.0
1	A	161	GLY	4.0
1	E	3	LYS	4.0
1	F	33	ASN	4.0
1	A	129	GLU	3.9
1	C	75	ARG	3.9
1	D	56	ILE	3.9
1	E	90	VAL	3.9
1	E	201	SER	3.9
1	F	129	GLU	3.9
1	B	227	ARG	3.9
1	B	127	LYS	3.9
1	F	153	TRP	3.9
1	F	218	THR	3.8
1	A	302	LEU	3.8
1	F	36	SER	3.8
1	F	151	VAL	3.8
1	A	269	TRP	3.8
1	F	122	LEU	3.8
1	E	4	SER	3.8
1	F	274	GLY	3.8
1	A	301	PHE	3.8
1	D	2	LEU	3.7
1	F	190	LYS	3.7
1	F	170	PHE	3.7
1	F	19	TRP	3.7
1	F	114	LEU	3.7
1	E	318	GLY	3.7
1	F	75	ARG	3.7
1	E	88	PHE	3.7
1	A	63	ILE	3.7
1	A	100	ILE	3.7
1	E	253	TRP	3.7
1	A	127	LYS	3.7
1	F	166	CYS	3.7
1	E	50	THR	3.6
1	F	73	ALA	3.6
1	F	113	ALA	3.6
1	E	186	SER	3.6
1	E	194	SER	3.6
1	E	70	LYS	3.6
1	E	159	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	70	LYS	3.6
1	D	5	VAL	3.5
1	F	235	TYR	3.5
1	A	88	PHE	3.5
1	E	84	VAL	3.5
1	F	223	ILE	3.5
1	A	156	GLY	3.5
1	E	105	ALA	3.5
1	F	115	ALA	3.5
1	A	130	GLU	3.5
1	A	49	VAL	3.5
1	F	84	VAL	3.5
1	A	56	ILE	3.5
1	A	164	SER	3.5
1	F	34	SER	3.5
1	B	191	LYS	3.5
1	F	27	LEU	3.5
1	F	80	PHE	3.4
1	D	7	VAL	3.4
1	F	65	SER	3.4
1	F	232	LYS	3.4
1	C	68	GLU	3.4
1	F	219	PHE	3.4
1	E	57	VAL	3.4
1	C	58	ILE	3.4
1	D	63	ILE	3.4
1	E	323	SER	3.4
1	A	25	GLU	3.4
1	E	206	GLU	3.4
1	E	5	VAL	3.4
1	D	6	THR	3.3
1	D	51	LEU	3.3
1	D	121	LEU	3.3
1	F	124	LEU	3.3
1	F	241	HIS	3.3
1	F	150	PHE	3.3
1	F	145	SER	3.3
1	D	306	GLU	3.3
1	E	103	GLY	3.3
1	A	188	LYS	3.3
1	B	188	LYS	3.3
1	D	139	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	127	LYS	3.3
1	F	15	VAL	3.3
1	F	161	GLY	3.3
1	F	109	ALA	3.3
1	A	5	VAL	3.3
1	F	147	PHE	3.3
1	F	195	ARG	3.2
1	A	314	LYS	3.2
1	F	271	HIS	3.2
1	E	127	LYS	3.2
1	F	207	LEU	3.2
1	F	47	THR	3.2
1	F	167	TYR	3.2
1	F	22	ARG	3.2
1	D	157	GLU	3.2
1	F	152	VAL	3.2
1	E	100	ILE	3.1
1	F	169	ILE	3.1
1	F	242	SER	3.1
1	E	80	PHE	3.1
1	C	69	MET	3.1
1	F	159	GLU	3.1
1	E	156	GLY	3.1
1	E	60	ASN	3.1
1	A	6	THR	3.1
1	E	23	GLY	3.1
1	A	90	VAL	3.1
1	C	158	ARG	3.1
1	F	90	VAL	3.1
1	D	92	VAL	3.1
1	D	65	SER	3.1
1	A	124	LEU	3.0
1	A	157	GLU	3.0
1	C	127	LYS	3.0
1	F	156	GLY	3.0
1	E	45	VAL	3.0
1	F	77	LEU	3.0
1	D	188	LYS	3.0
1	C	63	ILE	3.0
1	F	88	PHE	3.0
1	E	112	ALA	3.0
1	F	9	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	64	LEU	3.0
1	E	306	GLU	3.0
1	C	98	PHE	3.0
1	E	51	LEU	2.9
1	F	51	LEU	2.9
1	D	3	LYS	2.9
1	A	26	ARG	2.9
1	B	23	GLY	2.9
1	E	6	THR	2.9
1	F	14	ALA	2.9
1	D	57	VAL	2.9
1	B	91	LYS	2.9
1	F	270	ILE	2.9
1	A	76	VAL	2.9
1	A	122	LEU	2.9
1	E	104	LEU	2.9
1	F	126	LEU	2.9
1	A	233	LYS	2.9
1	E	193	SER	2.9
1	E	195	ARG	2.9
1	F	85	GLY	2.9
1	A	191	LYS	2.9
1	D	159	GLU	2.9
1	F	26	ARG	2.9
1	D	60	ASN	2.9
1	A	82	LYS	2.9
1	F	248	VAL	2.9
1	F	146	MET	2.8
1	E	91	LYS	2.8
1	E	165	TYR	2.8
1	F	174	TYR	2.8
1	C	324	ARG	2.8
1	D	158	ARG	2.8
1	E	30	PRO	2.8
1	C	188	LYS	2.8
1	F	134	ILE	2.8
1	F	32	ASN	2.8
1	A	61	ASP	2.8
1	A	160	ASP	2.8
1	B	157	GLU	2.8
1	E	59	VAL	2.8
1	D	69	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	256	PHE	2.8
1	D	75	ARG	2.8
1	C	57	VAL	2.8
1	C	95	LYS	2.7
1	F	155	LYS	2.7
1	D	322	LEU	2.7
1	E	202	ALA	2.7
1	F	95	LYS	2.7
1	A	322	LEU	2.7
1	C	2	LEU	2.7
1	A	55	ASN	2.7
1	E	69	MET	2.7
1	F	140	GLY	2.7
1	D	162	GLU	2.7
1	E	157	GLU	2.7
1	F	224	GLU	2.7
1	F	50	THR	2.7
1	F	116	PHE	2.7
1	A	99	PRO	2.7
1	A	128	SER	2.7
1	C	59	VAL	2.7
1	E	16	VAL	2.7
1	E	192	ILE	2.7
1	F	158	ARG	2.7
1	A	304	SER	2.7
1	E	54	LYS	2.7
1	F	49	VAL	2.7
1	E	61	ASP	2.7
1	F	137	LEU	2.6
1	D	88	PHE	2.6
1	E	67	ASP	2.6
1	F	236	TYR	2.6
1	E	126	LEU	2.6
1	F	31	LEU	2.6
1	A	95	LYS	2.6
1	F	68	GLU	2.6
1	E	131	LEU	2.6
1	F	144	ARG	2.6
1	D	95	LYS	2.6
1	E	196	LYS	2.6
1	C	7	VAL	2.6
1	E	142	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	168	GLN	2.6
1	F	226	ILE	2.6
1	A	75	ARG	2.6
1	E	158	ARG	2.6
1	E	85	GLY	2.6
1	F	20	GLY	2.6
1	F	16	VAL	2.6
1	E	154	ASN	2.6
1	A	83	ILE	2.5
1	E	43	LEU	2.5
1	C	309	ARG	2.5
1	C	157	GLU	2.5
1	D	84	VAL	2.5
1	B	67	ASP	2.5
1	B	158	ARG	2.5
1	C	227	ARG	2.5
1	E	48	LYS	2.5
1	F	2	LEU	2.5
1	F	237	LEU	2.5
1	B	25	GLU	2.5
1	F	25	GLU	2.5
1	F	209	GLU	2.5
1	A	85	GLY	2.5
1	E	102	ALA	2.5
1	E	12	ASN	2.5
1	F	244	SER	2.5
1	E	191	LYS	2.5
1	B	64	LEU	2.5
1	B	66	GLU	2.5
1	B	159	GLU	2.5
1	E	71	GLU	2.5
1	A	274	GLY	2.5
1	F	59	VAL	2.5
1	F	69	MET	2.5
1	A	2	LEU	2.5
1	E	199	ILE	2.5
1	E	227	ARG	2.5
1	F	37	ILE	2.5
1	F	121	LEU	2.5
1	F	194	SER	2.5
1	D	61	ASP	2.5
1	E	258	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	10	PRO	2.5
1	E	49	VAL	2.5
1	D	195	ARG	2.4
1	A	141	SER	2.4
1	E	248	VAL	2.4
1	F	70	LYS	2.4
1	D	50	THR	2.4
1	D	62	ARG	2.4
1	C	96	SER	2.4
1	D	48	LYS	2.4
1	F	54	LYS	2.4
1	D	49	VAL	2.4
1	F	57	VAL	2.4
1	D	98	PHE	2.4
1	A	126	LEU	2.4
1	A	119	ASN	2.4
1	F	4	SER	2.4
1	A	292	GLU	2.4
1	C	54	LYS	2.4
1	E	81	LYS	2.4
1	A	57	VAL	2.4
1	A	115	ALA	2.4
1	E	113	ALA	2.4
1	C	94	SER	2.4
1	F	163	ASP	2.4
1	F	249	ILE	2.3
1	A	50	THR	2.3
1	A	54	LYS	2.3
1	B	54	LYS	2.3
1	F	44	SER	2.3
1	C	90	VAL	2.3
1	F	76	VAL	2.3
1	B	126	LEU	2.3
1	A	89	HIS	2.3
1	E	252	SER	2.3
1	B	75	ARG	2.3
1	E	20	GLY	2.3
1	F	234	PHE	2.3
1	F	38	THR	2.3
1	A	146	MET	2.3
1	B	3	LYS	2.3
1	B	95	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	25	GLU	2.3
1	E	55	ASN	2.3
1	A	96	SER	2.3
1	B	194	SER	2.3
1	F	251	ASP	2.3
1	E	324	ARG	2.3
1	B	85	GLY	2.3
1	A	321	VAL	2.3
1	E	321	VAL	2.3
1	A	51	LEU	2.3
1	F	98	PHE	2.3
1	D	196	LYS	2.3
1	F	214	TYR	2.3
1	B	68	GLU	2.3
1	D	52	ASN	2.3
1	C	26	ARG	2.3
1	C	317	ASP	2.3
1	D	96	SER	2.3
1	F	117	SER	2.3
1	E	7	VAL	2.3
1	E	124	LEU	2.3
1	E	276	ALA	2.2
1	B	70	LYS	2.2
1	F	191	LYS	2.2
1	E	93	GLU	2.2
1	B	65	SER	2.2
1	E	139	SER	2.2
1	F	11	SER	2.2
1	C	161	GLY	2.2
1	A	131	LEU	2.2
1	F	321	VAL	2.2
1	A	134	ILE	2.2
1	E	46	ILE	2.2
1	E	115	ALA	2.2
1	E	241	HIS	2.2
1	D	93	GLU	2.2
1	F	206	GLU	2.2
1	A	65	SER	2.2
1	E	149	GLY	2.2
1	F	132	SER	2.2
1	A	114	LEU	2.2
1	F	7	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	86	LYS	2.2
1	A	69	MET	2.2
1	F	247	ALA	2.2
1	D	26	ARG	2.2
1	A	220	ASN	2.2
1	F	106	SER	2.2
1	A	135	ALA	2.2
1	A	195	ARG	2.2
1	F	210	CYS	2.2
1	F	28	ASN	2.2
1	F	228	ASN	2.2
1	D	91	LYS	2.2
1	A	58	ILE	2.2
1	E	89	HIS	2.2
1	F	83	ILE	2.2
1	A	109	ALA	2.1
1	D	66	GLU	2.1
1	F	71	GLU	2.1
1	E	254	PRO	2.1
1	A	118	LEU	2.1
1	E	121	LEU	2.1
1	D	83	ILE	2.1
1	E	226	ILE	2.1
1	E	317	ASP	2.1
1	F	108	ALA	2.1
1	B	87	GLU	2.1
1	F	231	GLU	2.1
1	F	279	THR	2.1
1	B	72	TYR	2.1
1	D	122	LEU	2.1
1	D	124	LEU	2.1
1	E	167	TYR	2.1
1	F	322	LEU	2.1
1	E	161	GLY	2.1
1	B	7	VAL	2.1
1	E	65	SER	2.1
1	F	87	GLU	2.1
1	B	195	ARG	2.1
1	C	321	VAL	2.1
1	B	98	PHE	2.1
1	B	71	GLU	2.1
1	B	324	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	129	GLU	2.1
1	D	324	ARG	2.1
1	E	144	ARG	2.1
1	E	19	TRP	2.1
1	A	275	LYS	2.1
1	F	82	LYS	2.1
1	C	6	THR	2.1
1	D	77	LEU	2.1
1	D	118	LEU	2.1
1	E	138	GLY	2.1
1	A	298	ILE	2.1
1	F	13	ILE	2.1
1	E	222	VAL	2.1
1	E	26	ARG	2.0
1	F	202	ALA	2.0
1	F	91	LYS	2.0
1	F	133	LYS	2.0
1	C	50	THR	2.0
1	F	6	THR	2.0
1	B	69	MET	2.0
1	A	64	LEU	2.0
1	D	220	ASN	2.0
1	E	83	ILE	2.0
1	C	49	VAL	2.0
1	F	171	ARG	2.0
1	F	61	ASP	2.0
1	F	67	ASP	2.0
1	D	54	LYS	2.0
1	E	233	LYS	2.0
1	E	39	LEU	2.0
1	E	250	LEU	2.0
1	F	29	LEU	2.0
1	F	250	LEU	2.0
1	B	56	ILE	2.0
1	D	59	VAL	2.0
1	E	22	ARG	2.0
1	E	76	VAL	2.0
1	F	229	ARG	2.0

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

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	E	401	5/5	0.86	0.13	67,67,72,77	0
2	SO4	B	401	5/5	0.90	0.12	59,60,64,68	0
2	SO4	A	401	5/5	0.90	0.13	50,51,64,66	0
2	SO4	F	401	5/5	0.91	0.13	54,65,67,69	0
2	SO4	D	401	5/5	0.92	0.14	59,60,63,66	0
2	SO4	C	401	5/5	0.94	0.12	65,66,70,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.