



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:02 AM UTC

PDB ID : 7CPN / pdb_00007cpn
Title : CRYSTAL STRUCTURE OF DODECAPRENYL DIPHOSPHATE SYNTHASE FROM THERMOBIFIDA FUSCA
Authors : Kurokawa, H.; Ambo, T.; Takahasi, S.; Koyama, T.
Deposited on : 2020-08-07
Resolution : 2.28 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

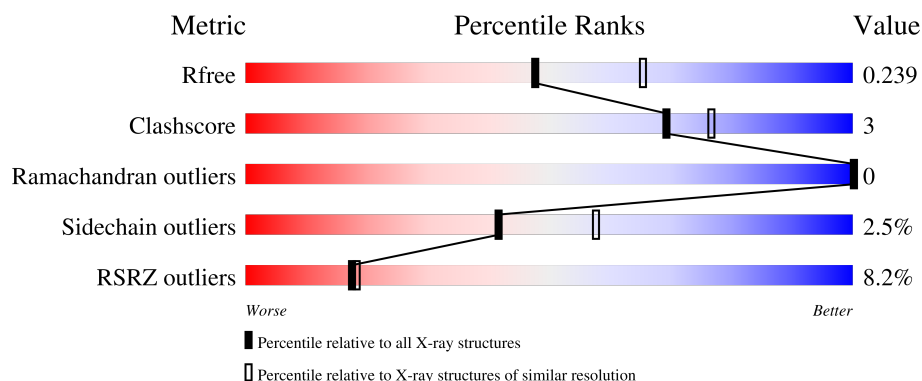
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	282	4% 78% 6% 16%
1	B	282	2% 76% 6% 18%
1	C	282	4% 76% 5% 18%
1	D	282	17% 72% 5% 22%
1	E	282	3% 73% 7% 18%

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Mol	Chain	Length	Quality of chain
1	F	282	11% 73% 8% 18%

2 Entry composition [i](#)

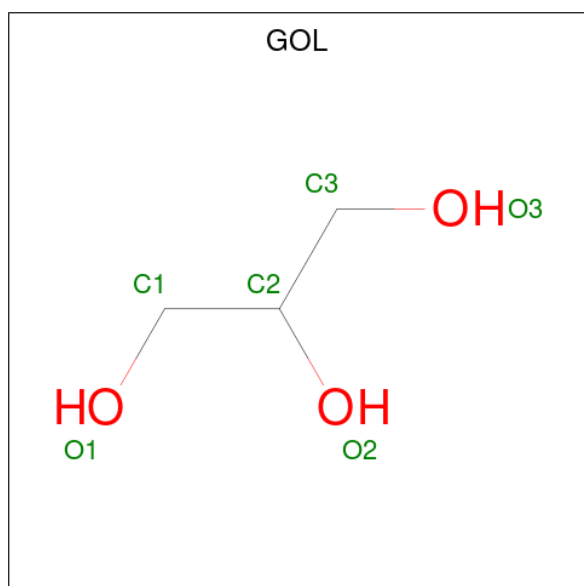
There are 4 unique types of molecules in this entry. The entry contains 22389 atoms, of which 10844 are hydrogens and 0 are deuteriums.

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 Trans,polycis-polyprenyl diphosphate synthase ((2Z,6E)-farnesyl diphosphate specific).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	238	Total	C	H	N	O	S	74	0	0
			3796	1213	1879	363	337	4			
1	B	232	Total	C	H	N	O	S	71	0	0
			3727	1192	1849	349	333	4			
1	C	231	Total	C	H	N	O	S	71	0	0
			3716	1187	1843	352	330	4			
1	D	221	Total	C	H	N	O	S	79	0	0
			3367	1087	1653	312	312	3			
1	E	230	Total	C	H	N	O	S	75	0	0
			3639	1170	1801	337	327	4			
1	F	231	Total	C	H	N	O	S	76	0	0
			3659	1176	1811	340	328	4			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

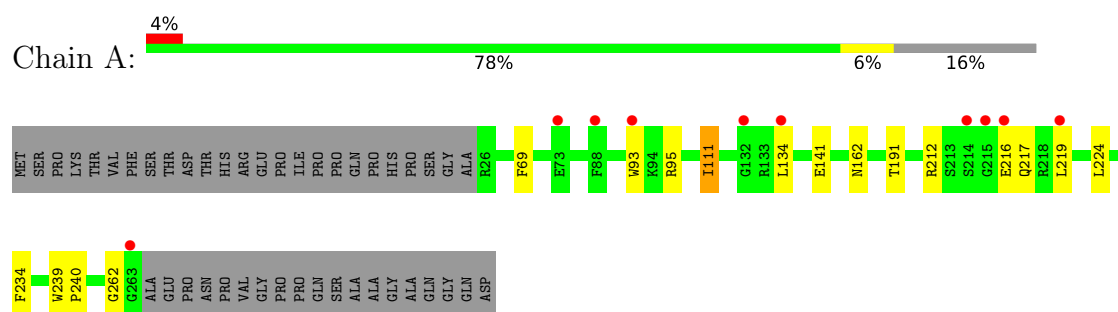
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	106	Total	O	0	0
			106	106		
4	C	70	Total	O	0	0
			70	70		
4	D	42	Total	O	0	0
			42	42		
4	E	45	Total	O	0	0
			45	45		
4	F	42	Total	O	0	0
			42	42		

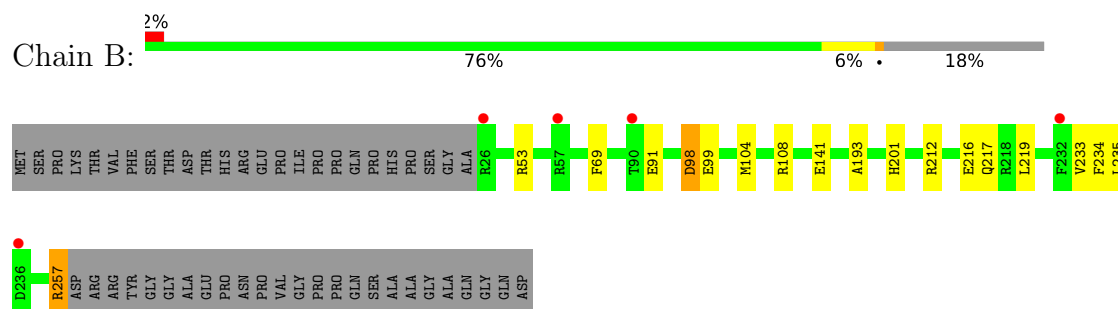
3 Residue-property plots [i](#)

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

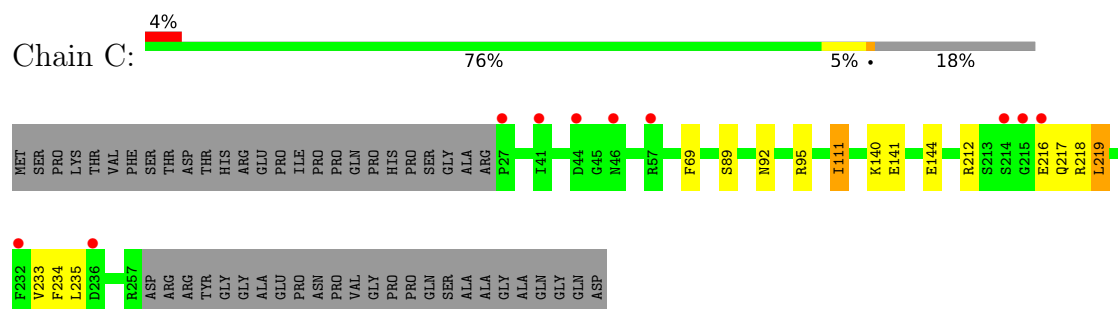
- Molecule 1: Trans,polycis-polyprenyl diphosphate synthase ((2Z,6E)-farnesyl diphosphate specific)



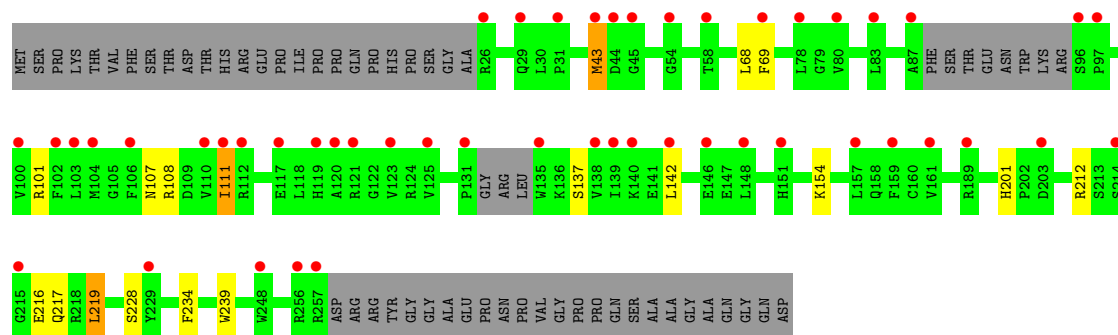
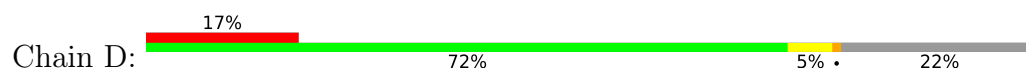
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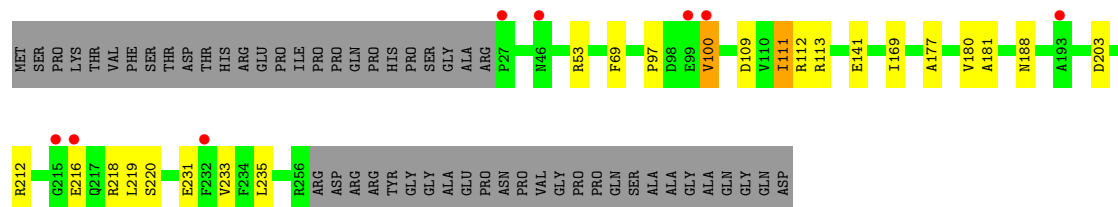
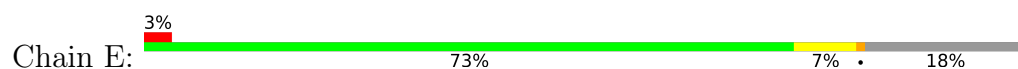
- Molecule 1: Trans,polycis-polyprenyl diphosphate synthase ((2Z,6E)-farnesyl diphosphate specific)



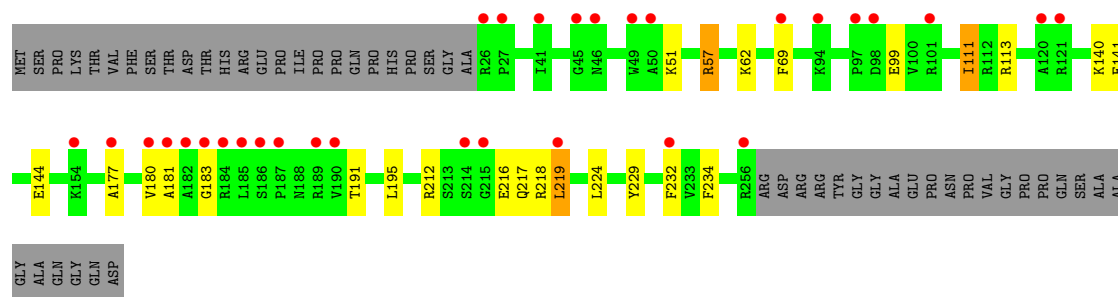
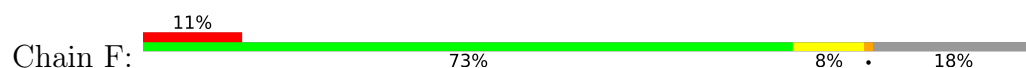
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.09Å 137.88Å 168.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.28 47.53 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.53-2.28) 99.9 (47.53-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.67 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.203 , 0.239 0.203 , 0.239	Depositor DCC
R_{free} test set	3885 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22389	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.07	0/1967	1.33	1/2668 (0.0%)
1	B	1.05	0/1927	1.38	2/2613 (0.1%)
1	C	0.99	0/1922	1.39	1/2606 (0.0%)
1	D	1.10	2/1756 (0.1%)	1.34	1/2393 (0.0%)
1	E	0.99	0/1887	1.33	1/2563 (0.0%)
1	F	1.01	0/1897	1.35	1/2577 (0.0%)
All	All	1.03	2/11356 (0.0%)	1.35	7/15420 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	LEU	C-O	-7.07	1.16	1.24
1	D	201	HIS	CE1-NE2	5.21	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	69	PHE	CA-CB-CG	-6.14	107.66	113.80
1	F	69	PHE	CA-CB-CG	-6.07	107.73	113.80
1	B	69	PHE	CA-CB-CG	-5.75	108.05	113.80
1	E	69	PHE	CA-CB-CG	-5.38	108.42	113.80
1	D	69	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	98	ASP	CA-CB-CG	-5.26	107.34	112.60

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	1917	1879	1858	12	0
1	B	1878	1849	1836	13	0
1	C	1873	1843	1831	13	0
1	D	1714	1653	1610	13	0
1	E	1838	1801	1781	21	0
1	F	1848	1811	1788	19	0
2	A	6	8	8	1	0
3	A	5	0	0	1	0
3	B	20	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	1	0
3	E	10	0	0	1	0
3	F	10	0	0	1	0
4	A	101	0	0	0	0
4	B	106	0	0	2	0
4	C	70	0	0	0	0
4	D	42	0	0	2	0
4	E	45	0	0	0	0
4	F	42	0	0	0	0
All	All	11545	10844	10712	76	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 3.

All (76) 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:C:219:LEU:HD11	1:D:219:LEU:HD11	1.36	1.04
1:D:107:ASN:O	1:D:111:ILE:HG12	1.74	0.88
1:B:193:ALA:HB3	1:F:183:GLY:HA3	1.69	0.74
1:C:233:VAL:HG12	1:C:235:LEU:CD1	2.19	0.73
1:E:233:VAL:HG12	1:E:235:LEU:CD1	2.20	0.72
1:B:233:VAL:HG12	1:B:235:LEU:CD1	2.20	0.71
1:E:180:VAL:HG12	1:F:181:ALA:HB2	1.72	0.71
1:A:93:TRP:O	1:F:191:THR:HG21	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:NH2	4:B:402:HOH:O	2.28	0.66
1:E:177:ALA:HB1	1:F:180:VAL:HG21	1.77	0.66
1:A:95:ARG:NH2	3:A:302:SO4:O1	2.31	0.63
1:E:181:ALA:HB2	1:F:180:VAL:HG12	1.81	0.63
1:E:109:ASP:HA	1:E:112:ARG:HG2	1.83	0.61
1:C:233:VAL:HG12	1:C:235:LEU:HD11	1.83	0.60
1:E:180:VAL:HG21	1:F:177:ALA:HB1	1.82	0.60
1:B:233:VAL:HG12	1:B:235:LEU:HD11	1.84	0.60
1:E:233:VAL:HG12	1:E:235:LEU:HD11	1.85	0.59
1:A:191:THR:HB	2:A:301:GOL:H11	1.84	0.59
1:B:212:ARG:HG2	1:B:216:GLU:O	2.02	0.58
1:D:101:ARG:HD3	4:D:436:HOH:O	2.03	0.58
1:C:219:LEU:HD11	1:D:219:LEU:CD1	2.23	0.57
1:D:101:ARG:HG3	1:E:203:ASP:HA	1.86	0.57
1:D:212:ARG:NH2	3:D:302:SO4:O2	2.37	0.56
1:D:212:ARG:HG2	1:D:216:GLU:O	2.05	0.56
1:B:193:ALA:CB	1:F:183:GLY:HA3	2.34	0.56
1:E:97:PRO:O	1:E:100:VAL:HG12	2.06	0.56
1:C:212:ARG:HG2	1:C:216:GLU:O	2.05	0.55
1:F:57:ARG:NH1	1:F:99:GLU:OE2	2.40	0.54
1:D:108:ARG:O	1:D:111:ILE:HG13	2.08	0.53
1:A:212:ARG:HG2	1:A:216:GLU:O	2.07	0.53
1:D:216:GLU:N	1:D:216:GLU:OE2	2.42	0.53
1:D:43:MET:HE1	1:D:68:LEU:HD13	1.90	0.53
1:E:231:GLU:OE2	1:F:218:ARG:NH1	2.42	0.52
1:E:233:VAL:HG12	1:E:235:LEU:HD12	1.90	0.52
1:C:233:VAL:HG12	1:C:235:LEU:HD12	1.91	0.52
1:D:154:LYS:CB	4:D:407:HOH:O	2.57	0.51
1:F:212:ARG:HG2	1:F:216:GLU:O	2.09	0.51
1:A:219:LEU:CD2	1:A:224:LEU:HD13	2.40	0.50
1:B:235:LEU:HD12	1:B:235:LEU:N	2.27	0.50
1:A:219:LEU:HD23	1:A:224:LEU:HD13	1.94	0.49
1:B:233:VAL:HG12	1:B:235:LEU:HD12	1.91	0.49
1:A:262:GLY:HA3	1:B:91:GLU:HB3	1.94	0.49
1:B:108:ARG:HG3	1:B:141:GLU:HG3	1.95	0.49
1:E:235:LEU:HD12	1:E:235:LEU:N	2.29	0.48
1:E:220:SER:OG	3:E:302:SO4:O1	2.28	0.47
1:F:140:LYS:HE2	1:F:144:GLU:OE1	2.14	0.47
1:B:217:GLN:HA	1:B:234:PHE:CE1	2.50	0.47
1:B:201:HIS:HE1	4:B:407:HOH:O	1.96	0.47
1:C:235:LEU:HD12	1:C:235:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:CG1	1:F:181:ALA:HB2	2.42	0.47
1:A:217:GLN:HA	1:A:234:PHE:CE1	2.50	0.46
1:F:219:LEU:HD12	1:F:232:PHE:CZ	2.52	0.45
1:F:219:LEU:HD22	1:F:224:LEU:HD13	1.99	0.45
1:D:217:GLN:HA	1:D:234:PHE:CE1	2.52	0.45
1:A:134:LEU:HD13	1:A:162:ASN:HB2	1.99	0.44
1:F:218:ARG:NE	3:F:302:SO4:O4	2.50	0.44
1:C:217:GLN:HA	1:C:234:PHE:CE1	2.52	0.44
1:E:109:ASP:HA	1:E:112:ARG:CG	2.46	0.44
1:A:219:LEU:CD2	1:A:224:LEU:CD1	2.95	0.44
1:E:109:ASP:O	1:E:112:ARG:HG3	2.18	0.44
1:F:217:GLN:HA	1:F:234:PHE:CE1	2.53	0.44
1:C:111:ILE:CG2	1:C:141:GLU:HB3	2.48	0.43
1:C:233:VAL:CG1	1:C:235:LEU:HD11	2.48	0.43
1:C:89:SER:HB3	1:C:92:ASN:OD1	2.19	0.43
1:C:140:LYS:HE3	1:C:144:GLU:OE1	2.19	0.43
1:E:111:ILE:CG2	1:E:141:GLU:HB3	2.49	0.42
1:E:212:ARG:HG2	1:E:216:GLU:O	2.20	0.42
1:E:220:SER:HA	1:F:229:TYR:CE1	2.55	0.42
1:B:233:VAL:CG1	1:B:235:LEU:HD11	2.49	0.41
1:E:233:VAL:CG1	1:E:235:LEU:HD11	2.50	0.41
1:F:111:ILE:CG2	1:F:141:GLU:HB3	2.49	0.41
1:D:43:MET:HE2	1:D:239:TRP:CH2	2.56	0.41
1:A:111:ILE:CG2	1:A:141:GLU:HB3	2.51	0.41
1:E:169:ILE:HG22	1:F:195:LEU:CD2	2.50	0.40
1:A:239:TRP:N	1:A:240:PRO:CD	2.85	0.40
1:C:95:ARG:NH2	3:C:301:SO4:O3	2.55	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	236/282 (84%)	231 (98%)	5 (2%)	0	100	100
1	B	230/282 (82%)	227 (99%)	3 (1%)	0	100	100
1	C	229/282 (81%)	225 (98%)	4 (2%)	0	100	100
1	D	215/282 (76%)	211 (98%)	4 (2%)	0	100	100
1	E	228/282 (81%)	225 (99%)	3 (1%)	0	100	100
1	F	229/282 (81%)	228 (100%)	1 (0%)	0	100	100
All	All	1367/1692 (81%)	1347 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	191/233 (82%)	190 (100%)	1 (0%)	81	89
1	B	191/233 (82%)	185 (97%)	6 (3%)	35	50
1	C	190/233 (82%)	187 (98%)	3 (2%)	55	71
1	D	167/233 (72%)	162 (97%)	5 (3%)	36	51
1	E	185/233 (79%)	178 (96%)	7 (4%)	29	42
1	F	185/233 (79%)	179 (97%)	6 (3%)	34	49
All	All	1109/1398 (79%)	1081 (98%)	28 (2%)	42	58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ILE
1	B	53	ARG
1	B	98	ASP
1	B	99	GLU
1	B	104	MET
1	B	219	LEU
1	B	257	ARG

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Mol	Chain	Res	Type
1	C	111	ILE
1	C	218	ARG
1	C	219	LEU
1	D	43	MET
1	D	111	ILE
1	D	137	SER
1	D	219	LEU
1	D	228	SER
1	E	53	ARG
1	E	100	VAL
1	E	111	ILE
1	E	113	ARG
1	E	188	ASN
1	E	218	ARG
1	E	219	LEU
1	F	51	LYS
1	F	57	ARG
1	F	62	LYS
1	F	111	ILE
1	F	113	ARG
1	F	219	LEU

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	246	HIS
1	B	107	ASN
1	B	158	GLN
1	B	201	HIS
1	B	246	HIS
1	C	61	HIS
1	C	217	GLN
1	C	246	HIS
1	D	61	HIS
1	D	217	GLN
1	D	246	HIS
1	E	246	HIS
1	F	119	HIS
1	F	246	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	SO4	B	303	-	4,4,4	0.32	0	6,6,6	0.20	0
2	GOL	A	301	-	5,5,5	0.20	0	5,5,5	0.68	0
3	SO4	D	302	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	B	301	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	A	302	-	4,4,4	0.20	0	6,6,6	0.24	0
3	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	D	301	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	F	302	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	E	301	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	C	301	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	C	302	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	F	301	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	304	-	4,4,4	0.31	0	6,6,6	0.16	0
3	SO4	E	302	-	4,4,4	0.25	0	6,6,6	0.15	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
2	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-O2
2	A	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	0
3	D	302	SO4	1	0
3	A	302	SO4	1	0
3	F	302	SO4	1	0
3	C	301	SO4	1	0
3	E	302	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	238/282 (84%)	0.16	10 (4%) 40 42	24, 46, 77, 131	0
1	B	232/282 (82%)	-0.05	5 (2%) 62 64	23, 40, 66, 94	0
1	C	231/282 (81%)	0.33	10 (4%) 40 41	27, 52, 88, 105	0
1	D	221/282 (78%)	1.15	49 (22%) 2 2	29, 68, 95, 121	0
1	E	230/282 (81%)	0.51	8 (3%) 47 49	30, 57, 95, 116	0
1	F	231/282 (81%)	0.94	31 (13%) 7 7	32, 67, 106, 119	0
All	All	1383/1692 (81%)	0.50	113 (8%) 17 18	23, 53, 94, 131	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	TRP	6.8
1	F	185	LEU	5.6
1	A	93	TRP	5.4
1	F	181	ALA	5.1
1	F	182	ALA	4.6
1	B	232	PHE	4.3
1	C	215	GLY	4.2
1	D	257	ARG	4.2
1	F	186	SER	4.2
1	D	106	PHE	4.2
1	F	189	ARG	4.0
1	D	142	LEU	3.9
1	D	159	PHE	3.9
1	F	26	ARG	3.9
1	A	216	GLU	3.8
1	F	41	ILE	3.8
1	F	180	VAL	3.8
1	A	215	GLY	3.8
1	D	26	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	98	ASP	3.6
1	D	125	VAL	3.6
1	F	219	LEU	3.5
1	D	214	SER	3.5
1	B	26	ARG	3.4
1	E	27	PRO	3.3
1	F	187	PRO	3.3
1	A	214	SER	3.2
1	D	139	ILE	3.2
1	F	183	GLY	3.2
1	A	263	GLY	3.1
1	D	148	LEU	3.1
1	D	138	VAL	3.1
1	F	46	ASN	3.0
1	F	120	ALA	3.0
1	C	214	SER	2.9
1	D	97	PRO	2.9
1	D	112	ARG	2.9
1	D	117	GLU	2.9
1	A	88	PHE	2.9
1	D	87	ALA	2.8
1	C	44	ASP	2.8
1	D	131	PRO	2.7
1	F	101	ARG	2.7
1	F	69	PHE	2.7
1	F	215	GLY	2.7
1	F	256	ARG	2.7
1	A	219	LEU	2.7
1	C	27	PRO	2.7
1	D	100	VAL	2.6
1	B	90	THR	2.6
1	F	177	ALA	2.6
1	D	111	ILE	2.6
1	F	214	SER	2.6
1	A	134	LEU	2.6
1	E	215	GLY	2.6
1	C	216	GLU	2.6
1	F	190	VAL	2.6
1	F	121	ARG	2.5
1	E	100	VAL	2.5
1	D	54	GLY	2.5
1	D	110	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	157	LEU	2.5
1	D	103	LEU	2.4
1	D	229	TYR	2.4
1	D	104	MET	2.4
1	E	216	GLU	2.4
1	D	151	HIS	2.4
1	D	256	ARG	2.4
1	D	215	GLY	2.4
1	D	58	THR	2.3
1	F	232	PHE	2.3
1	F	184	ARG	2.3
1	E	46	ASN	2.3
1	F	27	PRO	2.3
1	F	45	GLY	2.3
1	D	161	VAL	2.3
1	B	236	ASP	2.3
1	D	203	ASP	2.3
1	D	69	PHE	2.2
1	F	97	PRO	2.2
1	F	49	TRP	2.2
1	C	232	PHE	2.2
1	C	46	ASN	2.2
1	D	121	ARG	2.2
1	D	120	ALA	2.2
1	D	189	ARG	2.2
1	D	96	SER	2.2
1	D	83	LEU	2.1
1	D	80	VAL	2.1
1	D	123	VAL	2.1
1	D	31	PRO	2.1
1	F	50	ALA	2.1
1	C	41	ILE	2.1
1	D	248	TRP	2.1
1	D	146	GLU	2.1
1	D	45	GLY	2.1
1	B	57	ARG	2.1
1	C	57	ARG	2.1
1	F	94	LYS	2.0
1	D	43	MET	2.0
1	E	193	ALA	2.0
1	D	119	HIS	2.0
1	A	132	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	102	PHE	2.0
1	E	232	PHE	2.0
1	A	73	GLU	2.0
1	E	99	GLU	2.0
1	D	29	GLN	2.0
1	C	236	ASP	2.0
1	D	44	ASP	2.0
1	D	78	LEU	2.0
1	D	140	LYS	2.0
1	F	154	LYS	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(Å ²)	Q<0.9
3	SO4	C	302	5/5	0.52	0.12	136,137,139,145	0
3	SO4	D	301	5/5	0.52	0.15	105,113,124,125	0
3	SO4	D	302	5/5	0.61	0.10	113,117,120,120	0
3	SO4	E	301	5/5	0.63	0.14	80,98,109,114	0
3	SO4	C	301	5/5	0.74	0.11	88,92,111,115	0
3	SO4	F	302	5/5	0.75	0.12	95,97,108,112	0
3	SO4	F	301	5/5	0.79	0.10	75,83,92,98	0
3	SO4	E	302	5/5	0.79	0.10	73,78,93,95	0
3	SO4	A	302	5/5	0.83	0.10	64,64,82,88	0
3	SO4	B	301	5/5	0.83	0.10	64,71,75,77	0
2	GOL	A	301	6/6	0.87	0.13	48,59,79,79	2
3	SO4	B	303	5/5	0.87	0.09	62,63,80,80	0
3	SO4	B	302	5/5	0.94	0.15	49,61,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	304	5/5	0.95	0.10	47,49,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.