



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:16 PM UTC

PDB ID : 3TZX / pdb_00003tzx
Title : Crystal structure of a fragment containing the acyltransferase domain of Pks13 from Mycobacterium tuberculosis in tetragonal apo form at 2.3 Å
Authors : Bergeret, F.; Pedelacq, J.D.; Mourey, L.; Bon, C.
Deposited on : 2011-09-28
Resolution : 2.30 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

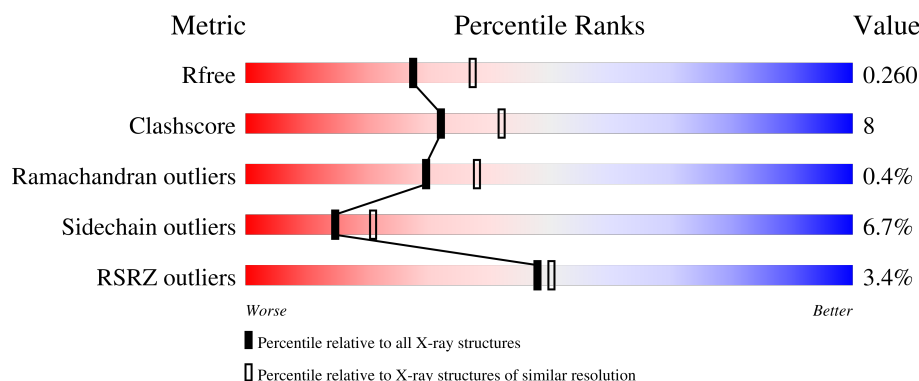
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	491	0% 75% 17% • 5%
1	B	491	3% 75% 16% • • 5%
2	C	12	25% 58% 17% 17% 8%
2	D	12	75% 25% 17% 33% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	6	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7524 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 Polyketide synthase PKS13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3479	2199	600	668	12			
1	B	467	Total	C	N	O	S	0	1	0
			3489	2210	610	657	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	572	GLY	-	expression tag	UNP O53579
A	573	SER	-	expression tag	UNP O53579
A	574	HIS	-	expression tag	UNP O53579
A	575	MET	-	expression tag	UNP O53579
B	572	GLY	-	expression tag	UNP O53579
B	573	SER	-	expression tag	UNP O53579
B	574	HIS	-	expression tag	UNP O53579
B	575	MET	-	expression tag	UNP O53579

- Molecule 2 is a protein called 12-mer peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	S	0	0	0
			94	60	15	18	1			
2	D	9	Total	C	N	O	S	0	0	0
			67	45	11	10	1			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

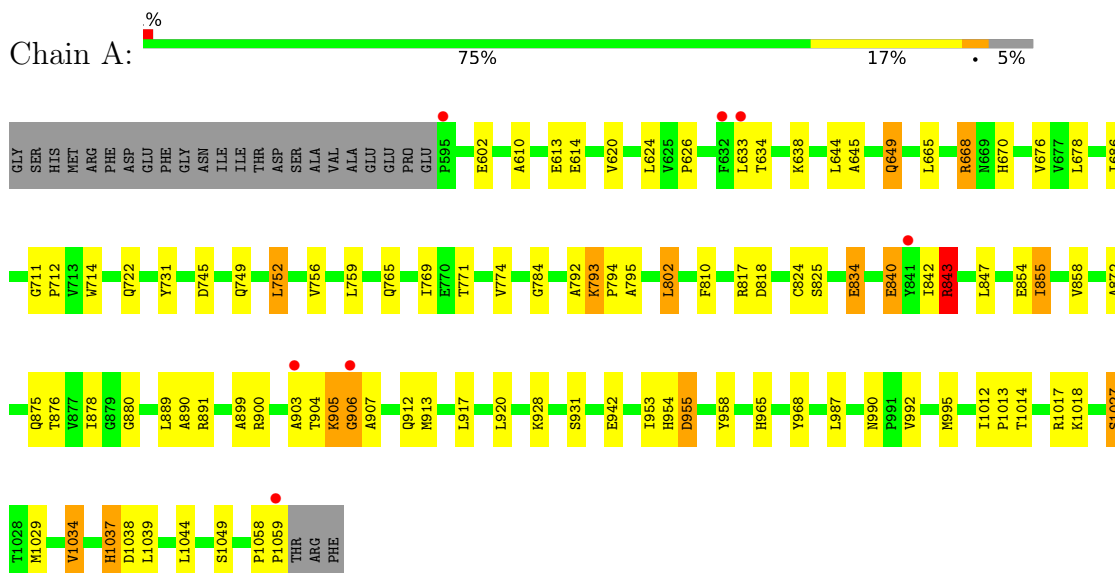
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	169	Total O 169 169	0	0
5	B	180	Total O 180 180	0	0
5	D	2	Total O 2 2	0	0

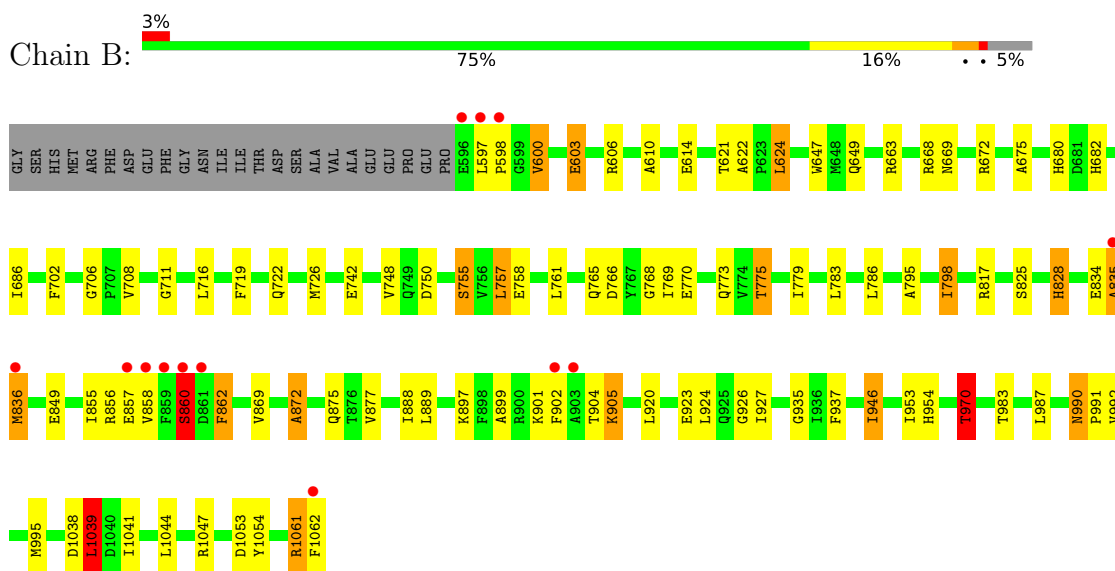
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Polyketide synthase PKS13



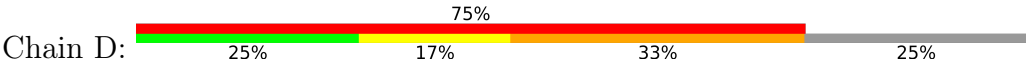
• Molecule 1: Polyketide synthase PKS13



• Molecule 2: 12-mer peptide



● Molecule 2: 12-mer peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.56Å 106.56Å 258.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.12 – 2.30 41.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (41.12-2.30) 96.9 (41.12-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.200 , 0.260 0.201 , 0.260	Depositor DCC
R_{free} test set	3291 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7524	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: SO4, GOL

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	1.29	6/3552 (0.2%)	1.29	16/4834 (0.3%)
1	B	1.37	16/3562 (0.4%)	1.33	20/4846 (0.4%)
2	C	1.59	1/96 (1.0%)	1.79	2/128 (1.6%)
2	D	1.62	1/69 (1.4%)	1.45	1/93 (1.1%)
All	All	1.34	24/7279 (0.3%)	1.32	39/9901 (0.4%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	954	HIS	CD2-NE2	-7.06	1.30	1.37
1	B	860	SER	N-CA	6.23	1.54	1.46
1	B	954	HIS	CG-ND1	-6.22	1.31	1.38
2	C	7	TRP	CA-C	-6.21	1.44	1.52
1	A	712	PRO	C-O	6.19	1.30	1.23
1	A	670	HIS	CE1-NE2	6.17	1.38	1.32
1	B	828	HIS	CG-ND1	-6.15	1.31	1.38
1	A	626	PRO	CA-C	5.93	1.60	1.52
2	D	5	ASN	N-CA	5.91	1.53	1.45
1	B	775	THR	N-CA	-5.78	1.39	1.46
1	A	1037	HIS	CG-ND1	-5.67	1.32	1.38
1	B	603	GLU	CA-C	5.62	1.59	1.52
1	B	828	HIS	CD2-NE2	-5.57	1.31	1.37
1	B	786	LEU	CA-C	5.52	1.59	1.52
1	A	1037	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	983	THR	CA-C	5.43	1.59	1.52
1	B	722	GLN	N-CA	5.42	1.52	1.46
1	B	773	GLN	N-CA	-5.39	1.39	1.46
1	B	647	TRP	NE1-CE2	-5.30	1.31	1.37
1	B	836	MET	CA-C	5.27	1.59	1.53
1	B	858	VAL	CA-C	5.19	1.59	1.52
1	A	906	GLY	C-O	5.19	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	748	VAL	CA-CB	5.19	1.61	1.54
1	B	682	HIS	ND1-CE1	5.12	1.37	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	953	ILE	CB-CA-C	-13.21	95.53	111.65
1	A	955	ASP	N-CA-CB	-11.50	93.82	110.26
1	B	927	ILE	N-CA-C	-8.43	100.86	110.05
1	B	905	LYS	N-CA-C	-7.89	103.16	114.12
1	B	862	PHE	CA-C-N	-7.80	111.96	121.00
1	B	862	PHE	C-N-CA	-7.80	111.96	121.00
1	B	970	THR	CB-CA-C	-7.75	97.93	110.79
1	B	857	GLU	N-CA-C	7.72	123.16	112.04
2	D	5	ASN	N-CA-C	7.32	120.45	110.35
1	B	992	VAL	N-CA-C	7.01	117.72	110.36
1	A	954	HIS	CB-CA-C	6.33	119.01	111.22
1	A	990	ASN	CA-C-N	-6.32	115.27	121.65
1	A	990	ASN	C-N-CA	-6.32	115.27	121.65
1	A	1012	ILE	N-CA-C	6.31	113.80	107.55
2	C	6	PHE	N-CA-C	6.29	120.42	112.87
1	B	935	GLY	N-CA-C	-6.14	104.35	112.82
1	B	765	GLN	N-CA-C	5.97	118.45	108.96
1	A	793	LYS	CA-C-N	-5.95	113.56	119.99
1	A	793	LYS	C-N-CA	-5.95	113.56	119.99
1	B	766	ASP	N-CA-C	-5.77	102.76	110.55
1	B	990	ASN	CB-CA-C	5.73	117.76	109.45
1	A	1014	THR	N-CA-CB	5.71	120.14	110.49
1	B	624	LEU	CA-C-N	-5.69	117.81	123.04
1	B	624	LEU	C-N-CA	-5.69	117.81	123.04
1	A	965	HIS	N-CA-C	5.67	118.86	110.46
1	B	856	ARG	N-CA-C	5.66	117.53	111.36
1	B	970	THR	N-CA-CB	5.53	118.24	110.12
1	A	906	GLY	CA-C-O	5.36	126.12	121.41
1	A	931	SER	CA-C-N	-5.31	114.77	120.03
1	A	931	SER	C-N-CA	-5.31	114.77	120.03
1	A	890	ALA	N-CA-C	-5.29	105.56	112.23
2	C	6	PHE	N-CA-CB	5.29	119.95	110.32
1	B	904	THR	N-CA-C	-5.27	101.28	109.24
1	B	872	ALA	CA-C-N	-5.27	113.61	119.19
1	B	872	ALA	C-N-CA	-5.27	113.61	119.19
1	A	1013	PRO	CB-CA-C	-5.19	103.07	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	MET	N-CA-C	5.08	118.57	110.70
1	B	926	GLY	N-CA-C	5.07	121.76	114.10
1	A	843	ARG	CG-CD-NE	-5.03	100.94	112.00

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	3479	0	3405	57	0
1	B	3489	0	3424	52	0
2	C	94	0	86	7	0
2	D	67	0	54	5	0
3	A	12	0	16	5	0
3	B	12	0	16	0	0
4	B	15	0	0	1	0
4	C	5	0	0	0	0
5	A	169	0	0	2	0
5	B	180	0	0	3	0
5	D	2	0	0	0	0
All	All	7524	0	7001	113	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 8.

All (113) 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:903:ALA:H	3:A:6:GOL:H12	1.23	0.98
1:A:840:GLU:O	1:A:840:GLU:HG3	1.61	0.97
1:B:680:HIS:HE1	2:C:6:PHE:HE2	1.26	0.80
1:A:842:ILE:HG21	1:A:905:LYS:HG2	1.66	0.78
1:A:987:LEU:N	1:A:987:LEU:HD12	1.98	0.78
1:A:676:VAL:HG23	1:A:1034:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:PHE:CE2	1:B:902:PHE:CE2	2.76	0.73
1:B:716:LEU:HD11	1:B:987:LEU:HD12	1.69	0.72
1:A:878:ILE:HD12	1:A:878:ILE:C	2.15	0.72
1:A:903:ALA:N	3:A:6:GOL:H12	2.02	0.70
1:A:610:ALA:O	1:A:614:GLU:HG3	1.92	0.69
1:A:878:ILE:HD12	1:A:878:ILE:O	1.95	0.67
1:A:842:ILE:HG21	1:A:905:LYS:CG	2.26	0.65
1:A:906:GLY:HA3	5:A:230:HOH:O	1.96	0.64
1:B:624:LEU:HD11	2:C:7:TRP:HZ3	1.61	0.64
1:B:834:GLU:HG3	1:B:905:LYS:HB2	1.79	0.64
1:B:649:GLN:HG3	1:B:686:ILE:HD13	1.81	0.63
2:D:5:ASN:OD1	2:D:9:MET:HG3	1.99	0.63
1:B:610:ALA:O	1:B:614:GLU:HG3	1.98	0.63
1:A:711:GLY:HA3	1:A:795:ALA:HB2	1.79	0.63
1:B:889:LEU:HD22	1:B:899:ALA:HB1	1.81	0.62
1:A:872:ALA:HB3	1:A:875:GLN:HB2	1.80	0.62
2:D:4:GLU:HA	2:D:9:MET:O	2.00	0.61
1:B:680:HIS:CE1	2:C:6:PHE:HE2	2.14	0.61
1:A:634:THR:HG22	1:A:638:LYS:HE3	1.82	0.61
1:B:603:GLU:OE1	1:B:606:ARG:NH1	2.34	0.60
1:A:784:GLY:HA3	1:A:810:PHE:CZ	2.37	0.59
1:A:889:LEU:HD23	1:A:899:ALA:HB1	1.85	0.59
1:B:663:ARG:HD2	1:B:1053:ASP:O	2.03	0.59
1:B:849:GLU:HB3	1:B:897:LYS:HB3	1.84	0.59
1:A:903:ALA:H	3:A:6:GOL:C1	2.07	0.58
1:B:600:VAL:HG21	1:B:742:GLU:HG2	1.85	0.58
1:B:680:HIS:HE1	2:C:6:PHE:CE2	2.15	0.58
1:B:719:PHE:CE2	1:B:902:PHE:HE2	2.20	0.58
1:B:1038:ASP:O	1:B:1039:LEU:HB2	2.02	0.58
1:B:1061:ARG:HG2	5:B:340:HOH:O	2.04	0.58
1:A:913:MET:HE2	1:A:913:MET:HA	1.86	0.57
1:B:860:SER:C	1:B:862:PHE:H	2.11	0.57
1:B:600:VAL:CG2	1:B:742:GLU:HG2	2.34	0.57
1:B:719:PHE:HE2	1:B:902:PHE:HE2	1.52	0.56
1:B:872:ALA:HA	1:B:970:THR:HG23	1.86	0.55
1:B:889:LEU:HD11	1:B:901:LYS:HB3	1.88	0.55
1:A:878:ILE:C	1:A:878:ILE:CD1	2.80	0.54
2:D:6:PHE:HD1	2:D:6:PHE:O	1.90	0.54
1:A:987:LEU:HD12	1:A:987:LEU:H	1.74	0.53
1:B:711:GLY:HA3	1:B:795:ALA:HB2	1.90	0.52
1:B:755:SER:OG	1:B:758:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LEU:CD1	2:C:7:TRP:HZ3	2.22	0.52
1:A:1029:MET:HE3	1:A:1044:LEU:HD22	1.92	0.51
1:B:726:MET:HE3	1:B:775:THR:HG22	1.94	0.50
1:B:597:LEU:HB3	1:B:598:PRO:HD2	1.94	0.49
1:A:668:ARG:NH1	5:A:213:HOH:O	2.27	0.49
1:A:843:ARG:HG2	1:A:880:GLY:C	2.37	0.49
1:A:752:LEU:HD22	1:A:824:CYS:SG	2.53	0.49
1:A:1017:ARG:O	1:A:1018:LYS:CB	2.61	0.49
1:A:722:GLN:HE22	3:A:6:GOL:H31	1.79	0.48
1:B:834:GLU:O	1:B:835:ALA:C	2.55	0.48
1:B:872:ALA:HB3	1:B:875:GLN:HB2	1.95	0.48
1:B:1047:ARG:NH2	4:B:11:SO4:S	2.87	0.48
1:B:672:ARG:O	1:B:706:GLY:HA2	2.15	0.47
1:A:987:LEU:N	1:A:987:LEU:CD1	2.71	0.47
1:B:622:ALA:O	1:B:680:HIS:HD2	1.97	0.47
1:B:825:SER:HB3	1:B:920:LEU:HD12	1.96	0.47
1:B:624:LEU:HD11	2:C:7:TRP:CZ3	2.46	0.46
2:C:9:MET:HB3	2:C:9:MET:HE3	1.07	0.46
1:A:825:SER:HB3	1:A:920:LEU:HD12	1.97	0.46
1:B:757:LEU:HD22	1:B:761:LEU:CD1	2.46	0.46
1:A:634:THR:O	1:A:638:LYS:HG3	2.16	0.46
1:A:745:ASP:O	1:A:749:GLN:HG3	2.16	0.45
1:A:802:LEU:HD23	1:A:802:LEU:C	2.41	0.45
1:A:792:ALA:O	1:A:793:LYS:HG3	2.16	0.45
1:A:714:TRP:CD2	1:A:794:PRO:HB3	2.51	0.45
1:A:955:ASP:HB3	1:A:958:TYR:H	1.82	0.45
1:A:913:MET:HE2	1:A:913:MET:CA	2.46	0.44
1:A:942:GLU:HA	1:A:968:TYR:CG	2.52	0.44
1:A:731:TYR:CD2	1:A:731:TYR:C	2.96	0.44
1:A:759:LEU:HD22	1:A:765:GLN:HG2	1.99	0.44
1:B:675:ALA:HA	1:B:702:PHE:O	2.18	0.44
1:A:678:LEU:HD13	1:A:1027:SER:HB2	1.99	0.43
1:A:722:GLN:HE22	3:A:6:GOL:C3	2.30	0.43
1:B:750:ASP:HB3	1:B:817:ARG:HH22	1.84	0.43
1:A:644:LEU:HD21	1:A:665:LEU:HD11	2.00	0.43
1:A:771:THR:HA	1:A:774:VAL:HG22	1.99	0.43
1:B:869:VAL:HB	1:B:877:VAL:HB	1.99	0.43
1:B:783:LEU:HD23	1:B:783:LEU:HA	1.83	0.43
1:B:946:ILE:HD12	1:B:953:ILE:HD13	2.01	0.43
1:A:854:GLU:O	1:A:858:VAL:HG23	2.19	0.43
1:A:855:ILE:HD13	1:A:876:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ILE:CD1	1:A:834:GLU:HG3	2.49	0.42
1:B:768:GLY:O	1:B:769:ILE:C	2.61	0.42
1:B:798:ILE:HG13	1:B:937:PHE:O	2.18	0.42
1:A:649:GLN:NE2	1:A:686:ILE:HD13	2.35	0.42
1:B:668:ARG:NE	5:B:197:HOH:O	2.30	0.42
1:A:1029:MET:HE3	1:A:1044:LEU:CD2	2.50	0.42
1:B:924:LEU:HD23	1:B:924:LEU:HA	1.88	0.42
1:B:779:ILE:O	1:B:783:LEU:HG	2.20	0.42
1:B:770:GLU:OE2	1:B:828:HIS:HA	2.20	0.41
1:B:1041:ILE:HG13	1:B:1044:LEU:HD22	2.02	0.41
1:B:990:ASN:HA	1:B:991:PRO:HD3	1.81	0.41
1:B:663:ARG:HG2	1:B:1054:TYR:CE1	2.54	0.41
1:B:849:GLU:O	1:B:849:GLU:HG2	2.20	0.41
1:A:847:LEU:HD11	1:A:875:GLN:HB3	2.02	0.41
1:A:645:ALA:O	1:A:649:GLN:HG2	2.20	0.41
1:A:624:LEU:CD1	2:D:7:TRP:HZ3	2.34	0.41
1:A:1058:PRO:HA	1:A:1059:PRO:HD3	1.83	0.41
1:B:902:PHE:HB3	5:B:162:HOH:O	2.20	0.41
1:B:716:LEU:HD13	1:B:987:LEU:HB2	2.03	0.41
1:A:1037:HIS:O	1:A:1038:ASP:C	2.63	0.40
1:A:711:GLY:HA3	1:A:795:ALA:CB	2.48	0.40
1:A:818:ASP:OD2	1:A:928:LYS:NZ	2.52	0.40
1:A:624:LEU:HD11	2:D:7:TRP:HZ3	1.86	0.40
1:A:907:ALA:HB3	1:A:912:GLN:HB3	2.04	0.40
1:A:917:LEU:HD23	1:A:917:LEU:HA	1.87	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	463/491 (94%)	447 (96%)	15 (3%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	466/491 (95%)	447 (96%)	17 (4%)	2 (0%)	30	38
2	C	10/12 (83%)	10 (100%)	0	0	100	100
2	D	7/12 (58%)	6 (86%)	0	1 (14%)	0	0
All	All	946/1006 (94%)	910 (96%)	32 (3%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	6	PHE
1	B	835	ALA
1	B	1039	LEU
1	A	1039	LEU

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	352/387 (91%)	329 (94%)	23 (6%)	15	22
1	B	348/387 (90%)	330 (95%)	18 (5%)	21	31
2	C	9/9 (100%)	5 (56%)	4 (44%)	0	0
2	D	5/9 (56%)	2 (40%)	3 (60%)	0	0
All	All	714/792 (90%)	666 (93%)	48 (7%)	15	21

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

Mol	Chain	Res	Type
1	A	602	GLU
1	A	613	GLU
1	A	620	VAL
1	A	633	LEU
1	A	649	GLN
1	A	668	ARG
1	A	752	LEU

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Mol	Chain	Res	Type
1	A	756	VAL
1	A	802	LEU
1	A	817	ARG
1	A	834	GLU
1	A	840	GLU
1	A	843	ARG
1	A	855	ILE
1	A	891	ARG
1	A	900	ARG
1	A	904	THR
1	A	905	LYS
1	A	992	VAL
1	A	995	MET
1	A	1027	SER
1	A	1034	VAL
1	A	1049	SER
1	B	600	VAL
1	B	621	THR
1	B	669	ASN
1	B	708	VAL
1	B	755	SER
1	B	757	LEU
1	B	798	ILE
1	B	836	MET
1	B	855	ILE
1	B	860	SER
1	B	888	ILE
1	B	923	GLU
1	B	946	ILE
1	B	970	THR
1	B	995	MET
1	B	1039	LEU
1	B	1061	ARG
1	B	1062	PHE
2	C	4	GLU
2	C	6	PHE
2	C	9	MET
2	C	11	VAL
2	D	7	TRP
2	D	9	MET
2	D	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	654	GLN
1	A	670	HIS
1	A	780	GLN
1	A	789	HIS
1	A	1010	GLN
1	A	1037	HIS
1	B	680	HIS
1	B	697	GLN
1	B	780	GLN
1	B	875	GLN
1	B	975	ASN
1	B	1007	HIS
1	B	1010	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
4	SO4	B	9	-	4,4,4	0.60	0	6,6,6	0.29	0
3	GOL	A	4	-	5,5,5	0.43	0	5,5,5	1.23	0
4	SO4	C	13	-	4,4,4	0.59	0	6,6,6	0.42	0
3	GOL	A	6	-	5,5,5	0.49	0	5,5,5	0.53	0
4	SO4	B	11	-	4,4,4	0.65	0	6,6,6	0.79	0
3	GOL	B	3	-	5,5,5	0.53	0	5,5,5	1.36	1 (20%)
3	GOL	B	2	-	5,5,5	1.08	0	5,5,5	1.06	0
4	SO4	B	12	-	4,4,4	0.59	0	6,6,6	0.41	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	GOL	B	2	-	-	2/4/4/4	-
3	GOL	A	4	-	-	2/4/4/4	-
3	GOL	A	6	-	-	4/4/4/4	-
3	GOL	B	3	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	GOL	C3-C2-C1	2.07	119.37	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4	GOL	C1-C2-C3-O3
3	A	6	GOL	O1-C1-C2-C3
3	B	2	GOL	C1-C2-C3-O3
3	A	4	GOL	O2-C2-C3-O3
3	A	6	GOL	O2-C2-C3-O3
3	A	6	GOL	C1-C2-C3-O3
3	A	6	GOL	O1-C1-C2-O2
3	B	2	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	6	GOL	5	0
4	B	11	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	465/491 (94%)	-0.17	7 (1%) 72 73	24, 36, 58, 100	0
1	B	467/491 (95%)	-0.27	13 (2%) 55 57	16, 34, 57, 83	1 (0%)
2	C	12/12 (100%)	1.56	3 (25%) 2 2	41, 48, 74, 75	0
2	D	9/12 (75%)	3.45	9 (100%) 0 0	72, 86, 94, 99	0
All	All	953/1006 (94%)	-0.16	32 (3%) 48 50	16, 36, 60, 100	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	858	VAL	6.0
2	D	7	TRP	5.3
1	A	595	PRO	5.3
1	A	1059	PRO	5.0
2	D	11	VAL	5.0
2	C	12	ALA	4.6
2	D	10	ALA	4.5
1	B	835	ALA	4.5
2	C	7	TRP	4.2
1	B	857	GLU	3.9
1	B	596	GLU	3.6
2	D	8	GLY	3.4
2	D	6	PHE	3.2
2	C	1	SER	3.1
1	A	906	GLY	2.9
1	B	597	LEU	2.8
1	B	902	PHE	2.8
2	D	4	GLU	2.7
1	A	841	TYR	2.6
1	B	598	PRO	2.6
1	B	861	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	903	ALA	2.5
1	A	632	PHE	2.5
2	D	9	MET	2.5
1	B	1062	PHE	2.4
1	B	903	ALA	2.4
2	D	5	ASN	2.3
1	B	860	SER	2.2
1	B	836	MET	2.1
2	D	3	LYS	2.1
1	B	859	PHE	2.1
1	A	633	LEU	2.1

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
4	SO4	B	12	5/5	0.73	0.13	83,84,87,101	0
4	SO4	B	11	5/5	0.74	0.13	88,91,100,102	0
3	GOL	B	2	6/6	0.81	0.21	54,57,67,71	0
3	GOL	A	6	6/6	0.86	0.14	62,67,69,70	0
3	GOL	B	3	6/6	0.87	0.13	45,48,52,59	0
4	SO4	B	9	5/5	0.88	0.09	73,73,77,79	0
3	GOL	A	4	6/6	0.91	0.12	39,50,51,56	0
4	SO4	C	13	5/5	0.96	0.10	52,52,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.