



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:29 AM UTC

PDB ID : 5E7Z / pdb_00005e7z
Title : 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase from Mycobacterium tuberculosis in complex with D/L-tryptophan and D-phenylalanine
Authors : Reichau, S.; Jiao, W.; Parker, E.J.
Deposited on : 2015-10-13
Resolution : 2.40 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

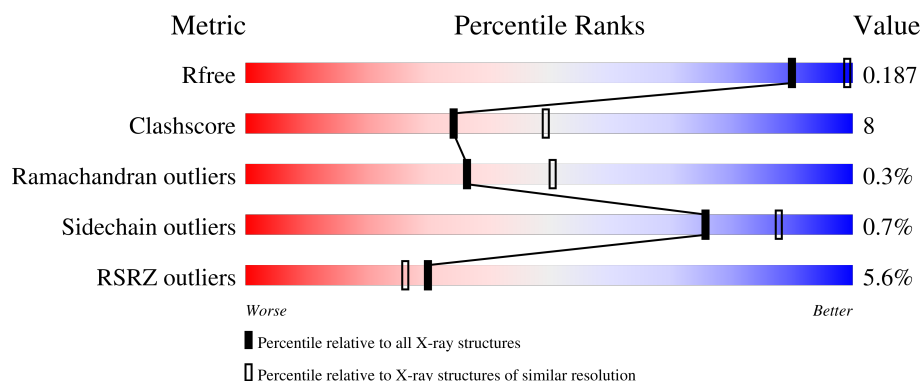
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	464	7% 81% 16% ..
1	B	464	4% 83% 16% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7281 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 3-deoxy-D-arabinoheptulosonate-7-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	1	0
			3527	2203	643	663	18			
1	B	456	Total	C	N	O	S	0	1	0
			3511	2192	640	661	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A0E8NFD1
A	0	ALA	-	expression tag	UNP A0A0E8NFD1
B	-1	GLY	-	expression tag	UNP A0A0E8NFD1
B	0	ALA	-	expression tag	UNP A0A0E8NFD1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

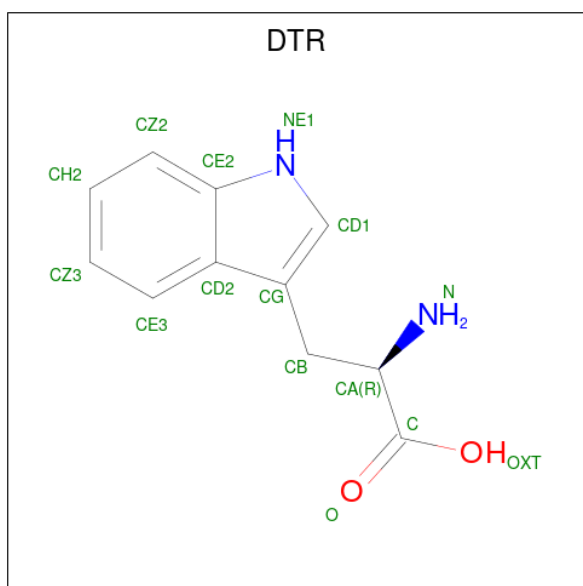


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

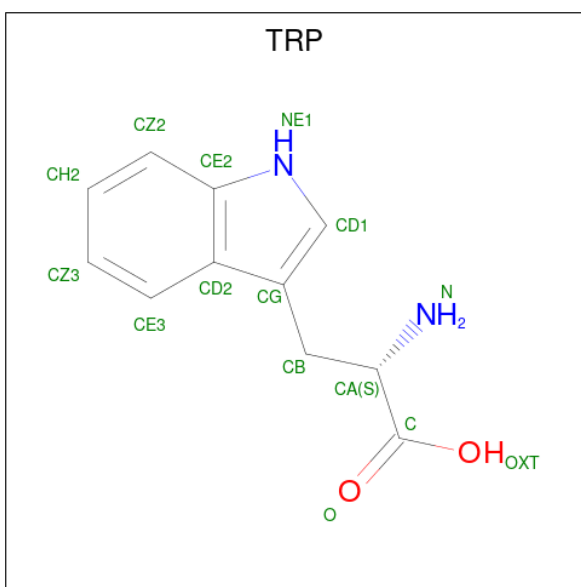
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is D-TRYPTOPHAN (CCD ID: DTR) (formula: C₁₁H₁₂N₂O₂).



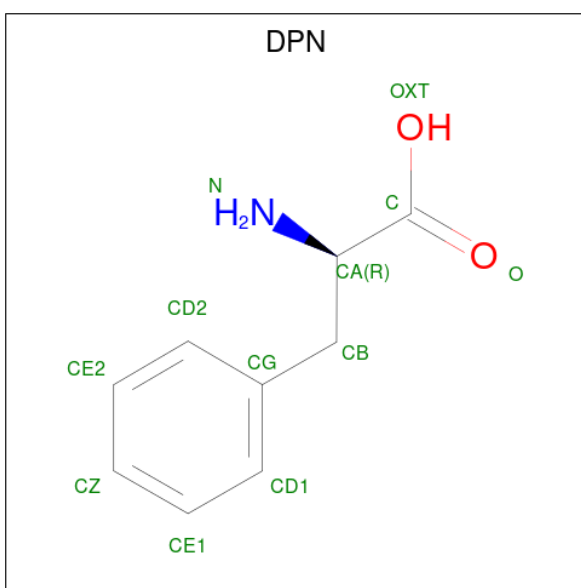
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 11 2 2	0	1
4	B	1	Total C N O 15 11 2 2	0	1

- Molecule 5 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



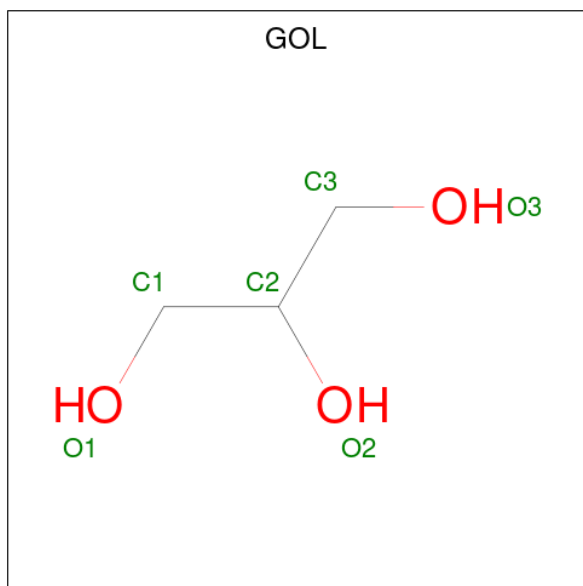
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			15	11	2	2		
5	B	1	Total	C	N	O	0	1
			15	11	2	2		

- Molecule 6 is D-PHENYLALANINE (CCD ID: DPN) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	9	1	2		
6	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

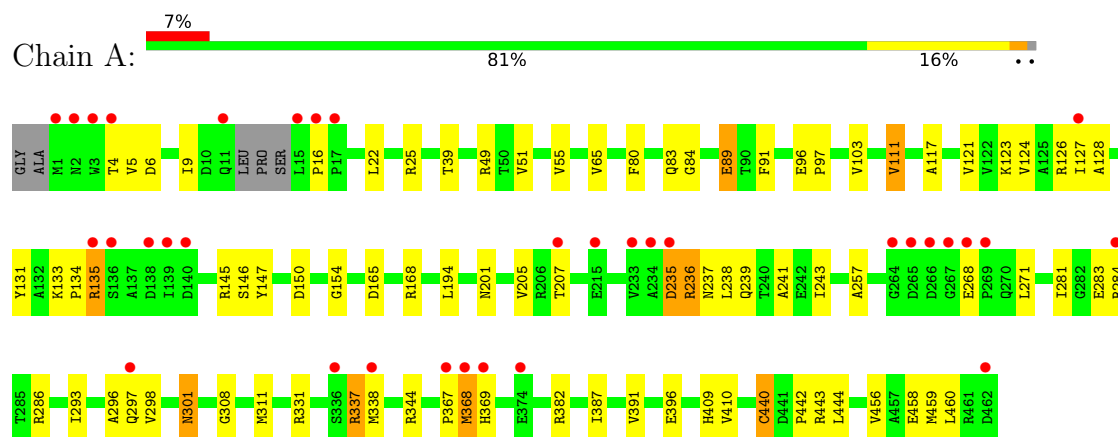
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	62	Total	O	0	0
			62	62		

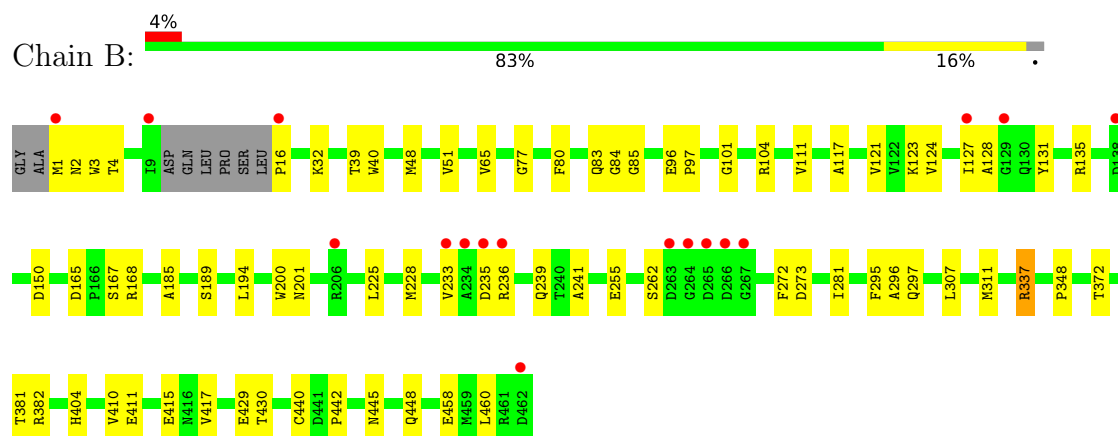
3 Residue-property plots [i](#)

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: 3-deoxy-D-arabinoheptulosonate-7-phosphate synthase



- Molecule 1: 3-deoxy-D-arabinoheptulosonate-7-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.36Å 206.36Å 66.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.55 – 2.40 47.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.55-2.40) 99.9 (47.55-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.137 , 0.161 0.169 , 0.187	Depositor DCC
R_{free} test set	3129 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
Reported twinning fraction	0.690 for H, K, L 0.310 for -h,-k,l	Depositor
Outliers	0 of 63886 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: DTR, GOL, DPN, SO4, MN

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	1.20	7/3602 (0.2%)	1.17	12/4900 (0.2%)
1	B	1.27	3/3586 (0.1%)	1.18	12/4877 (0.2%)
All	All	1.23	10/7188 (0.1%)	1.17	24/9777 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	GLN	CA-C	-6.13	1.44	1.52
1	A	147	TYR	C-O	-5.97	1.16	1.23
1	A	111	VAL	C-O	-5.48	1.17	1.24
1	A	165	ASP	C-O	-5.36	1.19	1.24
1	B	51	VAL	C-O	-5.26	1.18	1.24
1	B	3	TRP	CA-C	-5.24	1.46	1.52
1	A	154	GLY	N-CA	5.20	1.51	1.45
1	A	301	ASN	C-O	-5.14	1.17	1.23
1	A	16	PRO	CA-C	5.09	1.56	1.52
1	A	239	GLN	C-O	-5.03	1.17	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	MET	N-CA-C	10.29	122.50	111.28
1	A	207	THR	N-CA-C	8.92	122.67	111.69
1	A	369	HIS	N-CA-C	7.86	119.93	111.36
1	A	298	VAL	N-CA-C	6.57	117.32	110.62
1	A	16	PRO	CA-C-N	-6.33	114.14	120.21
1	A	16	PRO	C-N-CA	-6.33	114.14	120.21
1	B	16	PRO	CA-C-N	-6.27	113.82	120.03
1	B	16	PRO	C-N-CA	-6.27	113.82	120.03
1	A	135	ARG	N-CA-C	6.13	119.19	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	N-CA-C	5.97	119.35	110.52
1	A	55	VAL	CA-C-N	5.54	126.09	120.38
1	A	55	VAL	C-N-CA	5.54	126.09	120.38
1	A	146	SER	N-CA-C	5.48	117.80	110.35
1	B	430	THR	CB-CA-C	-5.32	102.53	110.88
1	B	40	TRP	N-CA-C	-5.26	103.48	108.22
1	B	348	PRO	CA-C-N	-5.25	113.51	119.28
1	B	348	PRO	C-N-CA	-5.25	113.51	119.28
1	B	429	GLU	CA-C-N	5.23	127.25	120.44
1	B	429	GLU	C-N-CA	5.23	127.25	120.44
1	A	89	GLU	N-CA-C	-5.17	102.83	110.48
1	B	32	LYS	CA-C-N	-5.03	114.58	119.76
1	B	32	LYS	C-N-CA	-5.03	114.58	119.76
1	B	39	THR	N-CA-C	-5.02	99.24	108.02
1	B	295	PHE	N-CA-C	-5.02	105.89	111.36

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	3527	0	3480	67	1
1	B	3511	0	3465	53	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	11	0	0
4	B	15	0	11	0	0
5	A	15	0	9	0	0
5	B	15	0	9	0	0
6	A	12	0	10	1	0
6	B	12	0	10	0	0
7	B	6	0	8	0	0
8	A	69	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	62	0	0	1	0
All	All	7281	0	7013	107	1

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 (107) 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:307:LEU:CD2	1:B:311:MET:HE3	1.64	1.24
1:B:307:LEU:HD22	1:B:311:MET:CE	1.79	1.12
1:A:456:VAL:HG22	1:A:459:MET:CE	1.97	0.93
1:A:5:VAL:CG1	1:B:48:MET:HE1	1.99	0.91
1:B:307:LEU:HD22	1:B:311:MET:HE3	0.86	0.86
1:A:5:VAL:HG13	1:B:48:MET:HE1	1.56	0.85
1:A:456:VAL:HA	1:A:459:MET:CE	2.07	0.84
1:A:133:LYS:NZ	1:A:440:CYS:SG	2.53	0.81
1:A:456:VAL:HG22	1:A:459:MET:HE1	1.63	0.80
1:B:48:MET:HE3	1:B:167:SER:HA	1.63	0.80
1:A:456:VAL:HA	1:A:459:MET:HE3	1.65	0.76
1:A:268:GLU:N	1:A:268:GLU:OE1	2.19	0.75
1:A:6:ASP:OD1	1:B:4:THR:HG22	1.87	0.75
1:A:293:ILE:O	1:A:297:GLN:HG3	1.89	0.72
1:A:39:THR:HB	1:A:145:ARG:HH22	1.56	0.71
1:B:48:MET:CE	1:B:167:SER:HA	2.20	0.70
1:A:5:VAL:HG11	1:B:48:MET:HE1	1.75	0.68
1:A:456:VAL:HA	1:A:459:MET:HE2	1.75	0.68
1:A:367:PRO:HB2	1:A:387:ILE:HG23	1.75	0.67
1:B:225:LEU:HD23	1:B:228:MET:HE3	1.77	0.65
1:A:368:MET:HE1	1:A:444:LEU:HG	1.79	0.65
1:A:117:ALA:HB2	1:A:460:LEU:HD13	1.79	0.63
1:B:307:LEU:CD2	1:B:311:MET:CE	2.56	0.62
1:A:22:LEU:HD23	1:A:25:ARG:NH1	2.15	0.62
1:A:235:ASP:O	1:A:237:ASN:N	2.33	0.61
1:B:445[B]:ASN:ND2	1:B:448:GLN:HG3	2.16	0.60
1:A:5:VAL:HG11	1:B:48:MET:SD	2.42	0.60
1:A:382:ARG:HD2	1:A:442:PRO:HG2	1.83	0.59
1:A:6:ASP:OD1	1:B:4:THR:CG2	2.50	0.59
1:A:308:GLY:C	1:A:338:MET:SD	2.87	0.58
1:B:228:MET:O	1:B:233:VAL:HG22	2.04	0.58
1:B:48:MET:HE3	1:B:167:SER:CA	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:CG1	1:B:48:MET:CE	2.78	0.57
1:B:1:MET:HG2	1:B:2:ASN:H	1.69	0.57
1:B:458:GLU:OE1	1:B:458:GLU:HA	2.03	0.57
1:B:104:ARG:HG3	1:B:200:TRP:CZ3	2.40	0.56
1:A:127:ILE:HG12	1:A:128:ALA:N	2.20	0.56
1:A:281:ILE:HD11	1:A:296:ALA:HB2	1.87	0.56
1:A:301:ASN:O	1:A:331:ARG:NH1	2.39	0.56
1:A:5:VAL:HG11	1:B:48:MET:CE	2.35	0.55
1:A:150:ASP:O	1:A:168:ARG:HD3	2.07	0.55
1:A:127:ILE:HG12	1:A:128:ALA:H	1.72	0.55
1:B:381:THR:HA	1:B:442:PRO:HG3	1.88	0.55
1:A:458:GLU:HA	1:A:458:GLU:OE1	2.07	0.54
1:A:443:ARG:HD3	8:A:646:HOH:O	2.07	0.53
1:A:9:ILE:HG21	1:A:51:VAL:HG21	1.91	0.53
1:A:39:THR:HB	1:A:145:ARG:NH2	2.23	0.52
1:A:131:TYR:OH	8:A:601:HOH:O	1.91	0.52
1:A:96:GLU:HB3	1:A:97:PRO:HD3	1.92	0.52
1:A:456:VAL:CG2	1:A:459:MET:CE	2.82	0.52
1:A:344:ARG:NH1	1:A:396:GLU:OE1	2.43	0.52
1:B:131:TYR:OH	8:B:602:HOH:O	2.15	0.51
1:A:4:THR:CG2	1:B:4:THR:HB	2.42	0.50
1:A:123:LYS:HE3	1:A:241:ALA:HB1	1.93	0.50
1:A:89:GLU:OE2	1:A:127:ILE:HG13	2.10	0.50
1:A:126:ARG:NH1	1:A:409:HIS:NE2	2.54	0.50
1:B:123:LYS:HE3	1:B:241:ALA:HB1	1.93	0.50
1:B:255:GLU:OE1	1:B:273:ASP:OD2	2.30	0.50
1:A:6:ASP:HA	1:B:4:THR:HG22	1.95	0.48
1:A:391:VAL:CG1	1:A:459:MET:HE1	2.44	0.48
1:B:127:ILE:HG12	1:B:128:ALA:N	2.29	0.48
1:A:4:THR:HG22	1:A:5:VAL:N	2.29	0.48
1:B:150:ASP:O	1:B:168:ARG:HD3	2.14	0.47
1:B:382:ARG:HD2	1:B:442:PRO:HG2	1.95	0.47
1:A:4:THR:HG21	1:B:4:THR:HB	1.97	0.47
1:A:111:VAL:HG23	1:A:194:LEU:HD11	1.98	0.46
1:A:49:ARG:HG2	1:A:257:ALA:HB2	1.98	0.46
1:A:84:GLY:HA2	1:A:410:VAL:O	2.15	0.46
1:A:235:ASP:C	1:A:237:ASN:N	2.73	0.46
1:A:5:VAL:HG13	1:B:48:MET:CE	2.37	0.46
1:B:337:ARG:O	1:B:337:ARG:HD3	2.16	0.46
1:A:91:PHE:O	6:A:506:DPN:N	2.49	0.45
1:A:135:ARG:HA	1:A:135:ARG:HD2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PHE:O	1:A:121:VAL:HA	2.17	0.44
1:A:22:LEU:HD13	1:A:271:LEU:HD13	1.99	0.44
1:B:117:ALA:HB2	1:B:460:LEU:HD13	1.98	0.44
1:A:311:MET:HA	1:A:311:MET:HE2	2.00	0.44
1:B:135:ARG:HD2	1:B:135:ARG:HA	1.64	0.44
1:B:111:VAL:HG23	1:B:194:LEU:HD11	2.00	0.44
1:A:194:LEU:HD23	1:A:238:LEU:HD22	2.00	0.44
1:A:283:GLU:CD	1:A:286:ARG:HH21	2.25	0.44
1:B:80:PHE:O	1:B:121:VAL:HA	2.18	0.43
1:A:337:ARG:HD3	1:A:337:ARG:O	2.17	0.43
1:A:9:ILE:CG2	1:A:51:VAL:HG21	2.48	0.43
1:A:103:VAL:HG13	1:A:243:ILE:HD12	2.00	0.43
1:B:101:GLY:HA2	1:B:104:ARG:NH2	2.33	0.43
1:B:372:THR:HA	1:B:382:ARG:HG2	2.01	0.43
1:A:133:LYS:CE	1:A:440:CYS:SG	3.06	0.43
1:A:236:ARG:NH2	1:B:236:ARG:HG2	2.34	0.43
1:B:96:GLU:HB3	1:B:97:PRO:HD3	2.01	0.43
1:B:127:ILE:HG12	1:B:128:ALA:H	1.84	0.43
1:B:165:ASP:OD1	1:B:167:SER:OG	2.36	0.42
1:A:83:GLN:HA	1:A:124:VAL:O	2.20	0.42
1:B:111:VAL:CG1	1:B:201:ASN:ND2	2.83	0.42
1:B:235:ASP:O	1:B:239:GLN:HG2	2.20	0.42
1:B:417:VAL:O	1:B:445[A]:ASN:OD1	2.38	0.42
1:B:281:ILE:HD11	1:B:296:ALA:HB2	2.00	0.42
1:A:391:VAL:HG11	1:A:459:MET:HE1	2.02	0.41
1:B:185:ALA:O	1:B:189:SER:HB2	2.20	0.41
1:B:83:GLN:HA	1:B:124:VAL:O	2.20	0.41
1:B:84:GLY:HA2	1:B:410:VAL:O	2.20	0.41
1:A:134:PRO:HB2	1:A:284:ARG:HD3	2.03	0.41
1:A:39:THR:HG22	1:A:39:THR:O	2.20	0.41
1:A:201:ASN:O	1:A:205:VAL:HG23	2.21	0.41
1:B:85:GLY:O	1:B:411:GLU:HA	2.21	0.40
1:B:262:SER:HB3	1:B:272:PHE:CE1	2.56	0.40
1:B:77:GLY:HA2	1:B:404:HIS:CG	2.57	0.40

All (1) 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:A:235:ASP:OD2	1:A:235:ASP:OD2[6_554]	1.88	0.32

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	456/464 (98%)	446 (98%)	8 (2%)	2 (0%)	30	43
1	B	453/464 (98%)	446 (98%)	6 (1%)	1 (0%)	43	58
All	All	909/928 (98%)	892 (98%)	14 (2%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ARG
1	B	440	CYS
1	A	440	CYS

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	370/376 (98%)	368 (100%)	2 (0%)	81	91
1	B	369/376 (98%)	366 (99%)	3 (1%)	73	86
All	All	739/752 (98%)	734 (99%)	5 (1%)	76	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	337	ARG
1	B	65	VAL

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	415	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	B	447	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](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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	DTR	B	505[A]	-	15,16,16	1.08	0	18,22,22	1.00	0
2	SO4	B	501	-	4,4,4	0.49	0	6,6,6	0.50	0
2	SO4	A	501	-	4,4,4	0.41	0	6,6,6	0.09	0
6	DPN	A	506	-	11,12,12	0.70	0	11,15,15	0.77	0
2	SO4	A	502	-	4,4,4	0.56	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DTR	A	504[A]	-	15,16,16	1.22	1 (6%)	18,22,22	1.00	1 (5%)
6	DPN	B	507	-	11,12,12	0.71	0	11,15,15	0.77	0
5	TRP	A	505[B]	-	15,16,16	0.67	0	18,22,22	0.41	0
2	SO4	B	502	-	4,4,4	0.76	0	6,6,6	0.92	0
7	GOL	B	504	-	5,5,5	0.81	0	5,5,5	0.66	0
5	TRP	B	506[B]	-	15,16,16	0.69	0	18,22,22	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
4	DTR	B	505[A]	-	-	2/8/8/8	0/2/2/2
6	DPN	A	506	-	-	1/8/8/8	0/1/1/1
6	DPN	B	507	-	-	1/8/8/8	0/1/1/1
4	DTR	A	504[A]	-	-	4/8/8/8	0/2/2/2
5	TRP	A	505[B]	-	-	1/8/8/8	0/2/2/2
7	GOL	B	504	-	-	2/4/4/4	-
5	TRP	B	506[B]	-	-	0/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504[A]	DTR	CH2-CZ2	2.06	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504[A]	DTR	CE3-CD2-CE2	2.12	121.04	118.84

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504[A]	DTR	N-CA-CB-CG
4	A	504[A]	DTR	O-C-CA-N
4	B	505[A]	DTR	O-C-CA-N
4	A	504[A]	DTR	OXT-C-CA-N
4	B	505[A]	DTR	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
7	B	504	GOL	C1-C2-C3-O3
4	A	504[A]	DTR	C-CA-CB-CG
7	B	504	GOL	O2-C2-C3-O3
5	A	505[B]	TRP	O-C-CA-N
6	B	507	DPN	C-CA-CB-CG
6	A	506	DPN	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	506	DPN	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	459/464 (98%)	0.08	34 (7%)	20 17	13, 34, 64, 109	2 (0%)
1	B	456/464 (98%)	-0.17	17 (3%)	45 41	16, 29, 58, 101	1 (0%)
All	All	915/928 (98%)	-0.04	51 (5%)	30 26	13, 31, 61, 109	3 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	LEU	6.6
1	A	234	ALA	6.4
1	B	267	GLY	5.5
1	B	234	ALA	5.4
1	A	235	ASP	5.4
1	A	16	PRO	5.3
1	B	16	PRO	5.2
1	A	336	SER	5.2
1	A	3	TRP	4.4
1	A	1	MET	4.4
1	B	235	ASP	4.4
1	A	269	PRO	4.1
1	B	138	ASP	3.9
1	B	9	ILE	3.7
1	A	11	GLN	3.6
1	B	462	ASP	3.6
1	A	4	THR	3.5
1	A	267	GLY	3.5
1	B	263	ASP	3.4
1	A	338	MET	3.4
1	A	17	PRO	3.4
1	B	1	MET	3.3
1	A	266	ASP	3.3
1	B	265	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	ASP	3.2
1	A	462	ASP	3.1
1	A	233	VAL	2.9
1	A	264	GLY	2.9
1	A	297	GLN	2.9
1	A	368	MET	2.9
1	B	206	ARG	2.8
1	B	264	GLY	2.8
1	A	284	ARG	2.8
1	A	138	ASP	2.7
1	A	127	ILE	2.6
1	B	233	VAL	2.6
1	A	136	SER	2.5
1	A	265	ASP	2.4
1	B	236	ARG	2.4
1	A	207	THR	2.3
1	A	135	ARG	2.3
1	A	2	ASN	2.2
1	B	127	ILE	2.2
1	A	215	GLU	2.2
1	B	129	GLY	2.1
1	A	374	GLU	2.1
1	A	369	HIS	2.1
1	A	140	ASP	2.1
1	A	367	PRO	2.1
1	A	139	ILE	2.0
1	A	268	GLU	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
2	SO4	A	501	5/5	0.81	0.23	48,54,64,66	0
5	TRP	A	505[B]	15/15	0.89	0.10	23,23,27,30	15
5	TRP	B	506[B]	15/15	0.90	0.09	19,19,23,24	15
4	DTR	B	505[A]	15/15	0.93	0.09	22,22,31,31	15
4	DTR	A	504[A]	15/15	0.94	0.09	25,27,38,44	15
6	DPN	A	506	12/12	0.94	0.10	22,24,28,28	0
2	SO4	B	502	5/5	0.95	0.12	39,48,53,59	0
6	DPN	B	507	12/12	0.95	0.09	28,31,34,36	0
7	GOL	B	504	6/6	0.96	0.09	37,40,42,43	0
3	MN	B	503	1/1	0.97	0.04	37,37,37,37	0
2	SO4	A	502	5/5	0.98	0.10	31,34,35,40	0
2	SO4	B	501	5/5	0.99	0.07	33,34,37,38	0
3	MN	A	503	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.