



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:21 PM UTC

PDB ID : 5DCC / pdb_00005dcc
Title : X-RAY CRYSTAL STRUCTURE OF a TEBIPENEM ADDUCT OF L,D
TRANSPEPTIDASE 2 FROM MYCOBACTERIUM TUBERCULOSIS
Authors : Pan, Y.; Basta, L.; Lamichhane, G.; Bianchet, M.A.
Deposited on : 2015-08-23
Resolution : 2.45 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

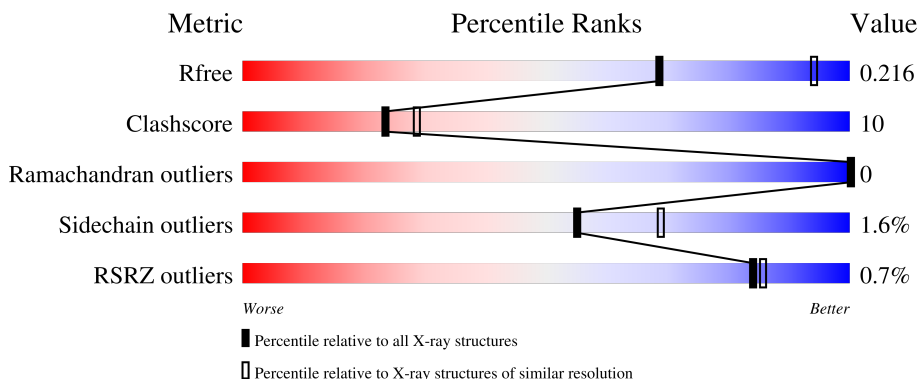
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


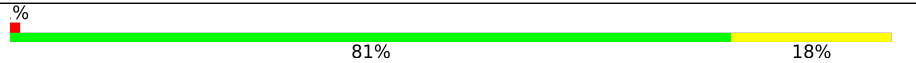
The reported resolution of this entry is 2.45 Å.

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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	353	 80% 19%
1	B	353	 81% 18%

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	SO4	A	506	-	-	X	-
4	PEG	A	508	-	-	X	-

2 Entry composition [i](#)

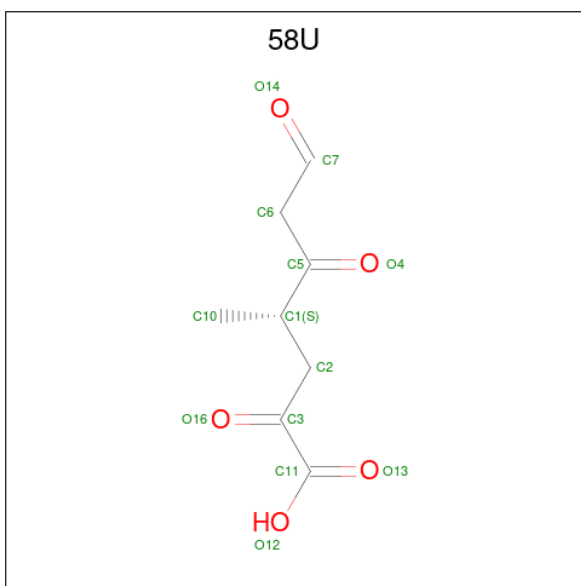
There are 8 unique types of molecules in this entry. The entry contains 6068 atoms, of which 48 are hydrogens and 0 are deuteriums.

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 L,D-transpeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	Total 2687	C 1685	N 473	O 521	S 8	0	4	0
1	B	353	Total 2708	C 1694	N 477	O 527	S 10	0	7	0

- Molecule 2 is (4S)-4-methyl-2,5,7-trioxoheptanoic acid (CCD ID: 58U) (formula: C₈H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 13	C 8	O 5	0	0
2	B	1	Total 13	C 8	O 5	0	0

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



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C H O 17 4 10 3	0	0
4	B	1	Total C H O 17 4 10 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



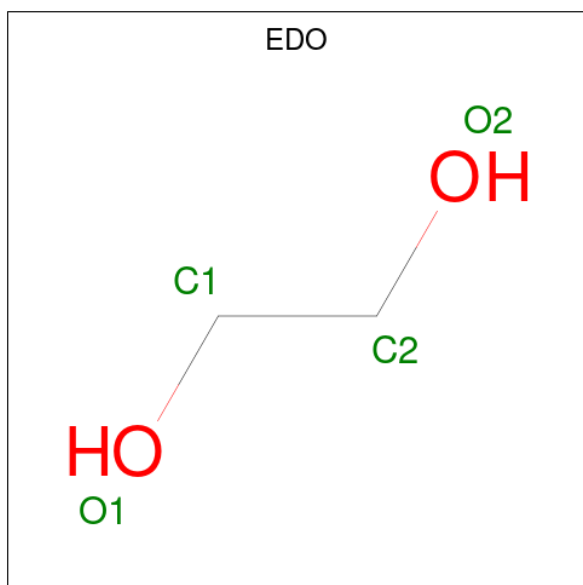
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C H O 24 6 14 4	0	0
5	A	1	Total C H O 24 6 14 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	2	1		
7	B	1	Total	C	O	0	0
			3	2	1		

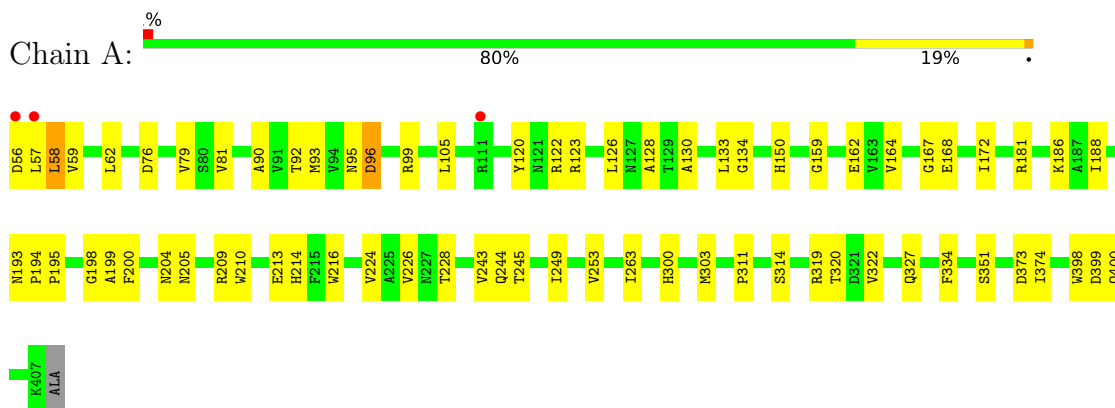
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	209	Total	O	0	0
			209	209		
8	B	200	Total	O	0	0
			200	200		

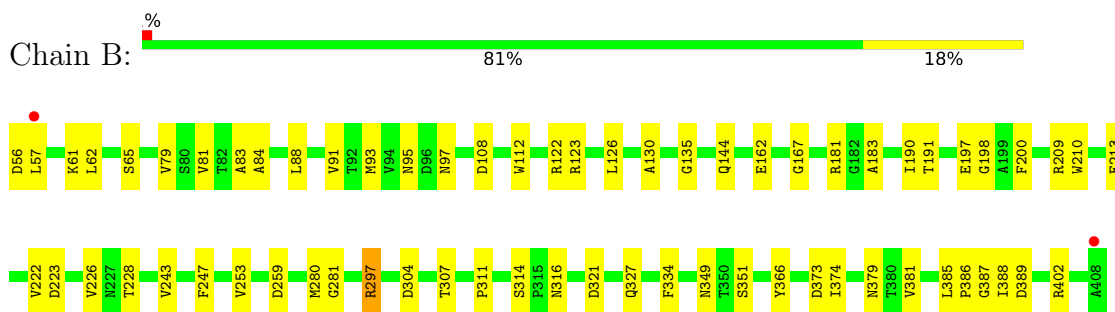
3 Residue-property plots [i](#)

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: L,D-transpeptidase 2



- Molecule 1: L,D-transpeptidase 2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.93Å 94.40Å 75.39Å 90.00° 92.88° 90.00°	Depositor
Resolution (Å)	43.16 – 2.45 43.16 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.1 (43.16-2.45) 99.0 (43.16-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.168 , 0.214 0.173 , 0.216	Depositor DCC
R_{free} test set	3112 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.090 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6068	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 58U, GOL, PEG, EDO, PGE, 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	0.31	0/2754	0.71	0/3770
1	B	0.31	0/2794	0.71	1/3820 (0.0%)
All	All	0.31	0/5548	0.71	1/7590 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLY	N-CA-C	5.19	118.31	111.52

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	2687	0	2585	62	1
1	B	2708	0	2584	46	1
2	A	13	0	0	3	0
2	B	13	0	0	1	0
3	A	25	0	0	3	0
3	B	20	0	0	1	0
4	A	15	0	20	12	0
4	B	30	20	40	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	40	28	56	7	0
5	B	30	0	42	2	0
6	A	12	0	16	1	0
6	B	12	0	16	0	0
7	A	3	0	3	0	0
7	B	3	0	3	0	0
8	A	209	0	0	10	1
8	B	200	0	0	6	0
All	All	6020	48	5365	112	2

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 10.

All (112) 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:199:ALA:HB1	4:A:508:PEG:H41	1.28	1.11
1:B:316:ASN:OD1	8:B:601:HOH:O	1.82	0.97
1:B:387:GLY:H	4:B:508:PEG:H42	1.31	0.94
1:A:210:TRP:HE1	4:A:509:PEG:H22	1.36	0.89
1:A:205:ASN:H	4:A:507:PEG:H32	1.46	0.81
1:B:123:ARG:HG3	1:B:144[A]:GLN:HG2	1.64	0.79
1:A:199:ALA:HB1	4:A:508:PEG:C4	2.14	0.75
1:A:204:ASN:HB2	4:A:507:PEG:H32	1.69	0.73
1:A:400:GLN:O	8:A:602:HOH:O	2.04	0.73
1:A:96:ASP:OD2	1:A:96:ASP:N	2.18	0.73
1:A:105:LEU:O	8:A:603:HOH:O	2.08	0.71
1:A:123:ARG:NH1	8:A:608:HOH:O	2.25	0.70
1:A:213:GLU:HG3	1:A:398:TRP:CG	2.27	0.68
1:A:351:SER:HB2	2:A:501:58U:C2	2.23	0.68
1:B:387:GLY:N	4:B:508:PEG:H42	2.07	0.68
1:B:181:ARG:HH22	5:B:514:PGE:H12	1.59	0.67
1:A:81:VAL:CG2	1:A:126[B]:LEU:HD21	2.27	0.65
1:A:92:THR:HA	5:A:512:PGE:H6	1.80	0.63
1:A:95:ASN:HD21	1:A:99:ARG:HB3	1.65	0.61
1:A:172:ILE:HD13	1:A:188:ILE:HD13	1.83	0.61
2:A:501:58U:O13	8:A:604:HOH:O	2.16	0.61
1:A:204:ASN:HB2	4:A:507:PEG:C3	2.30	0.61
1:B:81:VAL:CG2	1:B:126:LEU:HD21	2.31	0.61
1:A:93:MET:HE3	1:A:126[A]:LEU:HD21	1.82	0.60
1:B:297[A]:ARG:HG2	1:B:366:TYR:CD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:HB2	4:A:508:PEG:H32	1.85	0.58
1:B:281:GLY:O	8:B:602:HOH:O	2.17	0.58
3:A:505:SO4:O4	8:A:605:HOH:O	2.17	0.57
1:A:300:HIS:ND1	8:A:601:HOH:O	1.97	0.57
1:A:200:PHE:H	4:A:508:PEG:C3	2.18	0.57
5:A:513:PGE:H12	1:B:197:GLU:HA	1.88	0.56
1:B:167:GLY:HA3	1:B:374:ILE:HD11	1.88	0.56
1:A:199:ALA:CB	4:A:508:PEG:H41	2.20	0.55
1:A:200:PHE:H	4:A:508:PEG:H32	1.71	0.54
1:B:351:SER:HB2	2:B:501:58U:C2	2.37	0.54
1:A:210:TRP:NE1	4:A:509:PEG:H22	2.15	0.54
1:B:213:GLU:OE2	8:B:603:HOH:O	2.17	0.54
1:B:81:VAL:HG22	1:B:126:LEU:HD21	1.91	0.53
1:B:162:GLU:HG3	4:B:510:PEG:C2	2.39	0.53
1:B:183:ALA:HB1	4:B:511:PEG:H41	1.91	0.52
1:B:297[A]:ARG:HD3	8:B:632:HOH:O	2.09	0.52
1:A:263:ILE:HB	5:A:513:PGE:H62	1.92	0.52
1:A:92:THR:O	1:A:126[B]:LEU:HD12	2.09	0.52
1:A:90:ALA:O	1:A:128:ALA:HA	2.10	0.52
1:A:214:HIS:HB3	5:A:510:PGE:C3	2.40	0.51
1:B:122:ARG:NH1	3:B:503:SO4:O4	2.42	0.51
1:A:311:PRO:HB2	1:A:314:SER:OG	2.10	0.51
1:B:162:GLU:HG3	4:B:510:PEG:H22	1.92	0.51
1:B:259:ASP:HB3	1:B:379:ASN:O	2.10	0.51
1:A:226:VAL:HB	1:A:243:VAL:HG22	1.91	0.50
1:B:253:VAL:HB	1:B:373:ASP:CG	2.36	0.50
1:B:198:GLY:HA3	1:B:210:TRP:CZ2	2.47	0.50
1:A:181:ARG:HH12	6:A:514:GOL:HO1	1.55	0.50
1:A:79:VAL:HG11	1:A:93:MET:HE1	1.94	0.50
1:A:327:GLN:HB2	1:A:334:PHE:CE2	2.46	0.50
1:B:91:VAL:HG11	1:B:112:TRP:CD2	2.47	0.49
1:B:304:ASP:O	1:B:307:THR:HB	2.13	0.49
1:A:198:GLY:HA3	1:A:210:TRP:CZ2	2.49	0.48
1:A:263:ILE:HB	5:A:513:PGE:C6	2.43	0.48
1:B:190:ILE:HD13	1:B:210:TRP:CG	2.48	0.47
1:B:280:MET:O	1:B:349:ASN:HB3	2.14	0.47
1:A:193:ASN:HA	1:A:194:PRO:C	2.39	0.47
1:A:58:LEU:O	1:A:134:GLY:HA3	2.15	0.47
1:B:327:GLN:HB2	1:B:334:PHE:CE2	2.50	0.47
1:B:226:VAL:HB	1:B:243:VAL:CG2	2.45	0.47
1:A:164:VAL:HG21	1:A:168:GLU:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HB	1:A:373:ASP:CG	2.40	0.47
1:A:99:ARG:HD3	3:A:506:SO4:O4	2.15	0.47
1:A:93:MET:HE2	1:A:126[A]:LEU:HG	1.98	0.46
1:B:388:ILE:HG21	5:B:514:PGE:H52	1.97	0.46
1:A:216:TRP:HB3	1:A:249:ILE:HG13	1.97	0.46
1:A:226:VAL:HB	1:A:243:VAL:CG2	2.46	0.46
1:A:399:ASP:HB2	1:B:65:SER:HA	1.96	0.46
1:B:200:PHE:HA	1:B:209:ARG:O	2.17	0.45
1:A:159:GLY:O	1:A:162:GLU:HB2	2.17	0.45
1:A:200:PHE:HA	1:A:209:ARG:O	2.17	0.45
5:A:511:PGE:H32	5:A:511:PGE:H5	1.36	0.45
1:B:198:GLY:HA3	1:B:210:TRP:CH2	2.52	0.45
1:A:81:VAL:HG21	1:A:126[B]:LEU:HD21	1.96	0.45
1:A:320:THR:HG22	1:A:322:VAL:HG13	1.99	0.45
1:A:95:ASN:ND2	1:A:99:ARG:HB3	2.31	0.45
1:A:62:LEU:HD21	1:A:130:ALA:HB2	1.99	0.44
1:B:83:ALA:HB2	1:B:88:LEU:CD2	2.47	0.44
1:A:167:GLY:HA3	1:A:374:ILE:HD11	1.99	0.44
5:A:513:PGE:O4	8:A:606:HOH:O	2.17	0.43
1:B:316:ASN:HA	8:B:601:HOH:O	2.18	0.43
1:B:56:ASP:CG	1:B:57:LEU:H	2.25	0.43
1:A:224:VAL:HB	1:A:245:THR:HG22	2.00	0.43
4:A:509:PEG:H21	8:A:657:HOH:O	2.18	0.43
1:B:62:LEU:HD21	1:B:130:ALA:HB2	2.01	0.43
1:A:57:LEU:HD13	1:A:133:LEU:HB3	2.00	0.42
1:A:123:ARG:HD3	8:A:793:HOH:O	2.19	0.42
1:A:95:ASN:ND2	3:A:506:SO4:O4	2.50	0.42
1:A:194:PRO:HA	1:A:195:PRO:HD3	1.90	0.42
1:B:222:VAL:HG11	1:B:247:PHE:CZ	2.55	0.42
1:B:311:PRO:HB2	1:B:314:SER:OG	2.19	0.42
1:B:226:VAL:HB	1:B:243:VAL:HG22	2.00	0.42
1:B:61:LYS:HB2	1:B:84:ALA:HB3	2.02	0.42
1:A:93:MET:HB2	1:A:126[B]:LEU:HD13	2.01	0.42
1:B:381:VAL:HG22	8:B:696:HOH:O	2.18	0.41
1:B:79:VAL:HG11	1:B:93[B]:MET:HE1	2.01	0.41
1:B:297[A]:ARG:HH21	1:B:297[A]:ARG:HG3	1.85	0.41
1:A:244:GLN:O	1:A:244:GLN:HG3	2.20	0.41
1:A:56:ASP:N	1:A:56:ASP:OD1	2.53	0.41
1:A:120:TYR:O	1:A:122:ARG:HG3	2.21	0.41
1:B:191:THR:HB	1:B:223:ASP:HB3	2.03	0.41
1:A:303:MET:HE1	2:A:501:58U:C10	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HD12	1:B:386:PRO:HD2	2.03	0.41
1:A:319:ARG:NH1	8:A:625:HOH:O	2.51	0.40
1:A:76:ASP:OD1	1:A:76:ASP:N	2.54	0.40
1:B:95:ASN:C	1:B:97:ASN:H	2.29	0.40

All (2) 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)
8:A:744:HOH:O	8:A:748:HOH:O[1_556]	2.08	0.12
1:A:150[A]:HIS:ND1	1:B:321:ASP:OD2[1_656]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/353 (100%)	341 (97%)	12 (3%)	0	100	100
1	B	358/353 (101%)	347 (97%)	11 (3%)	0	100	100
All	All	711/706 (101%)	688 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/283 (101%)	281 (98%)	5 (2%)	53	67
1	B	290/283 (102%)	285 (98%)	5 (2%)	53	67
All	All	576/566 (102%)	566 (98%)	10 (2%)	55	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	59	VAL
1	A	96	ASP
1	A	186	LYS
1	A	228	THR
1	B	228	THR
1	B	297[A]	ARG
1	B	297[B]	ARG
1	B	389	ASP
1	B	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	B	150	HIS
1	B	316	ASN

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

33 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	A	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.10	0
4	PEG	A	509	-	6,6,6	0.46	0	5,5,5	0.35	0
6	GOL	B	515	-	5,5,5	0.40	0	5,5,5	0.26	0
3	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	B	506	-	3,3,6	0.42	0	2,2,5	0.38	0
4	PEG	B	508	-	3,3,6	0.44	0	2,2,5	0.37	0
4	PEG	A	508	-	3,3,6	0.40	0	2,2,5	0.34	0
4	PEG	B	507	-	3,3,6	0.43	0	2,2,5	0.37	0
3	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.04	0
3	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.07	0
4	PEG	A	507	-	3,3,6	0.42	0	2,2,5	0.37	0
3	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	505	-	4,4,4	0.23	0	6,6,6	0.07	0
5	PGE	B	514	-	9,9,9	0.33	0	8,8,8	0.27	0
3	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.07	0
5	PGE	B	513	-	9,9,9	0.34	0	8,8,8	0.22	0
2	58U	A	501	1	10,12,12	1.75	1 (10%)	10,15,15	1.52	2 (20%)
2	58U	B	501	1	10,12,12	1.75	1 (10%)	10,15,15	1.61	4 (40%)
6	GOL	A	515	-	5,5,5	0.34	0	5,5,5	0.36	0
6	GOL	B	516	-	5,5,5	0.35	0	5,5,5	0.33	0
5	PGE	B	512	-	9,9,9	0.32	0	8,8,8	0.30	0
5	PGE	A	511	-	9,9,9	0.32	0	8,8,8	0.30	0
5	PGE	A	513	-	9,9,9	0.33	0	8,8,8	0.17	0
5	PGE	A	510	-	9,9,9	0.33	0	8,8,8	0.32	0
6	GOL	A	514	-	5,5,5	0.38	0	5,5,5	0.19	0
7	EDO	B	517	-	2,2,3	0.79	0	1,1,2	0.52	0
5	PGE	A	512	-	9,9,9	0.35	0	8,8,8	0.32	0
4	PEG	B	510	-	6,6,6	0.46	0	5,5,5	0.21	0
3	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.08	0
7	EDO	A	516	-	2,2,3	0.81	0	1,1,2	0.54	0
4	PEG	B	511	-	6,6,6	0.48	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	B	509	-	3,3,6	0.44	0	2,2,5	0.37	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	PEG	A	509	-	-	1/4/4/4	-
6	GOL	B	515	-	-	2/4/4/4	-
4	PEG	B	506	-	-	1/1/1/4	-
4	PEG	B	508	-	-	0/1/1/4	-
4	PEG	A	508	-	-	0/1/1/4	-
4	PEG	B	507	-	-	0/1/1/4	-
4	PEG	A	507	-	-	0/1/1/4	-
5	PGE	B	514	-	-	3/7/7/7	-
5	PGE	B	513	-	-	4/7/7/7	-
2	58U	A	501	1	-	5/15/15/15	-
2	58U	B	501	1	-	4/15/15/15	-
6	GOL	A	515	-	-	4/4/4/4	-
6	GOL	B	516	-	-	2/4/4/4	-
5	PGE	B	512	-	-	4/7/7/7	-
5	PGE	A	511	-	-	4/7/7/7	-
5	PGE	A	513	-	-	3/7/7/7	-
5	PGE	A	510	-	-	5/7/7/7	-
6	GOL	A	514	-	-	4/4/4/4	-
5	PGE	A	512	-	-	3/7/7/7	-
4	PEG	B	510	-	-	3/4/4/4	-
4	PEG	B	511	-	-	2/4/4/4	-
4	PEG	B	509	-	-	0/1/1/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	58U	C3-C11	-4.68	1.46	1.53
2	B	501	58U	C3-C11	-4.32	1.47	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	58U	O14-C7-C6	-2.77	117.74	126.34
2	B	501	58U	O12-C11-C3	2.63	120.89	113.59
2	A	501	58U	O12-C11-C3	2.40	120.24	113.59
2	B	501	58U	C2-C3-C11	2.13	119.68	115.89
2	B	501	58U	O14-C7-C6	-2.09	119.86	126.34
2	B	501	58U	O12-C11-O13	-2.07	118.98	123.90

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	58U	O12-C11-C3-C2
2	A	501	58U	C5-C6-C7-O14
2	A	501	58U	C10-C1-C2-C3
2	B	501	58U	C5-C6-C7-O14
2	B	501	58U	C10-C1-C2-C3
6	A	514	GOL	O1-C1-C2-C3
6	A	515	GOL	O1-C1-C2-C3
6	A	515	GOL	C1-C2-C3-O3
6	B	515	GOL	O1-C1-C2-C3
6	B	516	GOL	C1-C2-C3-O3
5	A	511	PGE	C3-C4-O3-C5
5	A	511	PGE	O2-C3-C4-O3
6	A	514	GOL	O1-C1-C2-O2
5	B	512	PGE	O3-C5-C6-O4
5	A	513	PGE	O2-C3-C4-O3
5	A	510	PGE	O2-C3-C4-O3
6	A	514	GOL	C1-C2-C3-O3
5	A	510	PGE	O3-C5-C6-O4
5	A	513	PGE	O1-C1-C2-O2
6	B	515	GOL	O1-C1-C2-O2
6	B	516	GOL	O2-C2-C3-O3
4	B	511	PEG	O1-C1-C2-O2
4	B	510	PEG	O1-C1-C2-O2
5	B	513	PGE	O1-C1-C2-O2
6	A	515	GOL	O1-C1-C2-O2
6	A	515	GOL	O2-C2-C3-O3
5	B	514	PGE	O2-C3-C4-O3
5	A	511	PGE	C4-C3-O2-C2
2	B	501	58U	C10-C1-C5-O4
2	B	501	58U	C10-C1-C5-C6
4	B	510	PEG	O2-C3-C4-O4
5	A	511	PGE	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	512	PGE	C6-C5-O3-C4
5	B	512	PGE	C1-C2-O2-C3
5	A	510	PGE	C4-C3-O2-C2
5	B	514	PGE	C3-C4-O3-C5
2	A	501	58U	C10-C1-C5-O4
5	B	513	PGE	C4-C3-O2-C2
2	A	501	58U	C10-C1-C5-C6
5	A	512	PGE	O2-C3-C4-O3
5	B	514	PGE	C6-C5-O3-C4
4	B	506	PEG	O2-C3-C4-O4
4	B	511	PEG	C1-C2-O2-C3
5	A	513	PGE	C6-C5-O3-C4
4	B	510	PEG	C1-C2-O2-C3
5	B	512	PGE	C3-C4-O3-C5
4	A	509	PEG	O1-C1-C2-O2
5	A	512	PGE	O3-C5-C6-O4
5	B	513	PGE	O3-C5-C6-O4
5	A	510	PGE	C3-C4-O3-C5
5	B	512	PGE	O2-C3-C4-O3
5	A	510	PGE	C1-C2-O2-C3
6	A	514	GOL	O2-C2-C3-O3
5	B	513	PGE	C1-C2-O2-C3

There are no ring outliers.

17 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	PEG	3	0
3	A	506	SO4	2	0
4	B	508	PEG	2	0
4	A	508	PEG	6	0
3	A	505	SO4	1	0
4	A	507	PEG	3	0
5	B	514	PGE	2	0
3	B	503	SO4	1	0
2	A	501	58U	3	0
2	B	501	58U	1	0
5	A	511	PGE	1	0
5	A	513	PGE	4	0
5	A	510	PGE	1	0
6	A	514	GOL	1	0
5	A	512	PGE	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	510	PEG	2	0
4	B	511	PEG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	352/353 (99%)	-0.38	3 (0%) 81 82	8, 25, 38, 77	3 (0%)
1	B	353/353 (100%)	-0.43	2 (0%) 85 87	11, 24, 42, 69	6 (1%)
All	All	705/706 (99%)	-0.40	5 (0%) 84 86	8, 25, 40, 77	9 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	LEU	3.3
1	A	57	LEU	2.7
1	B	408	ALA	2.1
1	A	111[A]	ARG	2.1
1	A	56	ASP	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(\AA^2)	Q<0.9
5	PGE	A	511	10/10	0.62	0.30	74,77,78,78	0
5	PGE	A	512	10/10	0.68	0.22	60,73,81,81	0
5	PGE	B	512	10/10	0.71	0.25	67,68,69,69	0
4	PEG	A	509	7/7	0.73	0.24	58,60,61,61	0
3	SO4	A	503	5/5	0.74	0.16	93,93,93,93	0
3	SO4	B	505	5/5	0.74	0.14	89,89,89,89	0
3	SO4	A	504	5/5	0.75	0.25	118,118,118,118	0
4	PEG	A	507	4/7	0.75	0.19	60,60,60,60	0
5	PGE	A	513	10/10	0.76	0.19	45,54,57,57	0
4	PEG	B	509	4/7	0.76	0.16	41,41,41,41	0
6	GOL	B	516	6/6	0.77	0.17	57,58,59,59	0
3	SO4	B	503	5/5	0.78	0.18	70,71,71,71	0
4	PEG	B	511	7/7	0.78	0.29	43,51,59,59	0
5	PGE	A	510	10/10	0.78	0.20	39,45,49,49	0
5	PGE	B	514	10/10	0.78	0.16	53,54,54,54	0
2	58U	B	501	13/13	0.78	0.18	54,55,56,56	0
3	SO4	A	506	5/5	0.79	0.22	120,120,120,120	0
5	PGE	B	513	10/10	0.79	0.22	54,60,60,60	0
3	SO4	B	504	5/5	0.80	0.19	108,108,108,108	0
4	PEG	B	508	4/7	0.80	0.17	50,50,51,52	0
6	GOL	A	514	6/6	0.81	0.16	59,59,60,60	0
3	SO4	B	502	5/5	0.82	0.17	92,92,92,93	0
4	PEG	B	510	7/7	0.82	0.21	54,65,67,67	0
4	PEG	B	506	4/7	0.84	0.17	44,45,45,45	0
2	58U	A	501	13/13	0.86	0.15	48,49,52,53	13
7	EDO	A	516	3/4	0.87	0.25	45,45,45,45	0
7	EDO	B	517	3/4	0.87	0.29	47,47,48,48	0
6	GOL	A	515	6/6	0.88	0.11	39,40,40,40	0
4	PEG	B	507	4/7	0.89	0.14	49,49,50,50	0
6	GOL	B	515	6/6	0.90	0.14	34,38,39,40	0
3	SO4	A	505	5/5	0.91	0.11	55,55,55,56	5
4	PEG	A	508	4/7	0.92	0.16	36,36,37,37	0
3	SO4	A	502	5/5	0.94	0.11	52,52,53,53	0

6.5 Other polymers i

There are no such residues in this entry.