



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:05 am BST

PDB ID : 5MED
Title : Cyanothece lipxygenase 2 (CspLOX2)
Authors : Newie, J.; Neumann, P.; Werner, M.; Mata, R.A.; Ficner, R.; Feussner, I.
Deposited on : 2016-11-14
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

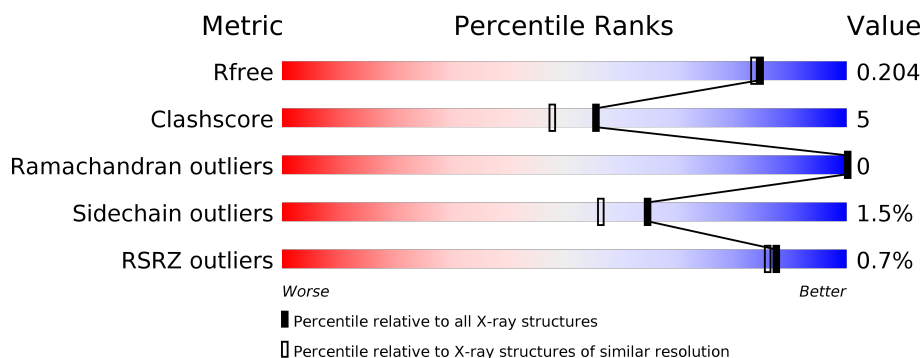
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	569	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 91% 9% </div> </div>
1	B	569	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 91% 8% .. </div> </div>

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	PGR	B	1009[B]	-	-	X	-
5	GOL	A	1005	-	-	X	-
6	HEZ	A	1006[A]	-	-	X	-
7	POL	A	1007	-	-	X	-
7	POL	B	1010	-	-	X	-
9	PDO	B	1011	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10296 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.

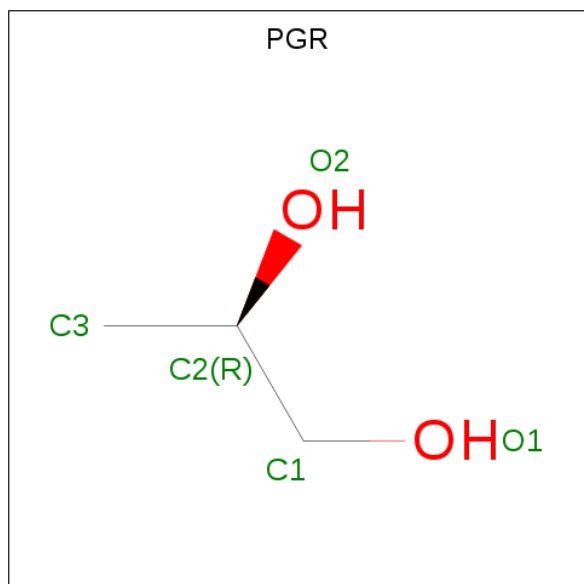
- Molecule 1 is a protein called Arachidonate 15-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	7	0
			4602	2947	782	858	15			
1	B	565	Total	C	N	O	S	0	3	0
			4537	2904	772	846	15			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

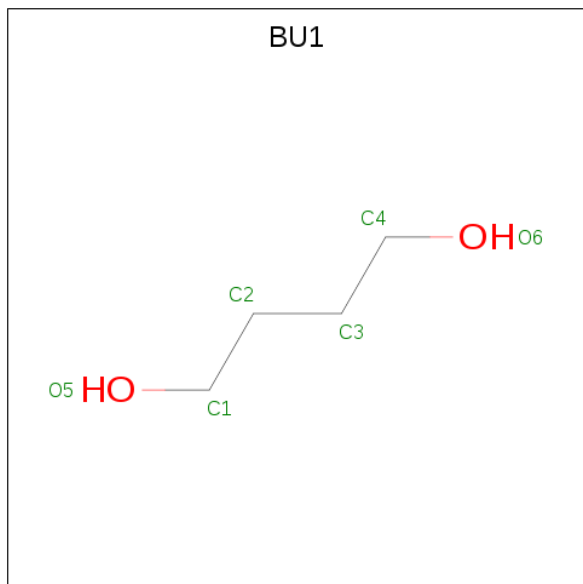
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	1
			10	6	4		

- Molecule 4 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: C₄H₁₀O₂).



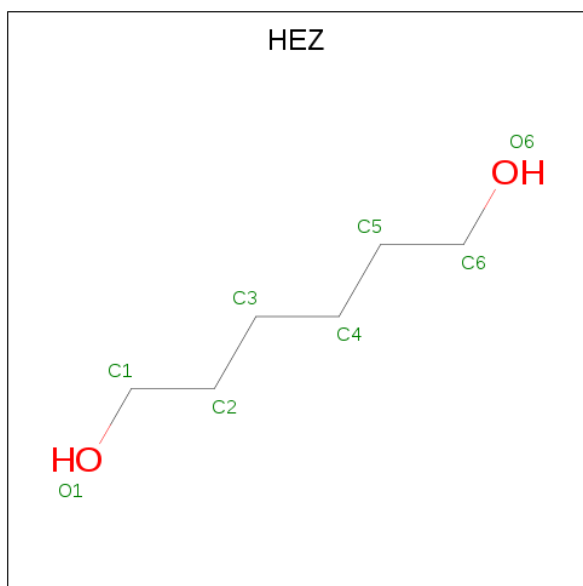
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



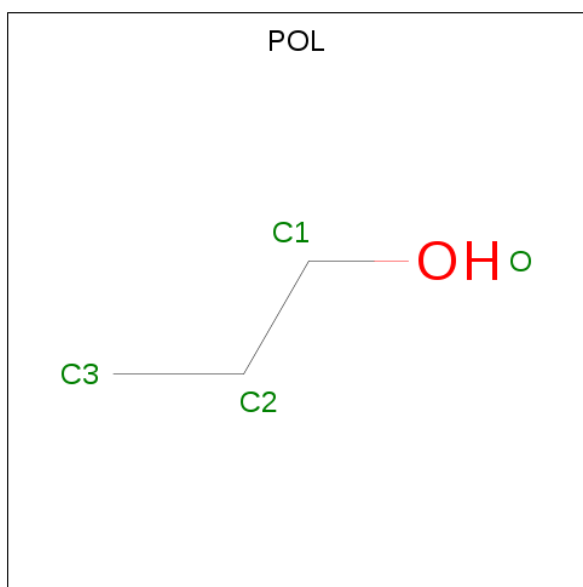
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



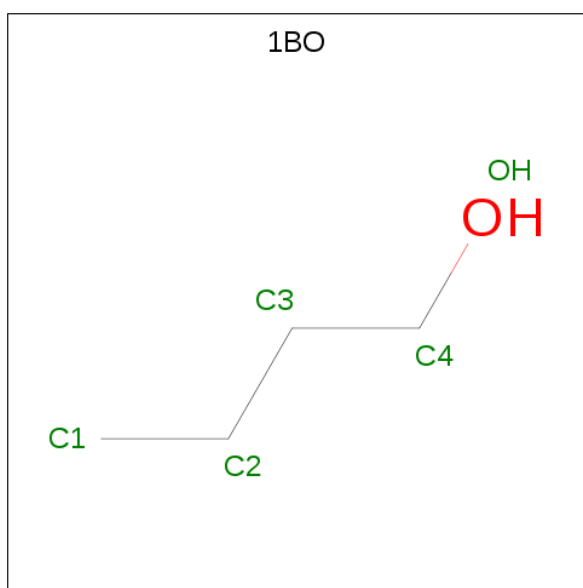
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			16	12	4		

- Molecule 7 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



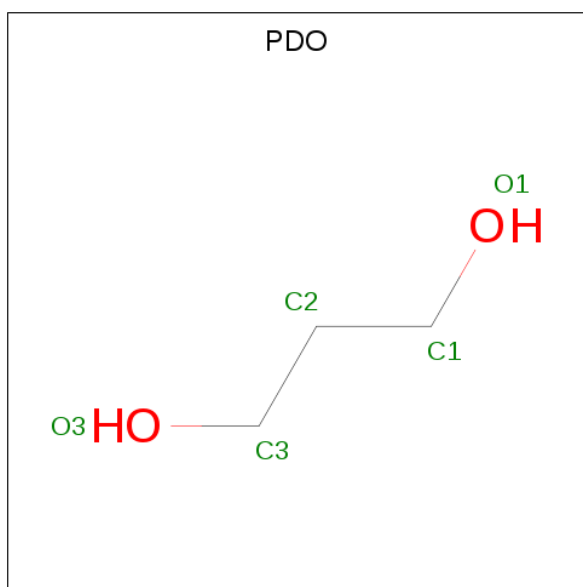
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	3	1		
7	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 8 is 1-BUTANOL (three-letter code: 1BO) (formula: $C_4H_{10}O$).



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

- Molecule 9 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			5	3	2		
9	B	1	Total	C	O	0	0
			5	3	2		

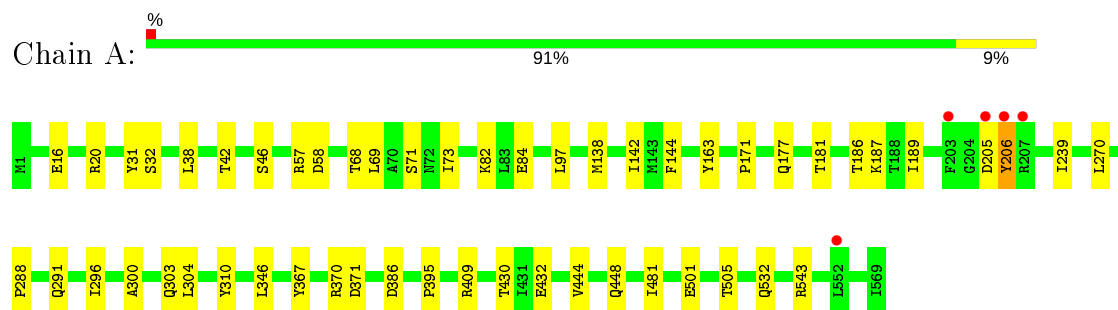
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	532	Total	O	0	2
			534	534		
10	B	514	Total	O	0	3
			517	517		

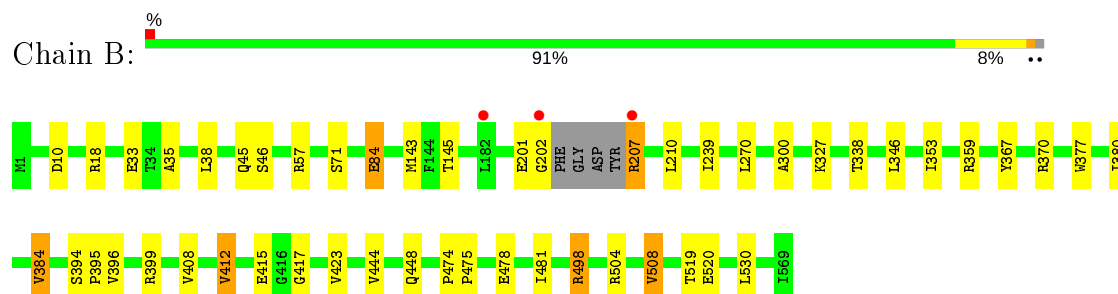
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Arachidonate 15-lipoxygenase



- Molecule 1: Arachidonate 15-lipoxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.50 Å 165.40 Å 166.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.55 – 1.80 41.55 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (41.55-1.80) 94.6 (41.55-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.79 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.173 , 0.203 0.174 , 0.204	Depositor DCC
R_{free} test set	6700 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.117 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10296	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: GOL, BU1, HEZ, PDO, POL, PGR, FE, 1BO

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	0.43	0/4709	0.61	0/6411
1	B	0.41	0/4641	0.62	2/6318 (0.0%)
All	All	0.42	0/9350	0.61	2/12729 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	498	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	210	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ASP	Peptide

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	4602	0	4592	49	0
1	B	4537	0	4533	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	8	2	0
3	B	30	0	48	10	0
4	A	12	0	16	2	0
4	B	12	0	17	2	0
5	A	6	0	8	5	0
6	A	16	0	28	10	0
7	A	4	0	8	8	0
7	B	4	0	8	4	0
8	B	5	0	10	0	0
9	B	10	0	16	8	0
10	A	534	0	0	10	0
10	B	517	0	0	7	0
All	All	10296	0	9292	94	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 5.

All (94) 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)
3:B:1004:PGR:H33	7:B:1010:POL:H22	1.64	0.80
1:B:300:ALA:HB2	7:B:1010:POL:H33	1.64	0.79
1:A:430:THR:HB	7:A:1007:POL:H22	1.67	0.76
9:B:1012:PDO:O1	10:B:1101:HOH:O	2.04	0.75
1:A:71[B]:SER:O	3:B:1009[B]:PGR:H33	1.86	0.75
3:B:1004:PGR:C3	7:B:1010:POL:H22	2.18	0.73
1:A:432:GLU:H	7:A:1007:POL:H21	1.54	0.73
1:A:371:ASP:OD1	10:A:1101:HOH:O	2.07	0.71
1:A:69:LEU:O	3:B:1009[B]:PGR:H31	1.89	0.70
1:A:300:ALA:HB2	6:A:1006[B]:HEZ:H22	1.75	0.69
1:B:530:LEU:HD23	4:B:1008:BU1:H12	1.75	0.68
5:A:1005:GOL:H11	10:A:1121:HOH:O	1.93	0.68
5:A:1005:GOL:O3	10:A:1103:HOH:O	2.13	0.67
3:B:1009[B]:PGR:H32	10:B:1300:HOH:O	1.97	0.65
1:B:239:ILE:HD12	1:B:481:ILE:HD13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLN:HB3	9:B:1011:PDO:H12	1.84	0.60
1:A:505[A]:THR:HG22	10:A:1423:HOH:O	2.01	0.60
1:B:338:THR:HG22	10:B:1525:HOH:O	2.02	0.59
1:A:163:TYR:HA	3:A:1002:PGR:H11	1.87	0.57
1:A:16:GLU:O	1:A:20:ARG:HG3	2.04	0.57
1:A:432:GLU:HB2	7:A:1007:POL:H31	1.88	0.56
1:B:46:SER:HA	9:B:1011:PDO:H32	1.87	0.55
1:A:432:GLU:H	7:A:1007:POL:C2	2.19	0.55
1:A:57:ARG:HH12	6:A:1006[A]:HEZ:C6	2.20	0.54
1:B:377:TRP:HZ2	3:B:1005:PGR:H2	1.72	0.54
1:A:543:ARG:NH2	10:A:1108:HOH:O	2.33	0.53
1:A:186:THR:HG22	1:A:187:LYS:O	2.10	0.53
1:B:415:GLU:HG2	10:B:1229:HOH:O	2.09	0.52
1:B:38:LEU:HD21	1:B:270:LEU:HD12	1.92	0.52
1:A:432:GLU:N	7:A:1007:POL:H21	2.25	0.52
5:A:1005:GOL:H2	10:A:1463:HOH:O	2.09	0.52
1:A:171:PRO:HB3	1:A:189:ILE:HG12	1.92	0.51
1:B:520:GLU:HG2	4:B:1008:BU1:H31	1.91	0.51
1:B:300:ALA:N	7:B:1010:POL:H31	2.25	0.51
1:A:138:MET:O	1:A:142:ILE:HD13	2.11	0.49
1:A:386:ASP:OD2	10:A:1104:HOH:O	2.18	0.49
1:A:239:ILE:HD12	1:A:481:ILE:HD13	1.95	0.49
1:B:71:SER:O	3:B:1009[B]:PGR:O1	2.29	0.49
1:B:71:SER:O	3:B:1009[A]:PGR:O2	2.31	0.49
1:B:143:MET:HB2	1:B:145:THR:HG22	1.93	0.49
1:B:417:GLY:HA2	9:B:1012:PDO:H31	1.95	0.48
1:B:46:SER:CA	9:B:1011:PDO:H32	2.44	0.48
1:A:57:ARG:HH12	6:A:1006[A]:HEZ:H62	1.78	0.48
1:A:71[B]:SER:OG	1:A:73:ILE:HG22	2.14	0.48
1:B:395:PRO:HB2	1:B:399:ARG:HH21	1.79	0.48
1:A:432:GLU:HG2	7:A:1007:POL:H31	1.95	0.47
4:A:1004:BU1:H32	10:A:1317:HOH:O	2.14	0.47
1:A:38[A]:LEU:HD21	1:A:270:LEU:HD12	1.97	0.47
1:A:501:GLU:O	1:A:505[A]:THR:HG23	2.15	0.47
1:B:380:ILE:O	1:B:384:VAL:HG13	2.14	0.47
1:B:504:ARG:O	1:B:508:VAL:HG22	2.14	0.47
3:A:1002:PGR:H31	4:A:1004:BU1:O6	2.15	0.47
1:B:519:THR:HG22	10:B:1473:HOH:O	2.15	0.46
1:A:82:LYS:HB3	1:A:84[A]:GLU:HG2	1.97	0.45
1:B:408:VAL:O	1:B:412:VAL:HG13	2.17	0.45
1:A:57:ARG:HH22	6:A:1006[A]:HEZ:H62	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:GLN:HB2	10:A:1102:HOH:O	2.17	0.45
1:A:31:TYR:HD1	1:A:38[B]:LEU:HD11	1.82	0.44
1:B:201:GLU:OE1	1:B:207:ARG:NH2	2.49	0.44
1:B:35:ALA:O	1:B:327:LYS:HD3	2.16	0.44
1:A:206:TYR:N	1:A:206:TYR:CD2	2.86	0.44
1:A:304:LEU:HD23	1:A:310:TYR:HB2	1.98	0.44
1:A:409:ARG:NH2	10:A:1128:HOH:O	2.49	0.44
1:A:46:SER:HA	9:B:1011:PDO:H31	1.99	0.44
1:B:45:GLN:HB3	9:B:1011:PDO:C1	2.47	0.44
1:B:84:GLU:HG3	10:B:1442:HOH:O	2.18	0.44
1:A:296:ILE:HG13	6:A:1006[B]:HEZ:H21	1.99	0.44
1:B:353:ILE:HG23	10:B:1404:HOH:O	2.18	0.43
1:B:415:GLU:CD	1:B:415:GLU:H	2.22	0.43
1:A:177:GLN:HA	1:A:181:THR:O	2.19	0.43
1:B:202:GLY:HA3	1:B:207:ARG:HA	2.01	0.43
1:A:288:PRO:HA	5:A:1005:GOL:H12	2.01	0.42
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.78	0.42
6:A:1006[A]:HEZ:H31	6:A:1006[A]:HEZ:H61	1.34	0.42
1:A:303:GLN:OE1	6:A:1006[A]:HEZ:H51	2.18	0.42
1:A:291:GLN:HB2	5:A:1005:GOL:H31	2.02	0.42
1:A:395:PRO:HB3	7:A:1007:POL:O	2.20	0.41
1:A:68:THR:O	3:B:1009[A]:PGR:O1	2.38	0.41
1:B:444:VAL:HA	1:B:448:GLN:HB3	2.01	0.41
1:A:304:LEU:HD12	6:A:1006[A]:HEZ:H22	2.03	0.41
1:B:394:SER:OG	1:B:396:VAL:HG12	2.20	0.41
1:A:58:ASP:OD2	1:B:57:ARG:NH2	2.50	0.41
1:A:73:ILE:O	3:B:1009[A]:PGR:H31	2.20	0.41
1:A:32:SER:O	1:A:38[B]:LEU:HD12	2.20	0.41
1:B:38:LEU:HB2	9:B:1012:PDO:H11	2.03	0.41
1:A:444:VAL:HA	1:A:448:GLN:HB3	2.03	0.41
1:A:432:GLU:CG	7:A:1007:POL:H31	2.51	0.41
1:A:346:LEU:HD13	1:A:370:ARG:HG3	2.02	0.40
1:A:296:ILE:CD1	6:A:1006[B]:HEZ:H31	2.52	0.40
1:A:304:LEU:HD12	6:A:1006[B]:HEZ:H22	2.03	0.40
1:B:10:ASP:OD2	1:B:18:ARG:HD2	2.21	0.40
1:B:346:LEU:HD13	1:B:370:ARG:HG3	2.02	0.40
1:B:395:PRO:CB	1:B:399:ARG:HH21	2.34	0.40
1:B:474:PRO:HA	1:B:475:PRO:HD3	2.00	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	574/569 (101%)	557 (97%)	17 (3%)	0	100	100
1	B	564/569 (99%)	552 (98%)	12 (2%)	0	100	100
All	All	1138/1138 (100%)	1109 (98%)	29 (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	499/493 (101%)	495 (99%)	4 (1%)	81	78
1	B	492/493 (100%)	481 (98%)	11 (2%)	52	39
All	All	991/986 (100%)	976 (98%)	15 (2%)	65	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	144	PHE
1	A	206	TYR
1	A	367	TYR
1	B	33	GLU
1	B	84	GLU
1	B	207	ARG
1	B	359	ARG

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Mol	Chain	Res	Type
1	B	367	TYR
1	B	384	VAL
1	B	412	VAL
1	B	423	VAL
1	B	478	GLU
1	B	498	ARG
1	B	508	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z > 2$
3	PGR	B	1006	-	3,4,4	0.90	0	1,4,4	0.31	0
8	1BO	B	1002	-	4,4,4	0.42	0	3,3,3	0.74	0
3	PGR	B	1009[A]	-	3,4,4	0.94	0	1,4,4	0.22	0
9	PDO	B	1011	-	4,4,4	0.38	0	3,3,3	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGR	B	1005	-	3,4,4	0.82	0	1,4,4	0.29	0
4	BU1	A	1004	-	5,5,5	0.85	0	4,4,4	0.65	0
6	HEZ	A	1006[B]	-	7,7,7	0.25	0	6,6,6	0.63	0
7	POL	B	1010	-	3,3,3	0.38	0	2,2,2	0.25	0
7	POL	A	1007	-	3,3,3	0.29	0	2,2,2	0.43	0
3	PGR	B	1004	-	3,4,4	1.02	0	1,4,4	0.36	0
4	BU1	B	1007	-	5,5,5	0.83	0	4,4,4	0.60	0
6	HEZ	A	1006[A]	-	7,7,7	0.27	0	6,6,6	0.51	0
3	PGR	A	1002	-	3,4,4	0.98	0	1,4,4	0.14	0
3	PGR	B	1003	-	3,4,4	0.87	0	1,4,4	0.47	0
4	BU1	B	1008	-	5,5,5	0.78	0	4,4,4	0.50	0
4	BU1	A	1003	-	5,5,5	0.90	0	4,4,4	0.35	0
3	PGR	B	1009[B]	-	3,4,4	1.13	0	1,4,4	0.89	0
5	GOL	A	1005	-	5,5,5	0.36	0	5,5,5	0.62	0
9	PDO	B	1012	-	4,4,4	0.30	0	3,3,3	0.56	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	PGR	B	1006	-	-	0/2/2/2	-
8	1BO	B	1002	-	-	2/2/2/2	-
3	PGR	B	1009[A]	-	-	1/2/2/2	-
9	PDO	B	1011	-	-	1/2/2/2	-
3	PGR	B	1005	-	-	0/2/2/2	-
4	BU1	A	1004	-	-	1/3/3/3	-
6	HEZ	A	1006[B]	-	-	2/5/5/5	-
7	POL	B	1010	-	-	0/1/1/1	-
7	POL	A	1007	-	-	0/1/1/1	-
3	PGR	B	1004	-	-	2/2/2/2	-
4	BU1	B	1007	-	-	1/3/3/3	-
6	HEZ	A	1006[A]	-	-	2/5/5/5	-
3	PGR	A	1002	-	-	0/2/2/2	-
3	PGR	B	1003	-	-	0/2/2/2	-
4	BU1	B	1008	-	-	0/3/3/3	-
4	BU1	A	1003	-	-	2/3/3/3	-
3	PGR	B	1009[B]	-	-	2/2/2/2	-
5	GOL	A	1005	-	-	2/4/4/4	-
9	PDO	B	1012	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1004	PGR	O1-C1-C2-C3
3	B	1004	PGR	O1-C1-C2-O2
3	B	1009[B]	PGR	O1-C1-C2-C3
3	B	1009[B]	PGR	O1-C1-C2-O2
9	B	1011	PDO	O1-C1-C2-C3
6	A	1006[A]	HEZ	C3-C4-C5-C6
6	A	1006[B]	HEZ	C1-C2-C3-C4
8	B	1002	1BO	C1-C2-C3-C4
4	A	1004	BU1	C1-C2-C3-C4
5	A	1005	GOL	O1-C1-C2-C3
8	B	1002	1BO	C2-C3-C4-OH
6	A	1006[B]	HEZ	C4-C5-C6-O6
6	A	1006[A]	HEZ	C4-C5-C6-O6
4	A	1003	BU1	C1-C2-C3-C4
4	A	1003	BU1	O5-C1-C2-C3
4	B	1007	BU1	C2-C3-C4-O6
5	A	1005	GOL	O1-C1-C2-O2
9	B	1012	PDO	C1-C2-C3-O3
3	B	1009[A]	PGR	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1009[A]	PGR	3	0
9	B	1011	PDO	5	0
3	B	1005	PGR	1	0
4	A	1004	BU1	2	0
6	A	1006[B]	HEZ	4	0
7	B	1010	POL	4	0
7	A	1007	POL	8	0
3	B	1004	PGR	2	0
6	A	1006[A]	HEZ	6	0
3	A	1002	PGR	2	0
4	B	1008	BU1	2	0
3	B	1009[B]	PGR	4	0
5	A	1005	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1012	PDO	3	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	569/569 (100%)	-0.32	5 (0%) 84 82	16, 26, 48, 106	0
1	B	565/569 (99%)	-0.36	3 (0%) 91 89	15, 26, 53, 94	0
All	All	1134/1138 (99%)	-0.34	8 (0%) 87 86	15, 26, 51, 106	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	ASP	7.7
1	A	206	TYR	6.6
1	A	207	ARG	4.3
1	A	203	PHE	2.9
1	B	207	ARG	2.5
1	B	202	GLY	2.5
1	B	182	LEU	2.2
1	A	552	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 carbohydrates 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	BU1	B	1008	6/6	0.70	0.23	45,52,54,62	0
3	PGR	B	1004	5/5	0.71	0.37	50,55,56,56	0
3	PGR	B	1006	5/5	0.72	0.15	61,62,62,65	0
4	BU1	A	1004	6/6	0.73	0.20	30,47,50,53	0
7	POL	B	1010	4/4	0.76	0.28	44,47,50,51	0
8	1BO	B	1002	5/5	0.78	0.21	42,45,49,55	0
4	BU1	A	1003	6/6	0.78	0.36	59,60,62,63	0
6	HEZ	A	1006[B]	8/8	0.83	0.24	36,40,42,42	8
6	HEZ	A	1006[A]	8/8	0.83	0.24	34,40,41,42	8
9	PDO	B	1012	5/5	0.83	0.29	35,43,53,57	0
9	PDO	B	1011	5/5	0.84	0.27	31,35,38,53	0
3	PGR	B	1005	5/5	0.85	0.32	37,42,47,55	0
3	PGR	B	1009[B]	5/5	0.86	0.17	17,28,30,31	5
3	PGR	B	1009[A]	5/5	0.86	0.17	18,26,30,32	5
5	GOL	A	1005	6/6	0.88	0.30	28,47,49,49	0
3	PGR	B	1003	5/5	0.89	0.12	44,45,49,50	0
7	POL	A	1007	4/4	0.90	0.21	31,36,37,47	0
4	BU1	B	1007	6/6	0.90	0.22	30,44,50,52	0
3	PGR	A	1002	5/5	0.94	0.21	31,36,46,46	0
2	FE	A	1001	1/1	1.00	0.10	20,20,20,20	0
2	FE	B	1001	1/1	1.00	0.09	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.