



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:11 PM UTC

PDB ID : 8AYF / pdb_00008ayf
Title : Crystal structure of human Sphingosine-1-phosphate lyase 1
Authors : Giardina, G.; Catalano, F.; Pampalone, G.; Cellini, B.
Deposited on : 2022-09-02
Resolution : 1.84 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

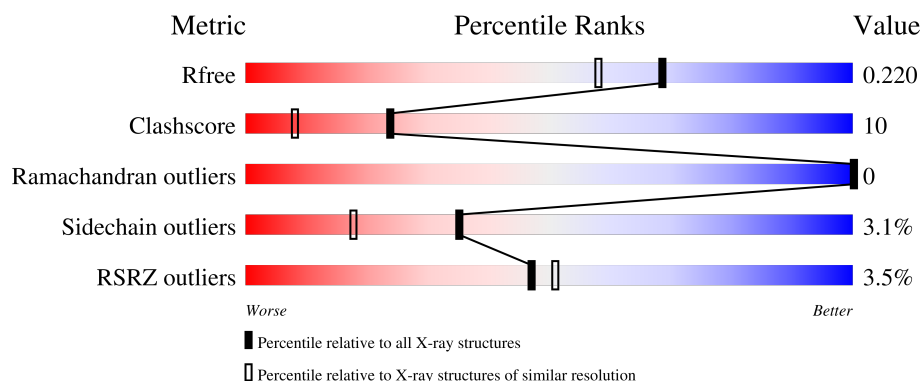
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

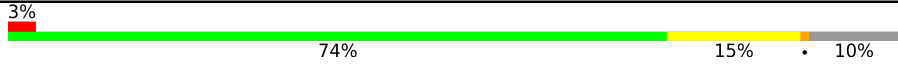
The reported resolution of this entry is 1.84 Å.

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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	494	
1	B	494	

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
2	ACT	A	601[A]	-	-	X	-
2	ACT	A	601[B]	-	-	X	-
2	ACT	B	601[A]	-	-	X	-
2	ACT	B	601[B]	-	-	X	-
3	GOL	B	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7239 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.

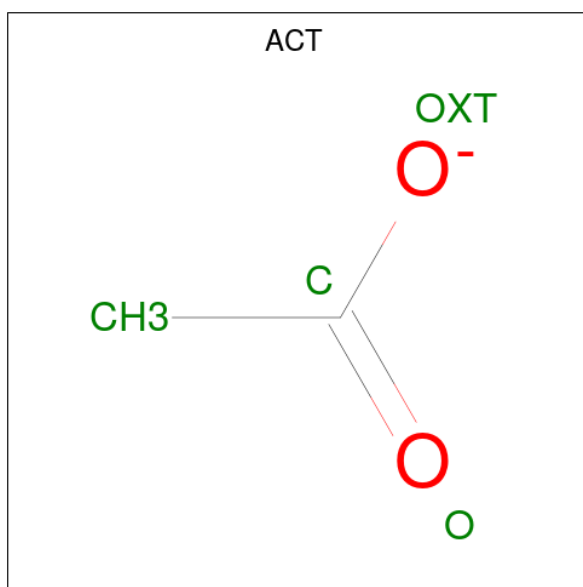
- Molecule 1 is a protein called Sphingosine-1-phosphate lyase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	P	S	3	3	0
			3449	2216	573	636	1	23			
1	B	448	Total	C	N	O	P	S	0	1	0
			3443	2208	574	638	1	22			

There are 12 discrepancies between the modelled and reference sequences:

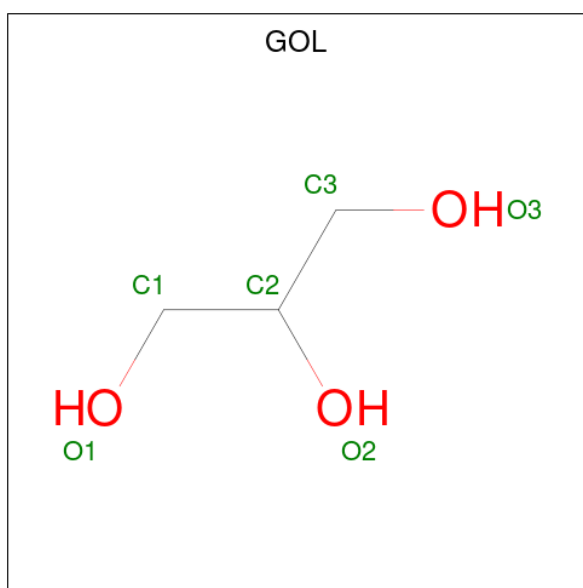
Chain	Residue	Modelled	Actual	Comment	Reference
A	569	HIS	-	expression tag	UNP O95470
A	570	HIS	-	expression tag	UNP O95470
A	571	HIS	-	expression tag	UNP O95470
A	572	HIS	-	expression tag	UNP O95470
A	573	HIS	-	expression tag	UNP O95470
A	574	HIS	-	expression tag	UNP O95470
B	569	HIS	-	expression tag	UNP O95470
B	570	HIS	-	expression tag	UNP O95470
B	571	HIS	-	expression tag	UNP O95470
B	572	HIS	-	expression tag	UNP O95470
B	573	HIS	-	expression tag	UNP O95470
B	574	HIS	-	expression tag	UNP O95470

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

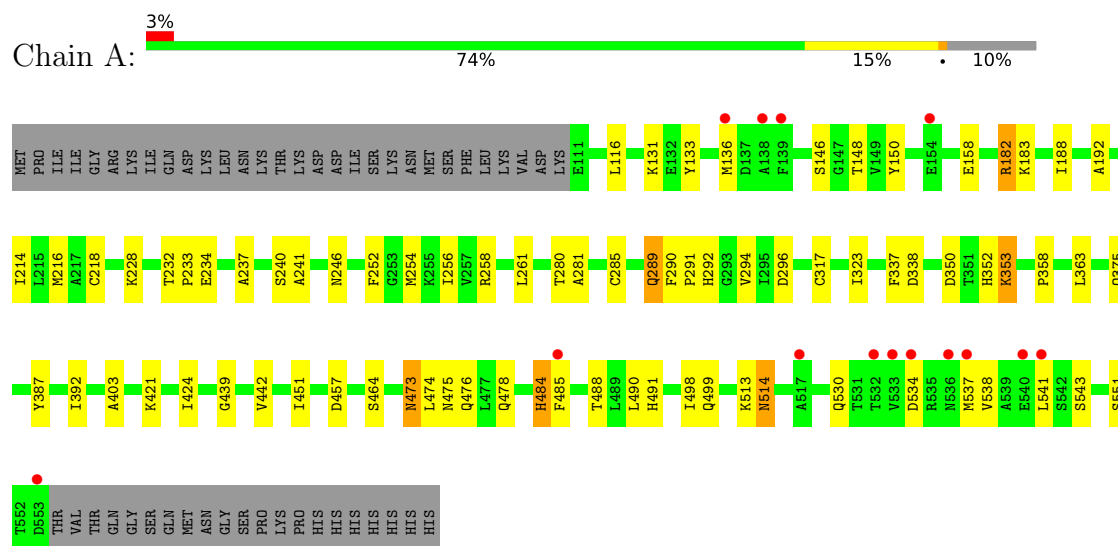
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total 148	O 148	0	0
4	B	171	Total 171	O 171	0	0

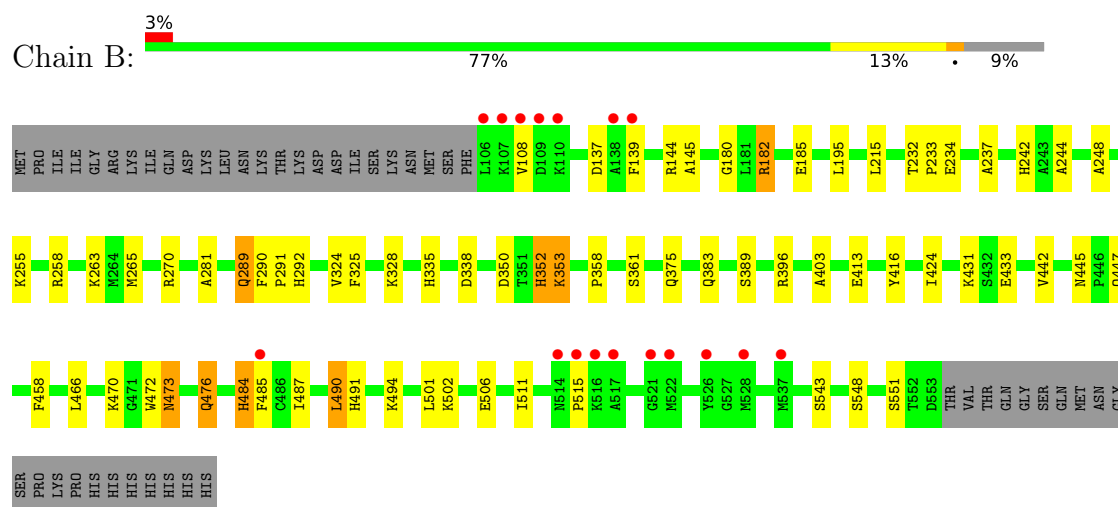
3 Residue-property plots

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: Sphingosine-1-phosphate lyase 1



• Molecule 1: Sphingosine-1-phosphate lyase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.16Å 127.41Å 66.95Å 90.00° 104.85° 90.00°	Depositor
Resolution (Å)	57.76 – 1.84 57.76 – 1.84	Depositor EDS
% Data completeness (in resolution range)	57.3 (57.76-1.84) 57.4 (57.76-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.214 0.198 , 0.220	Depositor DCC
R_{free} test set	2499 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7239	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.30% 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, ACT, LLP

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	0.62	0/3506	1.03	2/4749 (0.0%)
1	B	0.63	0/3499	1.01	2/4746 (0.0%)
All	All	0.62	0/7005	1.02	4/9495 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	485	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	338	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	158	GLU	CB-CA-C	-5.03	102.12	110.68

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	3449	0	3402	65	0
1	B	3443	0	3374	71	0
2	A	8	0	6	6	0
2	B	8	0	6	5	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	6	0
4	A	148	0	0	23	0
4	B	171	0	0	36	0
All	All	7239	0	6804	138	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 10.

All (138) 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)
2:A:601[B]:ACT:H1	4:A:839:HOH:O	1.43	1.18
2:A:601[B]:ACT:H2	4:A:841:HOH:O	1.51	1.08
1:A:317:CYS:SG	4:A:704:HOH:O	2.19	1.01
1:A:131:LYS:CG	4:A:817:HOH:O	2.13	0.94
1:B:442:VAL:HB	4:B:822:HOH:O	1.66	0.93
2:A:601[B]:ACT:CH3	4:A:841:HOH:O	2.15	0.86
1:B:144:ARG:HG2	4:B:794:HOH:O	1.76	0.84
1:B:144:ARG:CG	4:B:794:HOH:O	2.25	0.84
1:B:472:TRP:CZ3	4:B:794:HOH:O	2.32	0.83
1:B:466:LEU:HD22	4:B:755:HOH:O	1.78	0.83
1:A:352:HIS:CG	4:A:711:HOH:O	2.32	0.82
1:A:241:ALA:O	1:A:258:ARG:NH2	2.16	0.78
1:B:242:HIS:NE2	3:B:602:GOL:H32	2.00	0.77
1:B:353:LLP:H4'1	4:B:723:HOH:O	1.84	0.77
1:B:289:GLN:HE22	1:B:292:HIS:HD2	1.34	0.76
1:A:541:LEU:HB3	4:A:821:HOH:O	1.88	0.73
1:A:538:VAL:HA	4:A:821:HOH:O	1.86	0.73
1:B:470:LYS:HE3	4:B:755:HOH:O	1.89	0.72
1:B:515:PRO:HD2	4:B:859:HOH:O	1.90	0.71
1:B:335:HIS:HE1	4:B:728:HOH:O	1.73	0.70
1:A:352:HIS:CD2	4:A:711:HOH:O	2.42	0.69
1:A:534:ASP:OD2	1:A:537:MET:HB3	1.94	0.67
1:A:541:LEU:CB	4:A:821:HOH:O	2.43	0.67
1:A:214:ILE:HD11	4:A:704:HOH:O	1.93	0.67
1:B:476:GLN:NE2	4:B:706:HOH:O	2.28	0.66
1:A:232:THR:HG23	4:A:742:HOH:O	1.96	0.66
1:A:246:ASN:OD1	1:A:258:ARG:NH1	2.29	0.65
1:B:487:ILE:HA	1:B:491:HIS:HD2	1.61	0.65
1:A:218:CYS:HB3	1:A:254[A]:MET:HE1	1.79	0.65
1:B:137:ASP:O	4:B:701:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601[B]:ACT:H3	4:B:763:HOH:O	1.98	0.64
1:B:424:ILE:HG23	4:B:775:HOH:O	1.98	0.62
1:B:472:TRP:CH2	4:B:794:HOH:O	2.50	0.62
1:A:216:MET:HA	1:A:216:MET:HE2	1.80	0.62
1:B:144:ARG:CD	4:B:794:HOH:O	2.49	0.60
4:A:793:HOH:O	2:B:601[B]:ACT:H1	2.01	0.60
1:B:263:LYS:O	1:B:265:MET:HE2	2.01	0.60
1:B:242:HIS:CE1	3:B:602:GOL:H32	2.36	0.59
1:B:502:LYS:CE	1:B:506:GLU:OE2	2.51	0.59
1:A:289:GLN:HE22	1:A:292:HIS:HD2	1.48	0.59
1:A:498:ILE:HG12	4:A:746:HOH:O	2.03	0.59
1:A:252:PHE:HB2	1:A:254[A]:MET:HE2	1.85	0.58
1:B:289:GLN:HE22	1:B:292:HIS:CD2	2.19	0.58
4:A:793:HOH:O	2:B:601[B]:ACT:CH3	2.52	0.57
1:B:234:GLU:HG2	1:B:255:LYS:HB3	1.86	0.57
1:B:548:SER:HB3	4:B:720:HOH:O	2.04	0.57
1:A:353:LLP:H4'1	4:A:705:HOH:O	2.04	0.56
1:B:433:GLU:HG3	1:B:501:LEU:HD11	1.88	0.56
1:B:490:LEU:HD22	1:B:494:LYS:HG3	1.87	0.56
1:B:502:LYS:HE2	1:B:506:GLU:OE2	2.06	0.56
1:B:472:TRP:CE3	4:B:794:HOH:O	2.57	0.55
1:B:350:ASP:OD2	1:B:353:LLP:HE2	2.06	0.55
1:B:361:SER:HB2	4:B:716:HOH:O	2.07	0.55
1:B:431:LYS:NZ	1:B:445:ASN:OD1	2.36	0.55
1:A:289:GLN:HE22	1:A:292:HIS:CD2	2.26	0.54
1:A:353:LLP:C6	4:A:704:HOH:O	2.54	0.54
1:B:242:HIS:NE2	3:B:602:GOL:C3	2.69	0.54
1:A:148:THR:H	2:A:601[A]:ACT:H3	1.73	0.54
1:A:551:SER:O	1:B:182:ARG:NH1	2.42	0.53
1:B:442:VAL:CB	4:B:822:HOH:O	2.41	0.53
1:A:464:SER:HB2	1:A:476:GLN:HE21	1.73	0.53
1:A:131:LYS:CB	4:A:817:HOH:O	2.50	0.53
1:B:233:PRO:HB3	1:B:281:ALA:HB2	1.90	0.53
1:A:424:ILE:HB	4:A:822:HOH:O	2.09	0.52
1:A:240:SER:HA	1:B:383:GLN:HE21	1.75	0.52
1:B:358:PRO:HG2	4:B:716:HOH:O	2.09	0.52
1:B:265:MET:CE	4:B:846:HOH:O	2.57	0.51
1:B:265:MET:HE1	4:B:846:HOH:O	2.09	0.51
1:A:183:LYS:HE3	1:B:108:VAL:HG11	1.91	0.51
1:A:358:PRO:HG3	1:A:403:ALA:HB3	1.93	0.51
1:A:188:ILE:HG22	1:A:363:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD22	1:B:195:LEU:HD21	1.93	0.50
1:B:358:PRO:HG3	1:B:403:ALA:HB3	1.93	0.50
1:B:396:ARG:HD2	4:B:863:HOH:O	2.12	0.50
1:A:150:TYR:HA	1:A:488:THR:HB	1.93	0.50
1:A:133:TYR:O	1:B:180:GLY:HA3	2.12	0.50
1:A:484:HIS:C	1:A:484:HIS:CD2	2.89	0.50
1:A:350:ASP:OD2	1:A:353:LLP:HE2	2.11	0.49
1:A:387:TYR:CE1	3:B:602:GOL:H31	2.47	0.49
1:B:543[B]:SER:HB3	4:B:724:HOH:O	2.10	0.49
1:B:242:HIS:CE1	3:B:602:GOL:C3	2.95	0.49
1:B:325:PHE:CE2	1:B:416:TYR:HB3	2.47	0.49
1:A:352:HIS:CE1	4:A:711:HOH:O	2.66	0.49
1:A:289:GLN:HG3	1:A:294:VAL:O	2.14	0.48
1:B:215:LEU:HD23	1:B:248:ALA:HB2	1.95	0.48
1:B:237:ALA:O	1:B:258:ARG:HA	2.14	0.48
1:B:502:LYS:HE3	1:B:506:GLU:OE2	2.13	0.48
1:A:148:THR:N	2:A:601[A]:ACT:H3	2.30	0.47
1:B:145:ALA:HB3	4:B:798:HOH:O	2.14	0.47
2:B:601[A]:ACT:CH3	4:B:833:HOH:O	2.62	0.47
1:B:185:GLU:OE1	1:B:396:ARG:NH2	2.48	0.47
1:B:328:LYS:HE2	1:B:413:GLU:OE1	2.15	0.47
1:B:442:VAL:CG2	4:B:822:HOH:O	2.60	0.47
1:A:216:MET:HE3	1:A:392:ILE:CG1	2.45	0.46
1:A:490:LEU:C	1:A:490:LEU:HD23	2.41	0.46
1:A:234[B]:GLU:HG2	1:A:280:THR:HA	1.98	0.45
1:B:139:PHE:O	1:B:139:PHE:CD1	2.70	0.45
1:B:144:ARG:HA	4:B:794:HOH:O	2.16	0.45
1:A:451:ILE:HB	1:A:485[B]:PHE:CZ	2.51	0.45
1:A:192:ALA:CB	1:A:363:LEU:HD13	2.45	0.45
1:B:234:GLU:HA	1:B:255:LYS:O	2.17	0.45
1:B:361:SER:CB	4:B:716:HOH:O	2.65	0.45
1:A:182:ARG:NH1	1:B:551:SER:O	2.49	0.45
1:B:389:SER:HB3	4:B:712:HOH:O	2.15	0.45
1:A:464:SER:CB	1:A:476:GLN:HE21	2.30	0.45
2:B:601[A]:ACT:H1	4:B:833:HOH:O	2.16	0.45
1:B:139:PHE:CE1	1:B:473:ASN:HB2	2.52	0.44
1:A:473:ASN:C	1:A:473:ASN:HD22	2.25	0.44
1:A:421:LYS:HA	4:A:822:HOH:O	2.17	0.44
1:A:237:ALA:O	1:A:258:ARG:HA	2.18	0.44
1:A:387:TYR:HE1	3:B:602:GOL:H31	1.81	0.44
1:B:445:ASN:ND2	1:B:447:GLN:NE2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:HIS:CE1	1:A:353:LLP:OP3	2.70	0.43
2:A:601[A]:ACT:CH3	4:A:718:HOH:O	2.66	0.43
1:B:144:ARG:CB	4:B:794:HOH:O	2.63	0.43
1:A:323:ILE:HD12	1:A:337:PHE:CD1	2.52	0.43
1:B:491:HIS:O	4:B:704:HOH:O	2.21	0.43
1:A:261:LEU:HD11	1:B:383:GLN:HE22	1.84	0.42
1:B:242:HIS:HD1	1:B:244:ALA:H	1.68	0.42
1:A:513:LYS:C	1:A:514:ASN:ND2	2.77	0.42
1:A:478:GLN:HB2	1:A:530:GLN:HG2	2.01	0.42
1:B:270:ARG:HB3	4:B:733:HOH:O	2.19	0.42
1:A:464:SER:HB2	1:A:476:GLN:NE2	2.35	0.42
1:A:233:PRO:HB3	1:A:281:ALA:HB2	2.03	0.41
1:B:290:PHE:N	1:B:291:PRO:CD	2.84	0.41
1:A:228:LYS:HD3	4:A:794:HOH:O	2.20	0.41
1:A:439:GLY:HA2	1:A:457:ASP:OD2	2.20	0.41
1:B:458:PHE:CD1	1:B:511:ILE:HG21	2.55	0.41
1:B:484:HIS:CD2	1:B:484:HIS:C	2.98	0.41
1:A:290:PHE:N	1:A:291:PRO:CD	2.84	0.41
1:A:488:THR:H	1:A:491:HIS:HD2	1.69	0.41
1:A:488:THR:H	1:A:491:HIS:CD2	2.38	0.41
1:A:514:ASN:HD22	1:A:514:ASN:N	2.18	0.41
1:A:353:LLP:HE3	4:B:783:HOH:O	2.21	0.40
1:B:352:HIS:CD2	4:B:737:HOH:O	2.74	0.40
1:A:146:SER:OG	1:A:475:ASN:ND2	2.54	0.40
1:B:353:LLP:OP4	1:B:353:LLP:C4'	2.69	0.40
1:A:285:CYS:HB2	1:A:296:ASP:HB2	2.02	0.40

There are no symmetry-related clashes.

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	443/494 (90%)	433 (98%)	10 (2%)	0	100	100
1	B	446/494 (90%)	433 (97%)	13 (3%)	0	100	100
All	All	889/988 (90%)	866 (97%)	23 (3%)	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	360/414 (87%)	348 (97%)	12 (3%)	33	15
1	B	357/414 (86%)	347 (97%)	10 (3%)	38	20
All	All	717/828 (87%)	695 (97%)	22 (3%)	35	18

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	MET
1	A	182	ARG
1	A	256	ILE
1	A	289	GLN
1	A	375	GLN
1	A	442	VAL
1	A	473	ASN
1	A	474	LEU
1	A	484	HIS
1	A	499	GLN
1	A	514	ASN
1	A	543	SER
1	B	182	ARG
1	B	232	THR
1	B	289	GLN
1	B	324	VAL
1	B	352	HIS
1	B	375	GLN

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Mol	Chain	Res	Type
1	B	473	ASN
1	B	476	GLN
1	B	484	HIS
1	B	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	292	HIS
1	A	383	GLN
1	A	422	GLN
1	A	473	ASN
1	A	475	ASN
1	A	476	GLN
1	A	478	GLN
1	A	491	HIS
1	A	499	GLN
1	A	514	ASN
1	B	292	HIS
1	B	383	GLN
1	B	422	GLN
1	B	447	GLN
1	B	473	ASN
1	B	476	GLN
1	B	491	HIS
1	B	499	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	353	1	23,24,25	0.75	1 (4%)	25,32,34	1.16	2 (8%)
1	LLP	B	353	1	23,24,25	0.83	1 (4%)	25,32,34	1.12	1 (4%)

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
1	LLP	A	353	1	-	10/16/17/19	0/1/1/1
1	LLP	B	353	1	-	12/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	LLP	C4'-NZ	2.35	1.35	1.27
1	B	353	LLP	C4'-NZ	2.05	1.34	1.27

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	LLP	C5-C4-C4'	2.28	124.99	121.47
1	A	353	LLP	OP3-P-OP4	-2.17	101.00	106.67
1	A	353	LLP	OP3-P-OP2	2.04	115.46	107.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	353	LLP	C4-C4'-NZ-CE
1	A	353	LLP	C4-C5-C5'-OP4
1	A	353	LLP	C6-C5-C5'-OP4
1	A	353	LLP	C5'-OP4-P-OP2
1	A	353	LLP	C5'-OP4-P-OP3
1	A	353	LLP	O-C-CA-CB
1	B	353	LLP	C4-C4'-NZ-CE
1	B	353	LLP	C4-C5-C5'-OP4

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Mol	Chain	Res	Type	Atoms
1	B	353	LLP	C6-C5-C5'-OP4
1	B	353	LLP	C5'-OP4-P-OP1
1	B	353	LLP	C5'-OP4-P-OP2
1	B	353	LLP	C5'-OP4-P-OP3
1	B	353	LLP	O-C-CA-CB
1	B	353	LLP	CG-CD-CE-NZ
1	A	353	LLP	C5'-OP4-P-OP1
1	A	353	LLP	CD-CE-NZ-C4'
1	B	353	LLP	CD-CE-NZ-C4'
1	A	353	LLP	C3-C4-C4'-NZ
1	B	353	LLP	C3-C4-C4'-NZ
1	B	353	LLP	CE-CD-CG-CB
1	A	353	LLP	C5-C4-C4'-NZ
1	B	353	LLP	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	353	LLP	5	0
1	B	353	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
2	ACT	B	601[B]	-	3,3,3	0.76	0	3,3,3	0.94	0
2	ACT	A	601[B]	-	3,3,3	0.72	0	3,3,3	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	601[A]	-	3,3,3	0.95	0	3,3,3	0.78	0
3	GOL	B	602	-	5,5,5	0.20	0	5,5,5	0.68	0
2	ACT	B	601[A]	-	3,3,3	0.97	0	3,3,3	0.95	0
3	GOL	A	602	-	5,5,5	0.15	0	5,5,5	0.33	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	602	-	-	4/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601[B]	ACT	3	0
2	A	601[B]	ACT	3	0
2	A	601[A]	ACT	3	0
3	B	602	GOL	6	0
2	B	601[A]	ACT	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	442/494 (89%)	0.11	14 (3%)	50 54	9, 20, 41, 70	4 (0%)
1	B	447/494 (90%)	0.17	17 (3%)	44 48	11, 20, 46, 67	1 (0%)
All	All	889/988 (89%)	0.14	31 (3%)	47 51	9, 20, 43, 70	5 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	PHE	5.5
1	B	138	ALA	4.7
1	B	537	MET	4.3
1	B	107	LYS	3.7
1	A	533	VAL	3.6
1	A	534	ASP	3.6
1	B	109	ASP	3.6
1	B	108	VAL	3.4
1	B	517	ALA	3.4
1	B	106	LEU	3.3
1	A	532	THR	3.2
1	A	536	ASN	3.1
1	A	541	LEU	2.9
1	A	136	MET	2.7
1	A	485[A]	PHE	2.7
1	B	526	TYR	2.7
1	B	515	PRO	2.6
1	A	540	GLU	2.6
1	B	110	LYS	2.4
1	A	517	ALA	2.4
1	A	138	ALA	2.3
1	A	537	MET	2.3
1	B	522	MET	2.1
1	B	528	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	485	PHE	2.1
1	A	553	ASP	2.1
1	B	516	LYS	2.1
1	B	521	GLY	2.1
1	B	514	ASN	2.1
1	A	154	GLU	2.0
1	A	139	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	353	24/25	0.93	0.08	13,19,22,23	0
1	LLP	B	353	24/25	0.95	0.07	13,18,21,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	602	6/6	0.82	0.18	14,15,15,15	6
3	GOL	A	602	6/6	0.84	0.14	34,37,38,40	0
2	ACT	B	601[A]	4/4	0.91	0.10	17,17,18,18	4
2	ACT	B	601[B]	4/4	0.91	0.10	16,17,17,18	4
2	ACT	A	601[A]	4/4	0.95	0.08	12,12,12,12	4
2	ACT	A	601[B]	4/4	0.95	0.08	18,18,19,19	4

6.5 Other polymers [i](#)

There are no such residues in this entry.