



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:38 am BST

PDB ID : 3P53
Title : Structure of fascin
Authors : Jansen, S.; Dominguez, R.
Deposited on : 2010-10-07
Resolution : 2.00 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
buster-report : 1.1.7 (2018)
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

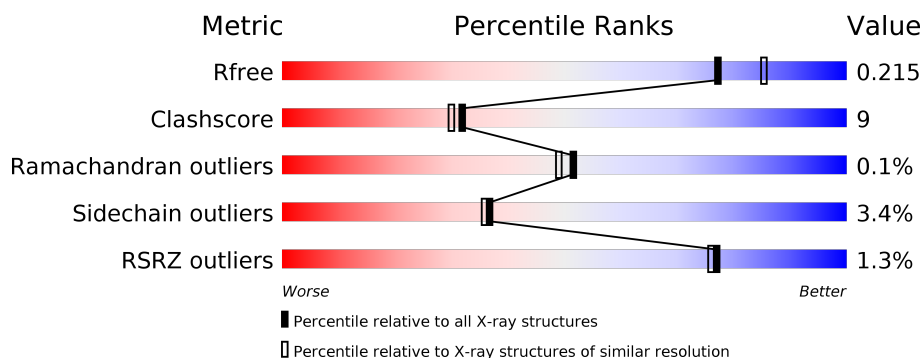
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	496	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	496	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </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
4	1PE	A	500	-	X	X	-
5	PG0	B	500	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8187 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 Fascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	8	0
			3834	2398	683	738	15			
1	B	484	Total	C	N	O	S	0	10	0
			3830	2398	684	733	15			

There are 6 discrepancies between the modelled and reference sequences:

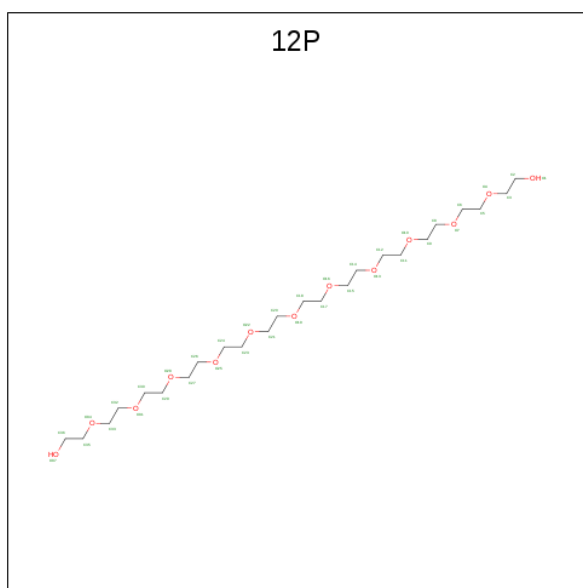
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP Q16658
A	-1	GLY	-	EXPRESSION TAG	UNP Q16658
A	0	HIS	-	EXPRESSION TAG	UNP Q16658
B	-2	ALA	-	EXPRESSION TAG	UNP Q16658
B	-1	GLY	-	EXPRESSION TAG	UNP Q16658
B	0	HIS	-	EXPRESSION TAG	UNP Q16658

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



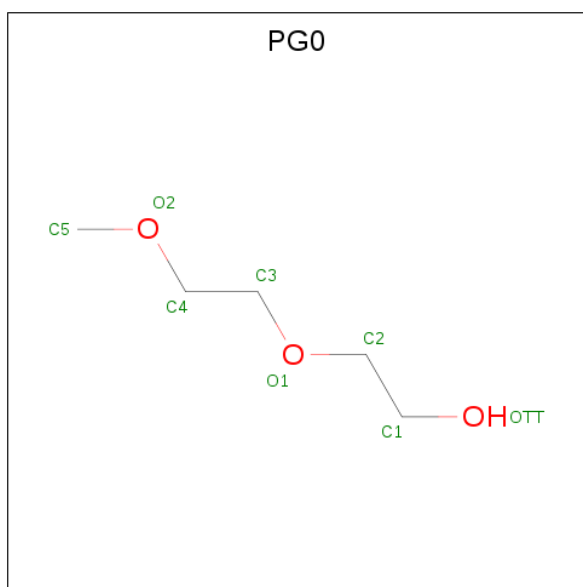
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



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

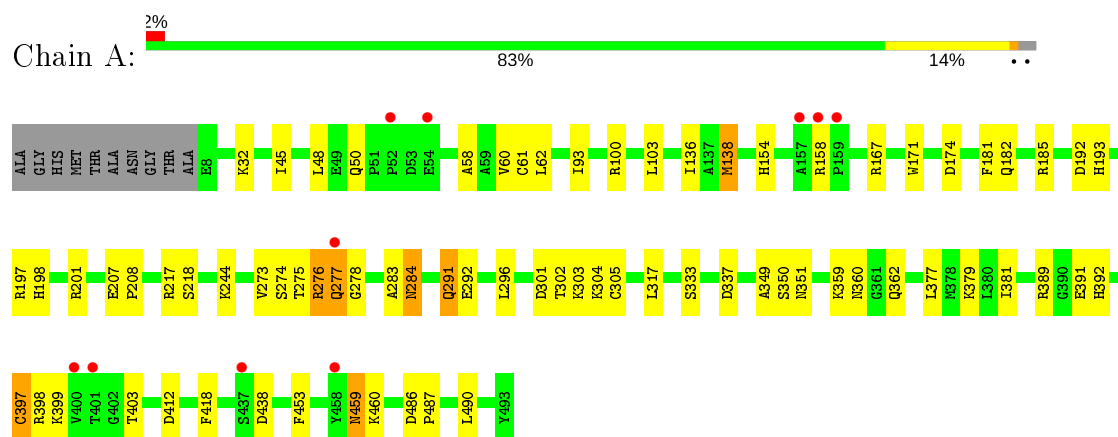
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total	O	0	0
			192	192		
6	B	204	Total	O	0	0
			204	204		

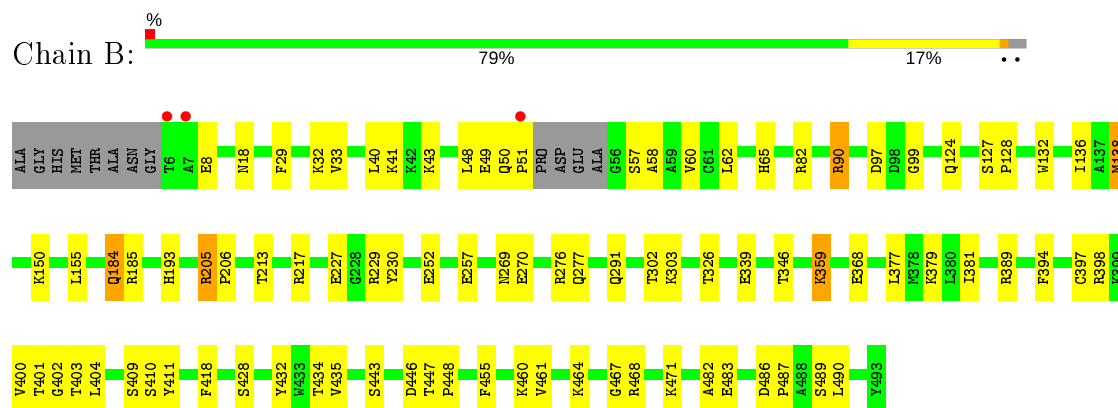
3 Residue-property plots [i](#)

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: Fascin



• Molecule 1: Fascin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.69 Å 71.01 Å 112.74 Å 90.00° 131.23° 90.00°	Depositor
Resolution (Å)	30.66 – 2.00 42.16 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.66-2.00) 95.8 (42.16-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.98 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.178 , 0.220 0.175 , 0.215	Depositor DCC
R_{free} test set	2000 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8187	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: 12P, GOL, PG0, 1PE

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	0.37	0/3939	0.51	0/5324
1	B	0.39	0/3939	0.53	0/5324
All	All	0.38	0/7878	0.52	0/10648

There are no bond length outliers.

There are no bond angle outliers.

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	3834	0	3736	71	0
1	B	3830	0	3746	64	0
2	A	24	0	32	1	0
2	B	24	0	32	2	0
3	A	25	0	33	4	0
4	A	27	0	35	14	0
4	B	20	0	26	3	0
5	B	7	0	9	3	0
6	A	192	0	0	3	0
6	B	204	0	0	5	0
All	All	8187	0	7649	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 9.

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)
1:B:90:ARG:HG3	1:B:90:ARG:HH11	1.17	1.08
1:A:276:ARG:HA	1:A:277:GLN:HB2	1.49	0.94
1:A:277:GLN:H	1:A:278:GLY:HA3	1.30	0.94
1:B:359:LYS:H	1:B:359:LYS:HD2	1.38	0.88
1:B:404:LEU:HD21	1:B:443:SER:HB2	1.56	0.86
1:B:359:LYS:N	1:B:359:LYS:HD2	1.93	0.84
1:A:277:GLN:N	1:A:278:GLY:HA3	1.93	0.83
1:B:90:ARG:NH1	1:B:90:ARG:HG3	1.89	0.80
1:A:100:ARG:NH2	3:A:498:12P:H112	1.97	0.78
1:A:167:ARG:NH1	1:A:174:ASP:OD1	2.23	0.72
1:A:351:ASN:HB3	4:A:499:1PE:H162	1.71	0.70
1:A:460:LYS:HE3	4:A:500:1PE:H251	1.71	0.69
1:A:296:LEU:HD12	1:A:305[B]:CYS:SG	2.33	0.68
1:A:459:ASN:HD22	1:A:459:ASN:H	1.42	0.67
1:B:486:ASP:HB2	1:B:487:PRO:HD2	1.78	0.65
1:A:453:PHE:O	2:A:495:GOL:H11	1.96	0.64
1:A:284:ASN:N	1:A:284:ASN:HD22	1.97	0.63
1:A:277:GLN:N	1:A:278:GLY:CA	2.61	0.62
1:B:184:GLN:HA	1:B:184:GLN:HE21	1.65	0.61
1:A:490:LEU:O	4:A:500:1PE:H252	2.00	0.61
1:A:460:LYS:CE	4:A:500:1PE:H251	2.30	0.61
1:A:284:ASN:HD22	1:A:284:ASN:H	1.47	0.61
4:A:501:1PE:H142	4:A:501:1PE:H261	1.82	0.60
1:B:434[A]:THR:HG22	1:B:435:VAL:N	2.17	0.59
1:A:276:ARG:CG	1:A:291:GLN:HG2	2.32	0.59
1:A:459:ASN:N	1:A:459:ASN:HD22	1.99	0.59
1:A:276:ARG:HA	1:A:277:GLN:CB	2.26	0.58
1:B:40:LEU:O	1:B:41:LYS:HD2	2.04	0.58
1:A:438:ASP:OD1	1:A:438:ASP:N	2.32	0.57
1:A:398:ARG:HE	1:A:403:THR:CG2	2.17	0.57
1:A:274[A]:SER:OG	1:A:292:GLU:HG3	2.05	0.57
1:B:394:PHE:CE1	5:B:500:PG0:H12	2.39	0.57
1:A:197:ARG:HD3	1:A:201:ARG:HH21	1.70	0.57
1:A:333:SER:HA	1:A:350:SER:OG	2.05	0.57
1:B:460:LYS:HE3	4:B:494:1PE:H141	1.88	0.56
1:A:276:ARG:HG2	1:A:291:GLN:HG2	1.87	0.56
1:B:490:LEU:O	4:B:494:1PE:H241	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:HG2	1:A:337:ASP:OD2	2.07	0.55
1:A:460:LYS:HE3	4:A:500:1PE:H151	1.89	0.54
1:A:389:ARG:HH21	4:A:501:1PE:H162	1.72	0.54
1:B:432:TYR:CD1	1:B:448:PRO:HB3	2.43	0.53
1:A:486:ASP:HB2	1:A:487:PRO:HD2	1.90	0.53
1:B:127:SER:HB2	1:B:128:PRO:HD2	1.89	0.53
1:A:296:LEU:CD1	1:A:305[B]:CYS:SG	2.96	0.53
1:A:486:ASP:HB2	1:A:487:PRO:CD	2.39	0.53
1:A:181:PHE:CE1	3:A:498:12P:H31	2.44	0.53
1:B:377:LEU:C	1:B:377:LEU:HD23	2.30	0.53
1:B:29:PHE:O	1:B:32:LYS:HG3	2.10	0.52
1:A:276:ARG:CA	1:A:277:GLN:HB2	2.31	0.52
1:B:58:ALA:HB1	1:B:217:ARG:HG3	1.92	0.52
1:B:400:VAL:HG23	1:B:401:THR:HG23	1.92	0.52
1:B:49:GLU:HG2	6:B:624:HOH:O	2.10	0.52
1:B:269:ASN:O	1:B:270:GLU:HB2	2.10	0.51
1:A:460:LYS:HE3	4:A:500:1PE:C15	2.41	0.51
1:A:197:ARG:CD	1:A:201:ARG:HH21	2.24	0.51
1:A:302:THR:O	1:A:303:LYS:HB2	2.10	0.51
4:B:494:1PE:H262	6:B:667:HOH:O	2.11	0.51
1:B:48:LEU:HD11	1:B:60:VAL:HG21	1.92	0.51
1:A:192:ASP:O	1:A:193:HIS:HB2	2.11	0.51
3:A:498:12P:H202	6:A:633:HOH:O	2.10	0.51
1:B:90:ARG:NH1	1:B:90:ARG:CG	2.66	0.50
1:A:154:HIS:HE1	1:A:158:ARG:HH12	1.57	0.50
1:B:99:GLY:HA2	1:B:213:THR:OG1	2.12	0.50
1:A:377:LEU:HD23	1:A:377:LEU:C	2.32	0.50
1:B:409:SER:O	5:B:500:PG0:H21	2.11	0.50
1:A:45:ILE:HD11	4:A:501:1PE:H141	1.93	0.50
1:B:379:LYS:HD3	1:B:418:PHE:CD2	2.47	0.50
1:A:277:GLN:O	1:A:277:GLN:HG3	2.12	0.49
1:B:302:THR:O	1:B:303:LYS:HB2	2.11	0.49
1:A:58:ALA:HB1	1:A:217:ARG:HG3	1.95	0.49
1:A:391:GLU:HG3	1:A:392:HIS:CD2	2.48	0.49
1:A:93:ILE:HG12	1:A:103:LEU:CD1	2.43	0.48
1:A:50:GLN:NE2	1:A:218:SER:O	2.47	0.48
1:B:33[B]:VAL:CG1	2:B:497:GOL:H11	2.44	0.48
1:A:460:LYS:HE3	4:A:500:1PE:C25	2.41	0.48
1:B:397[B]:CYS:SG	1:B:402:GLY:HA2	2.54	0.48
1:A:32:LYS:HB2	6:A:651:HOH:O	2.14	0.47
1:B:97:ASP:O	1:B:185[B]:ARG:NH2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HE	1:A:403:THR:HG21	1.79	0.46
1:A:389:ARG:NH2	4:A:501:1PE:H162	2.30	0.46
1:B:33[B]:VAL:HG12	2:B:497:GOL:H11	1.98	0.46
1:A:181:PHE:CD1	3:A:498:12P:H31	2.51	0.46
1:B:398:ARG:HD2	1:B:403:THR:OG1	2.16	0.46
1:A:284:ASN:N	1:A:284:ASN:ND2	2.63	0.45
1:A:61:CYS:C	1:A:62:LEU:HD12	2.37	0.45
1:B:434[A]:THR:HG22	1:B:435:VAL:H	1.79	0.45
1:B:43:LYS:HA	1:B:65:HIS:CD2	2.51	0.45
1:A:273:VAL:HA	1:A:283:ALA:HA	1.98	0.45
1:B:50:GLN:HB2	1:B:51:PRO:HA	1.97	0.45
1:B:8:GLU:HA	1:B:8:GLU:OE2	2.17	0.45
1:A:360:ASN:ND2	1:A:362:GLN:H	2.15	0.45
1:A:302:THR:HG21	1:A:304:LYS:HD2	1.99	0.45
1:B:447:THR:O	1:B:447:THR:HG23	2.17	0.44
1:B:468:ARG:NH1	1:B:483:GLU:HG2	2.32	0.44
1:B:276:ARG:HG2	1:B:291[A]:GLN:NE2	2.33	0.44
1:B:97:ASP:O	1:B:185[A]:ARG:NH2	2.50	0.44
1:B:18:ASN:HB3	1:B:132:TRP:CZ3	2.53	0.44
1:A:207:GLU:HB2	1:A:208:PRO:HD2	2.00	0.44
1:B:359:LYS:H	1:B:359:LYS:CD	2.18	0.44
1:A:276:ARG:HG3	1:A:291:GLN:HG2	2.00	0.44
1:A:275:THR:O	1:A:277:GLN:HA	2.18	0.44
1:B:136:ILE:HG23	1:B:138:MET:SD	2.58	0.44
1:B:257:GLU:OE1	6:B:664:HOH:O	2.21	0.44
1:B:471:LYS:HB3	1:B:489:SER:HB3	2.00	0.44
1:B:389[B]:ARG:NH2	6:B:508:HOH:O	2.51	0.43
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.87	0.43
1:A:397:CYS:HB2	1:A:412:ASP:OD1	2.18	0.43
1:B:339:GLU:HB2	1:B:346:THR:OG1	2.18	0.43
1:B:394:PHE:CD2	1:B:411:TYR:HB3	2.53	0.43
1:A:182:GLN:O	1:A:185:ARG:N	2.44	0.43
1:A:379:LYS:HD3	1:A:418:PHE:CD2	2.53	0.43
1:B:50:GLN:HA	1:B:51:PRO:C	2.39	0.43
1:A:359:LYS:HB3	6:A:670:HOH:O	2.18	0.43
1:B:381:ILE:C	1:B:381:ILE:HD12	2.39	0.43
1:B:230:TYR:HB2	1:B:252:GLU:HG2	2.01	0.43
1:A:136:ILE:HG23	1:A:138:MET:SD	2.59	0.42
1:A:303:LYS:HE3	1:B:400:VAL:O	2.19	0.42
4:A:501:1PE:C14	4:A:501:1PE:H261	2.48	0.42
1:B:205:ARG:HA	1:B:206:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PRO:CG	1:B:90:ARG:HE	2.32	0.42
1:A:459:ASN:N	1:A:459:ASN:ND2	2.67	0.42
1:B:62:LEU:N	1:B:62:LEU:HD12	2.35	0.42
1:B:434[A]:THR:CG2	1:B:435:VAL:N	2.82	0.42
1:B:410:SER:HA	6:B:544:HOH:O	2.20	0.41
1:B:217:ARG:HG2	1:B:217:ARG:HH21	1.86	0.41
1:A:291:GLN:HB3	1:A:292:GLU:OE1	2.21	0.41
1:B:471:LYS:HE3	1:B:482:ALA:HB2	2.03	0.41
1:B:464:LYS:HE2	1:B:467:GLY:HA2	2.03	0.41
1:A:317:LEU:HD22	1:A:349:ALA:HB1	2.02	0.41
1:B:51:PRO:HG3	1:B:90:ARG:HE	1.86	0.41
1:B:455:PHE:CD2	1:B:461[B]:VAL:CG1	3.04	0.41
1:A:389:ARG:O	4:A:500:1PE:H152	2.20	0.41
1:B:359:LYS:CD	1:B:359:LYS:N	2.74	0.41
1:A:381:ILE:C	1:A:381:ILE:HD12	2.42	0.41
1:A:389:ARG:HE	4:A:501:1PE:C16	2.33	0.41
1:A:48:LEU:HD11	1:A:60:VAL:HG21	2.03	0.41
1:B:193:HIS:CD2	1:B:193:HIS:N	2.89	0.40
1:B:409:SER:HA	5:B:500:PG0:O1	2.21	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	492/496 (99%)	464 (94%)	27 (6%)	1 (0%)	47	44
1	B	490/496 (99%)	467 (95%)	23 (5%)	0	100	100
All	All	982/992 (99%)	931 (95%)	50 (5%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	GLN

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	408/405 (101%)	398 (98%)	10 (2%)	47	49
1	B	408/405 (101%)	391 (96%)	17 (4%)	30	27
All	All	816/810 (101%)	789 (97%)	27 (3%)	37	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	A	171	TRP
1	A	198	HIS
1	A	276	ARG
1	A	284	ASN
1	A	291	GLN
1	A	301	ASP
1	A	397	CYS
1	A	399	LYS
1	A	459	ASN
1	B	57	SER
1	B	82	ARG
1	B	90	ARG
1	B	124	GLN
1	B	138	MET
1	B	150	LYS
1	B	155	LEU
1	B	184	GLN
1	B	205	ARG
1	B	227	GLU
1	B	229	ARG
1	B	277	GLN
1	B	326	THR

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Mol	Chain	Res	Type
1	B	359	LYS
1	B	368	GLU
1	B	428	SER
1	B	446	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	143	ASN
1	A	182	GLN
1	A	193	HIS
1	A	277	GLN
1	A	284	ASN
1	A	360	ASN
1	A	415	GLN
1	A	459	ASN
1	B	124	GLN
1	B	182	GLN
1	B	184	GLN
1	B	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	GOL	A	497	-	5,5,5	0.38	0	5,5,5	0.17	0
4	1PE	A	501	-	9,9,15	1.36	2 (22%)	8,8,14	1.68	2 (25%)
2	GOL	A	494	-	5,5,5	0.40	0	5,5,5	0.30	0
2	GOL	B	498	-	5,5,5	0.36	0	5,5,5	0.31	0
5	PG0	B	500	-	6,6,7	1.48	2 (33%)	5,5,6	2.23	2 (40%)
2	GOL	B	496	-	5,5,5	0.42	0	5,5,5	0.33	0
2	GOL	B	495	-	5,5,5	0.46	0	5,5,5	0.42	0
2	GOL	A	495	-	5,5,5	0.48	0	5,5,5	0.65	0
4	1PE	B	494	-	9,9,15	1.38	2 (22%)	8,8,14	1.39	2 (25%)
2	GOL	B	497	-	5,5,5	0.41	0	5,5,5	0.19	0
2	GOL	A	496	-	5,5,5	0.37	0	5,5,5	0.33	0
4	1PE	B	499	-	9,9,15	1.37	2 (22%)	8,8,14	1.51	2 (25%)
3	12P	A	498	-	24,24,36	1.04	2 (8%)	23,23,35	0.50	0
4	1PE	A	500	-	6,6,15	1.60	2 (33%)	5,5,14	1.98	2 (40%)
4	1PE	A	499	-	9,9,15	1.42	2 (22%)	8,8,14	1.45	2 (25%)

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
2	GOL	A	497	-	-	4/4/4/4	-
4	1PE	A	501	-	-	4/7/7/13	-
2	GOL	A	494	-	-	0/4/4/4	-
2	GOL	B	498	-	-	2/4/4/4	-
5	PG0	B	500	-	-	4/4/4/5	-
2	GOL	B	496	-	-	0/4/4/4	-
2	GOL	B	495	-	-	0/4/4/4	-
2	GOL	A	495	-	-	4/4/4/4	-
4	1PE	B	494	-	-	4/7/7/13	-
2	GOL	B	497	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	496	-	-	2/4/4/4	-
4	1PE	B	499	-	-	3/7/7/13	-
3	12P	A	498	-	-	7/22/22/34	-
4	1PE	A	500	-	-	3/4/4/13	-
4	1PE	A	499	-	-	3/7/7/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	499	1PE	C26-C16	-2.60	1.35	1.49
4	A	500	1PE	C26-C16	-2.55	1.35	1.49
4	A	501	1PE	C26-C16	-2.52	1.36	1.49
4	B	494	1PE	C26-C16	-2.52	1.36	1.49
4	A	499	1PE	C25-C15	-2.50	1.36	1.49
4	B	499	1PE	C26-C16	-2.50	1.36	1.49
4	A	500	1PE	C15-C25	-2.48	1.36	1.49
4	B	494	1PE	C25-C15	-2.45	1.36	1.49
4	B	499	1PE	C25-C15	-2.42	1.36	1.49
5	B	500	PG0	C2-C1	-2.42	1.36	1.49
5	B	500	PG0	C3-C4	-2.36	1.36	1.49
4	A	501	1PE	C25-C15	-2.32	1.37	1.49
3	A	498	12P	C11-C12	2.11	1.59	1.49
3	A	498	12P	C14-C15	2.07	1.59	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	PG0	O1-C3-C4	3.44	125.19	110.07
4	A	500	1PE	OH6-C15-C25	3.18	124.05	110.07
4	A	501	1PE	OH5-C25-C15	2.99	123.88	110.39
4	B	499	1PE	OH5-C25-C15	2.80	123.04	110.39
4	A	501	1PE	OH6-C15-C25	2.78	122.94	110.39
4	A	499	1PE	OH5-C25-C15	2.74	122.77	110.39
4	B	499	1PE	OH6-C15-C25	2.41	121.25	110.39
5	B	500	PG0	O2-C4-C3	2.38	125.63	111.81
4	A	499	1PE	OH6-C15-C25	2.37	121.10	110.39
4	B	494	1PE	OH5-C25-C15	2.33	120.90	110.39
4	A	500	1PE	OH5-C25-C15	2.17	124.39	111.81
4	B	494	1PE	OH6-C15-C25	2.11	119.92	110.39

There are no chirality outliers.

All (41) torsion outliers are listed below:

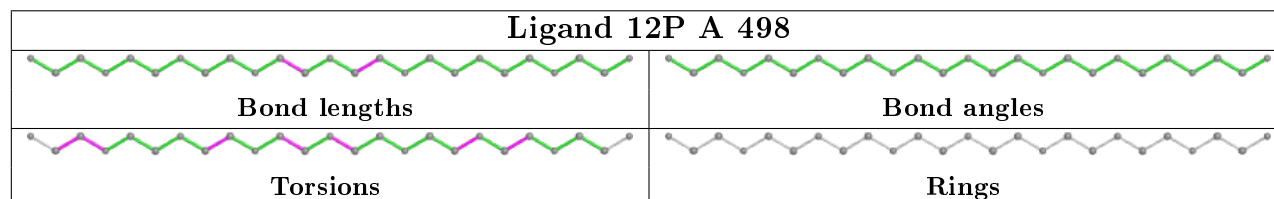
Mol	Chain	Res	Type	Atoms
2	A	497	GOL	O1-C1-C2-C3
2	A	495	GOL	O1-C1-C2-C3
2	A	495	GOL	C1-C2-C3-O3
2	A	496	GOL	O1-C1-C2-C3
4	A	501	1PE	C15-C25-OH5-C14
4	A	501	1PE	OH7-C16-C26-OH6
3	A	498	12P	O19-C20-C21-O22
3	A	498	12P	O10-C11-C12-O13
2	A	496	GOL	O1-C1-C2-O2
3	A	498	12P	O7-C8-C9-O10
4	B	499	1PE	OH5-C14-C24-OH4
5	B	500	PG0	O1-C3-C4-O2
3	A	498	12P	O1-C2-C3-O4
4	A	499	1PE	OH7-C16-C26-OH6
5	B	500	PG0	OTT-C1-C2-O1
4	B	494	1PE	OH5-C14-C24-OH4
2	A	497	GOL	C1-C2-C3-O3
2	B	498	GOL	O1-C1-C2-C3
2	B	497	GOL	O1-C1-C2-C3
4	A	499	1PE	OH6-C15-C25-OH5
4	A	500	1PE	OH6-C15-C25-OH5
2	A	497	GOL	O1-C1-C2-O2
2	A	497	GOL	O2-C2-C3-O3
2	A	495	GOL	O1-C1-C2-O2
2	A	495	GOL	O2-C2-C3-O3
5	B	500	PG0	C1-C2-O1-C3
4	B	494	1PE	OH6-C15-C25-OH5
4	B	499	1PE	OH6-C15-C25-OH5
2	B	498	GOL	O1-C1-C2-O2
4	A	501	1PE	C25-C15-OH6-C26
5	B	500	PG0	C4-C3-O1-C2
4	A	500	1PE	C25-C15-OH6-C26
4	B	494	1PE	C25-C15-OH6-C26
3	A	498	12P	C2-C3-O4-C5
3	A	498	12P	C17-C18-O19-C20
4	A	500	1PE	C16-C26-OH6-C15
4	A	501	1PE	C16-C26-OH6-C15
4	A	499	1PE	C16-C26-OH6-C15
4	B	499	1PE	C16-C26-OH6-C15
3	A	498	12P	C15-C14-O13-C12
4	B	494	1PE	OH7-C16-C26-OH6

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	1PE	6	0
5	B	500	PG0	3	0
2	A	495	GOL	1	0
4	B	494	1PE	3	0
2	B	497	GOL	2	0
3	A	498	12P	4	0
4	A	500	1PE	7	0
4	A	499	1PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	486/496 (97%)	-0.39	10 (2%) 63 62	26, 40, 76, 131	0
1	B	484/496 (97%)	-0.47	3 (0%) 89 88	22, 40, 70, 106	0
All	All	970/992 (97%)	-0.43	13 (1%) 77 76	22, 40, 73, 131	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	SER	4.3
1	A	159	PRO	4.1
1	A	277	GLN	4.0
1	A	157	ALA	3.8
1	B	51	PRO	3.3
1	B	6	THR	3.2
1	B	7	ALA	3.1
1	A	401	THR	3.0
1	A	400	VAL	2.4
1	A	52	PRO	2.3
1	A	158	ARG	2.3
1	A	458	TYR	2.2
1	A	54	GLU	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 ⓘ

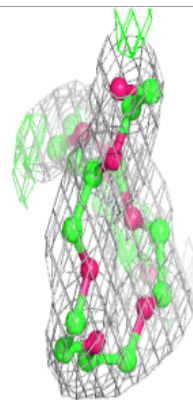
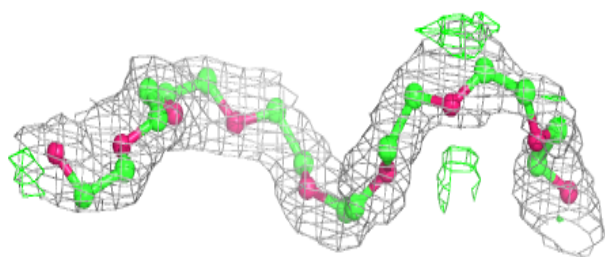
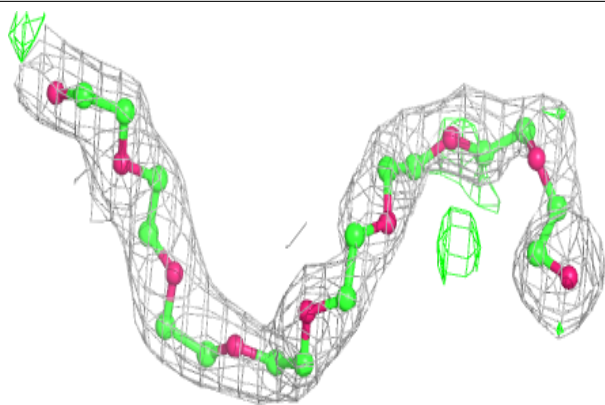
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1PE	A	501	10/16	0.75	0.21	71,83,85,88	0
5	PG0	B	500	7/8	0.77	0.18	46,50,59,65	0
4	1PE	A	500	7/16	0.78	0.19	50,54,65,68	0
4	1PE	B	494	10/16	0.79	0.17	48,67,87,87	0
2	GOL	A	495	6/6	0.80	0.18	33,43,53,60	0
4	1PE	B	499	10/16	0.82	0.20	56,76,96,97	0
3	12P	A	498	25/37	0.86	0.14	42,52,92,95	0
2	GOL	A	497	6/6	0.89	0.12	77,81,83,84	0
2	GOL	B	498	6/6	0.91	0.12	55,66,71,76	0
2	GOL	B	497	6/6	0.91	0.09	31,42,44,45	0
2	GOL	A	496	6/6	0.94	0.10	54,59,63,72	0
2	GOL	A	494	6/6	0.94	0.10	30,35,41,43	0
4	1PE	A	499	10/16	0.95	0.15	55,68,71,71	0
2	GOL	B	495	6/6	0.96	0.12	25,32,36,37	0
2	GOL	B	496	6/6	0.98	0.08	25,32,37,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 12P A 498:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.