



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:32 PM UTC

PDB ID : 3P53 / pdb\_00003p53  
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](mailto: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>.

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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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

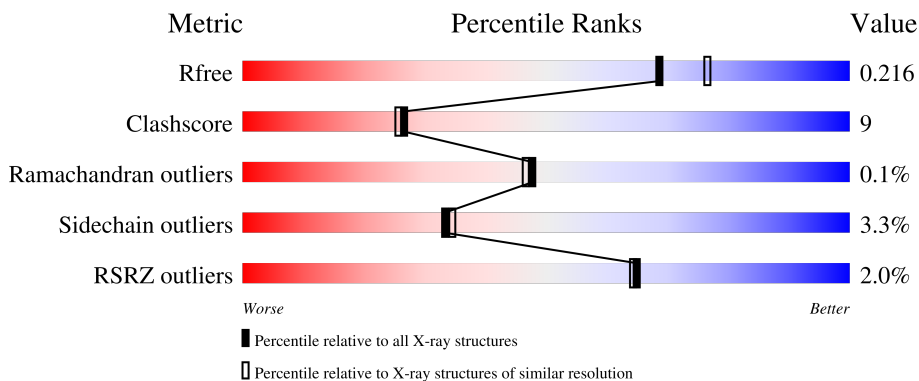
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 2% 82% 14% ..
1	B	496	 % 79% 17% ..

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.

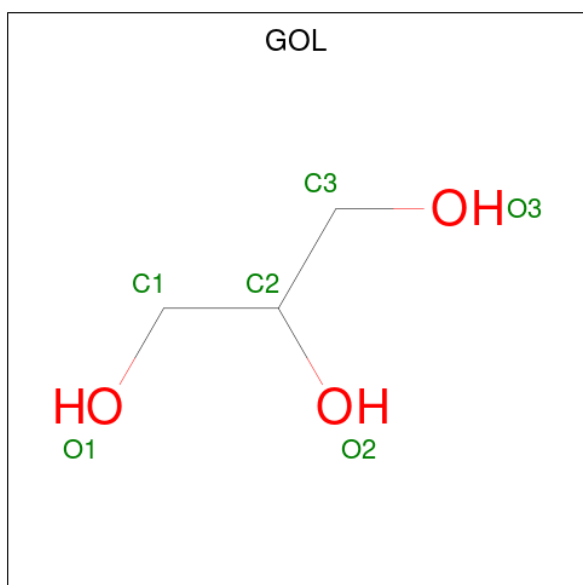
- Molecule 1 is a protein called Fascin.

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

There are 6 discrepancies between the modelled and reference sequences:

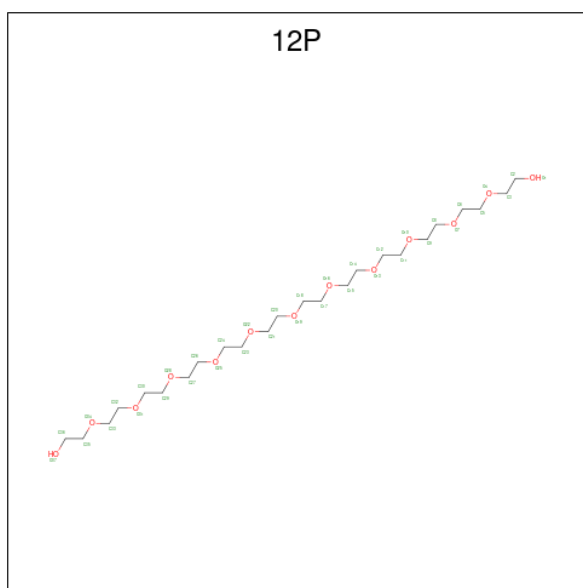
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q16658
A	-1	GLY	-	expression tag	UNP Q16658
A	0	HIS	-	expression tag	UNP Q16658
B	-2	ALA	-	expression tag	UNP Q16658
B	-1	GLY	-	expression tag	UNP Q16658
B	0	HIS	-	expression tag	UNP Q16658

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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 (CCD ID: 12P) (formula:  $C_{24}H_{50}O_{13}$ ).



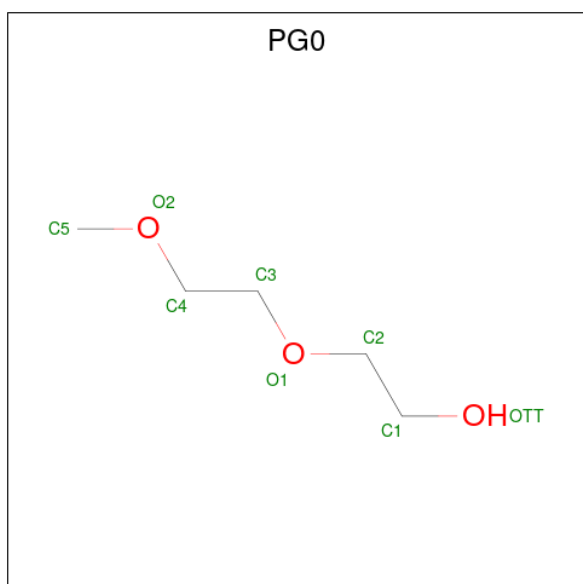
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		

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



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

- Molecule 5 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>3</sub>).



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

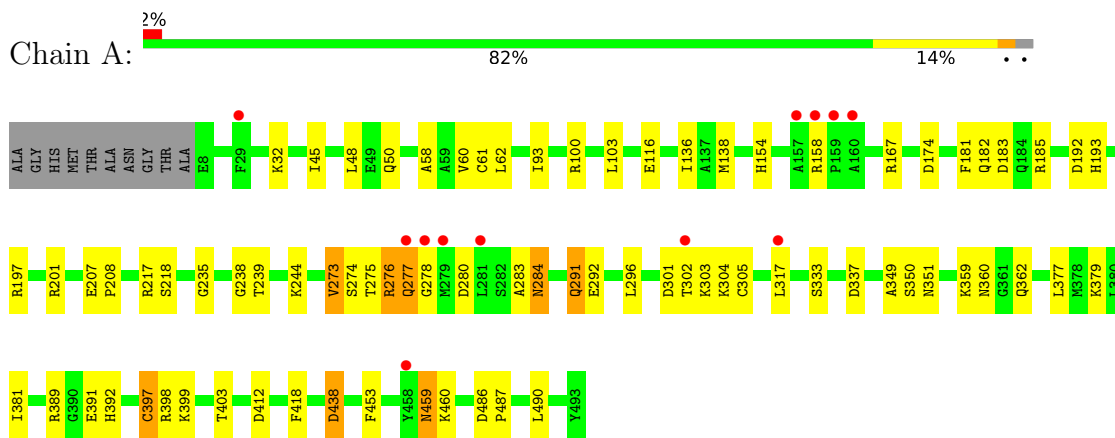
- Molecule 6 is water.

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

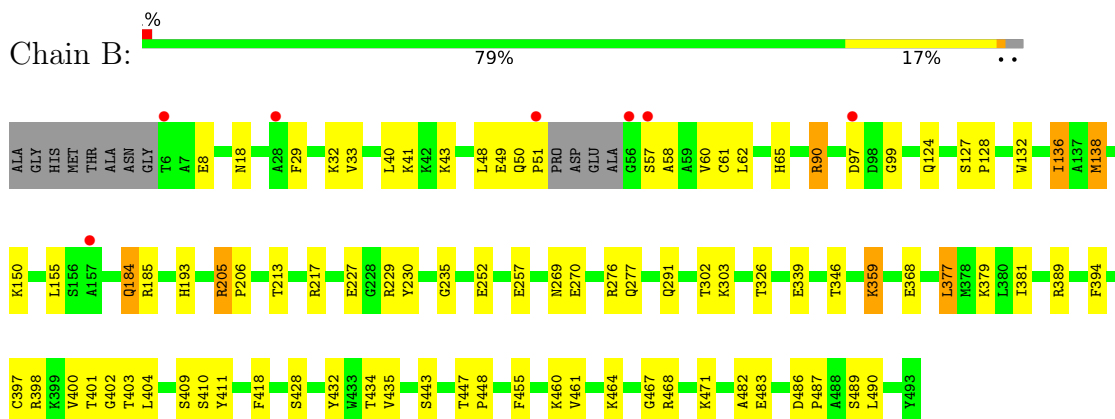
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Fascin



- Molecule 1: Fascin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.69Å 71.01Å 112.74Å 90.00° 131.23° 90.00°	Depositor
Resolution (Å)	30.66 – 2.00 30.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.66-2.00) 97.9 (30.66-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.178 , 0.220 0.176 , 0.216	Depositor DCC
$R_{free}$ test set	2000 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtrriage
Anisotropy	0.177	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.024 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 1PE, PG0, GOL, 12P

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	0.44	0/3939	0.77	3/5324 (0.1%)
1	B	0.46	0/3939	0.76	2/5324 (0.0%)
All	All	0.45	0/7878	0.77	5/10648 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLY	CA-C-N	6.36	126.11	119.05
1	A	235	GLY	C-N-CA	6.36	126.11	119.05
1	B	235	GLY	CA-C-N	6.05	125.27	118.97
1	B	235	GLY	C-N-CA	6.05	125.27	118.97
1	A	116	GLU	CB-CA-C	-5.22	110.54	116.54

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	74	0
1	B	3830	0	3746	66	0
2	A	24	0	32	1	0
2	B	24	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	143	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 (143) 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:HD2	1:B:359:LYS:N	1.93	0.84
1:A:277:GLN:N	1:A:278:GLY:HA3	1.93	0.83
1:B:90:ARG:HG3	1:B:90:ARG:NH1	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:HD22	1:A:284:ASN:N	1.97	0.63
1:A:277:GLN:N	1:A:278:GLY:CA	2.61	0.62
1:B:184:GLN:HE21	1:B:184:GLN:HA	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:HD22	1:A:459:ASN:N	1.99	0.59
1:A:276:ARG:HA	1:A:277:GLN:CB	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:377:LEU:HD23	1:B:377:LEU:C	2.30	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
1:A:377:LEU:C	1:A:377:LEU:HD23	2.32	0.55
1:A:304:LYS:HG2	1:A:337:ASP:OD2	2.07	0.55
1:A:389:ARG:HH21	4:A:501:1PE:H162	1.72	0.54
1:A:460:LYS:HE3	4:A:500:1PE:H151	1.89	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: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:136:ILE:HD12	1:B:138:MET:HE1	1.90	0.52
1:B:49:GLU:HG2	6:B:624:HOH:O	2.10	0.52
1:B:400:VAL:HG23	1:B:401:THR:HG23	1.92	0.52
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
1:B:269:ASN:O	1:B:270:GLU:HB2	2.10	0.51
1:B:48:LEU:HD11	1:B:60:VAL:HG21	1.92	0.51
4:B:494:1PE:H262	6:B:667:HOH:O	2.11	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:61:CYS:C	1:A:62:LEU:HD12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:302:THR:O	1:B:303:LYS:HB2	2.11	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:50:GLN:HA	1:B:51:PRO:C	2.39	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:B:381:ILE:C	1:B:381:ILE:HD12	2.39	0.47
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
1:A:389:ARG:NH2	4:A:501:1PE:H162	2.30	0.46
1:A:398:ARG:HE	1:A:403:THR:HG21	1.79	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:381:ILE:C	1:A:381:ILE:HD12	2.42	0.45
1:B:43:LYS:HA	1:B:65:HIS:CD2	2.51	0.45
1:B:434[A]:THR:HG22	1:B:435:VAL:H	1.79	0.45
1:A:273:VAL:HA	1:A:283:ALA:HA	1.98	0.45
1:B:8:GLU:OE2	1:B:8:GLU:HA	2.17	0.45
1:B:50:GLN:HB2	1:B:51:PRO:HA	1.97	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:HG23	1:B:447:THR:O	2.17	0.44
1:B:468:ARG:NH1	1:B:483:GLU:HG2	2.32	0.44
1:B:97:ASP:O	1:B:185[A]:ARG:NH2	2.50	0.44
1:B:276:ARG:HG2	1:B:291[A]:GLN:NE2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:359:LYS:HB3	6:A:670:HOH:O	2.18	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:H261	4:A:501:1PE:C14	2.48	0.42
1:B:61:CYS:C	1:B:62:LEU:HD12	2.44	0.42
1:B:51:PRO:CG	1:B:90:ARG:HE	2.32	0.42
1:B:205:ARG:HA	1:B:206:PRO:HD3	1.94	0.42
1:A:459:ASN:N	1:A:459:ASN:ND2	2.67	0.42
1:B:62:LEU:HD12	1:B:62:LEU:N	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:HH21	1:B:217:ARG:HG2	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:A:238:GLY:O	1:A:239:THR:C	2.63	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:A:278:GLY:C	1:A:280:ASP:H	2.29	0.41
1:A:389:ARG:O	4:A:500:1PE:H152	2.20	0.41
1:B:359:LYS:N	1:B:359:LYS:CD	2.74	0.41
1:B:455:PHE:CD2	1:B:461[B]:VAL:CG1	3.04	0.41
1:A:48:LEU:HD11	1:A:60:VAL:HG21	2.03	0.41
1:A:389:ARG:HE	4:A:501:1PE:C16	2.33	0.41
1:A:182:GLN:O	1:A:183:ASP:C	2.63	0.40
1:B:193:HIS:N	1:B:193:HIS:CD2	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%)	43	42
1	B	490/496 (99%)	467 (95%)	23 (5%)	0	100	100
All	All	982/992 (99%)	931 (95%)	50 (5%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	GLN

### 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	408/405 (101%)	399 (98%)	9 (2%)	45	50
1	B	408/405 (101%)	391 (96%)	17 (4%)	26	25
All	All	816/810 (101%)	790 (97%)	26 (3%)	33	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	VAL
1	A	276	ARG
1	A	284	ASN
1	A	291	GLN
1	A	301	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	397	CYS
1	A	399	LYS
1	A	438	ASP
1	A	459	ASN
1	B	57	SER
1	B	90	ARG
1	B	124	GLN
1	B	136	ILE
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
1	B	359	LYS
1	B	368	GLU
1	B	377	LEU
1	B	428	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	50	GLN
1	A	143	ASN
1	A	182	GLN
1	A	277	GLN
1	A	284	ASN
1	A	360	ASN
1	A	392	HIS
1	A	415	GLN
1	A	459	ASN
1	B	21	ASN
1	B	124	GLN
1	B	143	ASN
1	B	184	GLN
1	B	198	HIS
1	B	258	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
4	1PE	A	500	-	6,6,15	1.60	2 (33%)	5,5,14	1.96	2 (40%)
2	GOL	B	498	-	5,5,5	0.37	0	5,5,5	0.35	0
5	PG0	B	500	-	6,6,7	1.48	2 (33%)	5,5,6	2.21	2 (40%)
2	GOL	B	495	-	5,5,5	0.46	0	5,5,5	0.47	0
4	1PE	B	499	-	9,9,15	1.39	2 (22%)	8,8,14	1.50	2 (25%)
2	GOL	A	495	-	5,5,5	0.49	0	5,5,5	0.69	0
4	1PE	A	499	-	9,9,15	1.44	2 (22%)	8,8,14	1.44	2 (25%)
4	1PE	A	501	-	9,9,15	1.38	2 (22%)	8,8,14	1.67	2 (25%)
2	GOL	B	497	-	5,5,5	0.42	0	5,5,5	0.22	0
2	GOL	A	494	-	5,5,5	0.41	0	5,5,5	0.34	0
3	12P	A	498	-	24,24,36	1.06	2 (8%)	23,23,35	0.50	0
2	GOL	A	497	-	5,5,5	0.39	0	5,5,5	0.19	0
2	GOL	B	496	-	5,5,5	0.43	0	5,5,5	0.35	0
4	1PE	B	494	-	9,9,15	1.40	2 (22%)	8,8,14	1.38	2 (25%)
2	GOL	A	496	-	5,5,5	0.38	0	5,5,5	0.36	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	1PE	A	500	-	-	3/4/4/13	-
2	GOL	B	498	-	-	2/4/4/4	-
5	PG0	B	500	-	-	4/4/4/5	-
2	GOL	B	495	-	-	0/4/4/4	-
4	1PE	B	499	-	-	3/7/7/13	-
2	GOL	A	495	-	-	4/4/4/4	-
4	1PE	A	499	-	-	3/7/7/13	-
4	1PE	A	501	-	-	5/7/7/13	-
2	GOL	B	497	-	-	1/4/4/4	-
2	GOL	A	494	-	-	0/4/4/4	-
3	12P	A	498	-	-	7/22/22/34	-
2	GOL	A	497	-	-	4/4/4/4	-
2	GOL	B	496	-	-	0/4/4/4	-
4	1PE	B	494	-	-	4/7/7/13	-
2	GOL	A	496	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	499	1PE	C26-C16	-2.59	1.35	1.49
4	A	499	1PE	C25-C15	-2.58	1.36	1.49
4	A	500	1PE	C26-C16	-2.54	1.35	1.49
4	B	494	1PE	C25-C15	-2.53	1.36	1.49
4	A	501	1PE	C26-C16	-2.52	1.36	1.49
4	B	494	1PE	C26-C16	-2.51	1.36	1.49
4	B	499	1PE	C25-C15	-2.50	1.36	1.49
4	B	499	1PE	C26-C16	-2.49	1.36	1.49
4	A	500	1PE	C15-C25	-2.47	1.36	1.49
5	B	500	PG0	C2-C1	-2.41	1.36	1.49
4	A	501	1PE	C25-C15	-2.40	1.37	1.49
5	B	500	PG0	C3-C4	-2.35	1.36	1.49
3	A	498	12P	C11-C12	2.16	1.59	1.49
3	A	498	12P	C14-C15	2.11	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	3.42	125.19	110.11
4	A	500	1PE	OH6-C15-C25	3.16	124.05	110.11
4	A	501	1PE	OH5-C25-C15	2.97	123.88	110.35
4	B	499	1PE	OH5-C25-C15	2.78	123.04	110.35
4	A	501	1PE	OH6-C15-C25	2.76	122.94	110.35
4	A	499	1PE	OH5-C25-C15	2.72	122.77	110.35
4	B	499	1PE	OH6-C15-C25	2.39	121.25	110.35
4	A	499	1PE	OH6-C15-C25	2.36	121.10	110.35
5	B	500	PG0	O2-C4-C3	2.35	125.63	111.82
4	B	494	1PE	OH5-C25-C15	2.31	120.90	110.35
4	A	500	1PE	OH5-C25-C15	2.13	124.39	111.82
4	B	494	1PE	OH6-C15-C25	2.10	119.92	110.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

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

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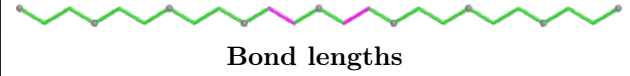
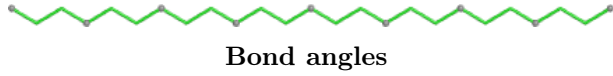
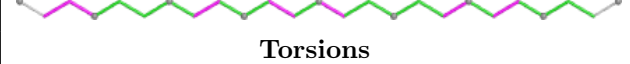

Mol	Chain	Res	Type	Atoms
4	B	494	1PE	OH6-C15-C25-OH5
4	B	499	1PE	OH6-C15-C25-OH5
2	B	498	GOL	O1-C1-C2-O2
5	B	500	PG0	C4-C3-O1-C2
4	A	500	1PE	C25-C15-OH6-C26
3	A	498	12P	C2-C3-O4-C5
4	B	494	1PE	C25-C15-OH6-C26
4	A	501	1PE	C25-C15-OH6-C26
3	A	498	12P	C17-C18-O19-C20
4	A	500	1PE	C16-C26-OH6-C15
4	A	501	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
4	A	501	1PE	OH5-C14-C24-OH4

There are no ring outliers.

8 monomers are involved in 27 short contacts:

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

Ligand 12P A 498	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	486/496 (97%)	0.02	12 (2%) 58 58	21, 39, 76, 131	8 (1%)
1	B	484/496 (97%)	-0.11	7 (1%) 73 73	15, 39, 70, 106	10 (2%)
All	All	970/992 (97%)	-0.04	19 (1%) 65 64	15, 39, 73, 131	18 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	PRO	4.0
1	A	277	GLN	3.7
1	A	278	GLY	3.6
1	B	157	ALA	3.1
1	A	458	TYR	3.0
1	B	57	SER	3.0
1	A	159	PRO	3.0
1	A	157	ALA	2.9
1	B	56	GLY	2.8
1	A	29	PHE	2.5
1	B	6	THR	2.4
1	A	279	MET	2.4
1	A	317	LEU	2.4
1	A	302	THR	2.2
1	A	160	ALA	2.2
1	B	28	ALA	2.2
1	A	158	ARG	2.2
1	A	281	LEU	2.1
1	B	97	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

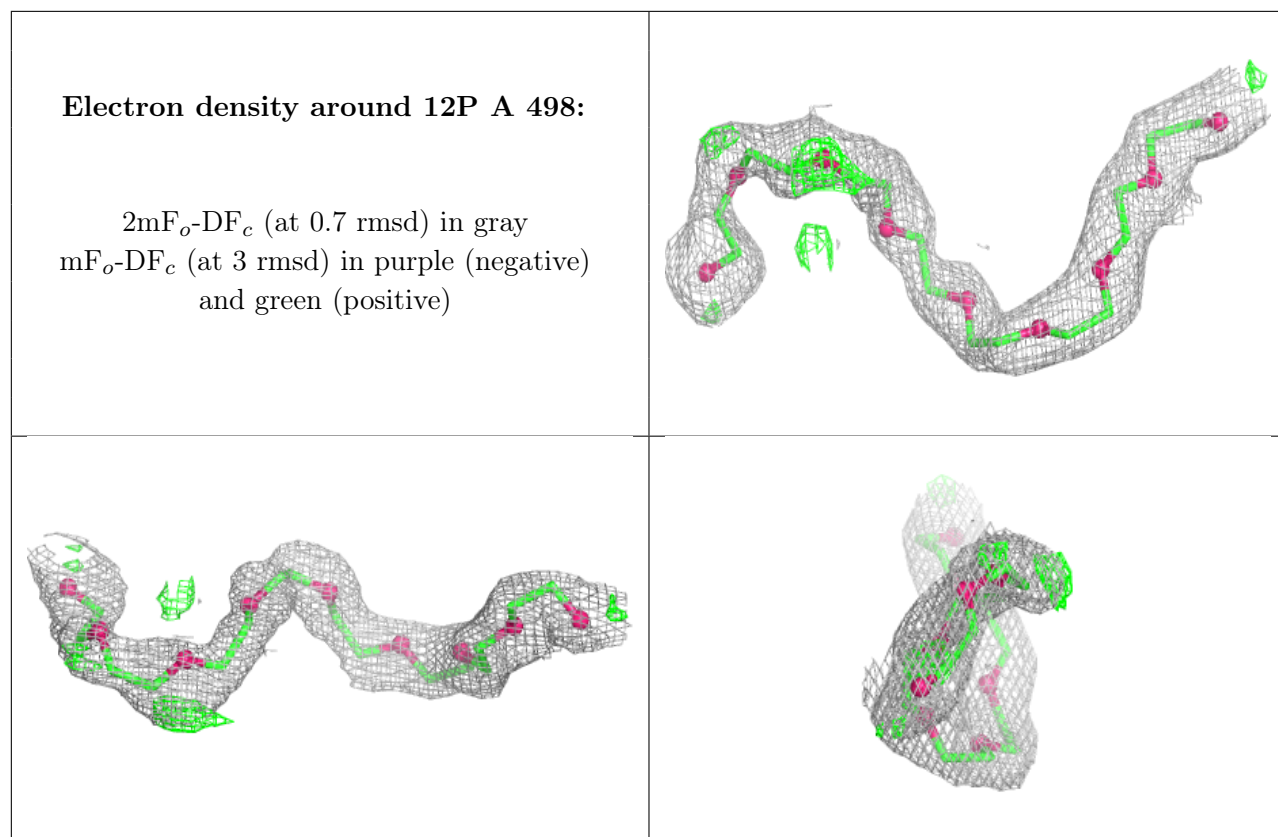
There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	1PE	A	500	7/16	0.75	0.16	50,54,65,68	0
4	1PE	A	501	10/16	0.75	0.18	71,83,85,88	0
2	GOL	A	497	6/6	0.78	0.11	77,81,83,84	0
4	1PE	B	494	10/16	0.79	0.15	48,67,87,87	0
2	GOL	A	495	6/6	0.82	0.17	33,43,53,60	0
5	PG0	B	500	7/8	0.82	0.17	46,50,59,65	0
2	GOL	A	496	6/6	0.86	0.11	54,59,63,72	0
3	12P	A	498	25/37	0.86	0.15	42,52,92,95	0
4	1PE	B	499	10/16	0.87	0.13	56,76,96,97	0
2	GOL	B	498	6/6	0.87	0.16	55,66,71,76	0
4	1PE	A	499	10/16	0.91	0.12	55,68,71,71	0
2	GOL	B	497	6/6	0.92	0.08	31,42,44,45	0
2	GOL	A	494	6/6	0.93	0.10	30,35,41,43	0
2	GOL	B	495	6/6	0.97	0.06	25,32,36,37	0
2	GOL	B	496	6/6	0.98	0.07	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.