



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2020 – 10:13 PM EDT

PDB ID : 6XLI
Title : CRYSTAL STRUCTURE OF ANTI-TAU ANTIBODY PT3
Fab+pT212/pT217-TAU PEPTIDE
Authors : Malia, T.J.; Teplyakov, A.; Luo, J.
Deposited on : 2020-06-28
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:

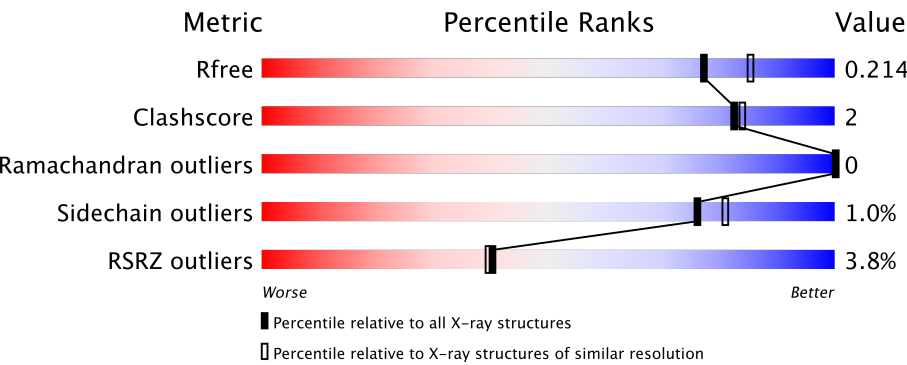
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4

1 Overall quality at a glance i

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	227	<div><div>2%</div><div></div><div>86%</div><div>5%</div><div>9%</div></div>
1	C	227	<div><div>6%</div><div></div><div>85%</div><div>7%</div><div>6%</div></div>
1	H	227	<div><div>9%</div><div></div><div>89%</div><div>5%</div><div>5%</div></div>
2	B	214	<div><div>%</div><div></div><div>95%</div><div>.</div><div>.</div></div>
2	D	214	<div><div></div><div></div><div>95%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	L	214	<div><div>%</div><div><div></div><div>93%</div><div>6%</div></div></div>
3	E	14	<div><div>14%</div><div><div></div><div>71%</div><div>21%</div><div>7%</div></div></div>
3	F	14	<div><div>7%</div><div><div></div><div>71%</div><div>21%</div><div>7%</div></div></div>
3	P	14	<div><div>7%</div><div><div></div><div>79%</div><div>14%</div><div>7%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10912 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 PT3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	1	0
			1570	1002	263	299	6			
1	C	213	Total	C	N	O	S	0	0	0
			1601	1022	270	303	6			
1	H	215	Total	C	N	O	S	0	2	0
			1636	1045	273	312	6			

- Molecule 2 is a protein called PT3 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1660	1042	277	334	7			
2	D	213	Total	C	N	O	S	0	1	0
			1669	1047	277	338	7			
2	L	213	Total	C	N	O	S	0	1	0
			1674	1050	279	338	7			

- Molecule 3 is a protein called Tau Phosphopeptide (Ac-SR(pT)PSLP(pT)PPTRE-OH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			109	61	19	27	2			
3	F	13	Total	C	N	O	P	0	0	0
			108	61	19	26	2			
3	P	13	Total	C	N	O	P	0	0	0
			109	61	19	27	2			

There are 3 discrepancies between the modelled and reference sequences:

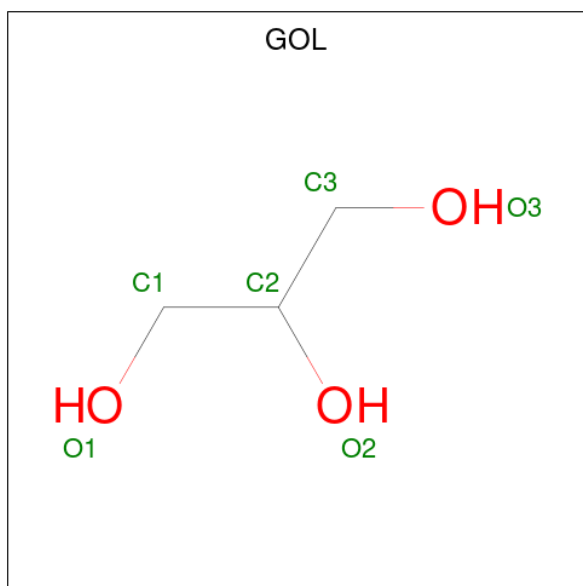
Chain	Residue	Modelled	Actual	Comment	Reference
E	209	ACE	-	acetylation	UNP P10636
F	209	ACE	-	acetylation	UNP P10636

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Chain	Residue	Modelled	Actual	Comment	Reference
P	209	ACE	-	acetylation	UNP P10636

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	123	Total	O	0	0
			123	123		
5	C	92	Total	O	0	0
			92	92		
5	D	136	Total	O	0	0
			136	136		
5	H	110	Total	O	0	0
			110	110		
5	L	138	Total	O	0	0
			138	138		

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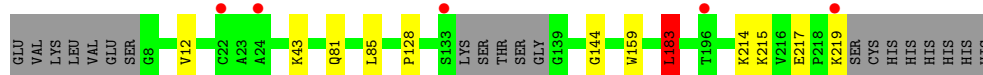
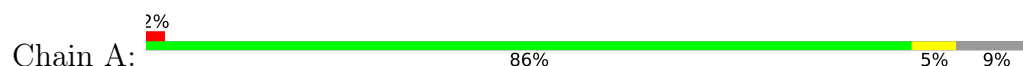
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	10	Total	O	0	0
			10	10		
5	F	13	Total	O	0	0
			13	13		
5	P	14	Total	O	0	0
			14	14		

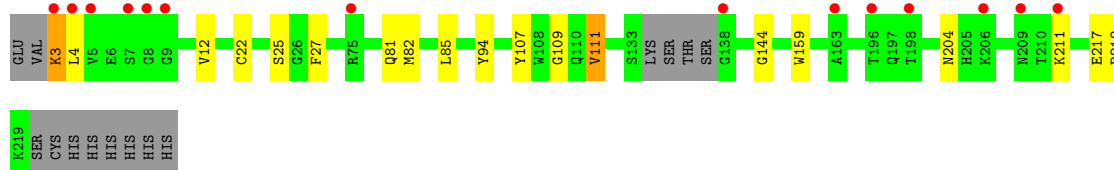
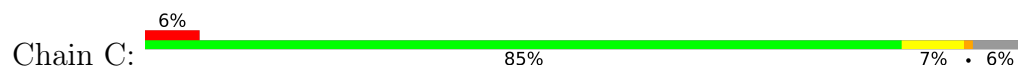
3 Residue-property plots

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.

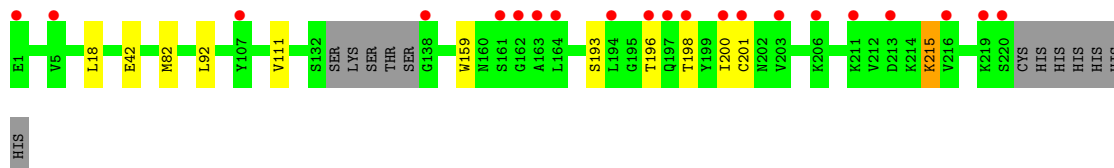
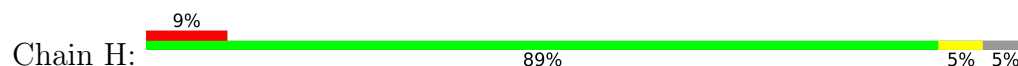
- Molecule 1: PT3 Fab Heavy Chain



- Molecule 1: PT3 Fab Heavy Chain



- Molecule 1: PT3 Fab Heavy Chain

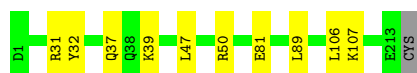


- Molecule 2: PT3 Fab Light Chain

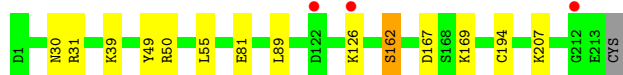
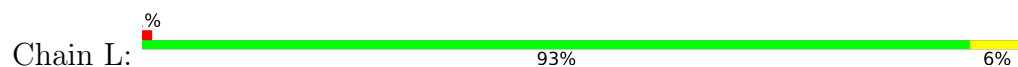


- Molecule 2: PT3 Fab Light Chain





- Molecule 2: PT3 Fab Light Chain



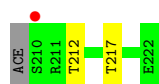
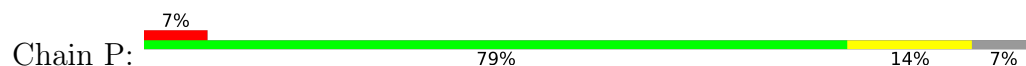
- Molecule 3: Tau Phosphopeptide (Ac-SR(pT)PSLP(pT)PPTRE-OH)



- Molecule 3: Tau Phosphopeptide (Ac-SR(pT)PSLP(pT)PPTRE-OH)



- Molecule 3: Tau Phosphopeptide (Ac-SR(pT)PSLP(pT)PPTRE-OH)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.24Å 83.66Å 166.87Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	36.16 – 2.00 41.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.16-2.00) 99.3 (41.83-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.213 0.190 , 0.214	Depositor DCC
R_{free} test set	2002 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10912	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: TPO, GOL

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	0.42	0/1615	0.55	1/2201 (0.0%)
1	C	0.43	0/1643	0.62	0/2237
1	H	0.44	0/1685	0.56	0/2294
2	B	0.44	0/1695	0.56	0/2294
2	D	0.42	0/1707	0.60	0/2311
2	L	0.46	0/1712	0.57	0/2317
3	E	0.34	0/88	0.60	0/114
3	F	0.43	0/87	0.60	0/114
3	P	0.40	0/88	0.50	0/114
All	All	0.43	0/10320	0.58	1/13996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	LEU	CA-CB-CG	5.49	127.93	115.30

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	1570	0	1536	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1601	0	1571	16	0
1	H	1636	0	1611	8	0
2	B	1660	0	1617	5	0
2	D	1669	0	1619	5	0
2	L	1674	0	1629	8	0
3	E	109	0	99	1	0
3	F	108	0	99	1	0
3	P	109	0	99	0	0
4	A	6	0	8	0	0
4	D	6	0	8	0	0
4	L	6	0	8	1	0
5	A	122	0	0	0	0
5	B	123	0	0	2	0
5	C	92	0	0	2	0
5	D	136	0	0	1	0
5	E	10	0	0	0	0
5	F	13	0	0	0	0
5	H	110	0	0	0	0
5	L	138	0	0	4	0
5	P	14	0	0	0	0
All	All	10912	0	9904	50	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 2.

All (50) 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:B:11:MET:SD	5:B:414:HOH:O	2.40	0.79
1:A:128:PRO:HD3	1:A:214:LYS:HE2	1.67	0.76
1:A:81:GLN:HG2	5:L:401:HOH:O	1.85	0.76
2:L:167:ASP:OD2	2:L:169:LYS:HG2	1.87	0.75
1:C:3:LYS:N	1:C:25:SER:O	2.22	0.71
1:H:42:GLU:OE1	1:H:42:GLU:N	2.25	0.69
2:L:126:LYS:HD2	2:L:126:LYS:N	2.08	0.68
1:C:4:LEU:HD21	1:C:27:PHE:HZ	1.60	0.66
1:H:92:LEU:HB3	1:H:111:VAL:HG21	1.80	0.63
1:A:12:VAL:HG11	1:A:85:LEU:HD13	1.83	0.60
2:L:162:SER:HB3	4:L:301:GOL:H12	1.85	0.59
1:H:200:ILE:HG12	1:H:215:LYS:HB2	1.87	0.57
2:L:30[B]:ASN:ND2	5:L:401:HOH:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:HD21	1:C:27:PHE:CZ	2.38	0.57
1:H:92:LEU:HB3	1:H:111:VAL:CG2	2.36	0.55
1:C:204:ASN:OD1	1:C:211:LYS:HE3	2.07	0.54
1:C:107:TYR:HE1	5:C:304:HOH:O	1.91	0.53
1:C:82:MET:HB3	1:C:85:LEU:HD21	1.89	0.53
5:D:458:HOH:O	3:F:221:ARG:HG3	2.09	0.53
2:L:49:TYR:HD1	2:L:55:LEU:HD22	1.73	0.53
1:A:219:LYS:NZ	2:B:122:ASP:OD2	2.40	0.52
1:C:12:VAL:HG11	1:C:85:LEU:HD13	1.92	0.51
1:C:94:TYR:CD2	1:C:111:VAL:HG13	2.47	0.49
1:C:81:GLN:OE1	5:C:301:HOH:O	2.20	0.48
2:B:45:LYS:NZ	5:B:303:HOH:O	2.46	0.48
1:C:94:TYR:CE2	1:C:111:VAL:HG13	2.48	0.48
1:A:43:LYS:HE3	1:A:43:LYS:HB2	1.58	0.46
1:C:3:LYS:HE3	1:C:3:LYS:HB3	1.69	0.46
2:L:39:LYS:HE2	2:L:81:GLU:O	2.16	0.46
2:D:32:TYR:CZ	2:D:50:ARG:NH2	2.84	0.46
1:A:183:LEU:C	1:A:183:LEU:HD12	2.36	0.46
1:C:4:LEU:HB2	1:C:109:GLY:HA3	1.97	0.45
2:D:39:LYS:HE2	2:D:81:GLU:O	2.16	0.45
1:C:4:LEU:HB3	1:C:22:CYS:SG	2.57	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.45
1:C:3:LYS:O	1:C:25:SER:N	2.43	0.45
1:H:159:TRP:CH2	1:H:201:CYS:HB3	2.53	0.44
1:H:18:LEU:HD23	1:H:82:MET:HE3	2.00	0.44
2:B:93:GLU:OE2	3:E:221:ARG:NH2	2.52	0.43
2:L:207:LYS:NZ	5:L:408:HOH:O	2.50	0.42
1:A:144:GLY:HA2	1:A:159:TRP:CH2	2.54	0.42
1:A:215:LYS:HE2	1:A:217:GLU:OE1	2.19	0.42
2:L:31:ARG:NH2	5:L:409:HOH:O	2.52	0.42
2:D:106:LEU:HD23	2:D:107:LYS:O	2.20	0.42
2:D:37:GLN:HB2	2:D:47:LEU:HD11	2.01	0.41
1:C:144:GLY:HA2	1:C:159:TRP:CH2	2.56	0.41
1:H:193:SER:HA	1:H:196:THR:HG22	2.02	0.41
2:D:31:ARG:O	2:D:50:ARG:HD3	2.21	0.40
1:H:198:THR:HG23	1:H:215:LYS:HD2	2.04	0.40
1:C:217:GLU:HA	1:C:218:PRO:HD3	1.96	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	204/227 (90%)	200 (98%)	4 (2%)	0	100	100
1	C	209/227 (92%)	204 (98%)	5 (2%)	0	100	100
1	H	213/227 (94%)	207 (97%)	6 (3%)	0	100	100
2	B	210/214 (98%)	208 (99%)	2 (1%)	0	100	100
2	D	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
2	L	212/214 (99%)	210 (99%)	2 (1%)	0	100	100
3	E	9/14 (64%)	9 (100%)	0	0	100	100
3	F	9/14 (64%)	9 (100%)	0	0	100	100
3	P	9/14 (64%)	9 (100%)	0	0	100	100
All	All	1287/1365 (94%)	1266 (98%)	21 (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	173/192 (90%)	172 (99%)	1 (1%)	86	90
1	C	175/192 (91%)	173 (99%)	2 (1%)	73	78
1	H	181/192 (94%)	180 (99%)	1 (1%)	86	90
2	B	189/191 (99%)	187 (99%)	2 (1%)	73	78
2	D	190/191 (100%)	189 (100%)	1 (0%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	191/191 (100%)	187 (98%)	4 (2%)	53	57
3	E	11/11 (100%)	11 (100%)	0	100	100
3	F	11/11 (100%)	11 (100%)	0	100	100
3	P	11/11 (100%)	11 (100%)	0	100	100
All	All	1132/1182 (96%)	1121 (99%)	11 (1%)	76	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
2	B	89	LEU
2	B	162	SER
1	C	3	LYS
1	C	111	VAL
2	D	89	LEU
1	H	215	LYS
2	L	50	ARG
2	L	89	LEU
2	L	162	SER
2	L	194	CYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
3	TPO	F	212	3	8,10,11	1.54	1 (12%)	10,14,16	1.46	1 (10%)
3	TPO	E	212	3	8,10,11	1.60	1 (12%)	10,14,16	1.53	1 (10%)
3	TPO	F	217	3	8,10,11	1.20	0	10,14,16	1.33	1 (10%)
3	TPO	P	212	3	8,10,11	1.21	0	10,14,16	1.51	2 (20%)
3	TPO	E	217	3	8,10,11	1.17	1 (12%)	10,14,16	1.49	1 (10%)
3	TPO	P	217	3	8,10,11	1.66	2 (25%)	10,14,16	1.37	2 (20%)

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	TPO	F	212	3	-	0/9/11/13	-
3	TPO	E	212	3	-	0/9/11/13	-
3	TPO	F	217	3	-	1/9/11/13	-
3	TPO	P	212	3	-	0/9/11/13	-
3	TPO	E	217	3	-	1/9/11/13	-
3	TPO	P	217	3	-	1/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	212	TPO	P-O1P	3.27	1.61	1.50
3	F	212	TPO	P-O1P	3.09	1.60	1.50
3	P	217	TPO	P-O1P	2.96	1.60	1.50
3	P	217	TPO	P-OG1	2.57	1.64	1.59
3	E	217	TPO	P-OG1	2.04	1.63	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	217	TPO	P-OG1-CB	-3.90	111.43	123.21
3	E	212	TPO	P-OG1-CB	-3.68	112.09	123.21
3	F	212	TPO	P-OG1-CB	-3.43	112.86	123.21
3	P	212	TPO	P-OG1-CB	-3.33	113.16	123.21
3	F	217	TPO	P-OG1-CB	-3.29	113.27	123.21
3	P	217	TPO	P-OG1-CB	-2.97	114.24	123.21
3	P	212	TPO	CG2-CB-CA	-2.41	108.41	113.16
3	P	217	TPO	O-C-CA	-2.31	118.72	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	217	TPO	O-C-CA-CB
3	E	217	TPO	O-C-CA-CB
3	P	217	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	GOL	D	301	-	5,5,5	0.32	0	5,5,5	0.43	0
4	GOL	L	301	-	5,5,5	0.38	0	5,5,5	0.50	0
4	GOL	A	301	-	5,5,5	0.36	0	5,5,5	0.74	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	GOL	D	301	-	-	0/4/4/4	-
4	GOL	L	301	-	-	3/4/4/4	-
4	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
4	L	301	GOL	O2-C2-C3-O3
4	A	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	L	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	207/227 (91%)	0.07	5 (2%) 59 57	28, 38, 57, 73	0
1	C	213/227 (93%)	0.34	14 (6%) 18 17	28, 41, 68, 81	3 (1%)
1	H	215/227 (94%)	0.58	21 (9%) 7 7	21, 40, 79, 92	0
2	B	212/214 (99%)	0.10	3 (1%) 75 74	26, 40, 53, 62	0
2	D	213/214 (99%)	-0.07	0 100 100	26, 38, 52, 66	0
2	L	213/214 (99%)	-0.03	3 (1%) 75 74	23, 37, 54, 68	0
3	E	11/14 (78%)	0.54	2 (18%) 1 1	34, 40, 63, 70	0
3	F	11/14 (78%)	0.34	1 (9%) 9 8	33, 37, 64, 64	0
3	P	11/14 (78%)	0.65	1 (9%) 9 8	24, 29, 57, 64	0
All	All	1306/1365 (95%)	0.17	50 (3%) 40 39	21, 39, 64, 92	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	GLY	7.9
1	H	200	ILE	5.2
1	H	219	LYS	5.1
1	C	3	LYS	4.9
2	L	212	GLY	4.8
3	P	210	SER	4.7
1	H	220	SER	4.6
1	C	5	VAL	4.5
1	C	7	SER	4.3
1	C	196	THR	4.2
1	C	4	LEU	3.9
1	H	197	GLN	3.8
1	A	133	SER	3.8
1	H	196	THR	3.5
1	C	138	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	163	ALA	3.4
1	H	194	LEU	3.4
1	C	209	ASN	3.2
3	F	222	GLU	3.0
1	H	201	CYS	2.9
1	H	1	GLU	2.9
1	A	219	LYS	2.8
1	A	22	CYS	2.8
1	C	206	LYS	2.7
1	H	216	VAL	2.7
1	C	9	GLY	2.6
2	B	212	GLY	2.5
1	H	198	THR	2.5
1	H	213	ASP	2.5
1	C	211	LYS	2.5
2	B	80	TYR	2.5
1	H	161	SER	2.4
1	H	107[A]	TYR	2.4
1	H	5	VAL	2.4
3	E	210	SER	2.3
1	H	162	GLY	2.3
2	B	210	ASN	2.3
2	L	122	ASP	2.3
3	E	222	GLU	2.3
1	A	24	ALA	2.2
1	H	164	LEU	2.2
1	H	203	VAL	2.2
1	A	196	THR	2.2
1	C	198	THR	2.2
1	H	138	GLY	2.2
1	H	206	LYS	2.1
1	H	211	LYS	2.1
2	L	126	LYS	2.1
1	C	75	ARG	2.1
1	C	163	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	TPO	F	212	11/12	0.97	0.13	33,36,38,40	0
3	TPO	E	217	11/12	0.97	0.12	33,35,41,41	0
3	TPO	F	217	11/12	0.98	0.10	32,33,35,36	0
3	TPO	P	212	11/12	0.98	0.10	30,37,42,43	0
3	TPO	E	212	11/12	0.98	0.10	37,39,42,46	0
3	TPO	P	217	11/12	0.99	0.13	21,24,28,32	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	301	6/6	0.82	0.21	35,41,45,47	0
4	GOL	L	301	6/6	0.92	0.10	37,41,43,43	0
4	GOL	D	301	6/6	0.93	0.12	38,42,43,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.