



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2021 – 04:09 PM JST

PDB ID : 7VUX
Title : Complex structure of PD1 and 609A-Fab
Authors : Huang, H.; Zhu, Z.; Zhao, J.; Jiang, L.; Yang, H.; Deng, L.; Meng, X.; Ding, J.; Yang, S.; Zhao, L.; Xu, W.; Wang, X.
Deposited on : 2021-11-04
Resolution : 1.64 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 : 2.23.2
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) : 2.23.2

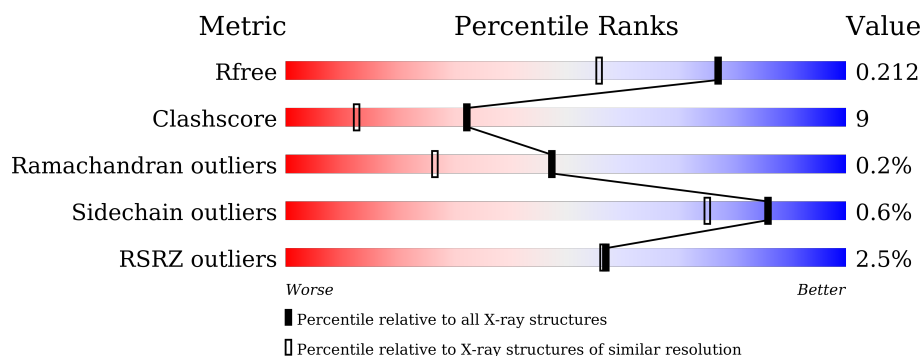
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	136	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
2	H	216	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
3	L	214	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</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
6	EDO	H	306	-	-	X	-
6	EDO	H	307	-	-	X	-
8	PEG	L	302	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5410 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 Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	7	0
			1028	634	193	196	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP Q15116
A	93	SER	CYS	conflict	UNP Q15116
A	161	GLU	-	expression tag	UNP Q15116
A	162	ASN	-	expression tag	UNP Q15116
A	163	LEU	-	expression tag	UNP Q15116
A	164	TYR	-	expression tag	UNP Q15116
A	165	PHE	-	expression tag	UNP Q15116
A	166	GLN	-	expression tag	UNP Q15116

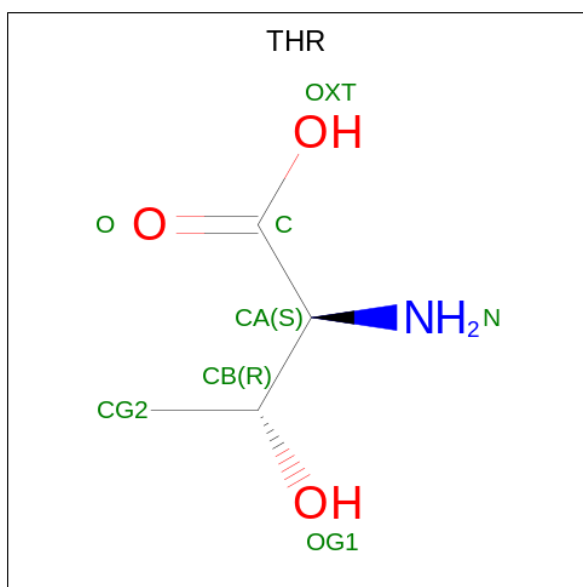
- Molecule 2 is a protein called Heavy chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	11	0
			1699	1065	286	335	13			

- Molecule 3 is a protein called Light chain of Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	21	0
			1800	1124	307	364	5			

- Molecule 4 is THREONINE (three-letter code: THR) (formula: C₄H₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

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



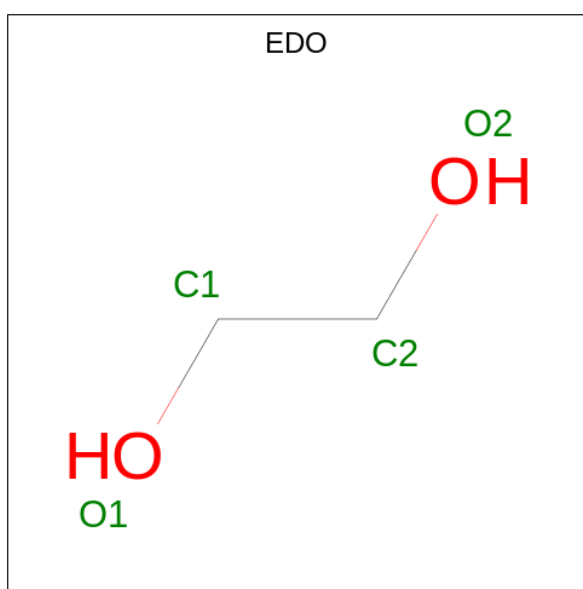
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	H	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

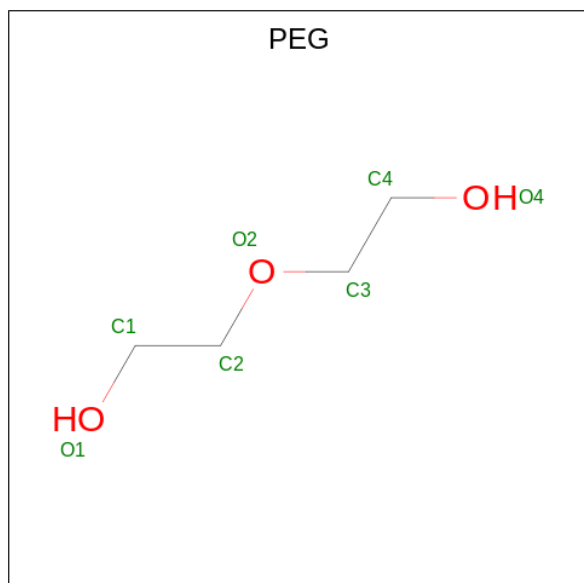


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total	Cl	0	0
			1	1		

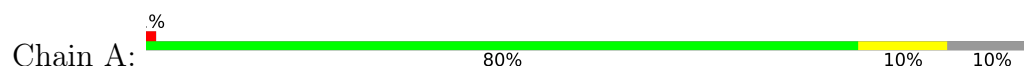
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	204	Total	O	0	0
			204	204		
10	H	251	Total	O	0	0
			251	251		
10	L	334	Total	O	0	0
			334	334		

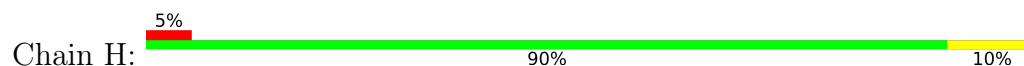
3 Residue-property plots

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: Programmed cell death protein 1



- Molecule 2: Heavy chain of Fab fragment



- Molecule 3: Light chain of Fab fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.29Å 68.41Å 77.31Å 90.00° 99.44° 90.00°	Depositor
Resolution (Å)	48.91 – 1.64 48.86 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-1.64) 99.7 (48.86-1.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.160 , 0.202 0.173 , 0.212	Depositor DCC
R_{free} test set	3529 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5410	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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: PEG, GOL, EDO, MG, CL

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	0.75	0/1050	1.00	1/1422 (0.1%)
2	H	0.75	0/1740	0.89	1/2369 (0.0%)
3	L	0.81	0/1840	0.93	0/2500
All	All	0.77	0/4630	0.93	2/6291 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	H	6	GLU	CB-CA-C	-5.71	98.99	110.40

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	1028	0	993	13	0
2	H	1699	0	1634	33	0
3	L	1800	0	1735	23	0
4	A	8	0	6	0	0
5	A	18	0	24	2	0
5	H	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	18	0	24	0	0
6	A	4	0	6	0	0
6	H	16	0	23	28	0
6	L	8	0	12	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	L	7	0	10	6	0
9	L	1	0	0	0	0
10	A	204	0	0	10	1
10	H	251	0	0	7	2
10	L	334	0	0	4	2
All	All	5410	0	4483	81	4

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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:202[A]:SER:OG	10:L:401:HOH:O	1.54	1.23
6:H:306:EDO:O1	6:H:307:EDO:H11	1.62	0.97
1:A:91[B]:GLN:OE1	10:A:301:HOH:O	1.90	0.90
2:H:183[A]:SER:H	6:H:306:EDO:H22	1.40	0.86
3:L:112:ALA:H	8:L:302:PEG:H42	1.41	0.86
2:H:182:LEU:HA	6:H:306:EDO:H21	1.57	0.84
3:L:28[A]:SER:OG	10:L:402:HOH:O	1.93	0.84
2:H:183[B]:SER:H	6:H:306:EDO:H22	1.40	0.83
2:H:115[B]:VAL:HG23	2:H:115[B]:VAL:O	1.80	0.80
3:L:72[B]:THR:HG22	10:L:403:HOH:O	1.82	0.78
2:H:183[A]:SER:H	6:H:306:EDO:C2	1.96	0.77
2:H:136:SER:OG	10:H:401:HOH:O	2.02	0.77
5:A:203[B]:GOL:O3	10:A:302:HOH:O	2.03	0.76
2:H:88:ALA:HA	2:H:115[B]:VAL:CG2	2.17	0.73
2:H:183[B]:SER:H	6:H:306:EDO:C2	2.01	0.72
2:H:171:PRO:O	6:H:306:EDO:C1	2.37	0.71
2:H:115[B]:VAL:O	2:H:115[B]:VAL:CG2	2.38	0.71
5:H:302:GOL:H12	10:H:437:HOH:O	1.91	0.68
2:H:216:GLU:HA	10:H:403:HOH:O	1.95	0.64
1:A:76[A]:THR:HG21	10:A:376:HOH:O	1.97	0.64
3:L:112:ALA:H	8:L:302:PEG:C4	2.09	0.63
2:H:91:THR:OG1	2:H:115[B]:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:PHE:HB2	6:H:306:EDO:H22	1.84	0.59
2:H:181:SER:HB3	6:H:307:EDO:H21	1.85	0.57
1:A:91[B]:GLN:NE2	10:A:301:HOH:O	2.36	0.57
3:L:200:GLY:CA	8:L:302:PEG:H21	2.34	0.57
6:H:304:EDO:H21	10:H:520:HOH:O	2.04	0.57
1:A:91[B]:GLN:CD	10:A:301:HOH:O	2.39	0.57
2:H:87:ARG:O	2:H:115[B]:VAL:HG21	2.05	0.57
2:H:182:LEU:HA	6:H:306:EDO:C2	2.31	0.57
3:L:24[A]:ARG:NH1	3:L:70:ASP:OD1	2.38	0.56
3:L:106[A]:ILE:HG22	3:L:107[A]:LYS:O	2.06	0.55
5:H:302:GOL:C1	10:H:437:HOH:O	2.51	0.55
2:H:182:LEU:CA	6:H:306:EDO:H21	2.35	0.54
2:H:88:ALA:HA	2:H:115[B]:VAL:HG21	1.86	0.54
3:L:138:ASN:ND2	10:L:404:HOH:O	2.34	0.54
1:A:69[B]:ARG:HD3	1:A:121:TYR:CE2	2.42	0.54
2:H:171:PRO:O	6:H:306:EDO:H12	2.08	0.53
3:L:24[A]:ARG:HD2	3:L:70:ASP:OD1	2.09	0.53
6:H:306:EDO:C1	6:H:307:EDO:H11	2.38	0.53
3:L:200:GLY:HA2	8:L:302:PEG:H21	1.91	0.53
3:L:2:ILE:HG12	3:L:27:GLN:CG	2.40	0.52
3:L:142:ARG:NH2	3:L:163[A]:VAL:HG21	2.27	0.50
6:H:306:EDO:C2	6:H:307:EDO:C1	2.91	0.49
3:L:58[B]:ILE:HD12	3:L:62:PHE:HB2	1.93	0.49
2:H:19:ARG:NH2	10:H:410:HOH:O	2.46	0.49
2:H:88:ALA:CA	2:H:115[B]:VAL:HG21	2.43	0.49
1:A:76[A]:THR:HG23	10:A:348:HOH:O	2.13	0.49
2:H:181:SER:CB	6:H:307:EDO:H21	2.42	0.49
2:H:183[A]:SER:N	6:H:306:EDO:C2	2.71	0.49
1:A:69[B]:ARG:HD3	1:A:121:TYR:CZ	2.48	0.48
1:A:149:ALA:O	10:A:303:HOH:O	2.20	0.48
2:H:131[B]:CYS:SG	3:L:119:PRO:HG3	2.54	0.47
2:H:171:PRO:O	6:H:306:EDO:H11	2.14	0.47
6:H:306:EDO:O2	6:H:307:EDO:H12	2.14	0.47
1:A:31:MET:N	1:A:133:GLN:HE21	2.13	0.47
6:H:306:EDO:O1	6:H:307:EDO:C1	2.50	0.47
2:H:183[A]:SER:N	6:H:306:EDO:H21	2.31	0.46
6:H:306:EDO:C2	6:H:307:EDO:H11	2.44	0.46
3:L:112:ALA:N	8:L:302:PEG:H42	2.21	0.46
1:A:62:SER:OG	10:A:304:HOH:O	2.21	0.45
2:H:87:ARG:C	2:H:115[B]:VAL:HG21	2.37	0.45
6:H:306:EDO:H21	6:H:307:EDO:C1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:183[B]:SER:N	6:H:306:EDO:H21	2.32	0.45
3:L:58[B]:ILE:O	3:L:58[B]:ILE:HG13	2.16	0.45
3:L:24[A]:ARG:CD	3:L:70:ASP:OD1	2.65	0.44
2:H:12:VAL:O	2:H:115[B]:VAL:HA	2.18	0.44
6:H:306:EDO:C2	6:H:307:EDO:H12	2.47	0.44
1:A:139[B]:ARG:NH1	10:A:310:HOH:O	2.47	0.43
1:A:147:ARG:HH12	5:A:203[B]:GOL:H11	1.84	0.43
1:A:89:PRO:O	10:A:305:HOH:O	2.21	0.43
6:H:307:EDO:H12	10:H:491:HOH:O	2.18	0.43
2:H:188:VAL:HB	2:H:189:PRO:HD2	2.01	0.42
3:L:31:ASN:O	3:L:50:TYR:HA	2.19	0.42
6:H:306:EDO:H12	3:L:162[A]:SER:OG	2.18	0.42
3:L:111:ALA:HA	8:L:302:PEG:H42	2.01	0.42
2:H:182:LEU:HA	6:H:306:EDO:C1	2.50	0.42
2:H:11:LEU:HD23	2:H:114:THR:HB	2.02	0.41
2:H:205:LYS:N	2:H:206:PRO:CD	2.83	0.41
3:L:159:SER:HA	3:L:178:THR:O	2.20	0.41
3:L:142:ARG:CZ	3:L:163[A]:VAL:HG21	2.52	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:531:HOH:O	10:H:583:HOH:O[2_645]	2.01	0.19
10:A:460:HOH:O	10:H:550:HOH:O[1_455]	2.03	0.17
10:L:685:HOH:O	10:L:715:HOH:O[1_455]	2.05	0.15
10:L:634:HOH:O	10:L:691:HOH:O[1_455]	2.11	0.09

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	127/136 (93%)	127 (100%)	0	0	100	100
2	H	226/216 (105%)	223 (99%)	2 (1%)	1 (0%)	34	15
3	L	233/214 (109%)	225 (97%)	8 (3%)	0	100	100
All	All	586/566 (104%)	575 (98%)	10 (2%)	1 (0%)	47	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	195	THR

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	114/120 (95%)	113 (99%)	1 (1%)	78	63
2	H	192/180 (107%)	189 (98%)	3 (2%)	62	39
3	L	208/188 (111%)	207 (100%)	1 (0%)	88	80
All	All	514/488 (105%)	509 (99%)	5 (1%)	86	59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
2	H	131[A]	CYS
2	H	131[B]	CYS
2	H	131[C]	CYS
3	L	105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	53	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	202	-	5,5,5	0.21	0	5,5,5	0.66	0
6	EDO	H	306	-	3,3,3	1.03	0	2,2,2	1.45	0
6	EDO	A	204	-	3,3,3	0.08	0	2,2,2	0.14	0
6	EDO	H	304	-	3,3,3	0.52	0	2,2,2	1.02	0
6	EDO	H	305	-	3,3,3	0.12	0	2,2,2	0.33	0
5	GOL	H	303	-	5,5,5	0.33	0	5,5,5	0.63	0
8	PEG	L	302	-	6,6,6	0.29	0	5,5,5	0.38	0
5	GOL	L	305	-	5,5,5	0.28	0	5,5,5	0.65	0
6	EDO	H	307	7	3,3,3	0.28	0	2,2,2	0.80	0
5	GOL	A	203[A]	-	5,5,5	0.17	0	5,5,5	0.69	0
5	GOL	L	306	-	5,5,5	0.12	0	5,5,5	0.31	0
4	THR	A	201	-	4,7,7	0.35	0	4,9,9	0.60	0
6	EDO	L	304	-	3,3,3	0.06	0	2,2,2	0.36	0
5	GOL	L	301	-	5,5,5	0.13	0	5,5,5	0.41	0
5	GOL	H	302	-	5,5,5	0.32	0	5,5,5	0.81	0
5	GOL	A	203[B]	-	5,5,5	0.12	0	5,5,5	0.27	0
6	EDO	L	303	-	3,3,3	0.04	0	2,2,2	0.26	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
5	GOL	A	202	-	-	0/4/4/4	-
6	EDO	H	306	-	-	0/1/1/1	-
6	EDO	A	204	-	-	1/1/1/1	-
6	EDO	H	304	-	-	1/1/1/1	-
6	EDO	H	305	-	-	1/1/1/1	-
5	GOL	H	303	-	-	0/4/4/4	-
8	PEG	L	302	-	-	1/4/4/4	-
5	GOL	L	305	-	-	2/4/4/4	-
6	EDO	H	307	7	-	0/1/1/1	-
5	GOL	A	203[A]	-	-	0/4/4/4	-
5	GOL	L	306	-	-	0/4/4/4	-
4	THR	A	201	-	-	0/4/8/8	-
6	EDO	L	304	-	-	1/1/1/1	-
5	GOL	L	301	-	-	1/4/4/4	-
5	GOL	H	302	-	-	3/4/4/4	-
5	GOL	A	203[B]	-	-	1/4/4/4	-
6	EDO	L	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	302	GOL	O1-C1-C2-C3
5	H	302	GOL	C1-C2-C3-O3
5	L	305	GOL	O1-C1-C2-C3
8	L	302	PEG	O1-C1-C2-O2
5	L	305	GOL	O1-C1-C2-O2
6	H	304	EDO	O1-C1-C2-O2
5	H	302	GOL	O2-C2-C3-O3
6	L	304	EDO	O1-C1-C2-O2
6	A	204	EDO	O1-C1-C2-O2
6	L	303	EDO	O1-C1-C2-O2
5	A	203[B]	GOL	O1-C1-C2-C3
6	H	305	EDO	O1-C1-C2-O2
5	L	301	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	306	EDO	24	0
6	H	304	EDO	1	0
8	L	302	PEG	6	0
6	H	307	EDO	11	0
5	H	302	GOL	2	0
5	A	203[B]	GOL	2	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	122/136 (89%)	-0.13	2 (1%) 72 73	11, 17, 33, 45	0
2	H	216/216 (100%)	0.04	10 (4%) 32 30	13, 21, 52, 85	0
3	L	213/214 (99%)	-0.24	2 (0%) 84 85	10, 15, 26, 54	0
All	All	551/566 (97%)	-0.11	14 (2%) 57 56	10, 18, 37, 85	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	194	GLY	5.1
2	H	133	ARG	5.1
1	A	151	VAL	4.7
2	H	216	GLU	4.5
2	H	195	THR	3.8
2	H	134	SER	3.8
1	A	149	ALA	3.7
2	H	131[A]	CYS	3.5
2	H	135	THR	3.4
2	H	136	SER	2.5
3	L	212	GLY	2.5
3	L	94[A]	TRP	2.5
2	H	132	SER	2.2
2	H	137	GLU	2.0

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

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

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
6	EDO	H	305	4/4	0.71	0.26	61,62,62,66	0
5	GOL	A	203[A]	6/6	0.79	0.24	14,16,17,17	6
5	GOL	A	203[B]	6/6	0.79	0.24	25,26,27,28	6
4	THR	A	201	8/8	0.79	0.19	27,35,42,43	0
6	EDO	H	304	4/4	0.80	0.22	32,37,38,41	0
6	EDO	A	204	4/4	0.80	0.14	50,51,52,53	0
5	GOL	L	305	6/6	0.84	0.12	28,40,44,47	0
5	GOL	L	301	6/6	0.84	0.11	28,34,35,44	0
6	EDO	H	307	4/4	0.84	0.20	35,36,38,42	0
8	PEG	L	302	7/7	0.85	0.23	30,38,42,43	0
6	EDO	L	303	4/4	0.90	0.14	54,56,59,61	0
6	EDO	L	304	4/4	0.92	0.16	34,40,44,55	0
5	GOL	H	302	6/6	0.93	0.13	22,31,38,38	0
7	MG	H	301	1/1	0.93	0.16	42,42,42,42	0
6	EDO	H	306	4/4	0.93	0.24	25,28,28,29	0
5	GOL	A	202	6/6	0.94	0.13	24,25,26,27	0
5	GOL	H	303	6/6	0.94	0.10	15,18,19,21	0
5	GOL	L	306	6/6	0.94	0.15	21,31,34,37	0
9	CL	L	308	1/1	0.95	0.08	54,54,54,54	0
7	MG	L	307	1/1	0.97	0.18	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.