



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 8D47 / pdb_00008d47
Title : fp.006 Fab in complex with SARS-CoV-2 Fusion Peptide
Authors : Abernathy, M.E.; Barnes, C.O.
Deposited on : 2022-06-01
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

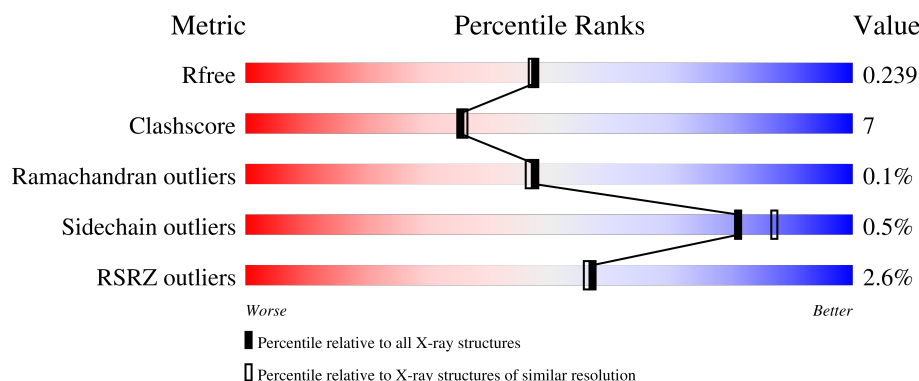
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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	215	4% 81% 18% .
1	L	215	88% 10% .
2	B	242	4% 86% 10% 5%
2	H	242	2% 76% 17% 7%
3	C	20	5% 80% 10% 10%

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Mol	Chain	Length	Quality of chain
3	D	20	55% 5% 40%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7759 atoms, of which 36 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 fp.006 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1609	1004	275	325	5			
1	A	213	Total	C	N	O	S	0	0	0
			1609	1004	275	325	5			

- Molecule 2 is a protein called fp.006 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	2	0
			1718	1083	295	331	9			
2	B	231	Total	C	N	O	S	0	2	0
			1744	1095	299	341	9			

- Molecule 3 is a protein called SARS-CoV-2 fusion peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	18	Total	C	N	O	0	0	0
			143	92	23	28			
3	D	12	Total	C	N	O	0	0	0
			103	67	17	19			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	212	Total	O	0	0
			212	212		
7	A	114	Total	O	0	0
			114	114		
7	H	200	Total	O	0	0
			200	200		
7	B	198	Total	O	0	0
			198	198		
7	C	13	Total	O	0	0
			13	13		
7	D	15	Total	O	0	0
			15	15		

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.

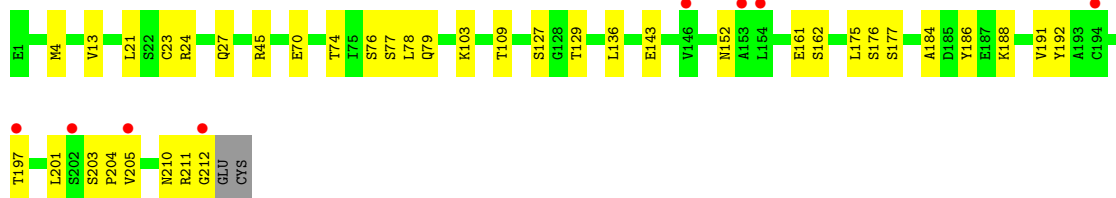
- Molecule 1: fp.006 light chain

Chain L: 



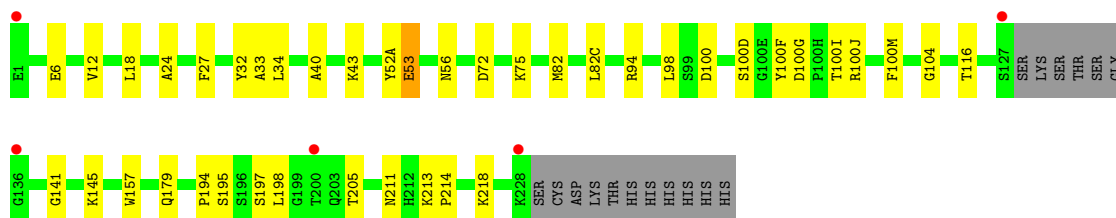
- Molecule 1: fp.006 light chain

Chain A: 



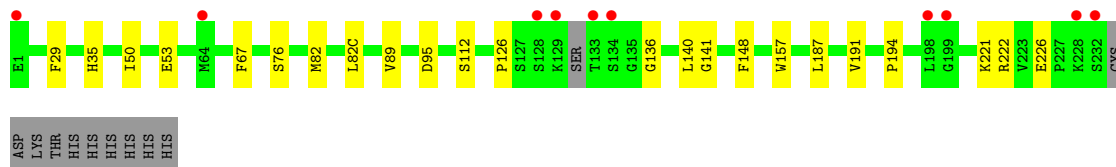
- Molecule 2: fp.006 heavy chain

Chain H: 

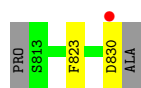
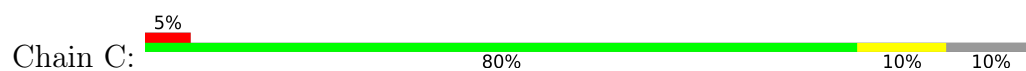


- Molecule 2: fp.006 heavy chain

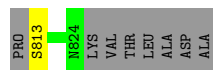
Chain B: 



- Molecule 3: SARS-CoV-2 fusion peptide



- Molecule 3: SARS-CoV-2 fusion peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.02Å 73.08Å 90.12Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	37.89 – 2.00 37.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.89-2.00) 97.6 (37.89-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.238 (Not available) , 0.239	Depositor DCC
R_{free} test set	3636 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7759	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: PO4, EDO, PEG

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	0.26	0/1643	0.47	0/2233
1	L	0.33	0/1643	0.52	0/2233
2	B	0.30	0/1785	0.47	0/2428
2	H	0.31	0/1759	0.49	0/2390
3	C	0.37	0/144	0.50	0/193
3	D	0.34	0/104	0.56	0/137
All	All	0.30	0/7078	0.49	0/9614

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	1609	0	1559	33	0
1	L	1609	0	1562	16	0
2	B	1744	0	1674	16	0
2	H	1718	0	1669	32	0
3	C	143	0	140	2	0
3	D	103	0	102	1	0
4	B	14	20	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	7	10	10	3	0
5	H	4	6	6	0	0
6	B	20	0	0	0	0
7	A	114	0	0	12	0
7	B	198	0	0	2	0
7	C	13	0	0	0	0
7	D	15	0	0	1	0
7	H	200	0	0	8	1
7	L	212	0	0	2	2
All	All	7723	36	6742	102	2

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 7.

All (102) 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:H:211:ASN:HD21	2:H:213:LYS:HE2	1.42	0.84
2:B:222:ARG:NH1	2:B:226:GLU:OE1	2.14	0.81
1:A:45:ARG:HD2	7:A:367:HOH:O	1.83	0.77
2:H:211:ASN:HB2	2:H:218:LYS:HE3	1.67	0.77
2:H:98:LEU:HD21	2:H:100(F):TYR:HD1	1.57	0.70
2:B:221:LYS:NZ	7:B:401:HOH:O	2.26	0.68
2:B:126:PRO:HG3	2:B:140:LEU:HB3	1.76	0.67
1:A:109:THR:HG23	7:A:311:HOH:O	1.96	0.65
1:A:177:SER:OG	7:A:301:HOH:O	2.14	0.65
1:A:201:LEU:HD22	1:A:205:VAL:HG23	1.80	0.63
2:H:72:ASP:CG	2:H:75:LYS:HG2	2.25	0.62
1:A:74:THR:HG23	7:A:395:HOH:O	2.00	0.61
2:H:211:ASN:ND2	2:H:213:LYS:HE2	2.12	0.61
1:A:24:ARG:HG3	1:A:70:GLU:OE1	2.00	0.59
1:A:13:VAL:HB	1:A:78:LEU:HD22	1.84	0.58
2:H:40:ALA:HB3	2:H:43:LYS:HD3	1.85	0.58
2:H:100(G):ASP:HB3	2:H:100(J):ARG:HD2	1.86	0.58
2:H:205:THR:HG23	7:H:494:HOH:O	2.03	0.58
1:A:161:GLU:HG3	1:A:175:LEU:HD21	1.86	0.57
1:L:33:LEU:HG	1:L:34:ALA:N	2.20	0.57
1:A:161:GLU:OE2	1:A:175:LEU:HD11	2.06	0.56
2:H:194:PRO:HG2	2:H:197:SER:OG	2.05	0.56
1:A:191:VAL:HG22	1:A:210:ASN:OD1	2.06	0.56
1:A:201:LEU:HD22	1:A:205:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:813:SER:N	7:D:901:HOH:O	2.38	0.55
2:H:116:THR:OG1	7:H:401:HOH:O	2.18	0.55
4:H:300:PEG:H42	7:H:558:HOH:O	2.06	0.54
2:B:67:PHE:CE2	2:B:82:MET:HE3	2.42	0.54
1:A:197:THR:HA	7:A:376:HOH:O	2.08	0.53
1:A:175:LEU:HD23	1:A:176:SER:N	2.24	0.53
1:L:190:LYS:HD2	1:L:210:ASN:HB3	1.91	0.53
2:B:112:SER:HB3	2:B:148:PHE:CZ	2.45	0.52
4:H:300:PEG:H12	7:H:558:HOH:O	2.09	0.52
2:H:43:LYS:HE2	7:H:563:HOH:O	2.11	0.51
2:B:35:HIS:CE1	2:B:50:ILE:HD12	2.46	0.51
1:L:185:ASP:HA	1:L:188:LYS:HE2	1.93	0.50
1:L:13:VAL:HB	1:L:78:LEU:HD22	1.92	0.50
1:L:1:GLU:HG2	1:L:93:ASP:OD2	2.11	0.50
2:H:100(I):THR:HG23	7:H:557:HOH:O	2.11	0.50
1:L:125:LEU:O	1:L:183:LYS:HD3	2.11	0.49
2:B:136:GLY:O	2:B:194:PRO:HA	2.12	0.49
1:L:13:VAL:HB	1:L:78:LEU:CD2	2.42	0.49
1:A:184:ALA:O	1:A:188:LYS:HG3	2.11	0.49
2:H:12:VAL:HG11	2:H:82(C):LEU:HD13	1.94	0.49
1:A:143:GLU:N	1:A:143:GLU:OE1	2.45	0.49
2:B:89:VAL:HG23	4:B:302:PEG:H31	1.95	0.48
2:B:112:SER:HB3	2:B:148:PHE:HZ	1.78	0.48
1:A:152:ASN:OD1	7:A:302:HOH:O	2.20	0.47
2:H:56:ASN:HB3	3:C:823:PHE:CD2	2.49	0.47
1:A:129:THR:HG21	7:A:400:HOH:O	2.13	0.47
2:H:33:ALA:C	2:H:34:LEU:HD22	2.40	0.47
1:L:4:MET:HE3	1:L:23:CYS:SG	2.54	0.46
2:B:187:LEU:HD12	2:B:187:LEU:C	2.40	0.46
1:A:24:ARG:HG3	1:A:70:GLU:CD	2.40	0.46
1:A:210:ASN:O	1:A:212:GLY:N	2.48	0.46
1:A:77:SER:O	1:A:79:GLN:NE2	2.49	0.46
2:H:72:ASP:OD2	2:H:75:LYS:HD3	2.16	0.46
1:A:175:LEU:HD23	1:A:175:LEU:C	2.40	0.46
4:B:301:PEG:H11	7:B:566:HOH:O	2.16	0.46
1:A:129:THR:CG2	7:A:400:HOH:O	2.64	0.46
2:B:35:HIS:CD2	2:B:95:ASP:HB2	2.51	0.45
1:A:127:SER:OG	1:A:129:THR:HG22	2.16	0.45
2:H:98:LEU:HD21	2:H:100(F):TYR:CD1	2.45	0.45
1:L:54:ARG:NH2	7:L:302:HOH:O	2.39	0.45
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:300:PEG:H21	7:H:556:HOH:O	2.16	0.44
1:L:175:LEU:C	1:L:175:LEU:HD23	2.42	0.44
2:H:56:ASN:HB3	3:C:823:PHE:CE2	2.52	0.44
1:A:186:TYR:HA	1:A:192:TYR:OH	2.16	0.44
1:A:4:MET:HE3	1:A:23:CYS:SG	2.58	0.44
2:H:98:LEU:HD23	7:H:425:HOH:O	2.17	0.44
2:B:29:PHE:CD2	2:B:76:SER:HA	2.53	0.44
1:A:76:SER:HB3	7:A:364:HOH:O	2.17	0.43
1:A:27:GLN:NE2	7:A:305:HOH:O	2.40	0.43
1:L:124:GLN:HE21	1:L:129:THR:HG23	1.82	0.43
1:A:103:LYS:NZ	7:A:303:HOH:O	2.31	0.43
1:L:190:LYS:HD3	1:L:190:LYS:HA	1.73	0.43
2:H:52(A):TYR:CE1	2:H:53:GLU:HG3	2.54	0.43
2:B:141:GLY:HA2	2:B:157:TRP:CH2	2.55	0.42
1:L:12:SER:OG	1:L:105:GLU:OE2	2.30	0.42
2:B:140:LEU:HD11	2:B:191:VAL:CG1	2.49	0.42
1:L:95(A):LEU:HD23	1:L:95(A):LEU:HA	1.86	0.42
1:L:207:LYS:NZ	7:L:307:HOH:O	2.46	0.42
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.55	0.41
2:H:32:TYR:O	2:H:34:LEU:HD22	2.20	0.41
2:H:198:LEU:HD23	2:H:198:LEU:HA	1.94	0.41
1:A:162:SER:HB2	7:A:321:HOH:O	2.21	0.41
2:H:145:LYS:NZ	2:H:179:GLN:OE1	2.51	0.41
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.20	0.41
2:H:34:LEU:HD22	2:H:34:LEU:N	2.35	0.41
2:H:94:ARG:O	2:H:100(M):PHE:HA	2.20	0.41
2:B:141:GLY:HA2	2:B:157:TRP:CZ2	2.55	0.41
2:H:213:LYS:HB2	2:H:214:PRO:HD3	2.03	0.41
1:A:21:LEU:HD12	1:A:21:LEU:N	2.35	0.41
1:A:136:LEU:HB2	1:A:175:LEU:HB3	2.03	0.40
2:H:100:ASP:OD2	2:H:100(D):SER:OG	2.33	0.40
2:H:141:GLY:HA2	2:H:157:TRP:CZ2	2.56	0.40
2:B:82:MET:HE2	2:B:82(C):LEU:HD21	2.03	0.40
1:L:124:GLN:HG2	1:L:129:THR:O	2.22	0.40
2:H:18:LEU:HD12	2:H:18:LEU:HA	1.95	0.40
1:A:175:LEU:HD23	1:A:176:SER:C	2.47	0.40
2:H:18:LEU:HB3	2:H:82:MET:HE3	2.03	0.40

All (2) 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)
7:L:508:HOH:O	7:H:593:HOH:O[1_545]	2.14	0.06
7:L:396:HOH:O	7:L:419:HOH:O[2_554]	2.17	0.03

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	211/215 (98%)	204 (97%)	6 (3%)	1 (0%)	24	21
1	L	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
2	B	229/242 (95%)	224 (98%)	5 (2%)	0	100	100
2	H	223/242 (92%)	221 (99%)	2 (1%)	0	100	100
3	C	16/20 (80%)	16 (100%)	0	0	100	100
3	D	10/20 (50%)	10 (100%)	0	0	100	100
All	All	899/954 (94%)	880 (98%)	18 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ARG

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	180/184 (98%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	181/184 (98%)	181 (100%)	0	100	100
2	B	193/205 (94%)	192 (100%)	1 (0%)	81	87
2	H	191/205 (93%)	189 (99%)	2 (1%)	68	75
3	C	16/18 (89%)	15 (94%)	1 (6%)	16	13
3	D	12/18 (67%)	12 (100%)	0	100	100
All	All	773/814 (95%)	769 (100%)	4 (0%)	81	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	53	GLU
2	H	195	SER
2	B	53	GLU
3	C	830	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	147	GLN
1	A	27	GLN
1	A	42	GLN
2	H	211	ASN
2	B	28	ASN
2	B	179	GLN
2	B	203	GLN
2	B	216	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	PEG	H	300	-	6,6,6	0.12	0	5,5,5	0.12	0
4	PEG	B	302	-	6,6,6	0.18	0	5,5,5	0.07	0
5	EDO	H	301	-	3,3,3	0.39	0	2,2,2	0.84	0
6	PO4	B	305	-	4,4,4	0.69	0	6,6,6	0.84	0
4	PEG	B	301	-	6,6,6	0.14	0	5,5,5	0.08	0
6	PO4	B	306	-	4,4,4	0.98	0	6,6,6	0.73	0
6	PO4	B	304	-	4,4,4	0.88	0	6,6,6	0.53	0
6	PO4	B	303	-	4,4,4	0.84	0	6,6,6	0.65	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	PEG	H	300	-	-	3/4/4/4	-
4	PEG	B	302	-	-	3/4/4/4	-
5	EDO	H	301	-	-	0/1/1/1	-
4	PEG	B	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	PEG	O1-C1-C2-O2
4	B	301	PEG	O1-C1-C2-O2
4	H	300	PEG	C1-C2-O2-C3
4	B	302	PEG	O2-C3-C4-O4
4	B	302	PEG	C4-C3-O2-C2
4	H	300	PEG	C4-C3-O2-C2
4	H	300	PEG	O1-C1-C2-O2
4	B	301	PEG	C4-C3-O2-C2
4	B	301	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	300	PEG	3	0
4	B	302	PEG	1	0
4	B	301	PEG	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	213/215 (99%)	0.32	8 (3%) 44 43	18, 36, 62, 68	0
1	L	212/215 (98%)	-0.32	0 100 100	14, 24, 44, 55	0
2	B	231/242 (95%)	-0.11	10 (4%) 40 39	13, 27, 55, 87	2 (0%)
2	H	225/242 (92%)	-0.21	5 (2%) 62 61	13, 27, 48, 68	2 (0%)
3	C	18/20 (90%)	0.17	1 (5%) 30 29	19, 27, 45, 63	0
3	D	12/20 (60%)	0.09	0 100 100	25, 30, 41, 45	0
All	All	911/954 (95%)	-0.07	24 (2%) 57 56	13, 28, 55, 87	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	133	THR	4.3
1	A	194	CYS	3.4
3	C	830	ASP	3.3
1	A	154	LEU	2.9
2	B	134	SER	2.9
2	B	128	SER	2.9
1	A	153	ALA	2.6
2	B	129	LYS	2.5
2	H	200	THR	2.3
2	H	1	GLU	2.3
2	B	232	SER	2.3
1	A	205	VAL	2.3
1	A	212	GLY	2.3
1	A	202	SER	2.2
1	A	146	VAL	2.2
2	B	228	LYS	2.2
1	A	197	THR	2.2
2	H	136	GLY	2.1
2	B	198	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1	GLU	2.1
2	B	199	GLY	2.1
2	H	228	LYS	2.1
2	H	127	SER	2.0
2	B	64	MET	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, 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	PEG	B	302	7/7	0.87	0.09	36,44,53,53	0
6	PO4	B	303	5/5	0.90	0.18	39,47,53,60	0
6	PO4	B	304	5/5	0.90	0.16	42,45,52,61	0
6	PO4	B	305	5/5	0.90	0.12	38,41,60,61	0
4	PEG	H	300	7/7	0.91	0.08	20,34,42,48	0
5	EDO	H	301	4/4	0.92	0.11	32,41,51,51	0
6	PO4	B	306	5/5	0.93	0.14	35,41,47,47	0
4	PEG	B	301	7/7	0.94	0.06	26,37,47,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.