Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 12:20 PM JST

PDB ID	:	7YI6
Title	:	bnAb 3D1 in complex with 6-mer HR1 peptide from HCoV-229E S protein
Authors	:	Yan, L.; Yang, G.
Deposited on	:	2022-07-15
Resolution	:	2.28 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 (i) 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 (i)) were used in the production of this report:

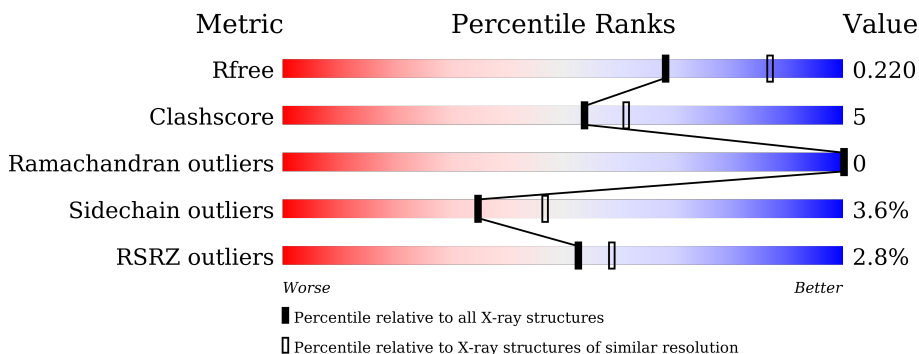|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.28 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		3.6%
RSRZ outliers		2.8%

Worse　　　　　　　　　　　　　　　　　　　　　　Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	7	29% / 71% 14% 14%
1	C	7	57% 14% 14% 14%
2	B	214	4% / 84% 13% ··
2	E	214	2% / 82% 14% ··
3	D	221	2% / 90% 9% ·
3	F	221	2% / 87% 10% ·

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	PEG	E	301	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6923 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	7	Total	C	N	O	0	0	1
			49	28	10	11			
1	C	6	Total	C	N	O	0	0	1
			41	24	9	8			

- Molecule 2 is a protein called light chain of 3D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	1	0
			1548	969	253	322	4			
2	E	210	Total	C	N	O	S	0	1	0
			1548	969	253	322	4			

- Molecule 3 is a protein called heavy chain of 3D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	221	Total	C	N	O	S	0	0	0
			1646	1046	271	323	6			
3	F	215	Total	C	N	O	S	0	0	0
			1605	1022	264	313	6			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 7	C 4	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total 4	O 4	0	0
7	B	98	Total 98	O 98	0	0
7	D	126	Total 126	O 126	0	0
7	C	4	Total 4	O 4	0	0
7	E	101	Total 101	O 101	0	0
7	F	125	Total 125	O 125	0	0

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.
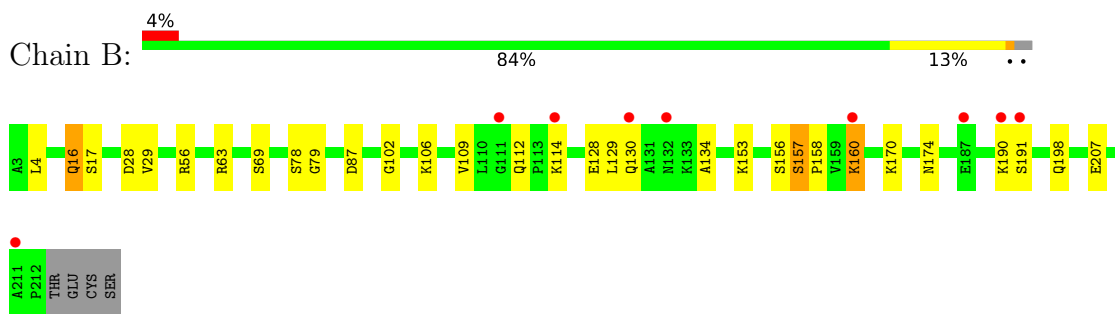
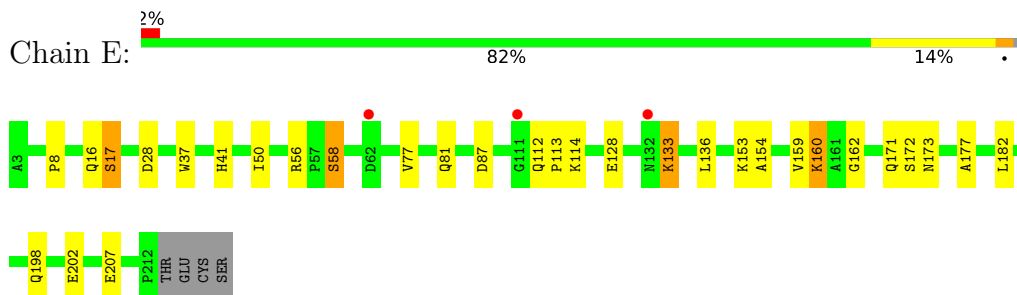• Molecule 1: Spike glycoprotein
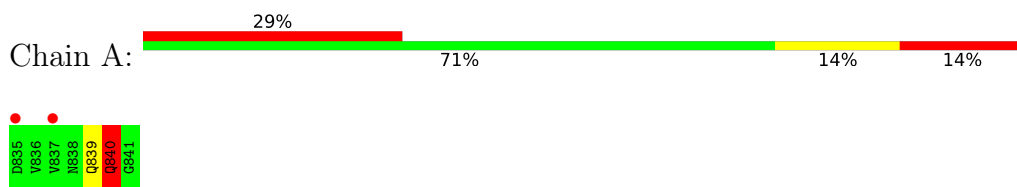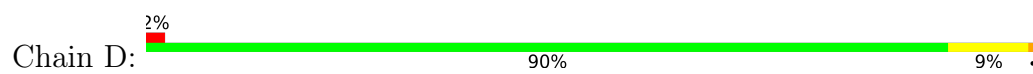
Chain A:

• Molecule 1: Spike glycoprotein

Chain C:

• Molecule 2: light chain of 3D1

Chain B:

• Molecule 2: light chain of 3D1

Chain E:

• Molecule 3: heavy chain of 3D1

Chain D:

2%

90%

9%

Q1 S33 Q62 Q100 P101 S120 V128 F129 P130 S135 K136 S137 T138 L145 H171 L177 S193 N204 K208 N211 V214 E219 P220 P221

• Molecule 3: heavy chain of 3D1

Chain F:

2%

87%

10%

Q1 S9 E10 L11 K12 K13 S25 W50 L115 A121 V128 F129 S134 SER LYS SER THR SER G140 P154 S168 H171 V188 S195 L196 N204 K208 K213 V214 D215 K216 E219 P220 PRO
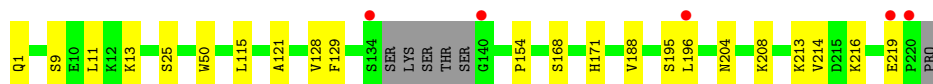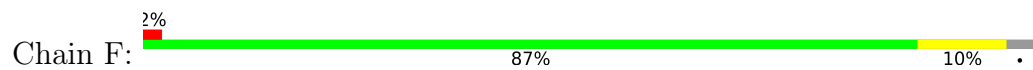
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.91Å　72.70Å　86.26Å 90.00°　109.54°　90.00°	Depositor
Resolution (Å)	45.86　–　2.28 45.85　–　2.28	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.86-2.28) 98.9 (45.85-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.193　,　0.220 0.193　,　0.220	Depositor DCC
R_{free} test set	2000 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9222e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, CL, EDO, PCA

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	3.19	1/48 (2.1%)	1.45	2/65 (3.1%)
1	C	3.33	1/40 (2.5%)	1.35	0/54
2	B	0.81	1/1590 (0.1%)	0.76	3/2173 (0.1%)
2	E	0.63	4/1590 (0.3%)	0.79	6/2173 (0.3%)
3	D	0.59	1/1684 (0.1%)	0.61	1/2304 (0.0%)
3	F	0.73	1/1641 (0.1%)	0.70	1/2244 (0.0%)
All	All	0.79	9/6593 (0.1%)	0.73	13/9013 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	GLN	C-N	-21.84	0.93	1.33
1	C	840	GLN	C-N	-18.27	1.00	1.33
2	B	17	SER	C-N	-7.32	1.17	1.34
2	E	58	SER	CB-OG	-6.09	1.34	1.42
2	E	17	SER	C-N	-6.03	1.20	1.34
2	E	202	GLU	CD-OE2	-5.50	1.19	1.25
2	E	16	GLN	C-N	-5.39	1.21	1.34
3	F	208	LYS	C-O	-5.39	1.13	1.23
3	D	129	PHE	C-O	-5.13	1.13	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	16	GLN	O-C-N	-10.41	106.04	122.70
2	B	16	GLN	O-C-N	-8.68	108.81	122.70
2	E	56	ARG	NE-CZ-NH2	-8.25	116.18	120.30
2	B	16	GLN	C-N-CA	8.24	142.29	121.70
2	E	16	GLN	C-N-CA	8.10	141.95	121.70
3	F	188	VAL	CG1-CB-CG2	7.12	122.29	110.90
1	A	839	GLN	O-C-N	-6.63	112.09	122.70
2	E	17	SER	O-C-N	-6.54	112.23	122.70
2	E	56	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	E	16	GLN	CA-C-N	6.42	131.33	117.20
1	A	840	GLN	O-C-N	-6.42	112.28	123.20
3	D	145	LEU	CB-CG-CD1	-6.27	100.34	111.00
2	B	16	GLN	CA-C-N	5.47	129.24	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	840	GLN	Mainchain
1	C	840	GLN	Mainchain

5.2 Too-close contacts ⓘ

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	49	0	43	2	0
1	C	41	0	39	1	0
2	B	1548	0	1492	22	0
2	E	1548	0	1492	23	0
3	D	1646	0	1604	19	0
3	F	1605	0	1561	7	0
4	B	8	0	12	5	0
4	D	8	0	12	2	0
4	E	4	0	6	1	0
5	B	1	0	0	0	0
6	E	7	0	9	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	0	0	0
7	B	98	0	0	4	0
7	C	4	0	0	0	0
7	D	126	0	0	3	0
7	E	101	0	0	4	0
7	F	125	0	0	1	0
All	All	6923	0	6270	67	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 5.

All (67) 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:63:ARG:HG2	4:B:302:EDO:H11	1.44	0.97
2:E:162:GLY:N	6:E:301:PEG:H32	1.94	0.83
2:E:171:GLN:HE21	2:E:177:ALA:HB2	1.46	0.80
3:D:219:GLU:HB3	3:D:220:PRO:HD2	1.63	0.80
3:D:219:GLU:CB	3:D:220:PRO:HD2	2.13	0.77
2:B:79:GLY:HA3	4:B:302:EDO:H22	1.66	0.76
2:E:162:GLY:H	6:E:301:PEG:H32	1.52	0.74
2:E:172:SER:H	4:E:302:EDO:H11	1.56	0.69
2:E:162:GLY:CA	6:E:301:PEG:H32	2.23	0.69
2:E:81:GLN:HB3	7:E:482:HOH:O	1.93	0.67
3:D:219:GLU:HB3	3:D:220:PRO:CD	2.25	0.66
3:D:138:THR:HB	3:D:193:SER:OG	1.95	0.66
3:D:177:LEU:HG	2:E:58:SER:HB2	1.79	0.63
2:B:114:LYS:NZ	7:B:403:HOH:O	2.31	0.63
2:B:56:ARG:NE	7:B:401:HOH:O	2.27	0.63
2:E:173:ASN:ND2	7:E:404:HOH:O	2.32	0.62
3:D:120:SER:H	4:D:302:EDO:H21	1.64	0.62
3:D:136:LYS:NZ	7:D:406:HOH:O	2.33	0.62
2:B:112:GLN:NE2	7:B:406:HOH:O	2.33	0.61
2:E:162:GLY:HA2	6:E:301:PEG:H32	1.84	0.59
2:E:171:GLN:NE2	2:E:177:ALA:HB2	2.16	0.58
2:B:109:VAL:O	4:B:301:EDO:H12	2.04	0.58
3:F:128:VAL:HG21	3:F:214:VAL:HG21	1.85	0.57
3:D:128:VAL:HG21	3:D:214:VAL:HG11	1.86	0.57
2:B:174:ASN:HB3	4:B:301:EDO:O1	2.06	0.56
3:D:208:LYS:O	3:D:211:ASN:ND2	2.38	0.56
3:D:219:GLU:CB	3:D:220:PRO:CD	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:159:VAL:C	2:E:160:LYS:HG2	2.26	0.56
2:B:28:ASP:OD1	2:B:29:VAL:N	2.27	0.55
2:B:63:ARG:CG	4:B:302:EDO:H11	2.26	0.55
3:F:11:LEU:HD21	3:F:121:ALA:O	2.06	0.55
2:B:128:GLU:HG3	3:D:129:PHE:CG	2.43	0.54
2:B:87:ASP:OD1	2:B:106:LYS:HG2	2.08	0.54
2:B:170:LYS:HE2	2:B:174:ASN:HA	1.89	0.54
2:E:154:ALA:HB2	2:E:159:VAL:CG2	2.38	0.53
2:B:129:LEU:HD23	2:B:134:ALA:HB2	1.90	0.53
3:D:120:SER:H	4:D:302:EDO:C2	2.21	0.53
2:E:37:TRP:HB2	2:E:50:ILE:HB	1.91	0.52
2:E:128:GLU:HG3	3:F:129:PHE:CE2	2.45	0.52
2:B:128:GLU:HG3	3:D:129:PHE:CD1	2.44	0.52
2:E:8:PRO:HG2	7:E:495:HOH:O	2.10	0.51
2:B:198:GLN:HG2	2:B:207:GLU:HG3	1.93	0.50
2:E:136:LEU:HD22	2:E:182:LEU:HD23	1.93	0.49
3:F:13:LYS:HG2	7:F:376:HOH:O	2.12	0.49
2:B:16:GLN:HB2	7:B:437:HOH:O	2.13	0.48
2:E:198:GLN:HG2	2:E:207:GLU:HG3	1.98	0.46
3:F:11:LEU:HB2	3:F:154:PRO:HG3	1.97	0.46
1:C:839:GLN:HB3	3:F:50:TRP:CD1	2.50	0.46
3:D:130:PRO:HD2	7:D:464:HOH:O	2.16	0.46
2:E:17:SER:HA	2:E:77:VAL:O	2.15	0.44
2:B:198:GLN:HE21	2:B:207:GLU:CD	2.20	0.44
2:E:153:LYS:HD2	2:E:198:GLN:OE1	2.18	0.44
2:E:133:LYS:HB2	2:E:133:LYS:HE2	1.90	0.43
2:B:129:LEU:CD2	2:B:134:ALA:HB2	2.48	0.43
3:F:9:SER:HB3	3:F:115:LEU:O	2.19	0.43
2:B:160:LYS:HD2	2:B:160:LYS:O	2.19	0.43
1:A:840:GLN:OE1	3:D:33:SER:CA	2.67	0.42
3:D:128:VAL:HG21	3:D:214:VAL:CG1	2.48	0.42
2:B:4:LEU:HB2	2:B:102:GLY:HA2	2.01	0.42
2:B:157:SER:HA	2:B:158:PRO:HD3	1.76	0.42
2:E:41:HIS:CE1	7:E:467:HOH:O	2.73	0.42
3:D:62:GLN:O	7:D:401:HOH:O	2.22	0.42
3:D:100:GLN:HG2	3:D:101:PRO:O	2.20	0.42
2:E:112:GLN:OE1	2:E:113:PRO:HD2	2.20	0.41
1:A:840:GLN:OE1	3:D:33:SER:N	2.54	0.40
2:E:185:THR:OG1	2:E:188:GLN:HG3	2.22	0.40
2:B:63:ARG:HD2	2:B:78:SER:O	2.21	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	5/7 (71%)	5 (100%)	0	0	100	100
1	C	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	B	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
2	E	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
3	D	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
3	F	211/221 (96%)	202 (96%)	9 (4%)	0	100	100
All	All	857/884 (97%)	819 (96%)	38 (4%)	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	6/6 (100%)	6 (100%)	0	100	100
1	C	5/6 (83%)	5 (100%)	0	100	100
2	B	176/180 (98%)	168 (96%)	8 (4%)	27	36
2	E	176/180 (98%)	170 (97%)	6 (3%)	37	49
3	D	184/184 (100%)	181 (98%)	3 (2%)	62	76
3	F	178/184 (97%)	169 (95%)	9 (5%)	24	31
All	All	725/740 (98%)	699 (96%)	26 (4%)	35	47

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

Mol	Chain	Res	Type
2	B	69	SER
2	B	130	GLN
2	B	153	LYS
2	B	156	SER
2	B	157	SER
2	B	160	LYS
2	B	190	LYS
2	B	191	SER
3	D	138	THR
3	D	171	HIS
3	D	204	ASN
2	E	28	ASP
2	E	87	ASP
2	E	114	LYS
2	E	133	LYS
2	E	160	LYS
2	E	191	SER
3	F	25	SER
3	F	168	SER
3	F	171	HIS
3	F	195	SER
3	F	196	LEU
3	F	204	ASN
3	F	213	LYS
3	F	216	LYS
3	F	219	GLU

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

Mol	Chain	Res	Type
2	E	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	PCA	F	1	3	7,8,9	1.99	2 (28%)	9,10,12	2.25	4 (44%)
3	PCA	D	1	3	7,8,9	2.26	2 (28%)	9,10,12	2.32	3 (33%)

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	PCA	F	1	3	-	0/0/11/13	0/1/1/1
3	PCA	D	1	3	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	PCA	CA-N	-4.55	1.41	1.46
3	F	1	PCA	CA-N	-3.65	1.42	1.46
3	D	1	PCA	OE-CD	-3.11	1.17	1.23
3	F	1	PCA	OE-CD	-2.81	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	PCA	CB-CA-C	-5.00	105.82	112.70
3	F	1	PCA	O-C-CA	-3.64	115.23	124.78
3	D	1	PCA	CB-CG-CD	-3.14	99.35	104.40
3	F	1	PCA	CB-CG-CD	-3.13	99.35	104.40
3	D	1	PCA	OE-CD-CG	-3.08	121.39	126.76
3	F	1	PCA	OE-CD-CG	-2.60	122.23	126.76
3	F	1	PCA	CB-CA-C	-2.48	109.30	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	#$|Z| > 2$
4	EDO	B	302	-	3,3,3	0.45	0	2,2,2	1.11	0
6	PEG	E	301	-	6,6,6	0.86	0	5,5,5	0.36	0
4	EDO	B	301	-	3,3,3	0.32	0	2,2,2	0.22	0
4	EDO	D	302	-	3,3,3	0.60	0	2,2,2	0.62	0
4	EDO	E	302	-	3,3,3	0.50	0	2,2,2	0.53	0
4	EDO	D	301	-	3,3,3	0.31	0	2,2,2	0.27	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	EDO	B	302	-	-	1/1/1/1	-
6	PEG	E	301	-	-	2/4/4/4	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	E	302	-	-	1/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-

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	B	301	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
6	E	301	PEG	C1-C2-O2-C3
6	E	301	PEG	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	E	302	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	EDO	3	0
6	E	301	PEG	4	0
4	B	301	EDO	2	0
4	D	302	EDO	2	0
4	E	302	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1
2	B	1
1	C	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	17:SER	C	18:VAL	N	1.20
1	B	17:SER	C	18:VAL	N	1.17
1	C	840:GLN	C	841:GLY	N	1.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	840:GLN	C	841:GLY	N	0.93

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	7/7 (100%)	1.21	2 (28%)	0	0	28, 34, 37, 60	0
1	C	6/7 (85%)	0.58	0	100	100	31, 36, 38, 41	0
2	B	210/214 (98%)	0.21	9 (4%)	35	40	20, 31, 56, 65	0
2	E	210/214 (98%)	0.26	4 (1%)	66	72	22, 35, 48, 58	0
3	D	220/221 (99%)	0.09	4 (1%)	68	74	20, 29, 47, 63	0
3	F	214/221 (96%)	0.16	5 (2%)	60	66	18, 26, 53, 81	0
All	All	867/884 (98%)	0.19	24 (2%)	53	59	18, 30, 52, 81	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	134	SER	7.7
3	D	220	PRO	4.4
3	D	135	SER	4.1
3	F	220	PRO	4.1
2	E	132	ASN	3.6
2	B	111	GLY	3.5
2	B	190	LYS	3.5
2	B	132	ASN	3.4
3	D	221	PRO	3.3
1	A	835	ASP	3.1
2	E	111	GLY	3.1
2	B	160	LYS	3.0
2	B	191	SER	3.0
3	D	138	THR	2.9
3	F	140	GLY	2.6
2	B	130	GLN	2.5
1	A	837	VAL	2.4
2	E	188	GLN	2.2
2	B	114	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	211	ALA	2.1
3	F	196	LEU	2.1
2	B	187	GLU	2.1
3	F	219	GLU	2.0
2	E	62	ASP	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(Å^2)	Q<0.9
3	PCA	D	1	8/9	0.93	0.12	28,30,36,38	0
3	PCA	F	1	8/9	0.94	0.13	31,32,36,38	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	D	301	4/4	0.83	0.21	32,41,42,46	0
6	PEG	E	301	7/7	0.86	0.18	38,48,53,55	0
4	EDO	B	301	4/4	0.91	0.45	48,53,53,54	0
4	EDO	E	302	4/4	0.92	0.13	40,51,55,57	0
5	CL	B	303	1/1	0.93	0.27	30,30,30,30	0
4	EDO	B	302	4/4	0.93	0.30	35,36,36,43	0
4	EDO	D	302	4/4	0.95	0.14	24,26,31,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

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