



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 7YI6 / pdb_00007yi6
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 ⓘ 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

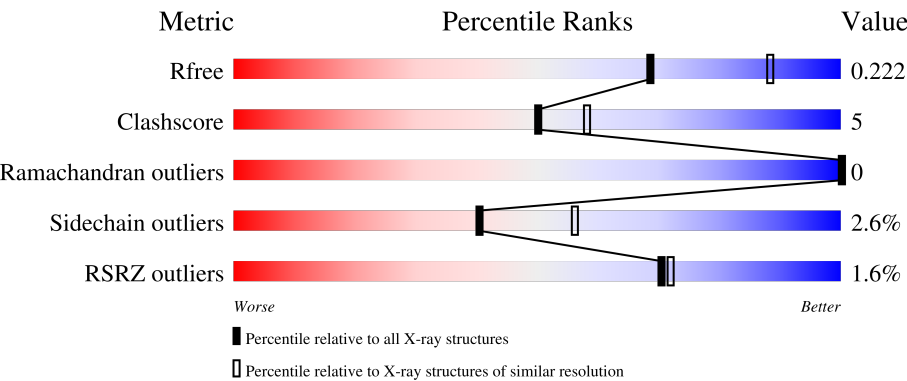
1 Overall quality at a glance i

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 $\leq 5\%$. 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	7	14% 71%14%14%
1	C	7	43%14%29%14%
2	B	214	% 78%17%..
2	E	214	% 83%14%..
3	D	221	2% 88%10%. .

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Mol	Chain	Length	Quality of chain
3	F	221	 2% 85% 11% ..

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 (CCD ID: EDO) (formula: C₂H₆O₂).

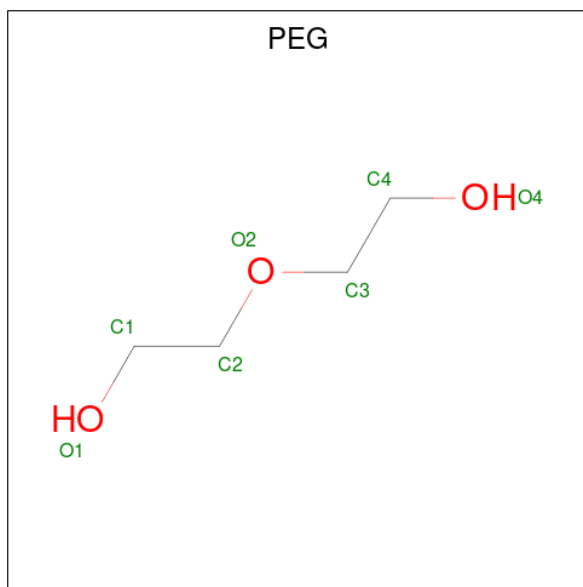


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 7 is water.

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

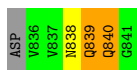
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

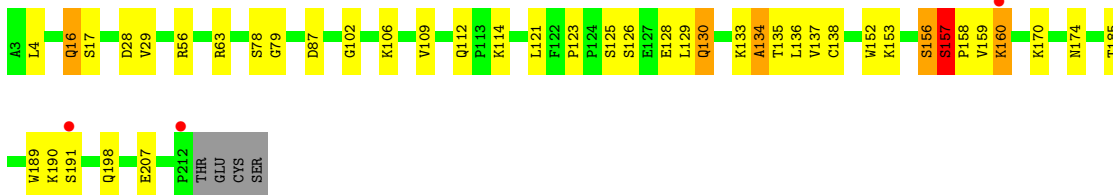
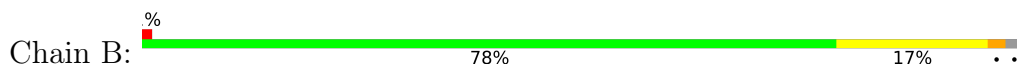
- Molecule 1: Spike glycoprotein



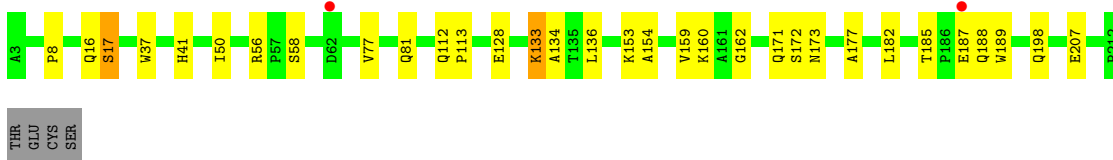
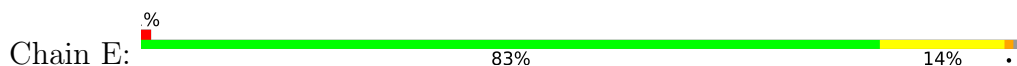
- Molecule 1: Spike glycoprotein



- Molecule 2: light chain of 3D1

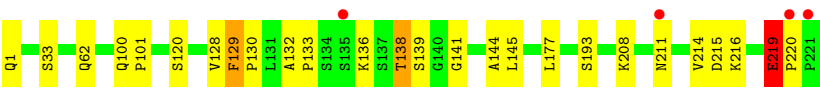


- Molecule 2: light chain of 3D1

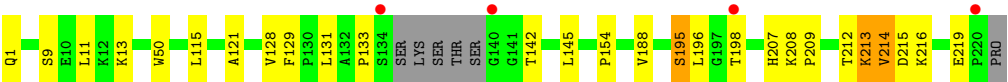
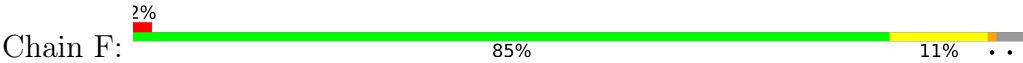


- Molecule 3: heavy chain of 3D1





● Molecule 3: heavy chain of 3D1



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 45.86 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.86-2.28) 98.9 (45.86-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.193 , 0.220 0.194 , 0.222	Depositor DCC
R_{free} test set	2000 reflections (5.07%)	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)	0.34 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: CL, PCA, PEG, EDO

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	4.13	1/48 (2.1%)	1.84	4/65 (6.2%)
1	C	4.42	2/40 (5.0%)	2.19	4/54 (7.4%)
2	B	1.05	17/1590 (1.1%)	0.93	5/2173 (0.2%)
2	E	0.73	5/1590 (0.3%)	0.91	8/2173 (0.4%)
3	D	0.79	7/1684 (0.4%)	0.65	5/2304 (0.2%)
3	F	0.99	11/1641 (0.7%)	0.74	2/2244 (0.1%)
All	All	1.02	43/6593 (0.7%)	0.84	28/9013 (0.3%)

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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	GLN	C-N	-28.30	0.93	1.33
1	C	840	GLN	C-N	-23.71	1.00	1.33
3	F	208	LYS	C-O	-11.94	1.13	1.24
2	B	17	SER	C-N	-11.41	1.17	1.33
3	D	129	PHE	C-O	-10.18	1.13	1.24
3	F	214	VAL	C-O	-9.11	1.14	1.24
2	E	17	SER	C-N	-8.53	1.20	1.33
2	B	121	LEU	C-O	-8.38	1.14	1.24
2	E	16	GLN	C-N	-8.20	1.21	1.33
3	F	213	LYS	C-O	-8.09	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	215	ASP	C-O	-8.05	1.14	1.24
2	E	134	ALA	C-O	-7.75	1.15	1.23
1	C	839	GLN	C-O	-6.95	1.16	1.24
2	B	135	THR	C-O	-6.70	1.16	1.23
2	B	138	CYS	C-O	-6.69	1.16	1.24
3	F	209	PRO	C-O	-6.68	1.15	1.24
2	E	56	ARG	C-O	-6.45	1.17	1.24
2	B	159	VAL	C-O	-6.43	1.17	1.24
3	D	144	ALA	C-O	-6.25	1.16	1.24
2	B	16	GLN	C-N	-6.23	1.24	1.33
3	F	215	ASP	C-O	-6.16	1.17	1.24
3	F	212	THR	C-O	-6.12	1.16	1.24
2	B	130	GLN	C-O	-6.10	1.16	1.24
2	B	189	TRP	C-O	-6.09	1.17	1.24
3	F	207	HIS	C-O	-5.79	1.15	1.23
3	D	139	SER	C-O	-5.73	1.16	1.24
2	B	152	TRP	C-O	-5.71	1.17	1.24
3	F	133	PRO	C-O	-5.71	1.16	1.24
3	D	216	LYS	C-O	-5.67	1.17	1.24
2	B	137	VAL	C-O	-5.64	1.18	1.24
2	E	187	GLU	C-O	-5.55	1.17	1.24
3	F	131	LEU	C-O	-5.55	1.17	1.23
3	D	133	PRO	C-O	-5.51	1.17	1.23
2	B	134	ALA	C-O	-5.48	1.17	1.23
2	B	185	THR	C-O	-5.40	1.18	1.24
3	D	216	LYS	CA-C	-5.38	1.46	1.52
2	B	136	LEU	C-O	-5.29	1.17	1.24
3	F	142	THR	CA-C	-5.15	1.46	1.52
2	B	126	SER	C-O	-5.11	1.18	1.24
2	B	156	SER	C-O	-5.10	1.16	1.24
2	B	123	PRO	C-O	-5.07	1.18	1.24
3	F	195	SER	C-O	-5.06	1.17	1.24
2	B	125	SER	C-O	-5.01	1.17	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	16	GLN	O-C-N	-13.51	106.04	122.65
2	E	16	GLN	CA-C-N	12.95	141.95	122.65
2	E	16	GLN	C-N-CA	12.95	141.95	122.65
2	B	16	GLN	CA-C-N	12.90	142.29	122.94
2	B	16	GLN	C-N-CA	12.90	142.29	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	GLN	O-C-N	-9.87	108.81	121.74
1	A	839	GLN	O-C-N	-9.69	112.09	122.07
2	E	17	SER	O-C-N	-9.37	112.23	123.19
2	E	189	TRP	N-CA-C	7.57	122.97	112.45
1	A	840	GLN	O-C-N	-6.70	112.28	123.00
2	B	157	SER	CA-C-N	6.46	126.38	119.85
2	B	157	SER	C-N-CA	6.46	126.38	119.85
1	C	838	ASN	CA-C-N	6.11	129.29	120.79
1	C	838	ASN	C-N-CA	6.11	129.29	120.79
2	E	17	SER	CA-C-N	6.07	132.86	122.67
2	E	17	SER	C-N-CA	6.07	132.86	122.67
2	E	187	GLU	CA-C-O	-6.00	114.52	120.70
3	F	195	SER	N-CA-C	5.70	119.33	112.38
3	D	219	GLU	CA-C-N	5.59	126.14	120.38
3	D	219	GLU	C-N-CA	5.59	126.14	120.38
1	A	839	GLN	CA-C-N	5.55	131.68	121.70
1	A	839	GLN	C-N-CA	5.55	131.68	121.70
3	F	188	VAL	CG1-CB-CG2	5.22	122.29	110.80
1	C	839	GLN	CA-C-N	5.18	131.02	121.70
1	C	839	GLN	C-N-CA	5.18	131.02	121.70
3	D	132	ALA	CA-C-N	5.13	125.54	119.99
3	D	132	ALA	C-N-CA	5.13	125.54	119.99
3	D	141	GLY	N-CA-C	5.04	119.97	113.27

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1548	0	1493	23	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	6	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
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	6271	68	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 (68) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLN:NE2	7:B:406:HOH:O	2.33	0.61
2:E:159:VAL:C	2:E:160:LYS:HG2	2.26	0.60
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
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
2:B:198:GLN:HE21	2:B:207:GLU:CD	2.20	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:E:153:LYS:HD2	2:E:198:GLN:OE1	2.18	0.44
2:B:174:ASN:HB3	4:B:301:EDO:HO1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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 [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	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%)	24	35
2	E	176/180 (98%)	175 (99%)	1 (1%)	78	87
3	D	184/184 (100%)	181 (98%)	3 (2%)	55	71
3	F	178/184 (97%)	171 (96%)	7 (4%)	28	41
All	All	725/740 (98%)	706 (97%)	19 (3%)	40	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	130	GLN
2	B	133	LYS
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	145	LEU
3	D	219	GLU
2	E	133	LYS
3	F	145	LEU
3	F	195	SER
3	F	196	LEU
3	F	198	THR
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	112	GLN
2	E	40	GLN
2	E	171	GLN

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Mol	Chain	Res	Type
3	F	39	GLN
3	F	77	ASN

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	2.03	2 (28%)	9,10,12	2.29	5 (55%)
3	PCA	D	1	3	7,8,9	2.32	3 (42%)	9,10,12	2.34	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	PCA	CA-N	-4.61	1.41	1.46
3	F	1	PCA	CA-N	-3.70	1.42	1.46
3	D	1	PCA	OE-CD	-3.18	1.17	1.23
3	F	1	PCA	OE-CD	-2.87	1.17	1.23
3	D	1	PCA	CD-N	-2.12	1.28	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	PCA	CB-CA-C	-4.99	105.82	112.66
3	F	1	PCA	O-C-CA	-3.71	115.23	124.77
3	D	1	PCA	CB-CG-CD	-3.27	99.35	104.41
3	F	1	PCA	CB-CG-CD	-3.27	99.35	104.41
3	D	1	PCA	OE-CD-CG	-2.99	121.39	126.72
3	F	1	PCA	OE-CD-CG	-2.51	122.23	126.72
3	F	1	PCA	CB-CA-C	-2.45	109.30	112.66
3	F	1	PCA	CB-CA-N	-2.01	97.71	103.24

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	301	-	3,3,3	0.29	0	2,2,2	0.23	0
4	EDO	D	302	-	3,3,3	0.61	0	2,2,2	0.62	0
6	PEG	E	301	-	6,6,6	0.87	0	5,5,5	0.35	0
4	EDO	E	302	-	3,3,3	0.51	0	2,2,2	0.54	0
4	EDO	B	301	-	3,3,3	0.31	0	2,2,2	0.16	0
4	EDO	B	302	-	3,3,3	0.46	0	2,2,2	1.07	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	D	301	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
6	PEG	E	301	-	-	2/4/4/4	-
4	EDO	E	302	-	-	1/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	B	302	-	-	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	D	301	EDO	O1-C1-C2-O2
4	B	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 13 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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
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%)	0.46	1 (14%) 6 6	28, 34, 37, 60	0
1	C	6/7 (85%)	0.44	0 100 100	31, 36, 38, 41	0
2	B	210/214 (98%)	0.15	3 (1%) 73 75	17, 31, 56, 65	1 (0%)
2	E	210/214 (98%)	0.22	2 (0%) 79 81	22, 35, 48, 58	1 (0%)
3	D	220/221 (99%)	-0.12	4 (1%) 67 69	20, 29, 47, 63	0
3	F	214/221 (96%)	-0.08	4 (1%) 66 68	18, 26, 53, 81	0
All	All	867/884 (98%)	0.05	14 (1%) 70 72	17, 30, 52, 81	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	220	PRO	4.5
3	F	134	SER	4.2
3	F	140	GLY	3.3
3	D	221	PRO	3.1
2	B	191	SER	2.5
2	B	160	LYS	2.4
3	F	198	THR	2.3
3	D	211	ASN	2.3
3	D	220	PRO	2.3
1	A	835	ASP	2.3
2	B	212	PRO	2.2
3	D	135	SER	2.2
2	E	187	GLU	2.0
2	E	62	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	PCA	F	1	8/9	0.93	0.07	31,32,36,38	0
3	PCA	D	1	8/9	0.95	0.07	28,30,36,38	0

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	EDO	D	301	4/4	0.81	0.18	32,41,42,46	0
4	EDO	B	301	4/4	0.82	0.20	48,53,53,54	0
6	PEG	E	301	7/7	0.83	0.14	38,48,53,55	0
4	EDO	E	302	4/4	0.88	0.12	40,51,55,57	0
4	EDO	B	302	4/4	0.89	0.18	35,36,36,43	0
5	CL	B	303	1/1	0.92	0.21	30,30,30,30	0
4	EDO	D	302	4/4	0.92	0.10	24,26,31,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.