



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 PM UTC

PDB ID : 8U0R / pdb_00008u0r
Title : The crystal structure of protein A21, a component of the conserved poxvirus entry-fusion complex
Authors : Diesterbeck, U.; Gittis, A.G.; Garboczi, D.N.; Moss, B.
Deposited on : 2023-08-29
Resolution : 2.30 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

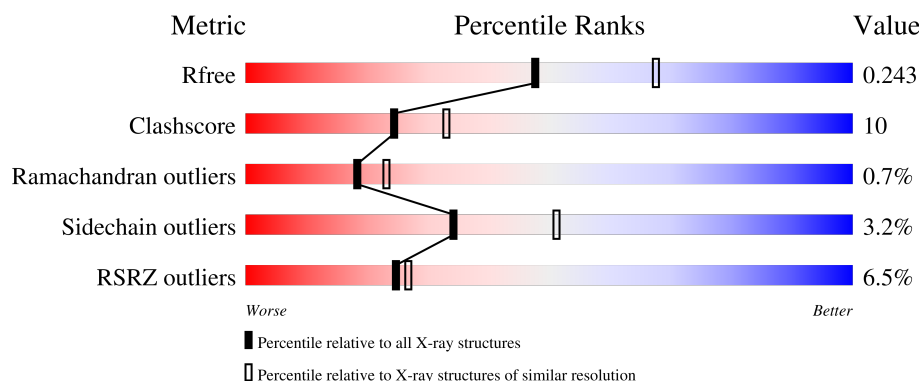
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	94	6% 65% 12% • 20%
1	B	94	5% 66% 15% 19%
1	C	94	4% 70% 7% • 21%
1	D	94	6% 61% 17% • 21%
1	E	94	4% 67% 12% 21%

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Mol	Chain	Length	Quality of chain
1	F	94	

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
15	GOL	F	201	-	-	X	-
2	EOH	F	203	-	-	X	-
3	EDO	B	202	-	-	X	-

2 Entry composition [i](#)

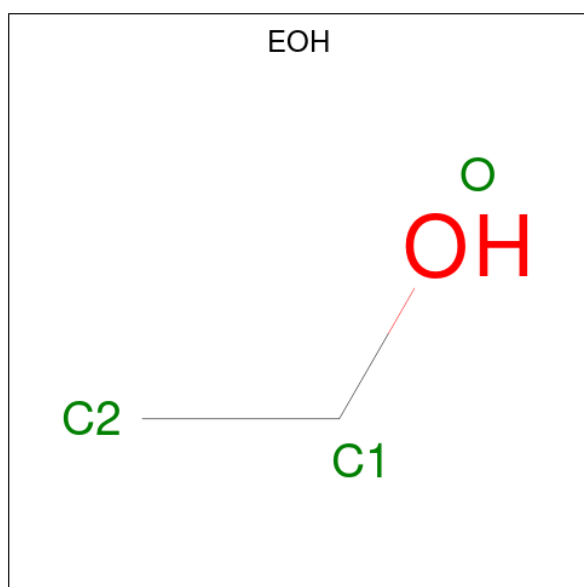
There are 17 unique types of molecules in this entry. The entry contains 3686 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Virion membrane protein A21.

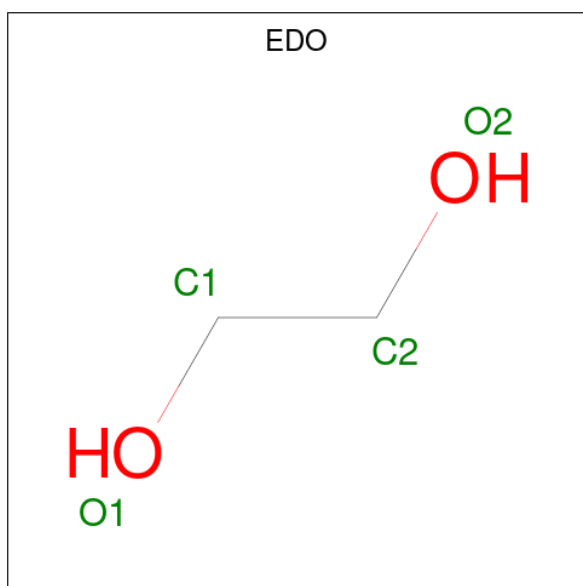
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	75	Total	C	N	O	S	0	0	0
			576	365	94	113	4			
1	B	76	Total	C	N	O	S	0	0	0
			578	364	97	113	4			
1	C	74	Total	C	N	O	S	0	0	0
			550	351	91	104	4			
1	D	74	Total	C	N	O	S	0	0	0
			552	350	90	108	4			
1	E	74	Total	C	N	O	S	0	0	0
			558	355	90	109	4			
1	F	75	Total	C	N	O	S	0	0	0
			575	361	99	111	4			

- Molecule 2 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 2 1	0	0
2	B	1	Total C O 3 2 1	0	0
2	D	1	Total C O 3 2 1	0	0
2	E	1	Total C O 3 2 1	0	0
2	F	1	Total C O 3 2 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



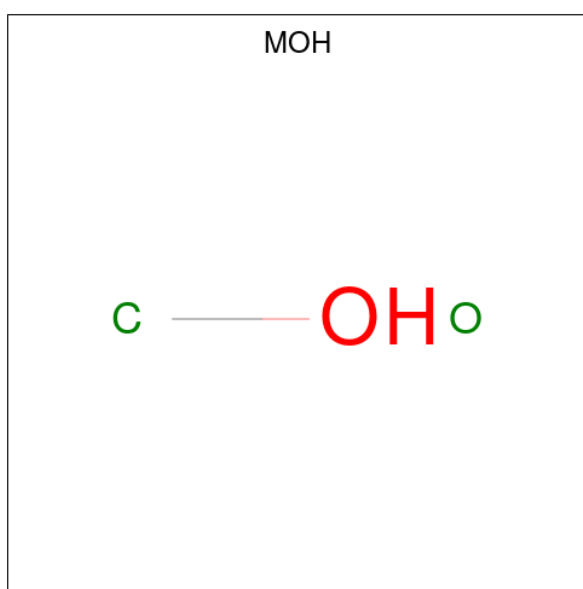
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

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

- Molecule 4 is METHANOL (CCD ID: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			2	1	1		
4	A	1	Total	C	O	0	0
			2	1	1		
4	A	1	Total	C	O	0	0
			2	1	1		
4	C	1	Total	C	O	0	0
			2	1	1		
4	C	1	Total	C	O	0	0
			2	1	1		
4	E	1	Total	C	O	0	0
			2	1	1		
4	F	1	Total	C	O	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			2	1	1		
4	F	1	Total	C	O	0	0
			2	1	1		

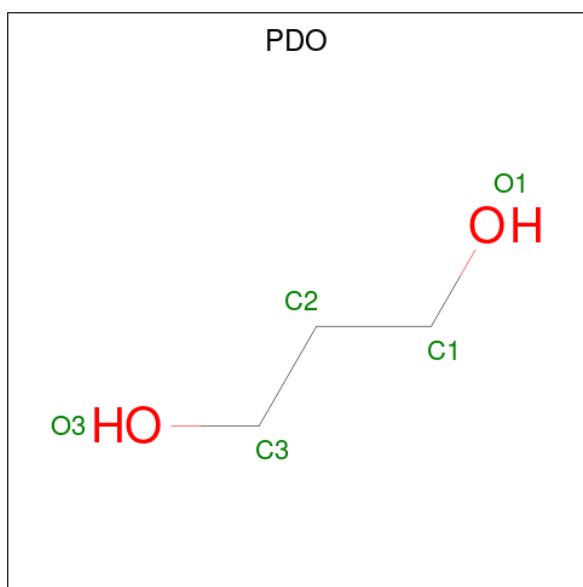
- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	I	0	0
			3	3		
5	B	6	Total	I	0	0
			6	6		
5	C	1	Total	I	0	0
			1	1		
5	D	2	Total	I	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

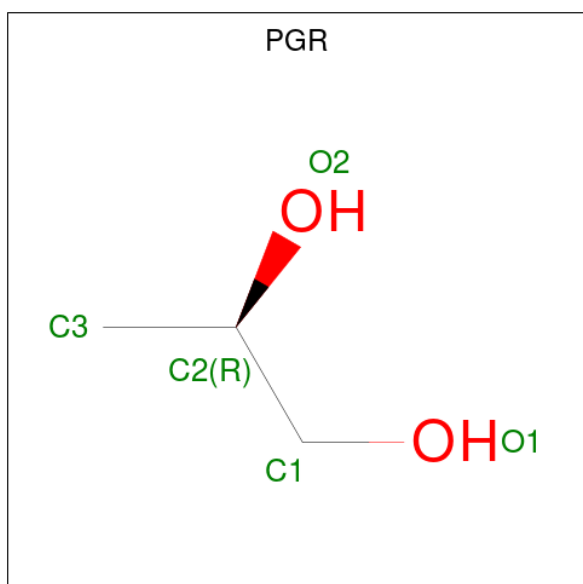
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cl	0	0
			3	3		
6	B	2	Total	Cl	0	0
			2	2		
6	C	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		
6	F	2	Total	Cl	0	0
			2	2		

- Molecule 7 is 1,3-PROPANDIOL (CCD ID: PDO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			5	3	2		
7	C	1	Total	C	O	0	0
			5	3	2		
7	D	1	Total	C	O	0	0
			5	3	2		
7	E	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: $C_3H_8O_2$).

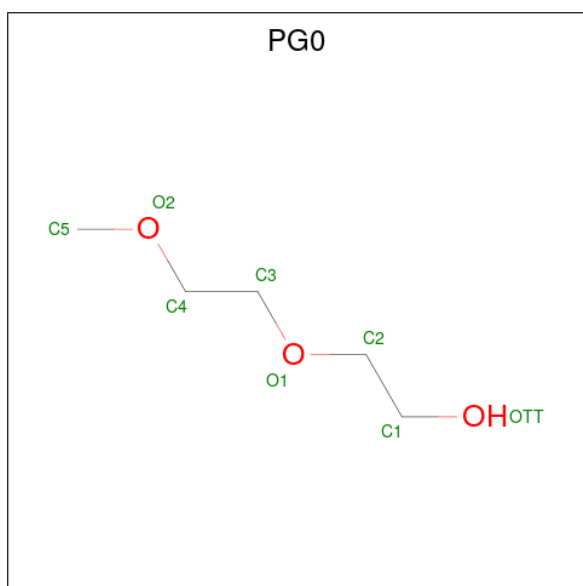


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

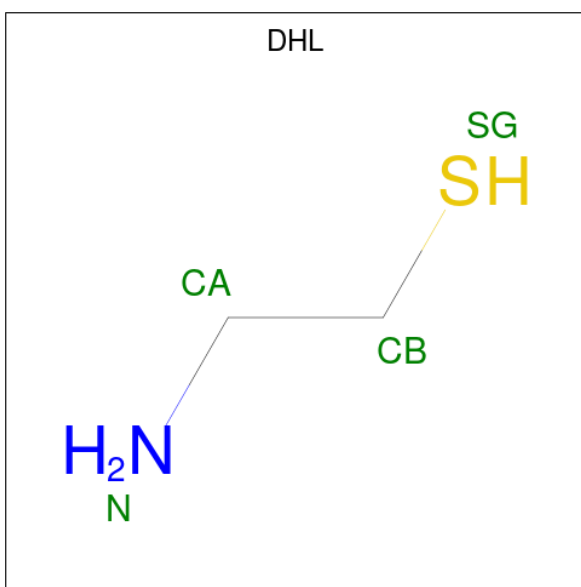
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Na	0	0
			1	1		
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



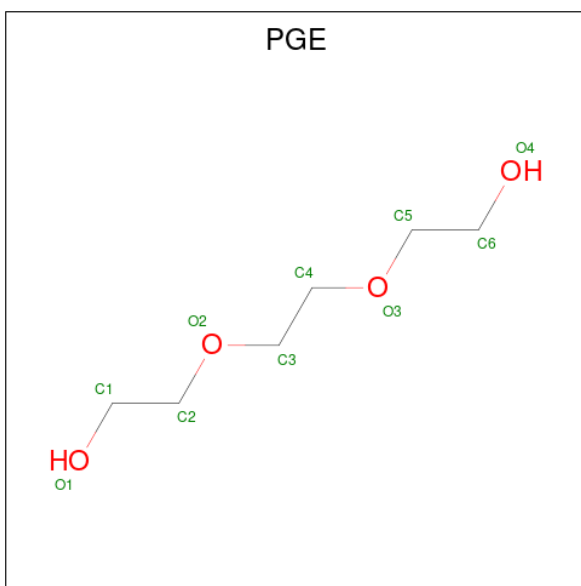
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 11 is 2-AMINO-ETHANETHIOL (CCD ID: DHL) (formula: C₂H₇NS).



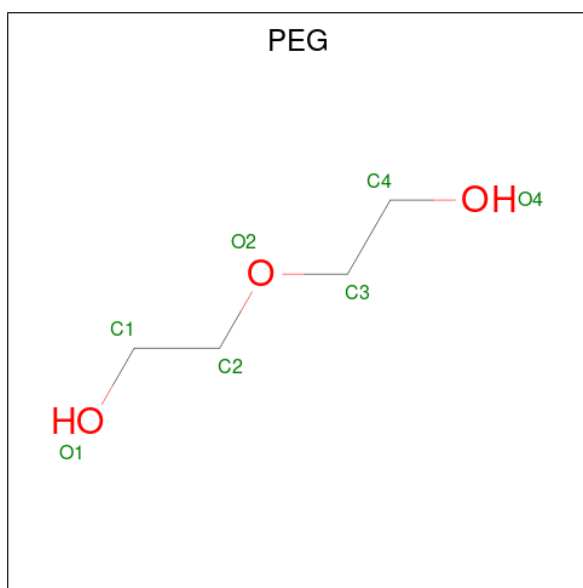
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	S	0	0
			4	2	1	1		
11	F	1	Total	C	N	S	0	0
			4	2	1	1		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



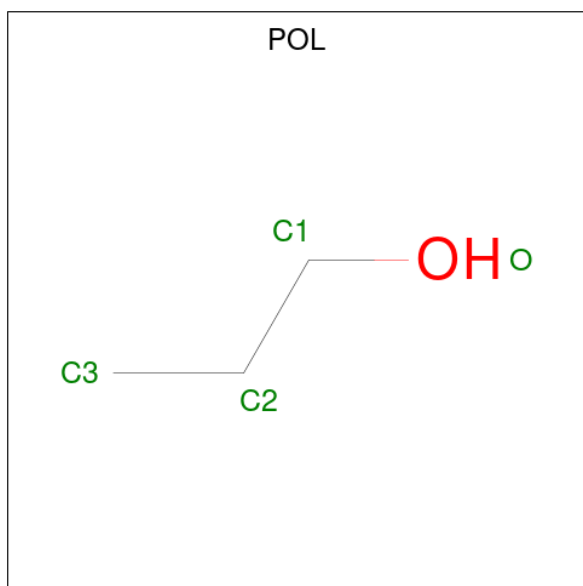
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			10	6	4		
12	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



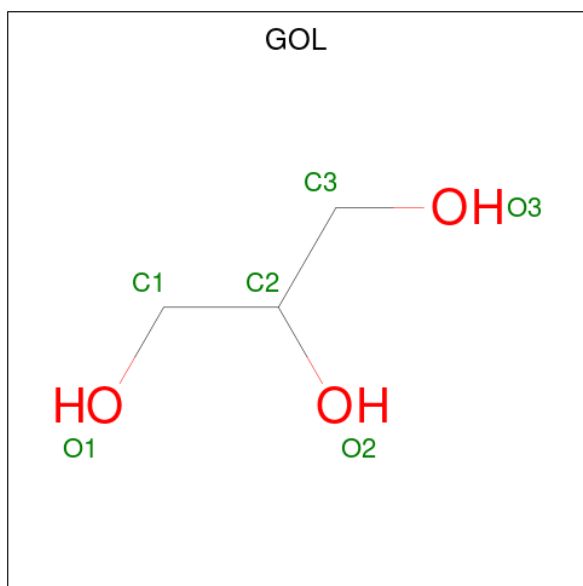
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			7	4	3		
13	D	1	Total	C	O	0	0
			7	4	3		
13	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 14 is N-PROPANOL (CCD ID: POL) (formula: C_3H_8O).



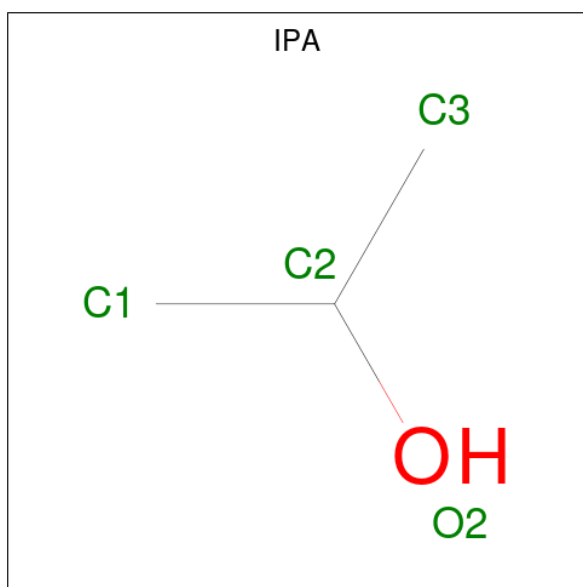
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			4	3	1		

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	E	1	Total	C	O	0	0
			6	3	3		
15	F	1	Total	C	O	0	0
			6	3	3		
15	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 16 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

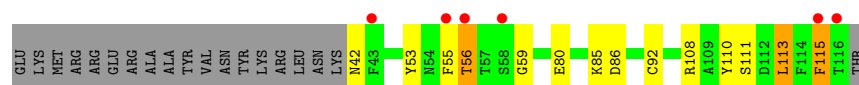
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	10	Total	O	0	0
			10	10		
17	B	16	Total	O	0	0
			16	16		
17	C	20	Total	O	0	0
			20	20		
17	D	11	Total	O	0	0
			11	11		
17	E	11	Total	O	0	0
			11	11		
17	F	16	Total	O	0	0
			16	16		

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: Virion membrane protein A21



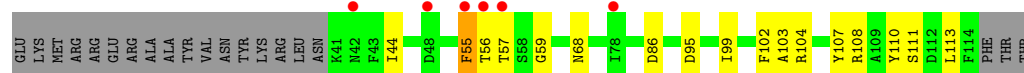
- Molecule 1: Virion membrane protein A21



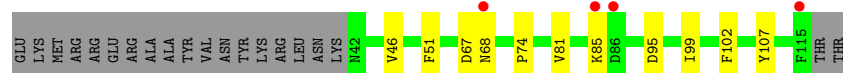
- Molecule 1: Virion membrane protein A21



- Molecule 1: Virion membrane protein A21



- Molecule 1: Virion membrane protein A21



- Molecule 1: Virion membrane protein A21



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.86Å 70.06Å 78.95Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	39.31 – 2.30 39.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.31-2.30) 99.3 (39.31-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.239 0.217 , 0.243	Depositor DCC
R_{free} test set	1810 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3686	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 30.02 % 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 1.4035e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, MOH, IPA, DHL, POL, PDO, PEG, EDO, PGE, NA, EOH, CL, GOL, PG0, PGR

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	0.55	0/588	0.83	0/798
1	B	0.49	0/590	0.72	1/802 (0.1%)
1	C	0.61	0/561	0.87	0/762
1	D	0.64	0/563	0.95	0/767
1	E	0.67	0/569	0.97	0/775
1	F	0.51	0/585	0.74	0/793
All	All	0.58	0/3456	0.85	1/4697 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	PHE	CB-CA-C	-6.48	99.17	109.80

There are no chirality outliers.

There are no planarity outliers.

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	576	0	511	13	0
1	B	578	0	506	14	0
1	C	550	0	491	6	0
1	D	552	0	481	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	558	0	502	9	0
1	F	575	0	529	12	0
2	A	3	0	6	1	0
2	B	3	0	6	1	0
2	D	3	0	6	0	0
2	E	3	0	6	0	0
2	F	3	0	6	2	0
3	A	8	0	12	0	0
3	B	4	0	6	5	0
3	C	12	0	18	0	0
3	D	8	0	12	2	0
3	E	8	0	12	0	0
3	F	4	0	6	1	0
4	A	6	0	0	1	0
4	C	4	0	0	0	0
4	E	2	0	0	0	0
4	F	6	0	0	0	0
5	A	3	0	0	0	0
5	B	6	0	0	1	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
7	B	10	0	16	0	0
7	C	5	0	8	0	0
7	D	5	0	8	2	0
7	E	5	0	8	1	0
8	B	5	0	8	1	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
10	B	8	0	12	1	0
11	B	4	0	7	0	0
11	F	4	0	7	1	0
12	C	10	0	14	2	0
12	F	10	0	14	1	0
13	C	7	0	10	3	0
13	D	7	0	10	1	0
13	F	7	0	10	1	0
14	D	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	6	0	8	1	0
15	F	12	0	16	6	0
16	E	4	0	8	1	0
17	A	10	0	0	0	0
17	B	16	0	0	1	0
17	C	20	0	0	0	0
17	D	11	0	0	1	0
17	E	11	0	0	0	0
17	F	16	0	0	0	0
All	All	3686	0	3288	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 10.

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)
1:F:103:ALA:HA	15:F:201:GOL:H32	1.51	0.93
1:A:53:TYR:CE2	1:A:113:LEU:HD22	2.24	0.72
1:A:108:ARG:HD3	4:A:206:MOH:C	2.19	0.72
1:B:45:CYS:HB3	3:B:202:EDO:H11	1.70	0.72
1:D:95:ASP:HB2	1:E:68:ASN:OD1	1.91	0.71
1:B:45:CYS:H	3:B:202:EDO:H22	1.61	0.66
1:F:90:LEU:HD12	1:F:99:ILE:HD11	1.77	0.65
1:A:92:CYS:HB3	3:D:203:EDO:H22	1.84	0.59
1:D:56:THR:HG23	3:D:203:EDO:O1	2.03	0.59
1:F:42:ASN:HB2	1:F:82:ASN:OD1	2.04	0.57
1:B:45:CYS:CB	3:B:202:EDO:H11	2.35	0.57
1:E:85:LYS:O	1:E:85:LYS:HG3	2.05	0.56
1:A:115:PHE:CD1	1:A:115:PHE:N	2.73	0.56
1:A:55:PHE:HE1	1:D:107:TYR:CE1	2.24	0.56
1:D:103:ALA:HB3	7:D:204:PDO:H22	1.88	0.55
1:A:110:TYR:CZ	1:D:59:GLY:HA2	2.41	0.55
1:B:49:ARG:HH21	8:B:205:PGR:H2	1.71	0.55
1:C:74:PRO:HD2	12:C:210:PGE:H2	1.89	0.54
1:D:103:ALA:H	7:D:204:PDO:H21	1.73	0.53
1:F:42:ASN:HA	1:F:85:LYS:HE2	1.89	0.53
1:F:103:ALA:CA	15:F:201:GOL:H32	2.33	0.53
1:B:68:ASN:ND2	17:B:302:HOH:O	2.42	0.53
1:C:73:ILE:HG12	12:C:210:PGE:H3	1.91	0.53
1:A:59:GLY:HA2	1:D:110:TYR:CZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:OD1	1:A:86:ASP:N	2.36	0.51
1:B:110:TYR:CZ	1:C:59:GLY:HA2	2.46	0.51
1:F:45:CYS:SG	15:F:202:GOL:H2	2.51	0.51
1:D:68:ASN:ND2	1:E:95:ASP:HB2	2.26	0.51
1:B:45:CYS:SG	5:B:206:IOD:I	3.39	0.51
2:B:201:EOH:H23	13:C:211:PEG:O4	2.11	0.51
1:C:55:PHE:CD1	1:C:55:PHE:C	2.88	0.50
1:D:108:ARG:HG2	13:D:209:PEG:O4	2.11	0.50
1:F:41:LYS:C	1:F:85:LYS:HZ3	2.20	0.49
1:F:92:CYS:HB3	15:F:201:GOL:C1	2.43	0.49
1:C:107:TYR:HB2	13:C:211:PEG:H42	1.95	0.48
1:E:67:ASP:HB2	16:E:207:IPA:H33	1.95	0.48
1:A:113:LEU:HD12	1:A:113:LEU:HA	1.65	0.48
1:D:86:ASP:OD1	1:D:86:ASP:N	2.42	0.48
1:A:42:ASN:N	1:A:85:LYS:HE2	2.28	0.48
12:F:210:PGE:H6	12:F:210:PGE:O2	2.13	0.47
1:D:99:ILE:HB	1:D:102:PHE:HB2	1.97	0.47
1:B:45:CYS:H	3:B:202:EDO:C2	2.27	0.47
1:D:55:PHE:CD1	1:D:55:PHE:N	2.83	0.46
1:F:45:CYS:HB2	15:F:202:GOL:H32	1.96	0.46
3:F:204:EDO:H21	13:F:211:PEG:C2	2.45	0.46
1:F:42:ASN:HB2	1:F:82:ASN:CG	2.40	0.46
1:E:74:PRO:HD2	15:E:201:GOL:H2	1.98	0.46
1:B:44:ILE:HD11	1:B:53:TYR:HE1	1.81	0.45
1:B:114:PHE:C	1:B:115:PHE:HD1	2.24	0.45
1:D:104:ARG:NH2	17:D:302:HOH:O	2.50	0.45
1:E:81:VAL:O	1:E:85:LYS:HB3	2.18	0.44
1:B:59:GLY:HA2	1:C:110:TYR:CZ	2.53	0.43
13:C:211:PEG:H41	13:C:211:PEG:H21	1.55	0.43
1:E:46:VAL:HB	1:E:51:PHE:CD2	2.54	0.43
1:A:111:SER:HA	1:D:55:PHE:HE2	1.82	0.43
1:B:47:ASP:O	1:B:48:ASP:HB2	2.17	0.43
1:E:99:ILE:HB	1:E:102:PHE:HB2	2.01	0.43
1:D:55:PHE:H	1:D:55:PHE:HD1	1.66	0.42
2:F:203:EOH:C2	11:F:212:DHL:HB3	2.49	0.42
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.83	0.41
1:F:47:ASP:H	2:F:203:EOH:H22	1.84	0.41
1:B:45:CYS:H	3:B:202:EDO:H11	1.85	0.41
10:B:215:PG0:H42	10:B:215:PG0:H22	1.86	0.41
1:A:56:THR:CA	2:A:201:EOH:O	2.69	0.41
1:E:107:TYR:CE2	7:E:206:PDO:H31	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:CYS:HB3	15:F:201:GOL:H12	2.01	0.41
1:A:55:PHE:CE1	1:D:107:TYR:CE1	3.06	0.41
1:B:90:LEU:HD13	1:B:96:ARG:CZ	2.51	0.41

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	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	9	9
1	B	74/94 (79%)	69 (93%)	5 (7%)	0	100	100
1	C	72/94 (77%)	67 (93%)	5 (7%)	0	100	100
1	D	72/94 (77%)	69 (96%)	2 (3%)	1 (1%)	9	9
1	E	72/94 (77%)	68 (94%)	4 (6%)	0	100	100
1	F	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	9	9
All	All	436/564 (77%)	407 (93%)	26 (6%)	3 (1%)	18	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	57	THR
1	A	56	THR
1	F	85	LYS

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	60/86 (70%)	57 (95%)	3 (5%)	22	33
1	B	60/86 (70%)	60 (100%)	0	100	100
1	C	54/86 (63%)	51 (94%)	3 (6%)	19	28
1	D	55/86 (64%)	52 (94%)	3 (6%)	19	28
1	E	58/86 (67%)	58 (100%)	0	100	100
1	F	60/86 (70%)	58 (97%)	2 (3%)	33	50
All	All	347/516 (67%)	336 (97%)	11 (3%)	34	51

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

Mol	Chain	Res	Type
1	A	80	GLU
1	A	113	LEU
1	A	115	PHE
1	C	54	ASN
1	C	55	PHE
1	C	57	THR
1	D	44	ILE
1	D	55	PHE
1	D	111	SER
1	F	41	LYS
1	F	83	ASN

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

Mol	Chain	Res	Type
1	C	54	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](#)

Of 67 ligands modelled in this entry, 23 are monoatomic - leaving 44 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	$\# Z > 2$
7	PDO	D	204	-	4,4,4	0.39	0	3,3,3	0.58	0
12	PGE	C	210	-	9,9,9	0.10	0	8,8,8	0.11	0
4	MOH	F	207	-	1,1,1	0.17	0	-		
7	PDO	C	206	-	4,4,4	0.16	0	3,3,3	0.12	0
4	MOH	E	205	-	1,1,1	0.11	0	-		
4	MOH	F	205	-	1,1,1	0.09	0	-		
4	MOH	A	206	-	1,1,1	0.11	0	-		
4	MOH	C	204	-	1,1,1	0.07	0	-		
3	EDO	A	203	-	3,3,3	0.56	0	2,2,2	0.04	0
4	MOH	A	204	-	1,1,1	0.21	0	-		
3	EDO	E	204	-	3,3,3	0.18	0	2,2,2	0.13	0
7	PDO	E	206	-	4,4,4	0.38	0	3,3,3	0.23	0
7	PDO	B	203	-	4,4,4	0.39	0	3,3,3	0.47	0
16	IPA	E	207	-	3,3,3	0.12	0	3,3,3	0.13	0
2	EOH	B	201	-	2,2,2	0.16	0	1,1,1	0.27	0
3	EDO	C	202	-	3,3,3	0.24	0	2,2,2	0.11	0
13	PEG	C	211	-	6,6,6	0.54	0	5,5,5	0.57	0
2	EOH	A	201	-	2,2,2	0.20	0	1,1,1	0.25	0
3	EDO	F	204	-	3,3,3	0.17	0	2,2,2	0.01	0
4	MOH	F	206	-	1,1,1	0.11	0	-		
10	PG0	B	215	-	7,7,7	0.54	0	6,6,6	0.49	0
7	PDO	B	204	-	4,4,4	0.38	0	3,3,3	0.36	0
15	GOL	F	201	-	5,5,5	0.18	0	5,5,5	0.39	0
13	PEG	F	211	-	6,6,6	0.50	0	5,5,5	0.24	0
3	EDO	D	202	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EOH	E	202	-	2,2,2	0.05	0	1,1,1	0.22	0
4	MOH	C	205	-	1,1,1	0.16	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PEG	D	209	-	6,6,6	0.57	0	5,5,5	0.50	0
14	POL	D	205	-	3,3,3	0.37	0	2,2,2	0.36	0
3	EDO	D	203	-	3,3,3	0.30	0	2,2,2	0.03	0
2	EOH	D	201	-	2,2,2	0.10	0	1,1,1	0.37	0
11	DHL	B	216	-	2,3,3	0.11	0	1,2,2	0.01	0
12	PGE	F	210	-	9,9,9	0.14	0	8,8,8	0.16	0
3	EDO	A	202	-	3,3,3	0.30	0	2,2,2	0.05	0
3	EDO	C	203	-	3,3,3	0.28	0	2,2,2	0.12	0
15	GOL	F	202	-	5,5,5	1.41	1 (20%)	5,5,5	0.92	0
3	EDO	C	201	-	3,3,3	0.24	0	2,2,2	0.19	0
4	MOH	A	205	-	1,1,1	0.15	0	-		
8	PGR	B	205	-	4,4,4	0.74	0	4,4,4	0.75	0
2	EOH	F	203	-	2,2,2	0.20	0	1,1,1	0.30	0
3	EDO	E	203	-	3,3,3	0.20	0	2,2,2	0.25	0
11	DHL	F	212	-	2,3,3	0.61	0	1,2,2	0.54	0
15	GOL	E	201	-	5,5,5	1.12	0	5,5,5	0.88	0
3	EDO	B	202	-	3,3,3	0.18	0	2,2,2	0.14	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
7	PDO	D	204	-	-	0/2/2/2	-
12	PGE	C	210	-	-	5/7/7/7	-
7	PDO	C	206	-	-	1/2/2/2	-
3	EDO	A	203	-	-	1/1/1/1	-
3	EDO	E	204	-	-	1/1/1/1	-
7	PDO	E	206	-	-	1/2/2/2	-
7	PDO	B	203	-	-	0/2/2/2	-
3	EDO	C	202	-	-	0/1/1/1	-
13	PEG	C	211	-	-	2/4/4/4	-
3	EDO	F	204	-	-	0/1/1/1	-
10	PG0	B	215	-	-	2/5/5/5	-
7	PDO	B	204	-	-	2/2/2/2	-
15	GOL	F	201	-	-	2/4/4/4	-
13	PEG	F	211	-	-	2/4/4/4	-
3	EDO	D	202	-	-	0/1/1/1	-
13	PEG	D	209	-	-	4/4/4/4	-
14	POL	D	205	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	203	-	-	1/1/1/1	-
11	DHL	B	216	-	-	0/1/1/1	-
12	PGE	F	210	-	-	4/7/7/7	-
3	EDO	A	202	-	-	1/1/1/1	-
3	EDO	C	203	-	-	1/1/1/1	-
15	GOL	F	202	-	-	2/4/4/4	-
3	EDO	C	201	-	-	1/1/1/1	-
8	PGR	B	205	-	-	2/2/2/2	-
11	DHL	F	212	-	-	1/1/1/1	-
3	EDO	E	203	-	-	1/1/1/1	-
15	GOL	E	201	-	-	2/4/4/4	-
3	EDO	B	202	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	202	GOL	C3-C2	2.38	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	204	PDO	O1-C1-C2-C3
7	B	204	PDO	C1-C2-C3-O3
7	C	206	PDO	C1-C2-C3-O3
7	E	206	PDO	O1-C1-C2-C3
15	E	201	GOL	O1-C1-C2-C3
15	F	202	GOL	O1-C1-C2-C3
13	C	211	PEG	C4-C3-O2-C2
12	C	210	PGE	O1-C1-C2-O2
13	C	211	PEG	O1-C1-C2-O2
13	F	211	PEG	O1-C1-C2-O2
15	F	201	GOL	C1-C2-C3-O3
13	D	209	PEG	O2-C3-C4-O4
13	D	209	PEG	O1-C1-C2-O2
3	B	202	EDO	O1-C1-C2-O2
3	D	203	EDO	O1-C1-C2-O2
3	E	203	EDO	O1-C1-C2-O2
15	F	202	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	B	205	PGR	O1-C1-C2-O2
12	F	210	PGE	O1-C1-C2-O2
3	C	203	EDO	O1-C1-C2-O2
8	B	205	PGR	O1-C1-C2-C3
15	E	201	GOL	O1-C1-C2-O2
12	C	210	PGE	C1-C2-O2-C3
10	B	215	PG0	C4-C3-O1-C2
12	F	210	PGE	C6-C5-O3-C4
13	F	211	PEG	C1-C2-O2-C3
12	C	210	PGE	O3-C5-C6-O4
10	B	215	PG0	O1-C3-C4-O2
15	F	201	GOL	O2-C2-C3-O3
13	D	209	PEG	C1-C2-O2-C3
3	C	201	EDO	O1-C1-C2-O2
3	E	204	EDO	O1-C1-C2-O2
12	C	210	PGE	C6-C5-O3-C4
3	A	202	EDO	O1-C1-C2-O2
12	F	210	PGE	O2-C3-C4-O3
12	C	210	PGE	C3-C4-O3-C5
3	A	203	EDO	O1-C1-C2-O2
13	D	209	PEG	C4-C3-O2-C2
12	F	210	PGE	C3-C4-O3-C5
11	F	212	DHL	N-CA-CB-SG

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	204	PDO	2	0
12	C	210	PGE	2	0
4	A	206	MOH	1	0
7	E	206	PDO	1	0
16	E	207	IPA	1	0
2	B	201	EOH	1	0
13	C	211	PEG	3	0
2	A	201	EOH	1	0
3	F	204	EDO	1	0
10	B	215	PG0	1	0
15	F	201	GOL	4	0
13	F	211	PEG	1	0
13	D	209	PEG	1	0
3	D	203	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	210	PGE	1	0
15	F	202	GOL	2	0
8	B	205	PGR	1	0
2	F	203	EOH	2	0
11	F	212	DHL	1	0
15	E	201	GOL	1	0
3	B	202	EDO	5	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(Å²)	Q<0.9	
1	A	75/94 (79%)	0.72	6 (8%)	18	20	35, 51, 69, 70	0
1	B	76/94 (80%)	0.54	5 (6%)	24	26	34, 44, 65, 78	0
1	C	74/94 (78%)	0.45	4 (5%)	31	33	31, 44, 64, 76	0
1	D	74/94 (78%)	0.84	6 (8%)	18	19	42, 56, 71, 77	0
1	E	74/94 (78%)	0.73	4 (5%)	31	33	39, 53, 72, 80	0
1	F	75/94 (79%)	0.49	4 (5%)	32	34	30, 45, 69, 78	0
All	All	448/564 (79%)	0.63	29 (6%)	25	27	30, 50, 70, 80	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	THR	3.9
1	A	115	PHE	3.7
1	F	114	PHE	3.4
1	A	58	SER	3.0
1	E	86	ASP	3.0
1	C	115	PHE	3.0
1	D	55	PHE	2.9
1	F	115	PHE	2.9
1	E	115	PHE	2.8
1	F	55	PHE	2.7
1	B	116	THR	2.7
1	B	114	PHE	2.6
1	D	42	ASN	2.5
1	C	57	THR	2.5
1	D	78	ILE	2.3
1	F	45	CYS	2.3
1	A	43	PHE	2.3
1	E	68	ASN	2.3
1	B	115	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	55	PHE	2.2
1	A	56	THR	2.2
1	B	57	THR	2.2
1	A	116	THR	2.1
1	D	57	THR	2.1
1	D	48	ASP	2.1
1	E	85	LYS	2.1
1	C	58	SER	2.1
1	C	97	ASP	2.1
1	B	58	SER	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	MOH	C	204	2/2	0.61	0.23	51,51,51,54	2
4	MOH	A	206	2/2	0.63	0.31	54,54,54,58	0
9	NA	C	209	1/1	0.68	0.13	76,76,76,76	0
4	MOH	E	205	2/2	0.70	0.20	56,56,56,56	0
2	EOH	E	202	3/3	0.70	0.22	51,51,52,63	0
3	EDO	E	204	4/4	0.72	0.15	60,66,70,75	0
7	PDO	B	203	5/5	0.74	0.18	56,57,59,61	5
13	PEG	D	209	7/7	0.74	0.16	61,62,72,74	0
4	MOH	C	205	2/2	0.75	0.21	50,50,50,51	0
14	POL	D	205	4/4	0.76	0.21	52,55,56,59	0
16	IPA	E	207	4/4	0.76	0.18	60,60,61,63	0
4	MOH	F	207	2/2	0.78	0.13	47,47,47,51	0
2	EOH	F	203	3/3	0.78	0.17	39,39,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MOH	A	204	2/2	0.79	0.17	56,56,56,60	0
2	EOH	D	201	3/3	0.80	0.19	62,62,63,71	0
4	MOH	F	205	2/2	0.80	0.16	57,57,57,58	0
4	MOH	A	205	2/2	0.81	0.19	60,60,60,65	0
3	EDO	F	204	4/4	0.82	0.14	57,62,64,69	0
12	PGE	F	210	10/10	0.82	0.13	60,64,72,73	0
13	PEG	C	211	7/7	0.82	0.15	48,50,59,66	7
3	EDO	C	201	4/4	0.83	0.13	59,62,65,68	0
7	PDO	E	206	5/5	0.83	0.19	52,59,62,64	0
10	PG0	B	215	8/8	0.84	0.15	43,48,56,63	0
15	GOL	E	201	6/6	0.84	0.14	51,56,58,59	6
3	EDO	A	202	4/4	0.84	0.15	56,58,62,65	0
13	PEG	F	211	7/7	0.85	0.14	49,55,61,64	7
3	EDO	C	203	4/4	0.85	0.15	49,57,61,67	0
4	MOH	F	206	2/2	0.85	0.15	49,49,49,56	0
7	PDO	B	204	5/5	0.85	0.16	50,58,59,61	0
2	EOH	A	201	3/3	0.86	0.17	55,55,58,65	0
12	PGE	C	210	10/10	0.87	0.14	44,50,59,59	10
3	EDO	B	202	4/4	0.88	0.12	43,45,46,52	4
3	EDO	D	203	4/4	0.88	0.12	51,56,60,67	0
15	GOL	F	202	6/6	0.90	0.13	33,47,48,52	0
2	EOH	B	201	3/3	0.90	0.22	45,45,45,56	0
5	IOD	D	206	1/1	0.91	0.10	70,70,70,70	1
15	GOL	F	201	6/6	0.91	0.14	41,48,54,61	0
7	PDO	C	206	5/5	0.91	0.10	53,53,55,60	0
7	PDO	D	204	5/5	0.91	0.12	44,47,54,55	0
6	CL	F	209	1/1	0.92	0.09	67,67,67,67	0
3	EDO	A	203	4/4	0.92	0.20	51,51,53,60	0
3	EDO	D	202	4/4	0.93	0.10	36,46,46,50	0
3	EDO	C	202	4/4	0.93	0.10	44,47,52,57	4
8	PGR	B	205	5/5	0.93	0.10	34,43,47,49	0
3	EDO	E	203	4/4	0.93	0.10	57,58,65,68	0
6	CL	A	211	1/1	0.93	0.09	71,71,71,71	0
5	IOD	A	209	1/1	0.94	0.08	76,76,76,76	1
11	DHL	B	216	4/4	0.94	0.13	50,54,54,56	0
6	CL	A	212	1/1	0.94	0.08	69,69,69,69	1
6	CL	C	208	1/1	0.94	0.10	66,66,66,66	0
9	NA	B	214	1/1	0.94	0.07	42,42,42,42	1
6	CL	D	208	1/1	0.94	0.07	67,67,67,67	0
6	CL	A	210	1/1	0.95	0.08	56,56,56,56	0
6	CL	B	213	1/1	0.96	0.08	66,66,66,66	0
5	IOD	C	207	1/1	0.96	0.06	75,75,75,75	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	B	212	1/1	0.96	0.07	55,55,55,55	0
5	IOD	A	207	1/1	0.97	0.05	56,56,56,56	1
5	IOD	A	208	1/1	0.98	0.04	61,61,61,61	1
11	DHL	F	212	4/4	0.98	0.09	34,37,38,42	0
6	CL	F	208	1/1	0.98	0.05	48,48,48,48	1
5	IOD	B	208	1/1	0.98	0.04	55,55,55,55	1
5	IOD	B	210	1/1	0.99	0.03	45,45,45,45	1
5	IOD	B	211	1/1	0.99	0.03	69,69,69,69	1
5	IOD	B	206	1/1	0.99	0.04	52,52,52,52	1
5	IOD	B	209	1/1	0.99	0.03	54,54,54,54	1
5	IOD	D	207	1/1	0.99	0.03	54,54,54,54	1
5	IOD	B	207	1/1	1.00	0.01	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.