WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:50 PM EDT

PDB ID	:	5NQP
Title	:	Structure of a fHbp(V1.4):PorA(P1.16) chimera. Fusion at fHbp position 151.
Authors	:	Johnson, S.; Hollingshead, S.; Lea, S.M.; Tang, C.M.
Deposited on	:	2017-04-20
Resolution	:	2.86 Å(reported)

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	:	2.37.1
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)	:	2.37.1

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 2.86 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		0.239
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.3%
RSRZ outliers		4.4%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
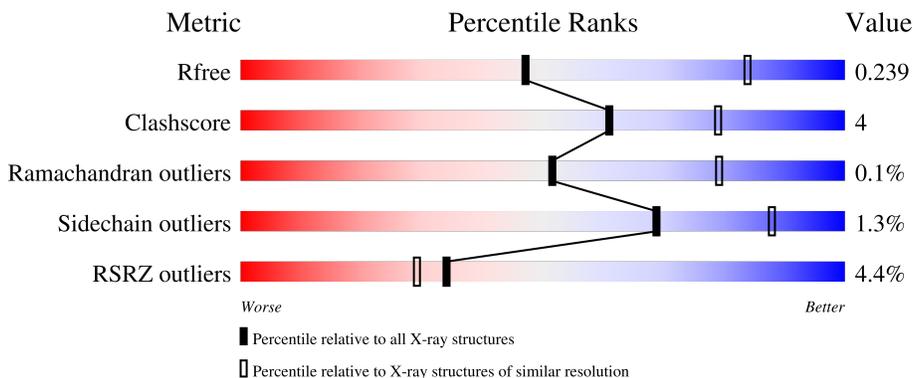
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	271	4% — 87% — 10% ·
1	B	271	3% — 81% — 12% · 6%
1	C	271	5% — 83% — 12% 5%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6007 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 Factor H binding protein variant B16_001,Major outer membrane protein P.IA,Factor H binding protein variant B16_001.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	257	Total 1963	C 1218	N 349	O 395	S 1	0	0	0
1	A	264	Total 2004	C 1243	N 356	O 404	S 1	0	0	0
1	B	255	Total 1949	C 1210	N 347	O 391	S 1	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	71	MET	-	initiating methionine	UNP Q6VS06
C	321	LEU	-	expression tag	UNP Q6VS06
C	322	GLU	-	expression tag	UNP Q6VS06
C	323	HIS	-	expression tag	UNP Q6VS06
C	324	HIS	-	expression tag	UNP Q6VS06
C	325	HIS	-	expression tag	UNP Q6VS06
C	326	HIS	-	expression tag	UNP Q6VS06
C	327	HIS	-	expression tag	UNP Q6VS06
C	328	HIS	-	expression tag	UNP Q6VS06
A	71	MET	-	initiating methionine	UNP Q6VS06
A	321	LEU	-	expression tag	UNP Q6VS06
A	322	GLU	-	expression tag	UNP Q6VS06
A	323	HIS	-	expression tag	UNP Q6VS06
A	324	HIS	-	expression tag	UNP Q6VS06
A	325	HIS	-	expression tag	UNP Q6VS06
A	326	HIS	-	expression tag	UNP Q6VS06
A	327	HIS	-	expression tag	UNP Q6VS06
A	328	HIS	-	expression tag	UNP Q6VS06
B	71	MET	-	initiating methionine	UNP Q6VS06
B	321	LEU	-	expression tag	UNP Q6VS06
B	322	GLU	-	expression tag	UNP Q6VS06
B	323	HIS	-	expression tag	UNP Q6VS06

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Chain	Residue	Modelled	Actual	Comment	Reference
B	324	HIS	-	expression tag	UNP Q6VS06
B	325	HIS	-	expression tag	UNP Q6VS06
B	326	HIS	-	expression tag	UNP Q6VS06
B	327	HIS	-	expression tag	UNP Q6VS06
B	328	HIS	-	expression tag	UNP Q6VS06

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
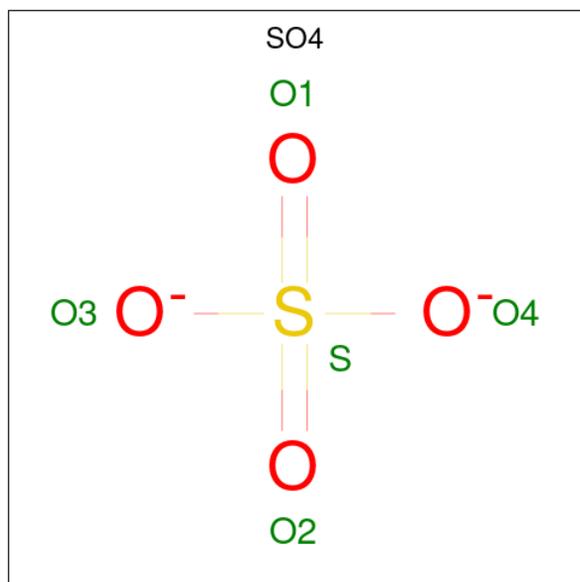
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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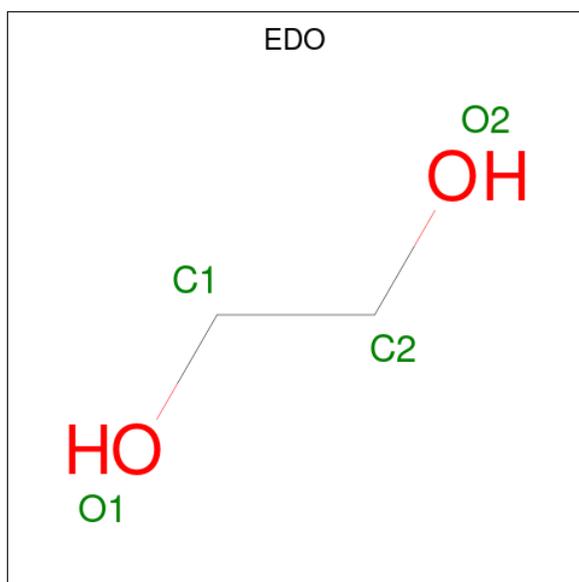
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	11	Total 11	O 11	0	0
5	A	10	Total 10	O 10	0	0
5	B	7	Total 7	O 7	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: Factor H binding protein variant B16_001,Major outer membrane protein P.IA,Factor H binding protein variant B16_001
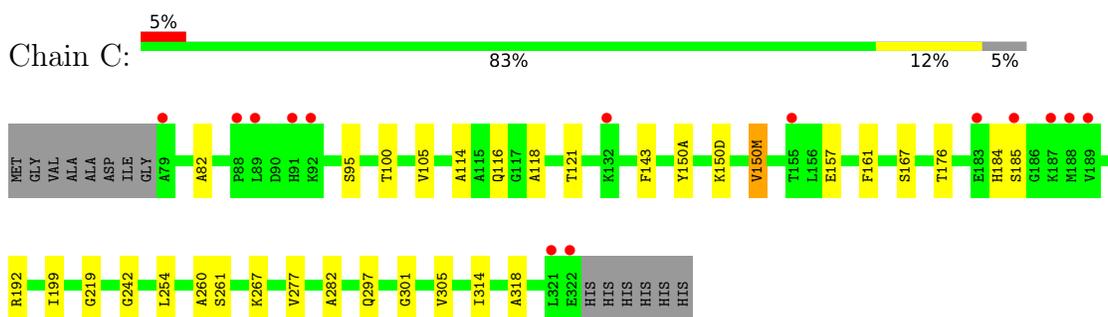
• Molecule 1: Factor H binding protein variant B16_001,Major outer membrane protein P.IA,Factor H binding protein variant B16_001
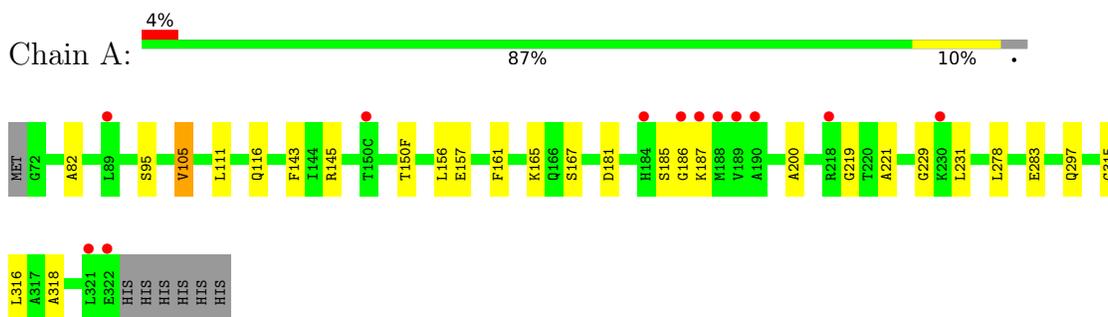
• Molecule 1: Factor H binding protein variant B16_001,Major outer membrane protein P.IA,Factor H binding protein variant B16_001
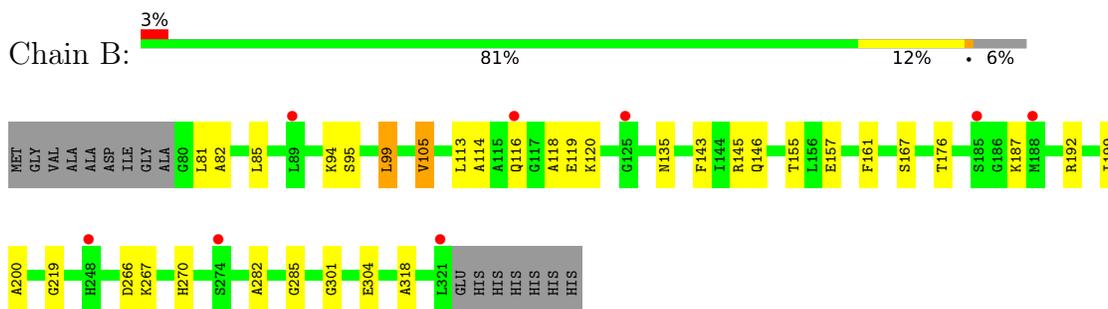
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	100.72Å 171.42Å 131.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.74 – 2.86 40.74 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.74-2.86) 99.0 (40.74-2.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.198 , 0.239 0.199 , 0.239	Depositor DCC
R_{free} test set	1240 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6007	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5　Model quality (i)

5.1　Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, SO4

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	0/2032	0.50	0/2735
1	B	0.25	0/1977	0.48	0/2660
1	C	0.25	0/1991	0.49	0/2679
All	All	0.26	0/6000	0.49	0/8074

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	2004	0	1984	15	0
1	B	1949	0	1933	19	0
1	C	1963	0	1944	20	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
3	A	8	0	12	0	0
3	B	12	0	18	1	0
3	C	24	0	36	4	0
4	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	1	0
5	A	10	0	0	0	0
5	B	7	0	0	0	0
5	C	11	0	0	0	0
All	All	6007	0	5927	53	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 4.

All (53) 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:A:95:SER:HB2	1:A:167:SER:HA	1.68	0.75
1:B:95:SER:HB2	1:B:167:SER:HA	1.68	0.74
1:C:95:SER:HB2	1:C:167:SER:HA	1.80	0.63
1:C:100:THR:H	3:C:404:EDO:H22	1.65	0.60
1:B:82:ALA:HB2	1:B:116:GLN:HB2	1.84	0.60
1:C:143:PHE:HB3	1:C:161:PHE:HB2	1.84	0.59
1:B:81:LEU:HB3	1:B:116:GLN:HG3	1.84	0.58
1:A:143:PHE:HB3	1:A:161:PHE:HB2	1.86	0.57
1:A:297:GLN:NE2	2:A:401:SO4:O4	2.31	0.57
1:B:99:LEU:HD12	1:B:200:ALA:HB3	1.89	0.55
1:C:261:SER:HA	3:C:405:EDO:H11	1.89	0.55
1:A:82:ALA:HB2	1:A:116:GLN:HB2	1.88	0.54
1:C:297:GLN:NE2	2:C:401:SO4:O3	2.41	0.54
1:B:94:LYS:HE3	1:B:135:ASN:OD1	2.08	0.54
1:B:199:ILE:HD13	1:B:301:GLY:HA2	1.90	0.53
1:C:157:GLU:OE2	1:C:176:THR:OG1	2.21	0.52
1:C:150(A):TYR:HB2	1:C:150(M):VAL:HG13	1.91	0.52
1:B:143:PHE:HB3	1:B:161:PHE:HB2	1.91	0.51
1:A:231:LEU:HD22	1:A:316:LEU:HB3	1.93	0.50
1:A:200:ALA:HB1	4:A:405:CL:CL	2.48	0.50
1:C:282:ALA:HB1	1:B:282:ALA:HB1	1.95	0.49
1:A:221:ALA:O	1:A:229:GLY:HA3	2.13	0.49
1:C:267:LYS:HG3	3:C:406:EDO:H21	1.95	0.48
1:B:114:ALA:HA	1:B:118:ALA:O	2.14	0.48
1:C:121:THR:HG21	3:C:402:EDO:H22	1.95	0.48
1:C:150(D):LYS:NZ	4:C:409:CL:CL	2.82	0.47
1:A:95:SER:OG	1:A:165:LYS:HE2	2.15	0.46
1:C:254:LEU:HD22	1:C:314:ILE:HD11	1.98	0.46
1:C:277:VAL:HG11	1:C:305:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ILE:HD13	1:C:301:GLY:HA2	1.98	0.46
1:B:219:GLY:HA3	1:B:318:ALA:HA	1.98	0.46
1:C:82:ALA:HB2	1:C:116:GLN:HB2	1.98	0.45
1:C:114:ALA:HA	1:C:118:ALA:O	2.16	0.45
1:B:157:GLU:OE2	1:B:176:THR:OG1	2.23	0.45
1:B:85:LEU:O	1:B:120:LYS:HD2	2.16	0.45
1:B:113:LEU:O	1:B:119:GLU:HA	2.17	0.44
1:A:145:ARG:O	1:A:156:LEU:N	2.48	0.43
1:B:146:GLN:HG2	1:B:155:THR:HA	1.99	0.43
1:B:176:THR:O	1:B:192:ARG:HA	2.19	0.43
1:A:105:VAL:HG22	1:A:111:LEU:HD22	2.01	0.43
1:A:143:PHE:HE1	1:A:157:GLU:HG3	1.85	0.42
1:A:221:ALA:HA	1:A:315:GLY:O	2.20	0.42
1:C:242:GLY:O	1:C:260:ALA:HA	2.19	0.42
1:A:278:LEU:HD23	1:A:283:GLU:HA	2.02	0.41
1:B:266:ASP:OD1	1:B:270:HIS:N	2.35	0.41
1:B:105:VAL:HA	1:B:145:ARG:HH12	1.85	0.41
1:A:219:GLY:HA3	1:A:318:ALA:HA	2.03	0.41
1:B:267:LYS:H	3:B:403:EDO:H21	1.86	0.41
1:C:219:GLY:HA3	1:C:318:ALA:HA	2.02	0.41
1:B:285:GLY:HA3	1:B:304:GLU:O	2.21	0.41
1:C:184:HIS:HB2	1:C:185:SER:H	1.65	0.41
1:A:185:SER:O	1:A:187:LYS:N	2.49	0.41
1:C:176:THR:O	1:C:192:ARG:HA	2.22	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	262/271 (97%)	245 (94%)	16 (6%)	1 (0%)	34	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	253/271 (93%)	244 (96%)	9 (4%)	0	100	100
1	C	255/271 (94%)	244 (96%)	11 (4%)	0	100	100
All	All	770/813 (95%)	733 (95%)	36 (5%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY

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	210/217 (97%)	207 (99%)	3 (1%)	67	86
1	B	206/217 (95%)	203 (98%)	3 (2%)	65	86
1	C	207/217 (95%)	205 (99%)	2 (1%)	76	91
All	All	623/651 (96%)	615 (99%)	8 (1%)	69	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	105	VAL
1	C	150(M)	VAL
1	A	105	VAL
1	A	150(F)	THR
1	A	181	ASP
1	B	99	LEU
1	B	105	VAL
1	B	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#|Z| > 2$
2	SO4	C	401	-	4,4,4	0.15	0	6,6,6	0.04	0
3	EDO	C	405	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	402	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.36	0
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	C	407	-	3,3,3	0.48	0	2,2,2	0.35	0
2	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.06	0
3	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	C	404	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	B	404	1	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	C	406	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	C	402	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	C	403	-	3,3,3	0.46	0	2,2,2	0.34	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
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	C	407	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	C	404	-	-	0/1/1/1	-
3	EDO	B	404	1	-	0/1/1/1	-
3	EDO	C	406	-	-	0/1/1/1	-
3	EDO	C	405	-	-	0/1/1/1	-
3	EDO	C	403	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SO4	1	0
3	C	405	EDO	1	0
2	A	401	SO4	1	0
3	B	403	EDO	1	0
3	C	404	EDO	1	0
3	C	406	EDO	1	0
3	C	402	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	264/271 (97%)	0.21	12 (4%) 33	28	55, 73, 124, 183	0
1	B	255/271 (94%)	0.26	8 (3%) 49	44	63, 87, 125, 166	0
1	C	257/271 (94%)	0.20	14 (5%) 25	21	46, 72, 115, 183	0
All	All	776/813 (95%)	0.22	34 (4%) 34	29	46, 77, 126, 183	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	GLU	5.0
1	A	322	GLU	4.9
1	B	185	SER	4.3
1	C	183	GLU	4.0
1	A	321	LEU	4.0
1	A	187	LYS	3.9
1	C	89	LEU	3.3
1	C	187	LYS	3.2
1	C	92	LYS	3.1
1	C	91	HIS	3.1
1	C	189	VAL	3.0
1	A	218	ARG	2.9
1	C	188	MET	2.9
1	C	132	LYS	2.8
1	A	186	GLY	2.8
1	A	89	LEU	2.8
1	A	230	LYS	2.6
1	A	188	MET	2.6
1	C	88	PRO	2.6
1	B	321	LEU	2.5
1	C	185	SER	2.5
1	B	125	GLY	2.5
1	A	150(C)	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	184	HIS	2.5
1	A	189	VAL	2.4
1	C	79	ALA	2.4
1	B	116	GLN	2.4
1	B	274	SER	2.3
1	B	188	MET	2.2
1	C	155	THR	2.2
1	B	248	HIS	2.2
1	C	321	LEU	2.1
1	B	89	LEU	2.0
1	A	190	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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
3	EDO	C	402	4/4	0.81	0.20	90,91,92,95	0
3	EDO	A	402	4/4	0.81	0.21	89,92,97,100	0
2	SO4	C	401	5/5	0.84	0.25	146,150,151,153	0
3	EDO	A	403	4/4	0.84	0.20	72,77,79,80	0
3	EDO	B	403	4/4	0.84	0.92	88,89,89,95	0
3	EDO	B	404	4/4	0.84	0.22	78,79,79,80	0
3	EDO	C	404	4/4	0.85	0.19	78,79,81,84	0
4	CL	A	404	1/1	0.87	0.43	94,94,94,94	0
3	EDO	C	407	4/4	0.88	0.58	83,83,86,87	0
4	CL	A	405	1/1	0.89	0.09	98,98,98,98	0
3	EDO	C	405	4/4	0.90	0.32	72,76,78,79	0
2	SO4	A	401	5/5	0.90	0.29	120,122,124,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	SO4	B	401	5/5	0.91	0.24	140,141,142,142	0
3	EDO	B	402	4/4	0.91	0.69	88,89,90,90	0
3	EDO	C	403	4/4	0.92	0.55	77,78,79,81	0
3	EDO	C	406	4/4	0.95	0.68	77,82,85,87	0
4	CL	C	409	1/1	0.95	0.23	63,63,63,63	0
4	CL	C	408	1/1	0.96	0.28	64,64,64,64	0

6.5　Other polymers ⓘ

There are no such residues in this entry.