Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 08:59 PM EST

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PDB ID	:	5DS8
Title	:	Context-independent anti-hypusine antibody FabHpu98 in complex with hypusine
Authors	:	Zhai, Q.; Carter, P.J.
Deposited on	:	2015-09-17
Resolution	:	1.95 Å(reported)

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 1.95 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.
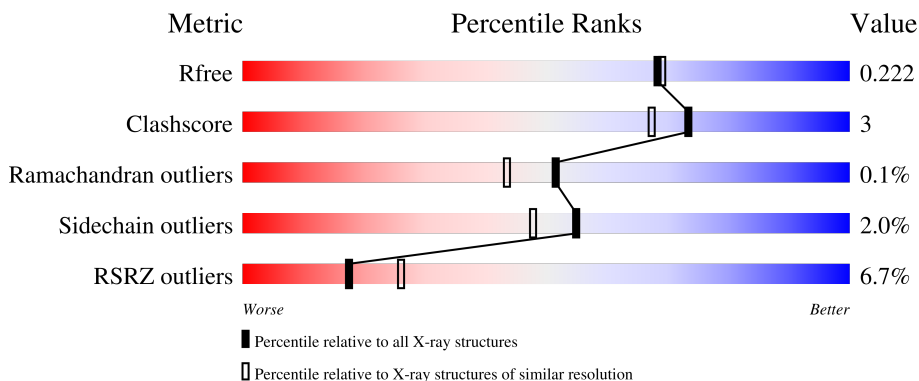
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	222	4% · 86% · 7% · 7%
1	H	222	8% · 79% · 12% · 8%
2	B	214	92% · 7% ·
2	L	214	13% · 85% · 14% ·
3	P	4	50% · 75% · 25%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6585 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 Fab Hpu98 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total 1556	C 984	N 254	O 312	S 6	0	1	0
1	H	204	Total 1542	C 976	N 251	O 306	S 9	0	3	0

- Molecule 2 is a protein called Fab Hou98 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total 1576	C 982	N 260	O 326	S 8	0	2	0
2	L	211	Total 1567	C 976	N 259	O 325	S 7	0	0	0

- Molecule 3 is a protein called Tetrapeptide GLY-HPU-GLY-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	4	Total 28	C 17	N 6	O 5	0	0	0

- 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	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0
4	H	1	Total 4	C 2	O 2	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
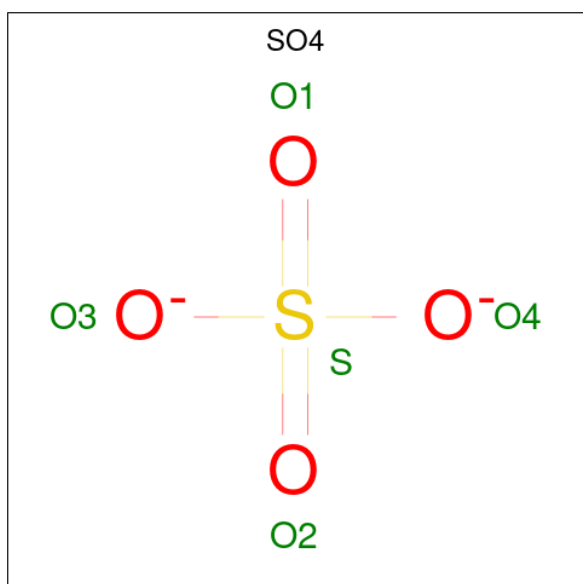
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 4	O 3	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0
5	L	1	Total 5	O 4	S 1	0	0
5	P	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	86	Total 86	O 86	0	0
6	B	95	Total 95	O 95	0	0
6	H	43	Total 43	O 43	0	0
6	L	18	Total 18	O 18	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: Fab Hpu98 Heavy Chain
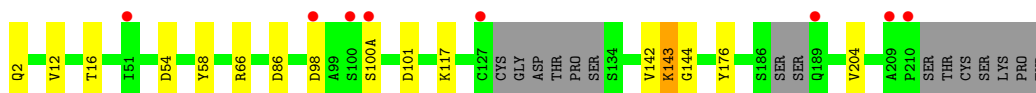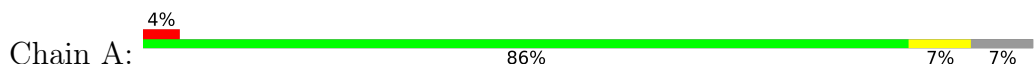
Chain A:

• Molecule 1: Fab Hpu98 Heavy Chain

Chain H:
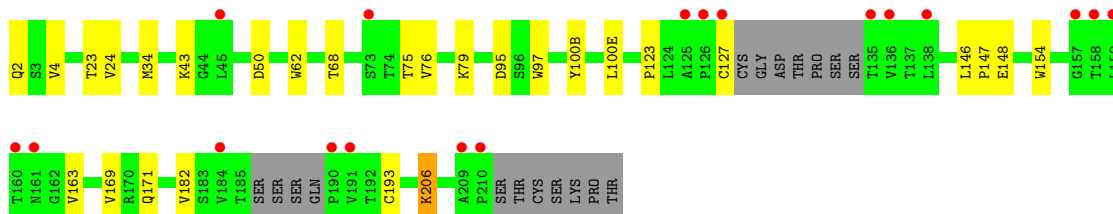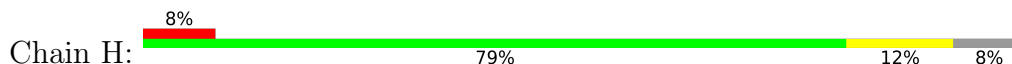
• Molecule 2: Fab Hou98 Light Chain
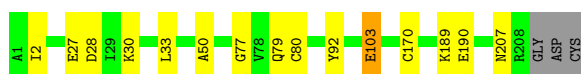
Chain B:

• Molecule 2: Fab Hou98 Light Chain

Chain L:
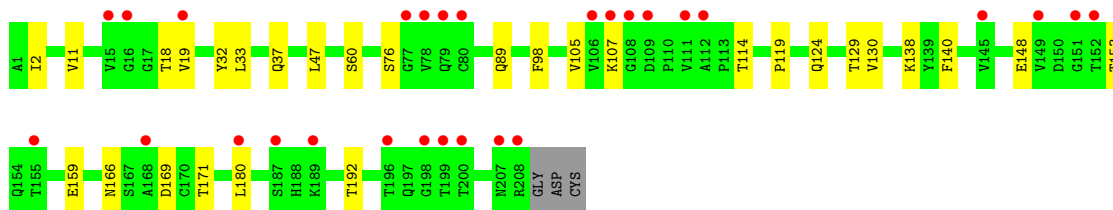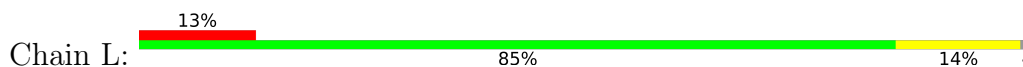
• Molecule 3: Tetrapeptide GLY-HPU-GLY-ALA

Chain P:

50%

75%

25%

G3 K4 G5 A6
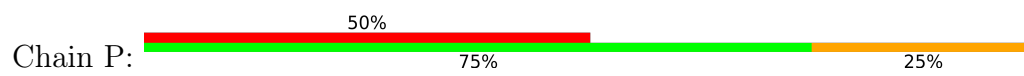
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	106.00Å 294.08Å 68.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 1.95 41.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.20-1.95) 99.7 (41.18-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.183 , 0.224 0.182 , 0.222	Depositor DCC
R_{free} test set	3972 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6585	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5CT, EDO, PCA, 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	0.83	0/1590	0.84	3/2183 (0.1%)
1	H	0.57	0/1576	0.69	0/2163
2	B	0.78	0/1612	0.76	0/2204
2	L	0.45	0/1597	0.58	0/2184
3	P	0.57	0/11	0.48	0/11
All	All	0.68	0/6386	0.72	3/8745 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	VAL	CG1-CB-CG2	5.52	119.73	110.90
1	A	101	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	204	VAL	CA-CB-CG1	5.04	118.46	110.90

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	1556	0	1518	8	0
1	H	1542	0	1499	19	0
2	B	1576	0	1538	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1567	0	1525	12	0
3	P	28	0	32	2	0
4	A	12	0	18	1	0
4	H	8	0	12	1	0
5	A	10	0	0	0	0
5	B	19	0	0	1	0
5	H	15	0	0	1	0
5	L	5	0	0	0	0
5	P	5	0	0	0	0
6	A	86	0	0	0	0
6	B	95	0	0	1	0
6	H	43	0	0	0	0
6	L	18	0	0	0	0
All	All	6585	0	6142	41	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 3.

All (41) 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:L:18:THR:HG22	2:L:76:SER:HA	1.68	0.73
2:B:189:LYS:HD2	2:B:207:ASN:HB3	1.75	0.67
1:H:68:THR:OG1	1:H:79:LYS:HB3	1.99	0.62
1:H:146:LEU:HD12	1:H:147:PRO:HA	1.86	0.57
2:B:80:CYS:SG	2:B:170[B]:CYS:HB3	2.45	0.56
1:H:95:ASP:HB3	1:H:100(E):LEU:HD23	1.89	0.55
2:B:92:TYR:OH	5:B:304:SO4:O4	2.13	0.54
1:H:127:CYS:HB2	2:L:119:PRO:HG3	1.88	0.54
1:H:4:VAL:HG12	1:H:24:VAL:HG22	1.89	0.54
1:A:66:ARG:NH2	1:A:86:ASP:OD1	2.41	0.53
1:A:117:LYS:HG2	1:A:144:GLY:O	2.09	0.53
1:A:100(A):SER:HB2	2:B:50:ALA:HB2	1.91	0.53
1:H:163:VAL:HG22	1:H:182:VAL:HG22	1.91	0.52
1:A:176:TYR:CE1	4:A:303:EDO:H21	2.45	0.52
1:H:23:THR:HG22	1:H:75:THR:HG22	1.92	0.51
1:H:169:VAL:HG11	2:L:159:GLU:HB3	1.94	0.49
2:L:166:ASN:HB3	2:L:169:ASP:HB2	1.94	0.49
1:H:34:MET:HG3	1:H:76:VAL:HG21	1.94	0.49
1:A:54:ASP:HB3	1:H:62:TRP:CD2	2.49	0.48
2:L:148:GLU:HB2	2:L:192:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:LYS:HB2	1:H:206:LYS:NZ	2.30	0.47
1:H:148:GLU:HG3	4:H:302:EDO:H12	1.97	0.46
2:L:89:GLN:HB2	2:L:98:PHE:CD1	2.51	0.46
1:H:97:TRP:CZ2	3:P:4:5CT:H9	2.50	0.46
2:L:124:GLN:HB3	2:L:130:VAL:HG12	1.98	0.45
1:A:143:LYS:HB3	1:A:143:LYS:HE3	1.68	0.45
1:A:58:TYR:CE2	1:H:43:LYS:HE3	2.52	0.44
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.00	0.44
2:B:28:ASP:OD2	2:B:30:LYS:HE3	2.16	0.44
1:H:50:ASP:OD2	3:P:4:5CT:H14	2.18	0.44
1:A:12:VAL:HG22	1:A:16:THR:HB	2.00	0.44
1:H:123:PRO:HG3	1:H:206:LYS:HD2	2.00	0.43
2:B:103:GLU:HG2	6:B:406:HOH:O	2.19	0.43
2:L:107:LYS:HA	2:L:140:PHE:CZ	2.53	0.43
2:B:77:GLY:O	2:B:79[A]:GLN:HG2	2.20	0.42
2:B:2:ILE:HD11	2:B:27:GLU:OE2	2.20	0.42
2:L:11:VAL:HG11	2:L:19:VAL:HG13	2.02	0.42
1:H:171:GLN:NE2	5:H:303:SO4:O2	2.45	0.42
1:H:100(B):TYR:HB2	2:L:32:TYR:CD2	2.56	0.41
2:L:169:ASP:HB3	2:L:171:THR:HG23	2.02	0.41
1:H:154:TRP:CH2	1:H:193[B]:CYS:HB2	2.57	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	202/222 (91%)	198 (98%)	4 (2%)	0	100	100
1	H	201/222 (90%)	198 (98%)	3 (2%)	0	100	100
2	B	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
2	L	209/214 (98%)	203 (97%)	5 (2%)	1 (0%)	29	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	1/4 (25%)	1 (100%)	0	0	100	100
All	All	824/876 (94%)	807 (98%)	16 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	138	LYS

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	178/191 (93%)	176 (99%)	2 (1%)	73	71
1	H	176/191 (92%)	175 (99%)	1 (1%)	86	85
2	B	179/179 (100%)	176 (98%)	3 (2%)	60	55
2	L	177/179 (99%)	169 (96%)	8 (4%)	27	15
All	All	710/740 (96%)	696 (98%)	14 (2%)	55	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	143	LYS
2	B	33	LEU
2	B	103	GLU
2	B	190	GLU
1	H	206	LYS
2	L	2	ILE
2	L	33	LEU
2	L	60	SER
2	L	105	VAL
2	L	114	THR
2	L	129	THR
2	L	153	THR

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Mol	Chain	Res	Type
2	L	180	LEU

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 ⓘ

3 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	5CT	P	4	3	13,14,15	0.49	0	9,15,17	1.21	1 (11%)
1	PCA	A	2	1	7,8,9	1.89	1 (14%)	9,10,12	2.46	5 (55%)
1	PCA	H	2	1	7,8,9	1.88	1 (14%)	9,10,12	1.86	4 (44%)

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	5CT	P	4	3	-	4/13/14/16	-
1	PCA	A	2	1	-	0/0/11/13	0/1/1/1
1	PCA	H	2	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	2	PCA	CD-N	4.74	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	PCA	CD-N	4.66	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	PCA	CB-CA-C	-4.36	106.70	112.70
1	A	2	PCA	CA-N-CD	-3.04	103.15	113.58
1	A	2	PCA	OE-CD-CG	-2.99	121.55	126.76
1	H	2	PCA	CA-N-CD	-2.94	103.52	113.58
1	H	2	PCA	CB-CA-N	2.75	111.18	103.30
1	A	2	PCA	CB-CA-N	2.60	110.76	103.30
3	P	4	5CT	C1-NZ-CE	-2.59	107.62	113.42
1	A	2	PCA	CG-CD-N	2.40	114.61	108.39
1	H	2	PCA	CG-CD-N	2.12	113.88	108.39
1	H	2	PCA	OE-CD-CG	-2.03	123.22	126.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	4	5CT	NZ-C1-C2-C3
3	P	4	5CT	NZ-C1-C2-O1
3	P	4	5CT	C1-C2-C3-C4
3	P	4	5CT	O1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	4	5CT	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.26	0
5	SO4	H	303	-	4,4,4	0.15	0	6,6,6	0.20	0
5	SO4	H	305	-	4,4,4	0.16	0	6,6,6	0.08	0
4	EDO	A	303	-	3,3,3	0.37	0	2,2,2	0.21	0
5	SO4	A	304	-	4,4,4	0.16	0	6,6,6	0.11	0
5	SO4	B	303	-	4,4,4	0.10	0	6,6,6	0.32	0
5	SO4	B	302	-	4,4,4	0.20	0	6,6,6	0.44	0
5	SO4	P	101	-	4,4,4	0.18	0	6,6,6	0.18	0
4	EDO	H	301	-	3,3,3	0.58	0	2,2,2	0.14	0
4	EDO	H	302	-	3,3,3	0.51	0	2,2,2	0.23	0
4	EDO	A	302	-	3,3,3	0.66	0	2,2,2	0.28	0
5	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.30	0
5	SO4	B	301	-	1,3,4	0.24	0	0,3,6	-	-
5	SO4	L	301	-	4,4,4	0.13	0	6,6,6	0.16	0
5	SO4	H	304	-	4,4,4	0.14	0	6,6,6	0.22	0
4	EDO	A	301	-	3,3,3	0.49	0	2,2,2	0.35	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	A	303	-	-	0/1/1/1	-
4	EDO	H	301	-	-	0/1/1/1	-
4	EDO	H	302	-	-	0/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	303	SO4	1	0
4	A	303	EDO	1	0
4	H	302	EDO	1	0
5	B	304	SO4	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	206/222 (92%)	0.32	8 (3%)	39	49	26, 37, 62, 85	0
1	H	203/222 (91%)	0.36	18 (8%)	9	15	34, 49, 76, 104	0
2	B	211/214 (98%)	-0.00	0	100	100	28, 39, 55, 67	0
2	L	211/214 (98%)	0.77	28 (13%)	3	5	37, 65, 99, 114	1 (0%)
3	P	3/4 (75%)	2.14	2 (66%)	0	0	67, 67, 68, 76	0
All	All	834/876 (95%)	0.37	56 (6%)	17	26	26, 46, 83, 114	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100(A)	SER	5.6
1	H	209	ALA	5.0
1	H	136	VAL	4.2
2	L	108	GLY	4.2
2	L	78	VAL	4.1
1	A	100	SER	4.0
2	L	199	THR	4.0
1	H	184	VAL	3.7
2	L	149	VAL	3.6
2	L	16	GLY	3.6
1	A	210	PRO	3.4
1	A	209	ALA	3.3
1	H	135	THR	3.2
2	L	79	GLN	3.1
2	L	151	GLY	3.0
2	L	187	SER	3.0
2	L	109	ASP	2.9
3	P	3	GLY	2.9
1	H	190	PRO	2.8
1	H	157	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLN	2.8
3	P	5	GLY	2.7
2	L	155	THR	2.7
1	H	160	THR	2.7
2	L	189	LYS	2.6
1	H	127	CYS	2.6
2	L	207	ASN	2.6
2	L	180	LEU	2.6
1	H	210	PRO	2.5
1	H	73	SER	2.5
2	L	111	VAL	2.5
2	L	77	GLY	2.5
2	L	198	GLY	2.5
2	L	112	ALA	2.4
1	H	161	ASN	2.4
2	L	19	VAL	2.4
2	L	168	ALA	2.4
1	A	51	ILE	2.3
2	L	208	ARG	2.3
1	H	125	ALA	2.3
2	L	200	THR	2.3
1	A	98	ASP	2.2
1	H	126	PRO	2.2
1	A	127	CYS	2.2
1	H	138	LEU	2.2
2	L	152	THR	2.2
1	H	191	VAL	2.2
2	L	15	VAL	2.2
2	L	107	LYS	2.1
2	L	106	VAL	2.1
1	H	159	LEU	2.1
1	H	158	THR	2.1
2	L	196	THR	2.1
2	L	145	VAL	2.1
1	H	45	LEU	2.1
2	L	80	CYS	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	5CT	P	4	15/16	0.86	0.18	47,57,61,62	0
1	PCA	H	2	8/9	0.95	0.15	45,56,64,67	0
1	PCA	A	2	8/9	0.96	0.09	38,42,48,54	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
5	SO4	H	304	5/5	0.86	0.23	65,69,71,80	3
4	EDO	H	302	4/4	0.88	0.21	41,44,47,48	2
5	SO4	B	304	5/5	0.88	0.19	55,60,62,63	3
4	EDO	A	301	4/4	0.88	0.22	45,50,51,56	0
5	SO4	A	305	5/5	0.90	0.15	76,79,81,83	2
5	SO4	B	302	5/5	0.93	0.14	50,50,52,57	3
5	SO4	B	303	5/5	0.93	0.23	68,69,70,74	3
4	EDO	A	302	4/4	0.95	0.16	35,37,39,39	3
5	SO4	H	303	5/5	0.96	0.10	77,78,79,80	2
5	SO4	A	304	5/5	0.96	0.17	80,80,81,82	2
4	EDO	A	303	4/4	0.97	0.12	29,31,32,34	3
4	EDO	H	301	4/4	0.97	0.10	46,47,53,57	1
5	SO4	H	305	5/5	0.97	0.16	62,62,63,64	5
5	SO4	P	101	5/5	0.97	0.09	70,70,71,73	3
5	SO4	L	301	5/5	0.98	0.10	61,62,63,64	4
5	SO4	B	301	4/5	0.98	0.24	46,46,50,55	1

6.5 Other polymers (i)

There are no such residues in this entry.