



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 07:30 AM EDT

PDB ID : 5OGI  
Title : Complex of a binding protein and human adenovirus C 5 hexon  
Authors : Schmid, M.; Ernst, P.; Honegger, A.; Suomalainen, M.; Zimmermann, M.; Braun, L.; Stauffer, S.; Thom, C.; Dreier, B.; Eibauer, M.; Kipar, A.; Vogel, V.; Greber, U.F.; Medalia, O.; Plueckthun, A.  
Deposited on : 2017-07-13  
Resolution : 2.80 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

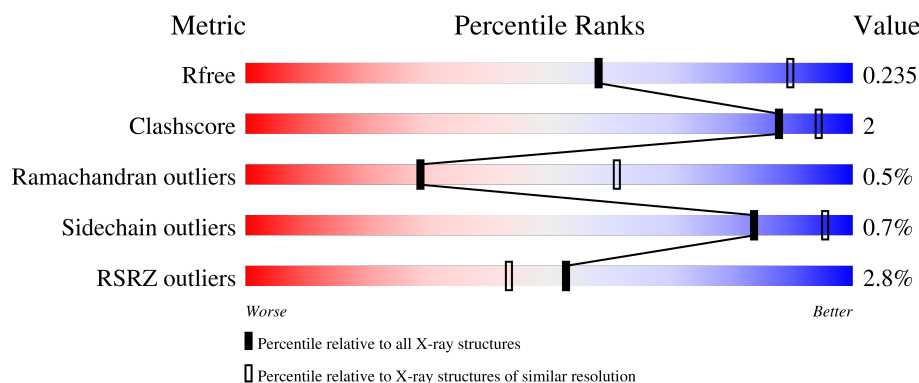
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	952	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
2	B	254	<div> <div>9%</div> <div>83%</div> <div>8%</div> <div>8%</div> </div>

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
4	DIO	A	1013	-	-	-	X
4	DIO	A	1015	-	-	-	X
5	EDO	A	1017	-	-	-	X
6	MES	A	1019	-	-	-	X
6	MES	A	1020	-	-	-	X
6	MES	A	1021	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18617 atoms, of which 8995 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 Hexon protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	921	Total	C	H	N	O	S	0	5	0
			14500	4701	7100	1258	1406	35			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	THR	conflict	UNP P04133
A	420	GLY	ILE	conflict	UNP P04133
A	422	ASN	THR	conflict	UNP P04133
A	423	SER	GLU	conflict	UNP P04133
A	425	TYR	LEU	conflict	UNP P04133

- Molecule 2 is a protein called scFv of 9C12 antibody.

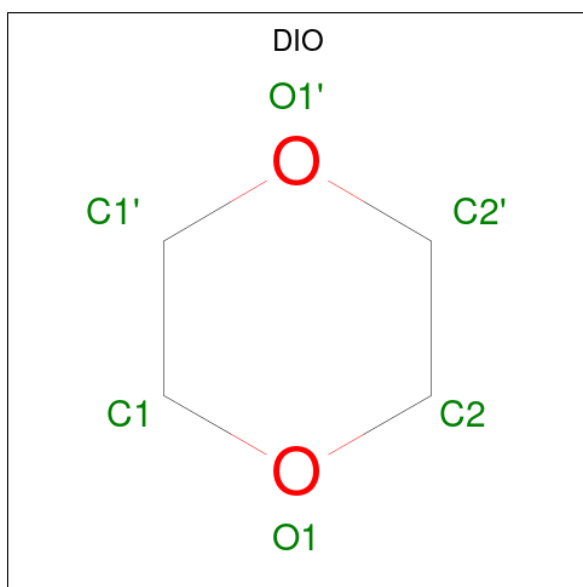
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	233	Total	C	H	N	O	S	0	2	0
			3567	1136	1757	310	357	7			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



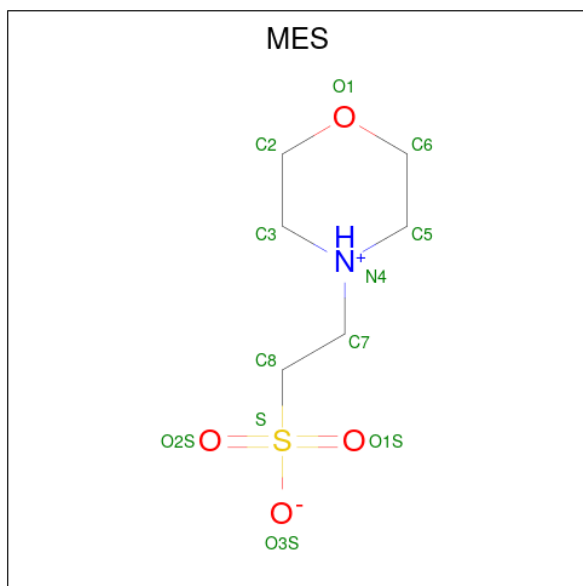
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 7 is water.

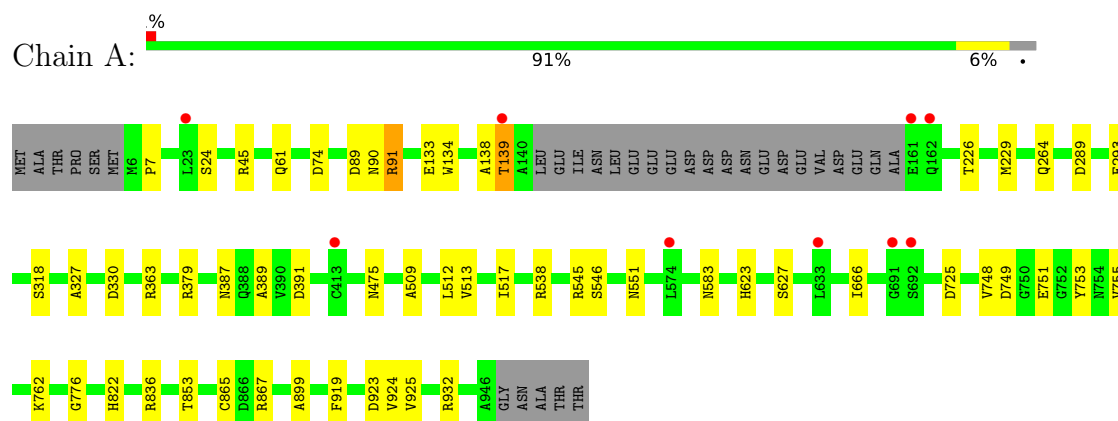
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	235	Total	O	0	0
			235	235		
7	B	30	Total	O	0	0
			30	30		



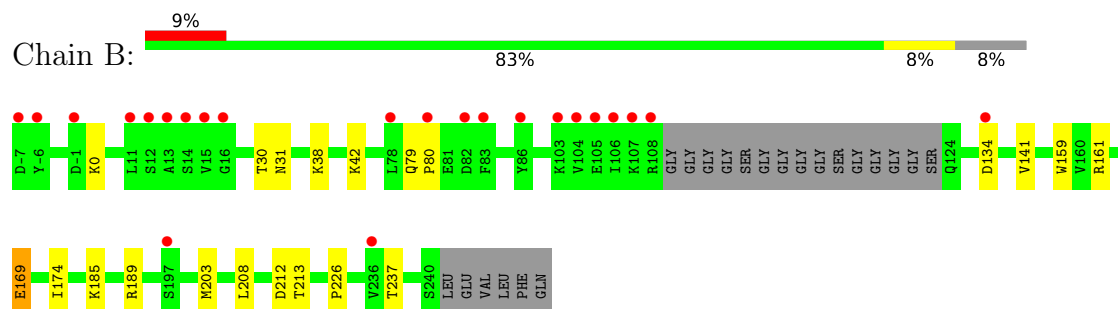
### 3 Residue-property plots [i](#)

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: Hexon protein



- Molecule 2: scFv of 9C12 antibody



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.19Å 158.19Å 140.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.80 49.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.80) 100.0 (49.09-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.198 , 0.235 0.198 , 0.235	Depositor DCC
$R_{free}$ test set	2463 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, DIO, MES, 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	0.25	0/7630	0.44	0/10373
2	B	0.26	0/1863	0.45	0/2522
All	All	0.26	0/9493	0.45	0/12895

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

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	7400	7100	7077	26	2
2	B	1810	1757	1747	11	1
3	A	35	0	0	2	0
4	A	54	72	72	0	0
4	B	6	8	8	0	0
5	A	4	6	6	0	0
6	A	48	52	52	0	0
7	A	235	0	0	0	0
7	B	30	0	0	0	0
All	All	9622	8995	8962	37	2

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 2.

All (37) 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:169:GLU:OE2	2:B:185:LYS:NZ	2.11	0.81
2:B:38:LYS:NZ	2:B:42:LYS:O	2.16	0.79
1:A:226:THR:OG1	1:A:289:ASP:OD1	2.08	0.71
1:A:389:ALA:O	1:A:545:ARG:NH1	2.25	0.70
1:A:725:ASP:N	1:A:899:ALA:O	2.27	0.67
1:A:751:GLU:N	1:A:751:GLU:OE1	2.34	0.61
2:B:161:ARG:NE	2:B:169:GLU:OE1	2.31	0.60
2:B:30:THR:OG1	2:B:31:ASN:N	2.36	0.58
1:A:749:ASP:OD2	1:A:753:TYR:N	2.39	0.56
1:A:90:ASN:OD1	1:A:627:SER:OG	2.24	0.56
1:A:89:ASP:OD2	1:A:932:ARG:NH1	2.44	0.51
1:A:755:VAL:HG21	1:A:762:LYS:HA	1.92	0.50
1:A:138:ALA:O	1:A:139:THR:OG1	2.30	0.49
1:A:475:ASN:OD1	1:A:538:ARG:NE	2.44	0.49
2:B:189:ARG:NH2	2:B:212:ASP:OD2	2.46	0.49
1:A:391:ASP:O	1:A:867:ARG:NH1	2.47	0.47
2:B:134:ASP:N	2:B:134:ASP:OD1	2.48	0.47
2:B:141:VAL:HG23	2:B:208:LEU:HD11	1.98	0.46
1:A:330:ASP:OD2	1:A:379:ARG:NH2	2.49	0.45
1:A:513:VAL:HA	1:A:517:ILE:HG21	1.98	0.45
1:A:822:HIS:O	1:A:822:HIS:ND1	2.49	0.45
1:A:134:TRP:HB3	1:A:229:MET:HE1	1.99	0.44
1:A:24:SER:OG	3:A:1006:SO4:S	2.76	0.43
1:A:363:ARG:NH1	1:A:923:ASP:OD2	2.51	0.43
2:B:174:ILE:O	2:B:174:ILE:HG23	2.20	0.41
1:A:666:ILE:HD11	1:A:919:PHE:CZ	2.55	0.41
2:B:79:GLN:CG	2:B:80:PRO:HD2	2.50	0.41
1:A:61:GLN:HG3	1:A:91:ARG:NH1	2.35	0.41
1:A:509:ALA:HB3	1:A:512:LEU:CD1	2.51	0.41
1:A:133:GLU:OE2	1:A:264:GLN:NE2	2.45	0.41
1:A:327:ALA:HB2	1:A:546:SER:HA	2.03	0.41
1:A:755:VAL:CG2	1:A:762:LYS:CG	2.99	0.41
1:A:551:ASN:OD1	1:A:551:ASN:N	2.53	0.40
2:B:159:TRP:CE2	2:B:203:MET:HB2	2.56	0.40
2:B:213:THR:HG23	2:B:237:THR:HA	2.03	0.40
1:A:623:HIS:ND1	3:A:1001:SO4:O2	2.51	0.40
1:A:924:VAL:HG12	1:A:925:VAL:N	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE2	1:A:853:THR:HG1[2_565]	1.56	0.04
1:A:583:ASN:OD1	2:B:0:LYS:NZ[6_665]	2.16	0.04

## 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	922/952 (97%)	870 (94%)	47 (5%)	5 (0%)	29 61
2	B	231/254 (91%)	218 (94%)	12 (5%)	1 (0%)	34 66
All	All	1153/1206 (96%)	1088 (94%)	59 (5%)	6 (0%)	29 61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	748	VAL
1	A	836	ARG
1	A	776	GLY
1	A	7	PRO
2	B	226	PRO

### 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	805/827 (97%)	799 (99%)	6 (1%)	84	95
2	B	199/206 (97%)	198 (100%)	1 (0%)	88	96
All	All	1004/1033 (97%)	997 (99%)	7 (1%)	84	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	74	ASP
1	A	91	ARG
1	A	318	SER
1	A	387	ASN
1	A	865	CYS
2	B	169	GLU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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	EDO	A	1017	-	3,3,3	0.49	0	2,2,2	0.24	0
4	DIO	A	1016	-	6,6,6	0.67	0	6,6,6	0.46	0
4	DIO	A	1011	-	6,6,6	0.66	0	6,6,6	0.46	0
3	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	A	1006	-	4,4,4	0.14	0	6,6,6	0.04	0
6	MES	A	1019	-	12,12,12	2.25	1 (8%)	14,16,16	1.54	4 (28%)
4	DIO	A	1013	-	6,6,6	0.67	0	6,6,6	0.40	0
3	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
4	DIO	B	301	-	6,6,6	0.67	0	6,6,6	0.58	0
6	MES	A	1018	-	12,12,12	2.26	1 (8%)	14,16,16	1.80	4 (28%)
4	DIO	A	1012	-	6,6,6	0.66	0	6,6,6	0.42	0
4	DIO	A	1015	-	6,6,6	0.67	0	6,6,6	0.55	0
3	SO4	A	1005	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	A	1001	-	4,4,4	0.12	0	6,6,6	0.05	0
3	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
4	DIO	A	1010	-	6,6,6	0.67	0	6,6,6	0.30	0
4	DIO	A	1008	-	6,6,6	0.69	0	6,6,6	0.38	0
4	DIO	A	1014	-	6,6,6	0.66	0	6,6,6	0.44	0
6	MES	A	1021	-	12,12,12	2.26	1 (8%)	14,16,16	1.69	4 (28%)
4	DIO	A	1009	-	6,6,6	0.66	0	6,6,6	0.56	0
6	MES	A	1020	-	12,12,12	2.17	1 (8%)	14,16,16	1.73	3 (21%)
3	SO4	A	1007	-	4,4,4	0.14	0	6,6,6	0.06	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	DIO	A	1013	-	-	-	0/1/1/1
4	DIO	A	1009	-	-	-	0/1/1/1
5	EDO	A	1017	-	-	0/1/1/1	-
4	DIO	A	1011	-	-	-	0/1/1/1
4	DIO	A	1015	-	-	-	0/1/1/1
4	DIO	B	301	-	-	-	0/1/1/1
6	MES	A	1018	-	-	5/6/14/14	0/1/1/1
6	MES	A	1020	-	-	5/6/14/14	0/1/1/1
4	DIO	A	1010	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DIO	A	1012	-	-	-	0/1/1/1
4	DIO	A	1016	-	-	-	0/1/1/1
4	DIO	A	1008	-	-	-	0/1/1/1
4	DIO	A	1014	-	-	-	0/1/1/1
6	MES	A	1019	-	-	1/6/14/14	0/1/1/1
6	MES	A	1021	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1018	MES	C8-S	-7.56	1.66	1.77
6	A	1019	MES	C8-S	-7.54	1.66	1.77
6	A	1021	MES	C8-S	-7.54	1.66	1.77
6	A	1020	MES	C8-S	-7.24	1.67	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1018	MES	C6-C5-N4	-4.11	103.87	110.10
6	A	1020	MES	O3S-S-C8	4.03	112.28	105.77
6	A	1021	MES	C6-C5-N4	-3.65	104.57	110.10
6	A	1018	MES	O3S-S-C8	2.70	110.14	105.77
6	A	1019	MES	O2S-S-C8	2.64	110.10	106.92
6	A	1019	MES	O1S-S-C8	2.43	109.84	106.92
6	A	1020	MES	C6-C5-N4	-2.39	106.48	110.10
6	A	1019	MES	C6-C5-N4	-2.25	106.69	110.10
6	A	1021	MES	O2S-S-C8	2.19	109.56	106.92
6	A	1021	MES	O1S-S-C8	2.18	109.54	106.92
6	A	1019	MES	O3S-S-C8	2.18	109.29	105.77
6	A	1021	MES	O3S-S-C8	2.14	109.22	105.77
6	A	1018	MES	C5-N4-C3	2.12	113.60	108.83
6	A	1020	MES	C5-N4-C3	2.11	113.58	108.83
6	A	1018	MES	O2S-S-C8	2.06	109.39	106.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1018	MES	C7-C8-S-O1S
6	A	1020	MES	N4-C7-C8-S
6	A	1020	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
6	A	1020	MES	C7-C8-S-O2S
6	A	1020	MES	C7-C8-S-O3S
6	A	1018	MES	C7-C8-S-O3S
6	A	1018	MES	C8-C7-N4-C3
6	A	1020	MES	C8-C7-N4-C3
6	A	1018	MES	C7-C8-S-O2S
6	A	1018	MES	C8-C7-N4-C5
6	A	1019	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1006	SO4	1	0
3	A	1001	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	921/952 (96%)	-0.03	9 (0%) 82 77	38, 74, 124, 188	0
2	B	233/254 (91%)	0.41	23 (9%) 7 4	63, 103, 151, 183	0
All	All	1154/1206 (95%)	0.06	32 (2%) 53 43	38, 80, 135, 188	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	83	PHE	4.5
1	A	161	GLU	4.2
2	B	-1	ASP	4.1
1	A	139	THR	4.1
2	B	86	TYR	4.0
2	B	15	VAL	3.7
2	B	104	VAL	3.3
1	A	633	LEU	3.2
2	B	106	ILE	3.2
2	B	105	GLU	3.0
2	B	103	LYS	3.0
1	A	413	CYS	2.8
2	B	-6	TYR	2.8
2	B	13	ALA	2.7
2	B	-7	ASP	2.6
2	B	107	LYS	2.6
1	A	692	SER	2.6
2	B	82	ASP	2.5
1	A	23	LEU	2.5
2	B	236	VAL	2.3
1	A	162	GLN	2.3
2	B	108	ARG	2.2
2	B	12	SER	2.2
1	A	691	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	574	LEU	2.2
2	B	11	LEU	2.2
2	B	14	SER	2.1
2	B	78	LEU	2.1
2	B	197	SER	2.1
2	B	134	ASP	2.1
2	B	16	GLY	2.0
2	B	80	PRO	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	MES	A	1021	12/12	0.44	0.52	196,199,237,237	0
6	MES	A	1019	12/12	0.67	0.42	191,200,234,236	0
5	EDO	A	1017	4/4	0.67	0.50	112,134,135,135	0
4	DIO	A	1015	6/6	0.68	0.62	134,160,165,165	0
4	DIO	A	1013	6/6	0.72	0.45	135,162,164,164	0
4	DIO	A	1014	6/6	0.72	0.20	143,172,176,176	0
6	MES	A	1020	12/12	0.77	0.72	174,184,213,216	0
3	SO4	A	1004	5/5	0.81	0.25	147,148,148,149	0
4	DIO	A	1010	6/6	0.83	0.55	112,135,139,139	0
4	DIO	A	1012	6/6	0.86	0.34	126,152,154,154	0
3	SO4	A	1005	5/5	0.87	0.14	128,129,139,140	0
3	SO4	A	1007	5/5	0.88	0.25	137,138,138,139	0
4	DIO	B	301	6/6	0.88	0.28	103,124,128,128	0
4	DIO	A	1008	6/6	0.88	0.62	123,148,150,150	0
3	SO4	A	1003	5/5	0.90	0.34	124,126,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1006	5/5	0.90	0.28	165,167,167,169	0
6	MES	A	1018	12/12	0.91	0.22	131,133,159,160	0
4	DIO	A	1009	6/6	0.92	0.20	107,128,131,131	0
3	SO4	A	1002	5/5	0.94	0.33	126,127,127,128	0
4	DIO	A	1016	6/6	0.94	0.24	109,130,133,133	0
4	DIO	A	1011	6/6	0.95	0.13	132,158,161,161	0
3	SO4	A	1001	5/5	0.95	0.10	119,121,122,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.