Preliminary Full wwPDB X-ray Structure Validation Report (i)

Sep 1, 2022 – 03:56 pm BST

Deposition ID : D_1292125369

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

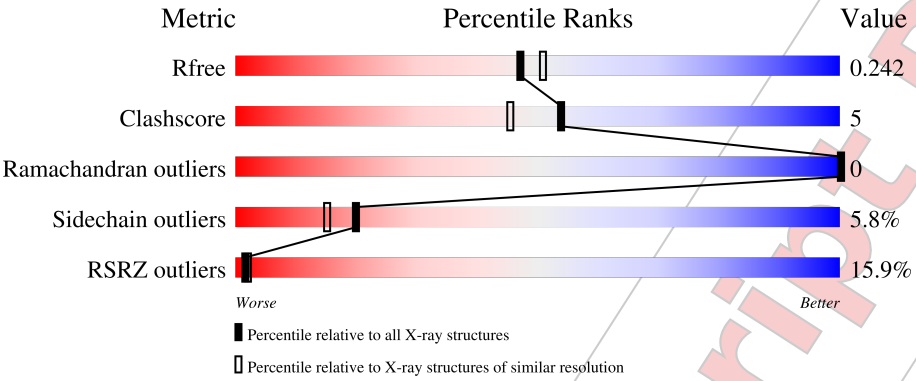
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	423	15% 84% 14%
2	B	411	17% 86% 12%

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
3	EDO	E	14	-	-	-	X
3	EDO	E	19	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7242 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.

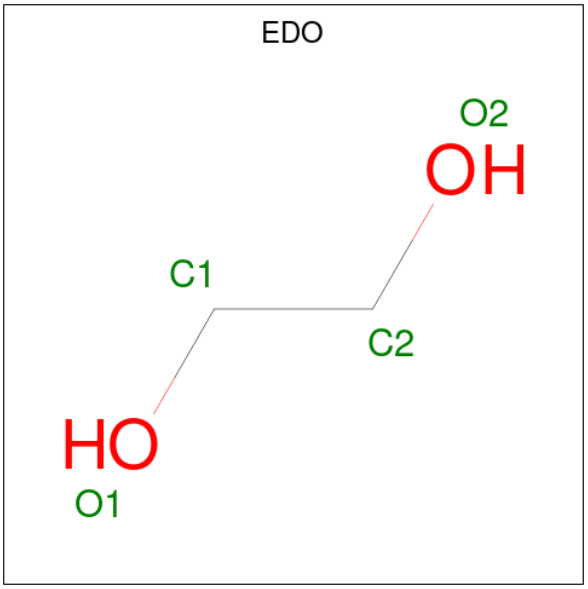
- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	423	3546	2265	608	654	19	0	2	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	411	3437	2194	586	640	17	0	1	0

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



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

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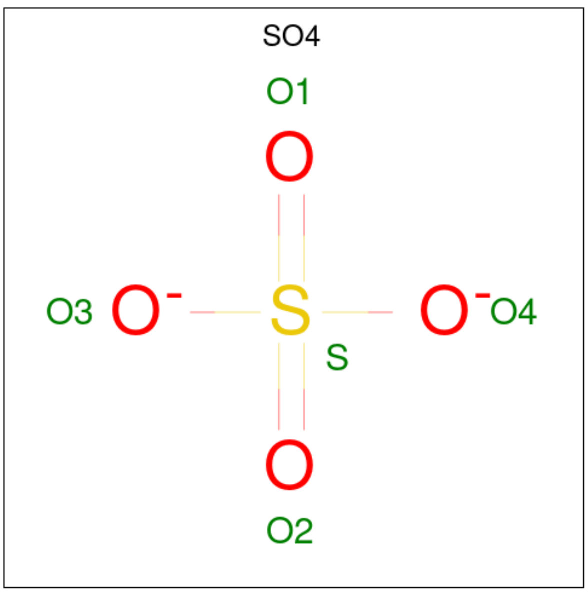
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

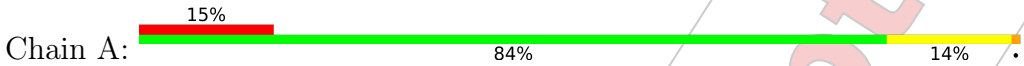
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	155	Total O 155 155	0	0

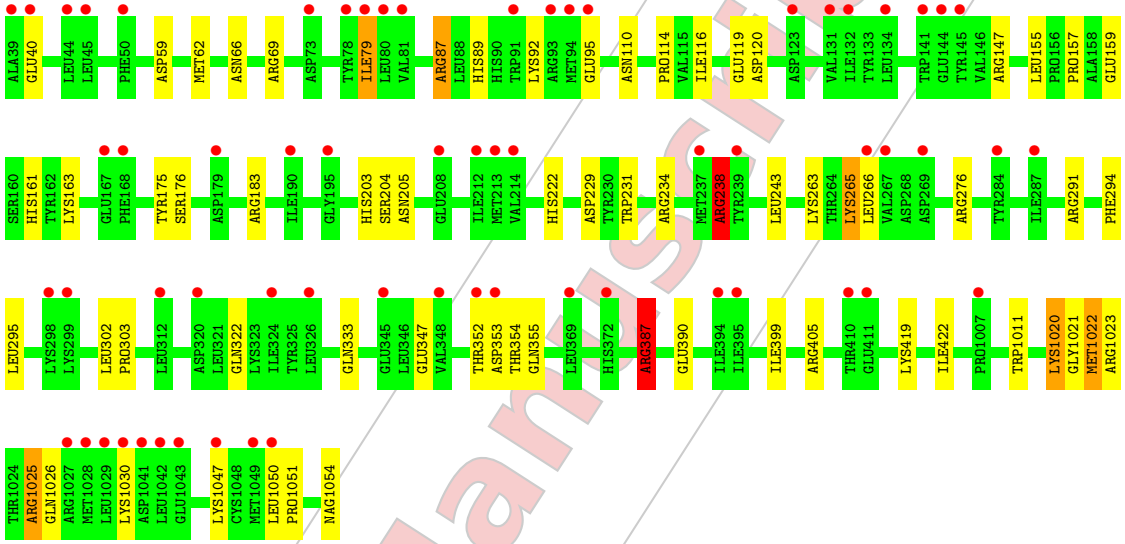
3 Residue-property plots (i)

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:

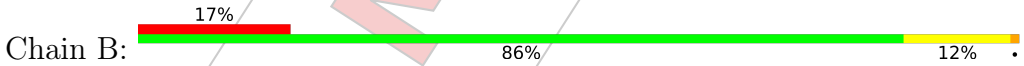
Chain A:

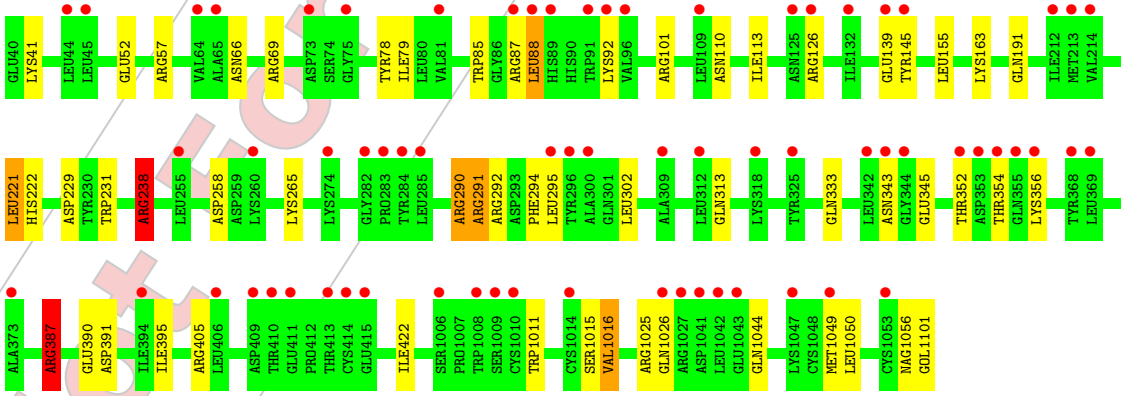




- Molecule 2:

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	156.85Å 156.85Å 80.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.13 19.90 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.90-2.13) 99.5 (19.90-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.194 , 0.240 0.201 , 0.242	Depositor DCC
R_{free} test set	2439 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7242	wwPDB-VP
Average B, all atoms (Å^2)	64.0	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.*

[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: EDO, NAG, GOL, 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	0.38	0/3627	0.75	4/4896 (0.1%)
2	B	0.38	0/3505	0.75	3/4734 (0.1%)
All	All	0.38	0/7132	0.75	7/9630 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	3
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	238	ARG	NE-CZ-NH2	-7.59	116.51	120.30
2	B	238	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	387	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	238	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	387	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	238	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	B	387	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1023	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	87	ARG	Sidechain
2	B	101	ARG	Sidechain
2	B	238	ARG	Sidechain
2	B	291	ARG	Sidechain

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	3546	0	3444	38	0
2	B	3437	0	3322	37	0
3	E	44	0	66	9	0
4	F	60	0	0	3	0
5	D	155	0	0	7	0
All	All	7242	0	6832	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (74) 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:290:ARG:HG3	2:B:290:ARG:HH11	1.34	0.90
2:B:85:TRP:HA	3:E:4:EDO:H12	1.65	0.77
1:A:234:ARG:HD3	3:E:19:EDO:H22	1.71	0.71
2:B:291:ARG:HG2	2:B:291:ARG:HH11	1.57	0.69
1:A:222:HIS:HD2	5:D:261:HOH:O	1.76	0.69
1:A:1011:TRP:CZ2	1:A:1025:ARG:HD2	2.28	0.68
1:A:59:ASP:HA	3:E:19:EDO:H11	1.77	0.67
1:A:203:HIS:HD2	1:A:205:ASN:H	1.42	0.67
1:A:1011:TRP:CH2	1:A:1025:ARG:HD2	2.33	0.64
1:A:79:ILE:HD11	1:A:116:ILE:HG22	1.80	0.62
2:B:139:GLU:OE2	2:B:191:GLN:NE2	2.33	0.62
1:A:79:ILE:HD11	1:A:116:ILE:CG2	2.29	0.62
2:B:222:HIS:HD2	5:D:440:HOH:O	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:LYS:NZ	5:D:241:HOH:O	2.34	0.58
1:A:399:ILE:HD12	1:A:419:LYS:HD2	1.87	0.57
2:B:57:ARG:HD3	3:E:4:EDO:H11	1.87	0.56
2:B:313:GLN:HE21	2:B:343:ASN:H	1.53	0.55
2:B:1011:TRP:CD2	2:B:1025:ARG:HG3	2.42	0.55
1:A:110[A]:ASN:ND2	1:A:114:PRO:HA	2.21	0.55
2:B:290:ARG:HH11	2:B:290:ARG:CG	2.11	0.55
2:B:290:ARG:NH1	2:B:292:ARG:O	2.41	0.54
2:B:69:ARG:NH2	4:F:14:SO4:O2	2.26	0.53
1:A:387:ARG:NH1	3:E:19:EDO:H21	2.24	0.53
2:B:52:GLU:OE1	2:B:1016:VAL:HG22	2.09	0.53
1:A:62:MET:SD	3:E:19:EDO:H11	2.50	0.52
2:B:387:ARG:NH2	5:D:378:HOH:O	2.21	0.52
2:B:291:ARG:NH2	4:F:16:SO4:O1	2.36	0.51
1:A:352:THR:C	1:A:354:THR:HG23	2.31	0.51
1:A:175:TYR:O	1:A:176:SER:OG	2.22	0.51
1:A:89:HIS:HB2	1:A:92:LYS:HD2	1.95	0.49
2:B:41:LYS:NZ	5:D:199:HOH:O	2.38	0.48
1:A:1050:LEU:HB3	1:A:1051:PRO:HD2	1.95	0.48
1:A:238:ARG:HD3	5:D:215:HOH:O	2.14	0.48
2:B:290:ARG:NE	2:B:1101:GOL:C1	2.76	0.48
2:B:352:THR:C	2:B:354:THR:HG23	2.34	0.47
1:A:387:ARG:HA	1:A:387:ARG:HD3	1.76	0.47
1:A:387:ARG:HH11	3:E:19:EDO:H21	1.80	0.47
2:B:387:ARG:HD3	2:B:390:GLU:OE1	2.14	0.47
2:B:221:LEU:HD12	2:B:1015:SER:HB3	1.97	0.47
2:B:1025:ARG:HH21	2:B:1044:GLN:HE22	1.63	0.46
2:B:391:ASP:O	2:B:395:ILE:HG12	2.16	0.46
1:A:265:LYS:HD3	1:A:266:LEU:N	2.30	0.46
1:A:1022:MET:HE3	1:A:1022:MET:HB3	1.77	0.46
1:A:157:PRO:HG2	1:A:161:HIS:CE1	2.51	0.45
1:A:183:ARG:HH11	1:A:183:ARG:HG3	1.82	0.45
2:B:291:ARG:HH11	2:B:291:ARG:CG	2.28	0.45
1:A:147:ARG:HH21	1:A:147:ARG:HG3	1.82	0.45
2:B:78:TYR:C	2:B:79:ILE:HD13	2.37	0.45
1:A:66:ASN:HD21	1:A:229:ASP:HB3	1.82	0.44
1:A:387:ARG:HD3	1:A:390:GLU:OE1	2.17	0.44
2:B:238:ARG:HD3	5:D:442:HOH:O	2.15	0.44
1:A:231:TRP:CE2	1:A:422:ILE:HA	2.53	0.44
1:A:69:ARG:NH2	4:F:17:SO4:O1	2.47	0.44
2:B:66:ASN:HD21	2:B:229:ASP:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:HD22	2:B:88:LEU:HA	1.86	0.43
2:B:1011:TRP:CE3	2:B:1025:ARG:HG3	2.53	0.43
1:A:291[B]:ARG:NH2	1:A:303:PRO:O	2.52	0.42
2:B:231:TRP:CE2	2:B:422:ILE:HA	2.53	0.42
1:A:116:ILE:HG12	1:A:120:ASP:HB2	2.01	0.42
1:A:294:PHE:O	1:A:1051:PRO:HG3	2.19	0.42
1:A:295:LEU:CD2	1:A:1050:LEU:HD12	2.50	0.42
2:B:290:ARG:HG3	2:B:290:ARG:NH1	2.14	0.41
1:A:66:ASN:ND2	1:A:229:ASP:HB3	2.34	0.41
2:B:57:ARG:CD	3:E:4:EDO:H11	2.48	0.41
2:B:345:GLU:OE2	2:B:345:GLU:N	2.47	0.41
1:A:1021:GLY:C	1:A:1022:MET:HG2	2.41	0.41
2:B:1025:ARG:HH21	2:B:1044:GLN:NE2	2.18	0.41
2:B:110[B]:ASN:HA	2:B:113:ILE:O	2.20	0.41
1:A:295:LEU:HD22	1:A:1050:LEU:HD12	2.02	0.41
1:A:40:GLU:HG3	3:E:16:EDO:H22	2.02	0.40
1:A:159:GLU:O	2:B:292:ARG:NH1	2.54	0.40
2:B:66:ASN:ND2	2:B:229:ASP:HB3	2.35	0.40
2:B:290:ARG:NH2	2:B:294:PHE:CE2	2.88	0.40
2:B:295:LEU:CD2	2:B:1050:LEU:HD12	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/423 (98%)	408 (98%)	8 (2%)	0	100	100
2	B	398/411 (97%)	391 (98%)	7 (2%)	0	100	100
All	All	814/834 (98%)	799 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	383/382 (100%)	358 (94%)	25 (6%)	17	11
2	B	373/372 (100%)	354 (95%)	19 (5%)	24	19
All	All	756/754 (100%)	712 (94%)	44 (6%)	20	15

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	87	ARG
1	A	95	GLU
1	A	119	GLU
1	A	155	LEU
1	A	163	LYS
1	A	204	SER
1	A	243	LEU
1	A	263	LYS
1	A	265	LYS
1	A	276	ARG
1	A	302	LEU
1	A	322	GLN
1	A	333	GLN
1	A	347	GLU
1	A	353	ASP
1	A	355	GLN
1	A	387	ARG
1	A	405	ARG
1	A	1020	LYS
1	A	1022	MET
1	A	1025	ARG
1	A	1026	GLN
1	A	1030	LYS
1	A	1047	LYS
2	B	87	ARG
2	B	88	LEU

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Mol	Chain	Res	Type
2	B	92	LYS
2	B	126	ARG
2	B	145	TYR
2	B	155	LEU
2	B	163	LYS
2	B	221	LEU
2	B	258	ASP
2	B	265	LYS
2	B	290	ARG
2	B	302	LEU
2	B	333	GLN
2	B	356	LYS
2	B	387	ARG
2	B	405	ARG
2	B	1016	VAL
2	B	1026	GLN
2	B	1049	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	161	HIS
1	A	203	HIS
1	A	222	HIS
1	A	322	GLN
1	A	333	GLN
1	A	372	HIS
2	B	66	ASN
2	B	222	HIS
2	B	313	GLN
2	B	322	GLN
2	B	333	GLN
2	B	1044	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1056	2	14,14,15	0.48	0	17,19,21	1.01	1 (5%)
1	NAG	A	1054	1	14,14,15	0.39	0	17,19,21	1.31	2 (11%)

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
2	NAG	B	1056	2	-	0/6/23/26	0/1/1/1
1	NAG	A	1054	1	-	4/6/23/26	0/1/1/1

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	1054	NAG	C1-O5-C5	4.15	117.81	112.19
1	A	1054	NAG	C1-C2-N2	2.64	115.00	110.49
2	B	1056	NAG	C2-N2-C7	-2.28	119.66	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1054	NAG	C4-C5-C6-O6
1	A	1054	NAG	O5-C5-C6-O6
1	A	1054	NAG	C8-C7-N2-C2
1	A	1054	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

23 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	$\#\|Z\| > 2$
4	SO4	F	14	-	4,4,4	0.44	0	6,6,6	0.10	0
3	EDO	E	26	-	3,3,3	0.41	0	2,2,2	0.88	0
4	SO4	F	11	-	4,4,4	0.35	0	6,6,6	0.13	0
3	EDO	E	10	-	3,3,3	0.19	0	2,2,2	0.50	0
4	SO4	F	12	-	4,4,4	0.30	0	6,6,6	0.20	0
3	EDO	E	12	-	3,3,3	0.37	0	2,2,2	0.16	0
3	EDO	E	4	-	3,3,3	0.31	0	2,2,2	0.89	0
4	SO4	F	8	-	4,4,4	0.37	0	6,6,6	0.08	0
3	EDO	E	8	-	3,3,3	0.28	0	2,2,2	0.25	0
3	EDO	E	2	-	3,3,3	0.23	0	2,2,2	0.15	0
4	SO4	F	2	-	4,4,4	0.42	0	6,6,6	0.13	0
4	SO4	F	18	-	4,4,4	0.37	0	6,6,6	0.21	0
3	EDO	E	7	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	E	14	-	3,3,3	0.14	0	2,2,2	0.32	0
3	EDO	E	25	-	3,3,3	0.21	0	2,2,2	0.64	0
4	SO4	F	13	-	4,4,4	0.40	0	6,6,6	0.12	0
4	SO4	F	17	-	4,4,4	0.40	0	6,6,6	0.19	0
4	SO4	F	9	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	F	10	-	4,4,4	0.32	0	6,6,6	0.18	0
4	SO4	F	16	-	4,4,4	0.36	0	6,6,6	0.09	0
4	SO4	F	15	-	4,4,4	0.32	0	6,6,6	0.14	0
3	EDO	E	16	-	3,3,3	0.16	0	2,2,2	0.34	0
3	EDO	E	19	-	3,3,3	0.23	0	2,2,2	0.59	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	E	12	-	-	1/1/1/1	-
3	EDO	E	4	-	-	0/1/1/1	-
3	EDO	E	26	-	-	1/1/1/1	-
3	EDO	E	7	-	-	1/1/1/1	-
3	EDO	E	8	-	-	1/1/1/1	-
3	EDO	E	14	-	-	0/1/1/1	-
3	EDO	E	25	-	-	1/1/1/1	-
3	EDO	E	2	-	-	1/1/1/1	-
3	EDO	E	10	-	-	1/1/1/1	-
3	EDO	E	16	-	-	1/1/1/1	-
3	EDO	E	19	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	12	EDO	O1-C1-C2-O2
3	E	16	EDO	O1-C1-C2-O2
3	E	19	EDO	O1-C1-C2-O2
3	E	26	EDO	O1-C1-C2-O2
3	E	2	EDO	O1-C1-C2-O2
3	E	10	EDO	O1-C1-C2-O2
3	E	8	EDO	O1-C1-C2-O2
3	E	7	EDO	O1-C1-C2-O2
3	E	25	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	14	SO4	1	0
3	E	4	EDO	3	0
4	F	17	SO4	1	0
4	F	16	SO4	1	0
3	E	16	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	19	EDO	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	6
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1053:CYS	C	1054:NAG	O3	30.55
1	B	1053:CYS	C	1056:NAG	O3	29.79
1	B	424:TYR	C	1006:SER	N	19.94
1	A	1030:LYS	C	1041:ASP	N	15.28
1	B	139:GLU	C	145:TYR	N	9.62
1	B	1027:ARG	C	1041:ASP	N	8.77
1	B	92:LYS	C	96:VAL	N	8.69
1	B	296:TYR	C	300:ALA	N	7.45
1	A	141:TRP	C	144:GLU	N	5.71

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	422/423 (99%)	0.81	64 (15%) 2 2	42, 58, 90, 127	0
2	B	409/411 (99%)	0.98	68 (16%) 1 2	44, 61, 105, 127	0
All	All	831/834 (99%)	0.89	132 (15%) 1 2	42, 59, 98, 127	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1042	LEU	11.2
2	B	1010	CYS	8.4
2	B	1041	ASP	8.1
2	B	1008	TRP	8.1
2	B	413	THR	7.9
2	B	92	LYS	7.4
2	B	355	GLN	7.2
1	A	1029	LEU	7.1
2	B	1049	MET	6.6
1	A	141	TRP	6.1
1	A	145	TYR	5.8
1	A	1042	LEU	5.6
1	A	1041	ASP	5.6
2	B	91	TRP	5.6
2	B	410	THR	5.4
1	A	168	PHE	5.3
2	B	343	ASN	5.2
1	A	352	THR	5.2
2	B	45	LEU	5.1
1	A	144	GLU	5.0
1	A	50	PHE	4.8
1	A	80	LEU	4.7
2	B	88	LEU	4.6
1	A	353	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	344	GLY	4.5
1	A	1030	LYS	4.4
2	B	1027	ARG	4.4
1	A	95	GLU	4.2
2	B	411	GLU	4.2
1	A	394	ILE	4.1
2	B	125	ASN	4.0
1	A	134	LEU	4.0
2	B	75	GLY	3.9
2	B	356	LYS	3.9
2	B	284	TYR	3.9
1	A	299	LYS	3.9
2	B	295	LEU	3.8
1	A	81	VAL	3.8
1	A	1049	MET	3.8
2	B	406	LEU	3.7
1	A	132	ILE	3.6
1	A	190	ILE	3.6
2	B	44	LEU	3.6
2	B	354	THR	3.5
1	A	179	ASP	3.5
1	A	91	TRP	3.5
2	B	274	LYS	3.5
1	A	131	VAL	3.4
2	B	81	VAL	3.4
1	A	298	LYS	3.3
2	B	132	ILE	3.3
2	B	260	LYS	3.2
1	A	345	GLU	3.2
2	B	255	LEU	3.2
2	B	1043	GLU	3.1
2	B	109	LEU	3.1
2	B	212	ILE	3.1
2	B	312	LEU	3.1
2	B	296	TYR	3.0
2	B	409	ASP	3.0
1	A	269	ASP	3.0
2	B	89	HIS	3.0
1	A	167	GLU	2.9
2	B	1006	SER	2.9
1	A	237	MET	2.9
2	B	73	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1027	ARG	2.9
1	A	287	ILE	2.8
1	A	1028	MET	2.8
2	B	415	GLU	2.8
1	A	73	ASP	2.8
2	B	145	TYR	2.8
1	A	324	ILE	2.8
2	B	318	LYS	2.8
1	A	45	LEU	2.8
1	A	94	MET	2.7
2	B	1014	CYS	2.7
2	B	213	MET	2.7
2	B	353	ASP	2.7
2	B	369	LEU	2.7
1	A	410	THR	2.7
1	A	213	MET	2.7
1	A	266	LEU	2.6
2	B	139	GLU	2.6
2	B	1009	SER	2.6
2	B	300	ALA	2.5
2	B	352	THR	2.5
1	A	372	HIS	2.5
2	B	342	LEU	2.5
1	A	214	VAL	2.5
2	B	64	VAL	2.5
2	B	96	VAL	2.5
2	B	1026	GLN	2.5
2	B	214	VAL	2.5
1	A	93	ARG	2.5
1	A	411	GLU	2.4
2	B	1047	LYS	2.4
1	A	79	ILE	2.4
1	A	1047	LYS	2.4
2	B	283	PRO	2.4
2	B	394	ILE	2.4
1	A	195	GLY	2.4
2	B	87	ARG	2.4
1	A	320	ASP	2.4
1	A	395	ILE	2.4
1	A	78	TYR	2.4
1	A	239	TYR	2.4
1	A	1050	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	267	VAL	2.3
2	B	126	ARG	2.3
2	B	1053	CYS	2.3
2	B	65	ALA	2.3
1	A	208	GLU	2.3
1	A	326	LEU	2.2
2	B	414	CYS	2.2
1	A	123	ASP	2.2
1	A	44	LEU	2.2
2	B	282	GLY	2.2
1	A	39	ALA	2.2
1	A	284	TYR	2.1
1	A	1043	GLU	2.1
1	A	212	ILE	2.1
1	A	312	LEU	2.1
2	B	285	LEU	2.1
1	A	40	GLU	2.1
1	A	1007	PRO	2.1
2	B	368	TYR	2.1
1	A	369	LEU	2.0
2	B	373	ALA	2.0
2	B	309	ALA	2.0
1	A	348	VAL	2.0
2	B	325	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	NAG	A	1054	14/?	0.86	0.16	63,78,86,91	0
2	NAG	B	1056	14/?	0.90	0.13	49,53,60,62	0

6.3 Carbohydrates (i)

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^{th} 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	E	16	4/?	0.54	0.31	75,92,92,97	0
3	EDO	E	14	4/?	0.58	0.43	57,75,77,83	0
3	EDO	E	4	4/?	0.66	0.33	74,82,91,94	0
3	EDO	E	10	4/?	0.67	0.26	73,75,75,76	0
3	EDO	E	26	4/?	0.68	0.31	65,68,69,72	0
3	EDO	E	2	4/?	0.76	0.16	79,79,87,100	0
4	SO4	F	9	5/?	0.76	0.24	129,137,148,151	0
3	EDO	E	8	4/?	0.81	0.94	60,76,77,78	0
3	EDO	E	7	4/?	0.84	0.53	65,66,71,81	0
4	SO4	F	11	5/?	0.86	0.38	118,123,135,143	0
4	SO4	F	18	5/?	0.86	0.26	93,103,120,123	0
4	SO4	F	15	5/?	0.87	0.29	91,97,109,113	0
3	EDO	E	25	4/?	0.89	0.19	70,73,76,78	0
3	EDO	E	19	4/?	0.91	0.32	50,63,66,66	0
3	EDO	E	12	4/?	0.93	0.33	62,68,71,75	0
4	SO4	F	16	5/?	0.94	0.24	80,85,97,101	0
4	SO4	F	14	5/?	0.94	0.10	73,85,97,101	0
4	SO4	F	8	5/?	0.95	0.12	83,101,102,111	0
4	SO4	F	13	5/?	0.96	0.12	71,73,88,89	0
4	SO4	F	2	5/?	0.97	0.11	67,69,75,92	0
4	SO4	F	10	5/?	0.97	0.14	79,85,98,103	0
4	SO4	F	17	5/?	0.98	0.12	72,79,83,96	0
4	SO4	F	12	5/?	0.98	0.21	60,65,71,83	0

6.5 Other polymers

There are no such residues in this entry.