



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:25 am BST

PDB ID : 5MHM
Title : FXIIIa in complex with the inhibitor ZED1630
Authors : Stieler, M.; Heine, A.; Klebe, G.
Deposited on : 2016-11-24
Resolution : 2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

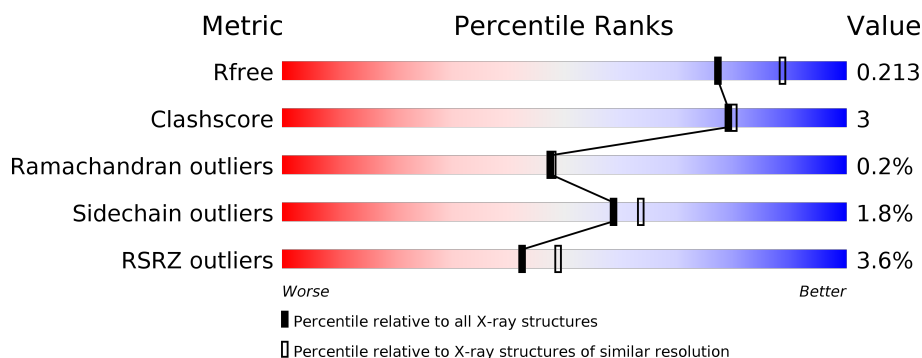
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>6% • 7%</div> </div> </div>
1	B	738	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>7% • 7%</div> </div> </div>
2	H	8	<div> <div></div> <div> <div></div> <div>88%</div> <div>13%</div> </div> </div>
2	O	8	<div> <div></div> <div> <div></div> <div>75%</div> <div>25%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11759 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 Coagulation factor XIII A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	6	0
			5328	3401	891	1010	26			
1	B	683	Total	C	N	O	S	0	5	0
			5396	3449	907	1012	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P00488
A	-5	HIS	-	expression tag	UNP P00488
A	-4	HIS	-	expression tag	UNP P00488
A	-3	HIS	-	expression tag	UNP P00488
A	-2	HIS	-	expression tag	UNP P00488
A	-1	HIS	-	expression tag	UNP P00488
A	0	HIS	-	expression tag	UNP P00488
A	649	ILE	THR	engineered mutation	UNP P00488
A	651	GLU	GLN	engineered mutation	UNP P00488
B	-6	MET	-	initiating methionine	UNP P00488
B	-5	HIS	-	expression tag	UNP P00488
B	-4	HIS	-	expression tag	UNP P00488
B	-3	HIS	-	expression tag	UNP P00488
B	-2	HIS	-	expression tag	UNP P00488
B	-1	HIS	-	expression tag	UNP P00488
B	0	HIS	-	expression tag	UNP P00488
B	649	ILE	THR	engineered mutation	UNP P00488
B	651	GLU	GLN	engineered mutation	UNP P00488

- Molecule 2 is a protein called inhibitor ZED1630.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	8	Total	C	N	O	S	0	0	1
			62	43	9	9	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	8	Total	C	N	O	S	0	0	1
			63	44	9	9	1			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

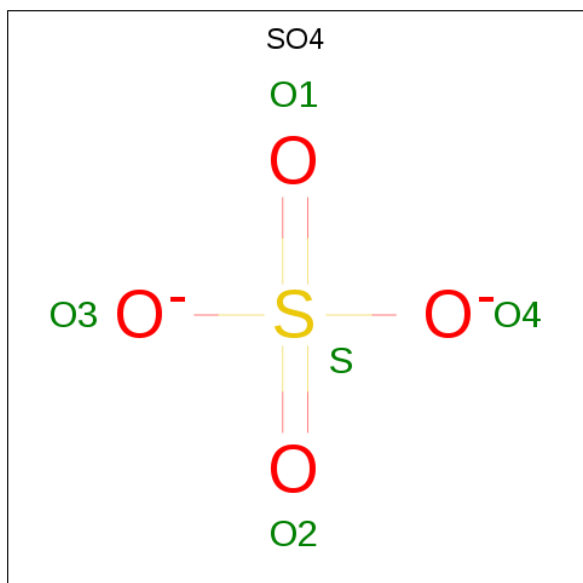


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	380	Total O 380 380	0	0
7	B	456	Total O 456 456	0	0

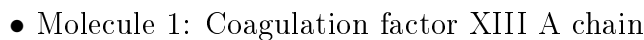
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	2	Total	O	0	0
			2	2		
7	O	3	Total	O	0	0
			3	3		

i


- Molecule 1: Coagulation factor XIII A chain



Chain H:  88% 13%



- Molecule 2: inhibitor ZED1630

Chain O:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.91Å 80.72Å 103.19Å 88.44° 76.60° 81.79°	Depositor
Resolution (Å)	24.88 – 2.12 24.87 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.9 (24.88-2.12) 96.9 (24.87-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.11Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.170 , 0.213 0.170 , 0.213	Depositor DCC
R_{free} test set	4903 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11759	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6613e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, CA, 1TX, NLE, 7NW, NH2, 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	0.40	0/5462	0.56	0/7438
1	B	0.42	1/5528 (0.0%)	0.57	0/7518
2	H	0.28	0/38	0.38	0/53
2	O	0.31	0/38	0.40	0/53
All	All	0.41	1/11066 (0.0%)	0.56	0/15062

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	CYS	CB-SG	-5.91	1.72	1.81

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	5328	0	5011	25	0
1	B	5396	0	5165	34	0
2	H	62	0	46	1	0
2	O	63	0	49	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	32	1	0
4	B	12	0	16	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	10	0	0	0	0
6	B	15	0	0	0	0
7	A	380	0	0	2	0
7	B	456	0	0	2	0
7	H	2	0	0	0	0
7	O	3	0	0	0	0
All	All	11759	0	10319	59	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 (59) 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:B:640:GLN:HB3	1:B:725:ILE:HG22	1.63	0.79
1:B:314:CYS:HB3	2:O:2:1TX:C25	2.21	0.70
1:B:245:ALA:HB2	1:B:265:MET:HG3	1.75	0.68
1:A:314:CYS:HB3	2:H:2:1TX:C25	2.29	0.63
1:B:245:ALA:HB2	1:B:265:MET:CG	2.28	0.62
1:B:711:SER:O	1:B:715:ARG:NH2	2.36	0.59
1:B:18:ASN:HD22	1:B:18:ASN:C	2.05	0.58
1:B:541:ASN:HB2	1:B:577:LEU:HG	1.86	0.57
1:B:524:VAL:HG22	1:B:535:LEU:HD12	1.87	0.56
1:A:151:LYS:NZ	7:A:903:HOH:O	2.36	0.56
1:A:275:LEU:HD11	1:A:316:VAL:HG12	1.89	0.54
1:B:398:THR:HG21	2:O:2:1TX:H13	1.90	0.53
1:A:704:LYS:NZ	1:A:720:GLU:OE1	2.37	0.52
1:A:20:ASN:O	4:A:807:GOL:H32	2.11	0.51
1:B:214:TYR:HB2	1:B:372:TYR:CZ	2.46	0.51
1:B:344:ASN:ND2	7:B:907:HOH:O	2.43	0.50
1:B:214:TYR:HB2	1:B:372:TYR:CE1	2.47	0.50
1:B:703:ARG:HG3	1:B:725:ILE:HD11	1.94	0.49
1:A:637:ARG:HG2	1:A:647:THR:HB	1.93	0.49
1:B:640:GLN:HG2	1:B:646:MET:SD	2.53	0.49
1:A:214:TYR:HB2	1:A:372:TYR:CZ	2.48	0.48
1:A:630:PRO:HB2	1:A:717:VAL:HG11	1.96	0.48
1:B:664:TRP:CE2	1:B:679:MET:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HD13	1:B:379:TRP:CE2	2.49	0.47
1:A:214:TYR:HB2	1:A:372:TYR:CE1	2.49	0.47
1:A:186:PRO:HG2	1:A:205:VAL:HG21	1.96	0.47
1:B:443:THR:O	1:B:450:HIS:HA	2.15	0.47
1:B:153:ILE:HD11	1:B:250:SER:HA	1.96	0.47
1:A:134:ILE:HG21	1:A:137:ARG:HD3	1.97	0.47
1:A:524:VAL:HG22	1:A:535:LEU:HD12	1.98	0.46
1:B:372:TYR:OH	2:O:1:7NW:N3	2.50	0.45
1:B:349:GLN:HA	1:B:437:SER:HB2	1.98	0.45
1:B:489:GLU:H	1:B:489:GLU:CD	2.20	0.45
1:A:637:ARG:NH2	1:A:692:GLU:OE2	2.50	0.45
1:B:15:PRO:HA	1:B:16:PRO:HD3	1.85	0.45
1:B:565:LYS:HG3	1:B:599:LEU:CD2	2.47	0.45
1:A:195:LEU:O	1:A:201:ARG:NH1	2.47	0.45
1:A:436:ASN:ND2	7:A:915:HOH:O	2.50	0.45
1:A:29:VAL:HG12	1:A:31:LEU:HG	1.98	0.44
1:A:349:GLN:HA	1:A:437:SER:HB2	2.00	0.43
1:B:310:ARG:HA	1:B:311:TYR:HA	1.82	0.43
1:B:396:ASP:HB3	1:B:409:CYS:HB3	2.01	0.43
1:B:189:GLU:HA	1:B:194:TYR:CD1	2.54	0.42
1:B:529:LEU:HD13	1:B:629:ILE:HG23	2.00	0.42
1:B:387:VAL:HG12	7:B:1184:HOH:O	2.19	0.42
1:B:186:PRO:HG2	1:B:205:VAL:HG21	2.00	0.42
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.54	0.42
1:B:189:GLU:HA	1:B:194:TYR:CG	2.55	0.42
1:A:396:ASP:HB3	1:A:409:CYS:HB3	2.02	0.42
1:B:565:LYS:HG3	1:B:599:LEU:HD21	2.02	0.42
1:A:235:LEU:HA	1:A:327:CYS:SG	2.60	0.41
1:A:385:LEU:HD22	1:A:424:PHE:HB3	2.02	0.41
1:A:189:GLU:HA	1:A:194:TYR:CG	2.56	0.41
1:A:704:LYS:HE3	1:A:720:GLU:HB2	2.03	0.41
1:B:598:LEU:HD23	1:B:598:LEU:HA	1.85	0.41
1:A:217:VAL:HG13	1:A:338:TYR:HB3	2.02	0.40
1:B:639:THR:O	1:B:646:MET:HB3	2.21	0.40
1:A:489:GLU:CD	1:A:489:GLU:H	2.25	0.40
1:A:565:LYS:HE3	1:A:599:LEU:HD21	2.03	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	682/738 (92%)	666 (98%)	14 (2%)	2 (0%)	41	40
1	B	678/738 (92%)	661 (98%)	16 (2%)	1 (0%)	51	53
2	H	4/8 (50%)	4 (100%)	0	0	100	100
2	O	4/8 (50%)	4 (100%)	0	0	100	100
All	All	1368/1492 (92%)	1335 (98%)	30 (2%)	3 (0%)	47	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ASN
1	B	669	GLY
1	A	669	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	553/651 (85%)	544 (98%)	9 (2%)	62	68
1	B	572/651 (88%)	561 (98%)	11 (2%)	57	61
2	H	3/4 (75%)	3 (100%)	0	100	100
2	O	3/4 (75%)	3 (100%)	0	100	100
All	All	1131/1310 (86%)	1111 (98%)	20 (2%)	59	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	137	ARG
1	A	140	ARG
1	A	211	VAL
1	A	217	VAL
1	A	321	PHE
1	A	484	GLN
1	A	599	LEU
1	A	695	CYS
1	B	18	ASN
1	B	20	ASN
1	B	137	ARG
1	B	216	GLU
1	B	321	PHE
1	B	387	VAL
1	B	565	LYS
1	B	581	SER
1	B	599	LEU
1	B	695	CYS
1	B	725	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	666	HIS
1	B	18	ASN
1	B	344	ASN
1	B	484	GLN
1	B	601	GLN
1	B	640	GLN
1	B	716	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	1TX	O	2	1,2	10,11,12	0.46	0	7,12,14	0.51	0
2	1TX	H	2	1,2	10,11,12	0.44	0	7,12,14	0.58	0
2	NLE	H	3	2	3,4,8	0.77	0	2,4,9	0.87	0
2	NLE	O	3	2	4,5,8	0.66	0	1,5,9	1.70	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
2	1TX	O	2	1,2	-	1/10/11/13	-
2	1TX	H	2	1,2	-	1/10/11/13	-
2	NLE	H	3	2	-	0/0/2/8	-
2	NLE	O	3	2	-	1/3/4/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	2	1TX	C22-C23-C24-C25
2	H	2	1TX	C22-C23-C24-C25
2	O	3	NLE	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	2	1TX	2	0
2	H	2	1TX	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\# Z > 2$
6	SO4	A	810	-	4,4,4	0.15	0	6,6,6	0.19	0
6	SO4	B	808	-	4,4,4	0.19	0	6,6,6	0.13	0
4	GOL	B	803	-	5,5,5	0.31	0	5,5,5	0.39	0
4	GOL	B	804	-	5,5,5	0.31	0	5,5,5	0.40	0
4	GOL	A	804	-	5,5,5	0.43	0	5,5,5	0.56	0
6	SO4	B	806	-	4,4,4	0.39	0	6,6,6	0.26	0
4	GOL	A	807	-	5,5,5	0.27	0	5,5,5	0.82	0
6	SO4	B	807	-	4,4,4	0.15	0	6,6,6	0.14	0
6	SO4	A	809	-	4,4,4	0.17	0	6,6,6	0.18	0
4	GOL	A	806	-	5,5,5	0.40	0	5,5,5	0.30	0
4	GOL	A	805	-	5,5,5	0.42	0	5,5,5	0.23	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	GOL	B	803	-	-	0/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
4	GOL	A	807	-	-	4/4/4/4	-
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	807	GOL	O1-C1-C2-C3
4	A	804	GOL	O1-C1-C2-C3
4	A	807	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	805	GOL	O1-C1-C2-C3
4	A	804	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-O2
4	A	805	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-O2
4	A	807	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	GOL	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, 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(Å ²)	Q<0.9
1	A	684/738 (92%)	-0.01	25 (3%) 41 48	13, 28, 58, 82	0
1	B	683/738 (92%)	-0.08	25 (3%) 41 48	13, 27, 54, 83	0
2	H	4/8 (50%)	0.48	0 100 100	33, 34, 39, 40	0
2	O	4/8 (50%)	0.50	0 100 100	31, 32, 38, 39	0
All	All	1375/1492 (92%)	-0.04	50 (3%) 42 49	13, 27, 57, 83	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	699	VAL	5.7
1	B	698	TRP	5.2
1	A	699	VAL	4.7
1	B	700	SER	4.4
1	A	698	TRP	4.0
1	A	695	CYS	3.7
1	A	643	GLY	3.6
1	A	353	PHE	3.4
1	B	695	CYS	3.1
1	A	685	PRO	3.1
1	A	637	ARG	3.1
1	A	659	THR	2.9
1	A	645	ASP	2.9
1	B	701	GLY	2.9
1	B	443	THR	2.8
1	B	328	LEU	2.6
1	B	671	GLY	2.6
1	B	325	LEU	2.5
1	B	15	PRO	2.5
1	B	360	VAL	2.5
1	A	470	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	330	ILE	2.4
1	B	560	TYR	2.4
1	A	154	VAL	2.4
1	A	638	GLY	2.3
1	A	364	LEU	2.3
1	A	127	SER	2.3
1	B	470	GLY	2.3
1	B	127	SER	2.3
1	B	374	CYS	2.3
1	A	712	ASP	2.3
1	A	325	LEU	2.3
1	B	433	ALA	2.3
1	B	320	VAL	2.3
1	B	16	PRO	2.3
1	A	57	TRP	2.2
1	B	444	ALA	2.2
1	A	701	GLY	2.2
1	B	451	VAL	2.1
1	B	364	LEU	2.1
1	A	452	VAL	2.1
1	A	321	PHE	2.1
1	B	702	HIS	2.1
1	A	697	PRO	2.1
1	B	686	ASN	2.1
1	A	442	ILE	2.1
1	A	601	GLN	2.0
1	A	454	ASN	2.0
1	A	330	ILE	2.0
1	B	694	VAL	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(\AA^2)	Q<0.9
2	NLE	H	3	5/9	0.92	0.10	27,30,33,36	0
2	NLE	O	3	6/9	0.93	0.10	28,31,33,34	0
2	1TX	O	2	12/13	0.94	0.10	21,25,39,39	0
2	1TX	H	2	12/13	0.94	0.12	19,29,32,33	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	806	6/6	0.81	0.21	41,50,57,60	0
4	GOL	A	807	6/6	0.89	0.20	23,35,40,45	6
6	SO4	A	809	5/5	0.92	0.12	37,41,49,58	5
6	SO4	B	806	5/5	0.93	0.10	17,23,32,38	5
6	SO4	A	810	5/5	0.93	0.23	28,35,37,38	5
6	SO4	B	808	5/5	0.94	0.23	24,32,34,38	5
4	GOL	A	805	6/6	0.94	0.16	43,44,46,49	0
4	GOL	A	804	6/6	0.95	0.14	21,26,32,32	0
6	SO4	B	807	5/5	0.96	0.16	32,38,41,46	5
4	GOL	B	804	6/6	0.96	0.12	30,34,35,35	0
3	CA	A	803	1/1	0.97	0.04	27,27,27,27	0
3	CA	A	802	1/1	0.98	0.06	39,39,39,39	0
4	GOL	B	803	6/6	0.98	0.08	22,24,26,30	0
3	CA	B	805	1/1	0.99	0.04	22,22,22,22	0
3	CA	B	802	1/1	0.99	0.04	29,29,29,29	0
3	CA	B	801	1/1	1.00	0.09	18,18,18,18	0
5	CL	A	808	1/1	1.00	0.04	21,21,21,21	0
3	CA	A	801	1/1	1.00	0.07	17,17,17,17	0
5	CL	B	809	1/1	1.00	0.04	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.