



Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 04:39 PM JST

Deposition ID : D_1300024349

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 ⓘ 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	:	2.23.1
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)	:	2.23.1

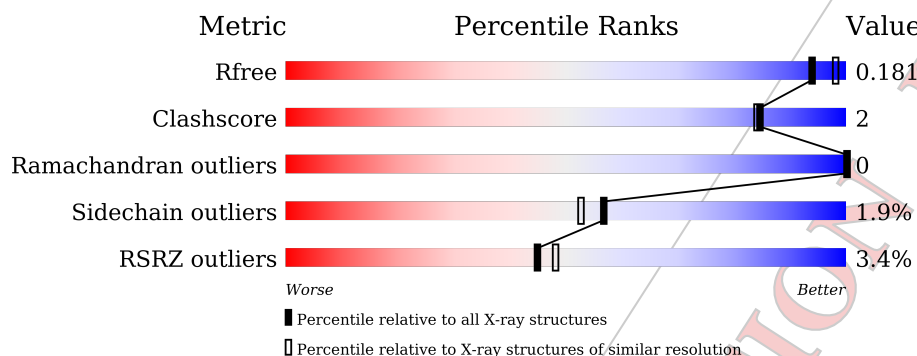
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	884	3% 89% 8%

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
5	ACT	F	1	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7628 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 Alanine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	859	6808	4287	1196	1308	17	0	9	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A4F9D7
A	-22	GLY	-	expression tag	UNP A4F9D7
A	-21	SER	-	expression tag	UNP A4F9D7
A	-20	SER	-	expression tag	UNP A4F9D7
A	-19	HIS	-	expression tag	UNP A4F9D7
A	-18	HIS	-	expression tag	UNP A4F9D7
A	-17	HIS	-	expression tag	UNP A4F9D7
A	-16	HIS	-	expression tag	UNP A4F9D7
A	-15	HIS	-	expression tag	UNP A4F9D7
A	-14	HIS	-	expression tag	UNP A4F9D7
A	-13	HIS	-	expression tag	UNP A4F9D7
A	-12	HIS	-	expression tag	UNP A4F9D7
A	-11	HIS	-	expression tag	UNP A4F9D7
A	-10	HIS	-	expression tag	UNP A4F9D7
A	-9	SER	-	expression tag	UNP A4F9D7
A	-8	SER	-	expression tag	UNP A4F9D7
A	-7	GLY	-	expression tag	UNP A4F9D7
A	-6	LEU	-	expression tag	UNP A4F9D7
A	-5	VAL	-	expression tag	UNP A4F9D7
A	-4	PRO	-	expression tag	UNP A4F9D7
A	-3	ARG	-	expression tag	UNP A4F9D7
A	-2	GLY	-	expression tag	UNP A4F9D7
A	-1	SER	-	expression tag	UNP A4F9D7
A	0	HIS	-	expression tag	UNP A4F9D7
A	1	VAL	-	expression tag	UNP A4F9D7

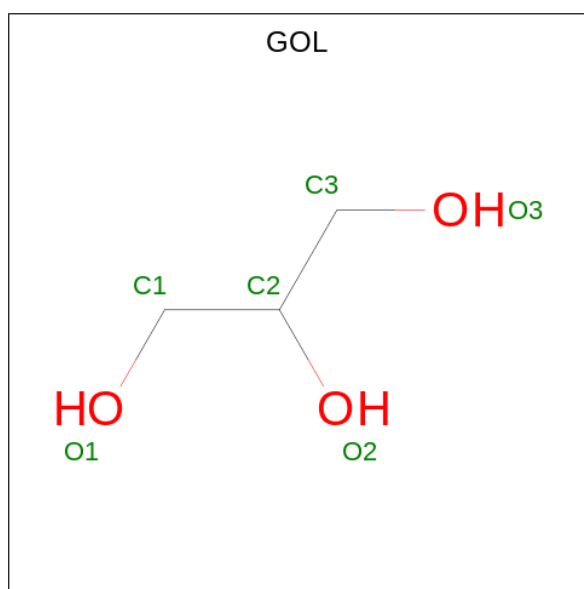
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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

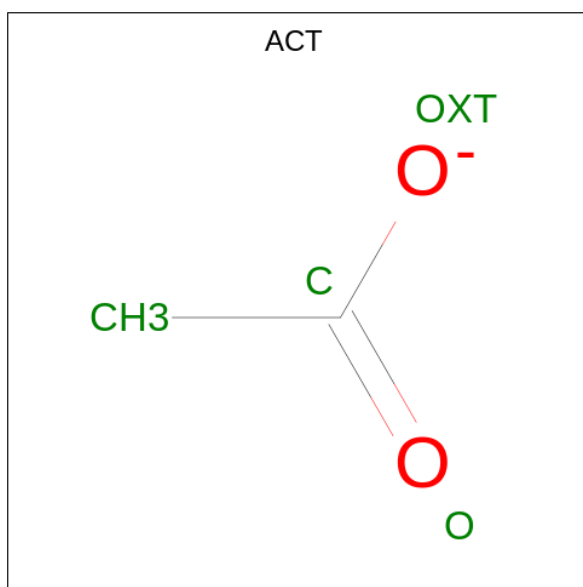
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		

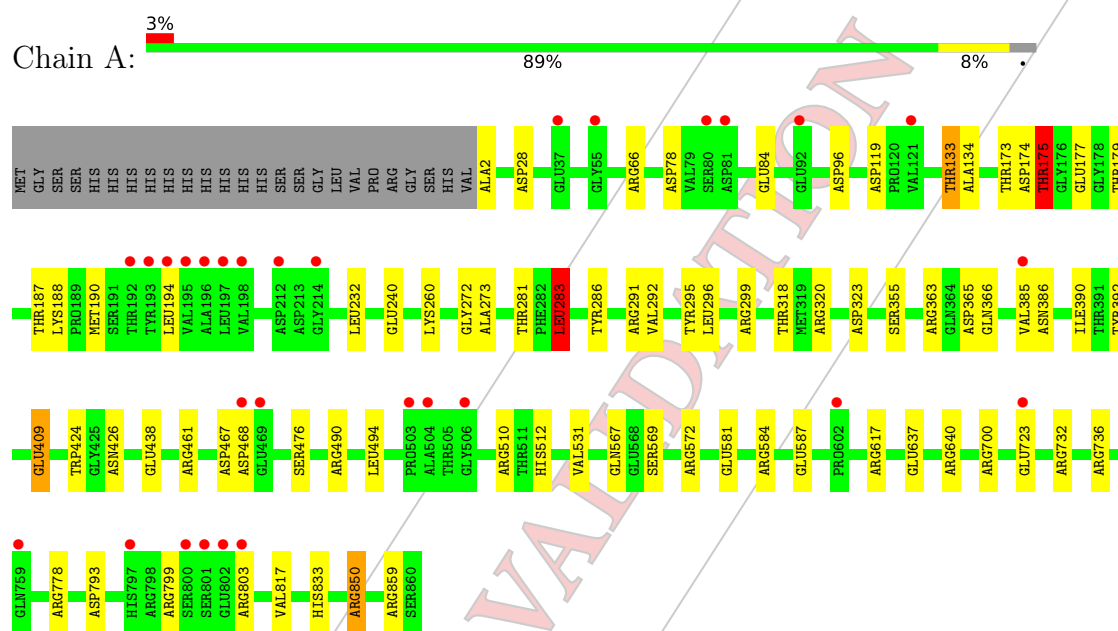
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	796	Total	O	0	0
			796	796		

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: Alanine aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	153.58Å 153.58Å 98.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.08 – 1.90 32.08 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.08-1.90) 100.0 (32.08-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.2 3874	Depositor
R, R_{free}	0.154 , 0.181 0.154 , 0.181	Depositor DCC
R_{free} test set	2000 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7628	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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, ACT, CA, ZN

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	1.11	10/6972 (0.1%)	1.04	34/9500 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	GLU	CD-OE1	15.23	1.42	1.25
1	A	569	SER	CB-OG	-8.49	1.31	1.42
1	A	409	GLU	CG-CD	7.84	1.63	1.51
1	A	581	GLU	CG-CD	6.83	1.62	1.51
1	A	392	TYR	CB-CG	6.53	1.61	1.51
1	A	409	GLU	CB-CG	6.02	1.63	1.52
1	A	850	ARG	CZ-NH2	5.94	1.40	1.33
1	A	240	GLU	CD-OE2	5.79	1.32	1.25
1	A	272	GLY	CA-C	5.22	1.60	1.51
1	A	438	GLU	CG-CD	5.04	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	850	ARG	NE-CZ-NH2	13.84	127.22	120.30
1	A	850	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	A	736	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	859	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	A	859	ARG	NE-CZ-NH2	8.71	124.66	120.30
1	A	778	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	736	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	467	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	510	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	320	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	A	778	ARG	NE-CZ-NH1	6.21	123.41	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	732	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	175	THR	OG1-CB-CG2	5.60	122.88	110.00
1	A	96	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	617	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	78	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	78	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	467	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	119	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	28	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	803	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	28	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	323	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	174	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	291	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	283	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	A	799	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	617	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	572	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	320	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	490	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	175	THR	N-CA-CB	-5.03	100.73	110.30
1	A	365	ASP	CB-CG-OD1	5.02	122.82	118.30

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	6808	0	6550	31	0
2	B	1	0	0	0	0
3	C	1	0	0	0	0
4	E	18	0	24	1	0
5	F	4	0	3	3	0
6	S	796	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7628	0	6577	31	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 2.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:HG2	6:S:83:HOH:O	1.92	0.68
1:A:175:THR:HG21	1:A:179:THR:OG1	1.92	0.68
1:A:175:THR:HG22	1:A:177:GLU:H	1.59	0.68
1:A:173:THR:HG23	6:S:821:HOH:O	1.96	0.64
1:A:133:THR:HG21	6:S:81:HOH:O	1.97	0.63
1:A:567:GLN:NE2	6:S:858:HOH:O	2.36	0.58
1:A:188:LYS:H	5:F:1:ACT:CH3	2.17	0.57
1:A:187:THR:HA	5:F:1:ACT:H2	1.87	0.56
1:A:584:ARG:NH1	6:S:492:HOH:O	2.27	0.54
1:A:295:TYR:CE1	1:A:299:ARG:HD3	2.44	0.51
1:A:175:THR:CG2	1:A:177:GLU:H	2.22	0.50
1:A:295:TYR:CZ	1:A:299:ARG:HD3	2.46	0.50
1:A:188:LYS:H	5:F:1:ACT:H3	1.77	0.49
1:A:188:LYS:HD3	1:A:424:TRP:CH2	2.48	0.47
1:A:292:VAL:HB	1:A:296:LEU:HD12	1.97	0.47
1:A:318:THR:O	1:A:426:ASN:HA	2.14	0.47
1:A:637:GLU:OE1	1:A:640[A]:ARG:NH1	2.48	0.47
1:A:175:THR:HG21	1:A:179:THR:HG1	1.82	0.44
1:A:494:LEU:C	1:A:494:LEU:HD12	2.37	0.44
1:A:133:THR:CG2	1:A:134:ALA:N	2.80	0.44
1:A:385:VAL:HG23	1:A:386:ASN:OD1	2.18	0.44
1:A:512[B]:HIS:CD2	1:A:531:VAL:HG13	2.53	0.44
1:A:793:ASP:OD2	1:A:833:HIS:CE1	2.71	0.43
1:A:817:VAL:O	4:E:3:GOL:H2	2.19	0.42
1:A:366:GLN:OE1	1:A:584:ARG:NH2	2.46	0.42
1:A:363:ARG:O	1:A:850:ARG:NH1	2.50	0.42
1:A:2:ALA:N	1:A:84:GLU:OE1	2.52	0.42
1:A:273:ALA:HA	1:A:281:THR:O	2.20	0.41
1:A:190:MET:CE	1:A:194:LEU:HB2	2.49	0.41
1:A:133:THR:HG23	1:A:134:ALA:N	2.35	0.41
1:A:283:LEU:HD23	1:A:286:TYR:CD2	2.56	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	866/884 (98%)	846 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	704/717 (98%)	689 (98%)	15 (2%)	53	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	133	THR
1	A	175	THR
1	A	232[A]	LEU
1	A	232[B]	LEU
1	A	260	LYS
1	A	283	LEU
1	A	355	SER
1	A	390	ILE
1	A	461[A]	ARG
1	A	461[B]	ARG
1	A	468	ASP
1	A	476	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	587	GLU
1	A	723	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	HIS

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
5	ACT	F	1	-	1,3,3	7.48	1 (100%)	0,3,3	0.00	-
4	GOL	E	3	-	5,5,5	0.71	0	5,5,5	0.68	0
4	GOL	E	2	-	5,5,5	0.36	0	5,5,5	0.87	0
4	GOL	E	1	-	5,5,5	0.91	0	5,5,5	0.93	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	E	3	-	-	4/4/4/4	-
4	GOL	E	2	-	-	1/4/4/4	-
4	GOL	E	1	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	ACT	CH3-C	-7.48	1.39	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	3	GOL	C1-C2-C3-O3
4	E	2	GOL	O1-C1-C2-C3
4	E	3	GOL	O1-C1-C2-C3
4	E	3	GOL	O2-C2-C3-O3
4	E	3	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	ACT	3	0
4	E	3	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	859/884 (97%)	-0.14	29 (3%) 45 48	14, 24, 44, 71	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	PRO	3.3
1	A	468	ASP	3.2
1	A	800	SER	3.2
1	A	195	VAL	3.2
1	A	385	VAL	3.2
1	A	194	LEU	2.9
1	A	55	GLY	2.7
1	A	469	GLU	2.6
1	A	759	GLN	2.5
1	A	803	ARG	2.5
1	A	602	PRO	2.5
1	A	196	ALA	2.4
1	A	801	SER	2.4
1	A	92	GLU	2.4
1	A	80	SER	2.4
1	A	37	GLU	2.3
1	A	193	TYR	2.3
1	A	214	GLY	2.3
1	A	506	GLY	2.2
1	A	504	ALA	2.2
1	A	81	ASP	2.2
1	A	797	HIS	2.2
1	A	212	ASP	2.2
1	A	192	THR	2.2
1	A	121	VAL	2.2
1	A	198	VAL	2.1
1	A	197	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	802	GLU	2.1
1	A	723	GLU	2.1

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

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

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($\text{\AA}^2$)	Q<0.9
4	GOL	E	3	6/?	0.87	0.33	39,49,52,56	0
5	ACT	F	1	4/?	0.92	0.11	15,26,32,34	0
4	GOL	E	2	6/?	0.93	0.21	29,39,41,52	0
4	GOL	E	1	6/?	0.97	0.07	20,28,35,44	0
3	CA	C	3	1/?	0.98	0.04	26,26,26,26	1
2	ZN	B	4	1/?	1.00	0.06	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.