



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2023 – 06:07 PM EDT

PDB ID : 7UVH
Title : Pfs230 domain 1 bound by RUPA-32 Fab
Authors : Ivanochko, D.; Newton, J.; Julien, J.P.
Deposited on : 2022-05-02
Resolution : 2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

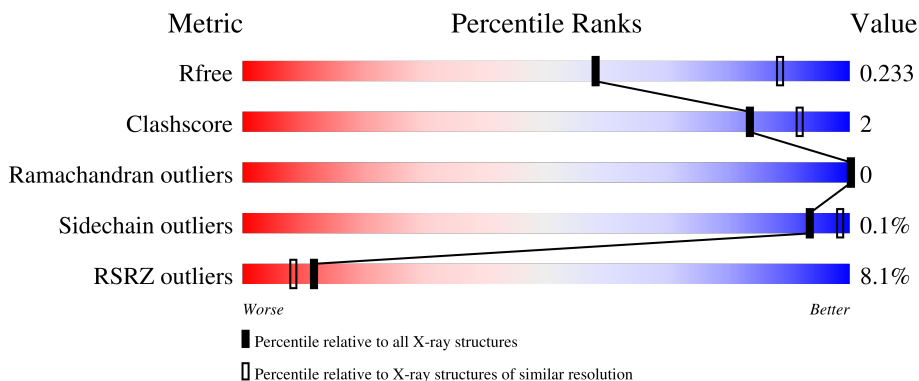
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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.



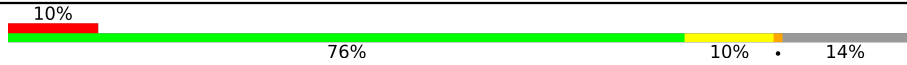
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	225	 3% 94% 5%
1	D	225	 13% 93% 5%
2	B	215	 93% 7%
2	E	215	 9% 86% 12%
3	C	199	 11% 80% 17%

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Mol	Chain	Length	Quality of chain
3	F	199	 <p>10% 76% 10% • 14%</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9382 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 RUPA-32 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total 1648	C 1040	N 276	O 325	S 7	0	0	0
1	D	222	Total 1648	C 1040	N 276	O 325	S 7	0	0	0

- Molecule 2 is a protein called RUPA-32 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	215	Total 1653	C 1032	N 283	O 332	S 6	0	0	0
2	E	211	Total 1623	C 1016	N 276	O 326	S 5	0	0	0

- Molecule 3 is a protein called Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	165	Total 1316	C 844	N 206	O 262	S 4	0	0	0
3	F	171	Total 1366	C 875	N 212	O 275	S 4	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

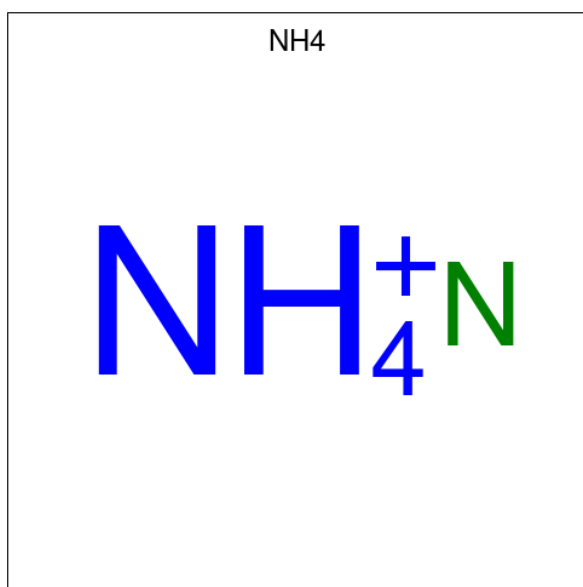
Chain	Residue	Modelled	Actual	Comment	Reference
C	585	GLN	ASN	conflict	UNP P68874
C	732	GLY	-	expression tag	UNP P68874
C	733	SER	-	expression tag	UNP P68874
C	734	LEU	-	expression tag	UNP P68874
C	735	LYS	-	expression tag	UNP P68874
C	736	GLU	-	expression tag	UNP P68874
C	737	ASN	-	expression tag	UNP P68874
C	738	LEU	-	expression tag	UNP P68874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	739	TYR	-	expression tag	UNP P68874
C	740	PHE	-	expression tag	UNP P68874
C	741	GLN	-	expression tag	UNP P68874
C	742	GLY	-	expression tag	UNP P68874
C	743	TRP	-	expression tag	UNP P68874
C	744	SER	-	expression tag	UNP P68874
C	745	HIS	-	expression tag	UNP P68874
C	746	PRO	-	expression tag	UNP P68874
C	747	GLN	-	expression tag	UNP P68874
C	748	PHE	-	expression tag	UNP P68874
C	749	GLU	-	expression tag	UNP P68874
C	750	LYS	-	expression tag	UNP P68874
F	585	GLN	ASN	conflict	UNP P68874
F	732	GLY	-	expression tag	UNP P68874
F	733	SER	-	expression tag	UNP P68874
F	734	LEU	-	expression tag	UNP P68874
F	735	LYS	-	expression tag	UNP P68874
F	736	GLU	-	expression tag	UNP P68874
F	737	ASN	-	expression tag	UNP P68874
F	738	LEU	-	expression tag	UNP P68874
F	739	TYR	-	expression tag	UNP P68874
F	740	PHE	-	expression tag	UNP P68874
F	741	GLN	-	expression tag	UNP P68874
F	742	GLY	-	expression tag	UNP P68874
F	743	TRP	-	expression tag	UNP P68874
F	744	SER	-	expression tag	UNP P68874
F	745	HIS	-	expression tag	UNP P68874
F	746	PRO	-	expression tag	UNP P68874
F	747	GLN	-	expression tag	UNP P68874
F	748	PHE	-	expression tag	UNP P68874
F	749	GLU	-	expression tag	UNP P68874
F	750	LYS	-	expression tag	UNP P68874

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	D	1	Total N 1 1	0	0

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

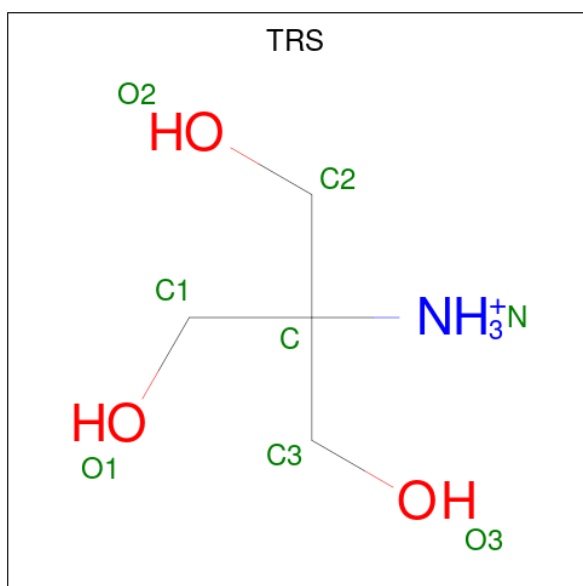
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	4	Total Cl 4 4	0	0
5	D	3	Total Cl 3 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			8	4	1	3		
7	F	1	Total	C	N	O	0	0
			8	4	1	3		

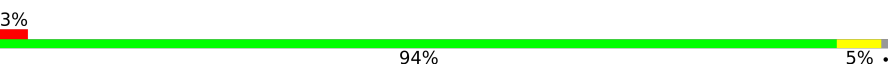
- Molecule 8 is water.

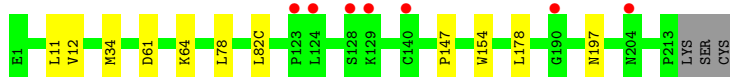
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	27	Total	O	0	0
			27	27		
8	C	9	Total	O	0	0
			9	9		
8	D	14	Total	O	0	0
			14	14		
8	E	10	Total	O	0	0
			10	10		
8	F	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

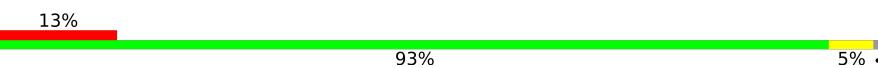
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

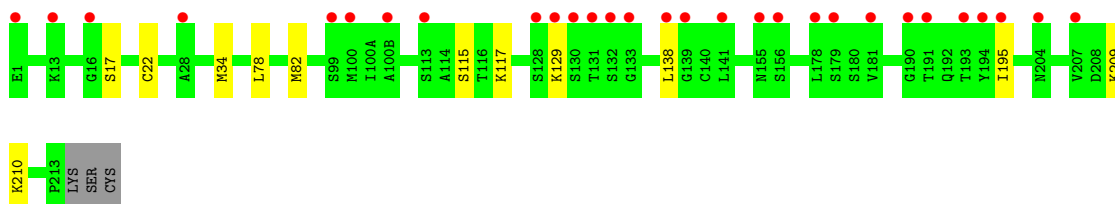
- Molecule 1: RUPA-32 Fab Heavy Chain

Chain A: 



- Molecule 1: RUPA-32 Fab Heavy Chain

Chain D: 




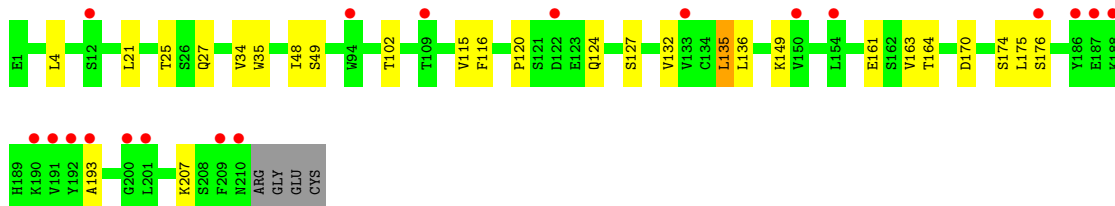
- Molecule 2: RUPA-32 Fab Light Chain

Chain B: 

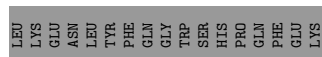
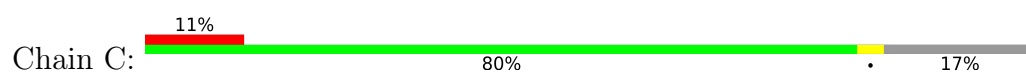


- Molecule 2: RUPA-32 Fab Light Chain

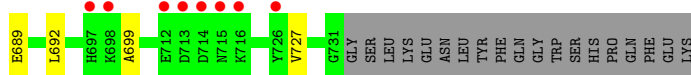
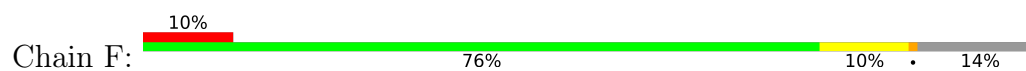
Chain E: 



- Molecule 3: Gametocyte surface protein P230



- Molecule 3: Gametocyte surface protein P230



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.87Å 80.47Å 124.96Å 90.00° 111.81° 90.00°	Depositor
Resolution (Å)	29.43 – 2.59 29.43 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.43-2.59) 100.0 (29.43-2.59)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.196 , 0.233 0.196 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9382	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: TRS, NH4, CL, EDO

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	0.56	0/1688	0.77	1/2296 (0.0%)
1	D	0.52	0/1688	0.75	1/2296 (0.0%)
2	B	0.60	1/1689 (0.1%)	0.81	2/2297 (0.1%)
2	E	0.52	0/1659	0.76	2/2258 (0.1%)
3	C	0.58	0/1341	0.77	0/1813
3	F	0.56	0/1392	0.79	1/1883 (0.1%)
All	All	0.56	1/9457 (0.0%)	0.77	7/12843 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	CYS	CB-SG	-6.07	1.72	1.82

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	666	LEU	CA-CB-CG	7.13	131.70	115.30
2	B	170	ASP	CB-CG-OD1	6.58	124.22	118.30
2	B	47	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	D	138	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	178	LEU	CA-CB-CG	5.36	127.63	115.30

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	1648	0	1617	5	0
1	D	1648	0	1617	7	0
2	B	1653	0	1617	6	0
2	E	1623	0	1590	15	0
3	C	1316	0	1331	3	0
3	F	1366	0	1373	10	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	D	3	0	0	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
6	E	4	0	6	0	0
7	C	8	0	12	0	0
7	F	8	0	12	0	0
8	A	24	0	0	0	0
8	B	27	0	0	1	0
8	C	9	0	0	1	0
8	D	14	0	0	0	0
8	E	10	0	0	0	0
8	F	4	0	0	0	0
All	All	9382	0	9187	44	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.

The worst 5 of 44 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)
3:F:666:LEU:HD12	3:F:667:ILE:HG13	1.86	0.57
3:F:568:GLU:HG2	3:F:657:LYS:HD3	1.86	0.56
3:C:707:ASP:OD2	3:C:720:ARG:NH1	2.40	0.54
2:E:4:LEU:HD22	2:E:25:THR:HG22	1.91	0.53
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.91	0.52

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	220/225 (98%)	214 (97%)	6 (3%)	0	100	100
1	D	220/225 (98%)	217 (99%)	3 (1%)	0	100	100
2	B	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
2	E	209/215 (97%)	207 (99%)	2 (1%)	0	100	100
3	C	163/199 (82%)	159 (98%)	4 (2%)	0	100	100
3	F	169/199 (85%)	163 (96%)	6 (4%)	0	100	100
All	All	1194/1278 (93%)	1169 (98%)	25 (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	184/187 (98%)	184 (100%)	0	100	100
1	D	184/187 (98%)	184 (100%)	0	100	100
2	B	189/189 (100%)	189 (100%)	0	100	100
2	E	186/189 (98%)	186 (100%)	0	100	100
3	C	154/185 (83%)	154 (100%)	0	100	100
3	F	160/185 (86%)	159 (99%)	1 (1%)	86	95
All	All	1057/1122 (94%)	1056 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	579	TYR

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](#)

Of 17 ligands modelled in this entry, 2 are modelled with single atom and 10 are monoatomic - leaving 5 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	EDO	E	301	-	3,3,3	0.59	0	2,2,2	0.19	0
6	EDO	C	801	-	3,3,3	0.43	0	2,2,2	0.41	0
6	EDO	B	301	-	3,3,3	0.64	0	2,2,2	0.26	0
7	TRS	C	802	-	7,7,7	0.58	0	9,9,9	0.54	0
7	TRS	F	801	-	7,7,7	0.32	0	9,9,9	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
6	EDO	E	301	-	-	0/1/1/1	-
6	EDO	C	801	-	-	1/1/1/1	-
6	EDO	B	301	-	-	0/1/1/1	-
7	TRS	C	802	-	-	4/9/9/9	-
7	TRS	F	801	-	-	5/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	802	TRS	C2-C-C3-O3
7	C	802	TRS	N-C-C3-O3
7	F	801	TRS	N-C-C1-O1
7	F	801	TRS	N-C-C2-O2
7	F	801	TRS	C2-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	222/225 (98%)	0.28	7 (3%) 47 40	42, 65, 102, 127	0
1	D	222/225 (98%)	0.68	29 (13%) 3 2	49, 78, 134, 237	0
2	B	215/215 (100%)	0.05	1 (0%) 91 89	46, 60, 87, 104	0
2	E	211/215 (98%)	0.60	19 (9%) 9 6	47, 85, 127, 141	0
3	C	165/199 (82%)	0.75	22 (13%) 3 2	50, 72, 135, 178	0
3	F	171/199 (85%)	0.85	20 (11%) 4 3	55, 81, 120, 154	0
All	All	1206/1278 (94%)	0.51	98 (8%) 12 8	42, 72, 122, 237	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	573	ALA	8.7
3	F	715	ASN	6.5
1	D	131	THR	6.1
3	C	656	THR	6.1
1	D	132	SER	6.0

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(Å ²)	Q<0.9
7	TRS	F	801	8/8	0.68	0.34	103,103,103,103	0
7	TRS	C	802	8/8	0.73	0.29	89,89,89,89	0
5	CL	B	302	1/1	0.82	0.12	93,93,93,93	0
6	EDO	C	801	4/4	0.82	0.26	82,82,82,82	0
6	EDO	B	301	4/4	0.86	0.27	59,59,59,59	0
5	CL	B	304	1/1	0.90	0.09	89,89,89,89	0
5	CL	B	303	1/1	0.92	0.13	80,80,80,80	0
6	EDO	E	301	4/4	0.92	0.22	66,66,67,70	0
4	NH4	D	301	1/1	0.93	0.45	39,39,39,39	0
5	CL	D	303	1/1	0.94	0.06	83,83,83,83	0
5	CL	A	303	1/1	0.95	0.06	76,76,76,76	0
5	CL	A	302	1/1	0.95	0.07	68,68,68,68	0
5	CL	D	302	1/1	0.95	0.08	61,61,61,61	1
5	CL	A	304	1/1	0.96	0.09	81,81,81,81	0
5	CL	D	304	1/1	0.97	0.05	81,81,81,81	0
5	CL	B	305	1/1	0.97	0.24	64,64,64,64	0
4	NH4	A	301	1/1	0.98	0.56	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.