wwPDB X-ray Structure Validation Summary Report (i)

Sep 23, 2020 – 10:33 PM BST

PDB ID	:	6ZEJ
Title	:	Structure of PP1-Phactr1 chimera [PP1(7-304) + linker (SGSGS) + Phactr1(526-580)]
Authors	:	Mouilleron, S.; Treisman, R.; Fedoryshchak, R.; Lee, R.; Butler, A.M.; Prechova, M.
Deposited on	:	2020-06-16
Resolution	:	1.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

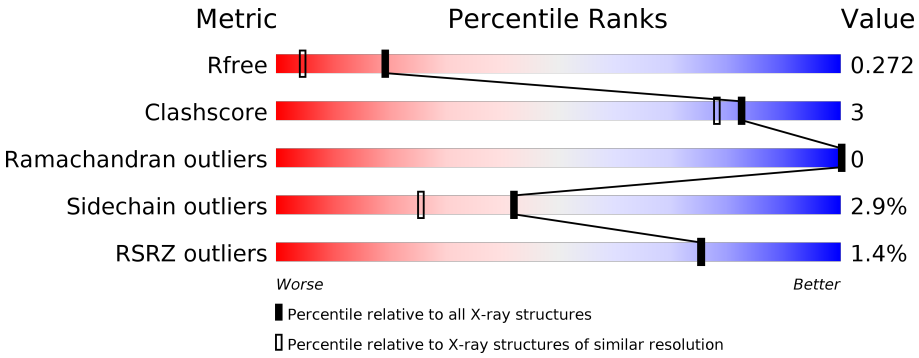
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	363	84% 12%
1	D	363	88% 7%
1	F	363	87% 9%
1	I	363	88% 8%
1	L	363	86% 9%
1	O	363	91% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33602 atoms, of which 16188 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	348	Total	C	H	N	O	S	0	1	0
			5456	1768	2686	475	507	20			
1	A	348	Total	C	H	N	O	S	0	1	0
			5518	1782	2724	481	513	18			
1	F	348	Total	C	H	N	O	S	0	1	0
			5443	1767	2674	471	511	20			
1	I	351	Total	C	H	N	O	S	0	0	0
			5448	1771	2669	470	519	19			
1	L	348	Total	C	H	N	O	S	0	0	0
			5433	1765	2668	470	512	18			
1	O	351	Total	C	H	N	O	S	0	1	0
			5522	1786	2717	482	518	19			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP P62136
D	2	HIS	-	expression tag	UNP P62136
D	3	MET	-	expression tag	UNP P62136
D	4	GLY	-	expression tag	UNP P62136
D	5	SER	-	expression tag	UNP P62136
D	305	SER	-	linker	UNP P62136
D	306	GLY	-	linker	UNP P62136
D	307	SER	-	linker	UNP P62136
D	308	GLY	-	linker	UNP P62136
D	309	SER	-	linker	UNP P62136
A	1	GLY	-	expression tag	UNP P62136
A	2	HIS	-	expression tag	UNP P62136
A	3	MET	-	expression tag	UNP P62136
A	4	GLY	-	expression tag	UNP P62136
A	5	SER	-	expression tag	UNP P62136
A	305	SER	-	linker	UNP P62136

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Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLY	-	linker	UNP P62136
A	307	SER	-	linker	UNP P62136
A	308	GLY	-	linker	UNP P62136
A	309	SER	-	linker	UNP P62136
F	1	GLY	-	expression tag	UNP P62136
F	2	HIS	-	expression tag	UNP P62136
F	3	MET	-	expression tag	UNP P62136
F	4	GLY	-	expression tag	UNP P62136
F	5	SER	-	expression tag	UNP P62136
F	305	SER	-	linker	UNP P62136
F	306	GLY	-	linker	UNP P62136
F	307	SER	-	linker	UNP P62136
F	308	GLY	-	linker	UNP P62136
F	309	SER	-	linker	UNP P62136
I	1	GLY	-	expression tag	UNP P62136
I	2	HIS	-	expression tag	UNP P62136
I	3	MET	-	expression tag	UNP P62136
I	4	GLY	-	expression tag	UNP P62136
I	5	SER	-	expression tag	UNP P62136
I	305	SER	-	linker	UNP P62136
I	306	GLY	-	linker	UNP P62136
I	307	SER	-	linker	UNP P62136
I	308	GLY	-	linker	UNP P62136
I	309	SER	-	linker	UNP P62136
L	1	GLY	-	expression tag	UNP P62136
L	2	HIS	-	expression tag	UNP P62136
L	3	MET	-	expression tag	UNP P62136
L	4	GLY	-	expression tag	UNP P62136
L	5	SER	-	expression tag	UNP P62136
L	305	SER	-	linker	UNP P62136
L	306	GLY	-	linker	UNP P62136
L	307	SER	-	linker	UNP P62136
L	308	GLY	-	linker	UNP P62136
L	309	SER	-	linker	UNP P62136
O	1	GLY	-	expression tag	UNP P62136
O	2	HIS	-	expression tag	UNP P62136
O	3	MET	-	expression tag	UNP P62136
O	4	GLY	-	expression tag	UNP P62136
O	5	SER	-	expression tag	UNP P62136
O	305	SER	-	linker	UNP P62136
O	306	GLY	-	linker	UNP P62136
O	307	SER	-	linker	UNP P62136

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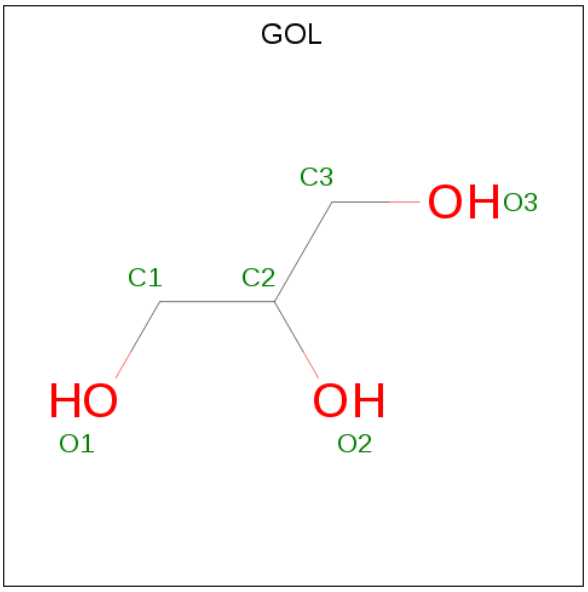
Chain	Residue	Modelled	Actual	Comment	Reference
O	308	GLY	-	linker	UNP P62136
O	309	SER	-	linker	UNP P62136

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	O	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 12 3 6 3	0	0
3	A	1	Total C H O 13 3 7 3	0	0

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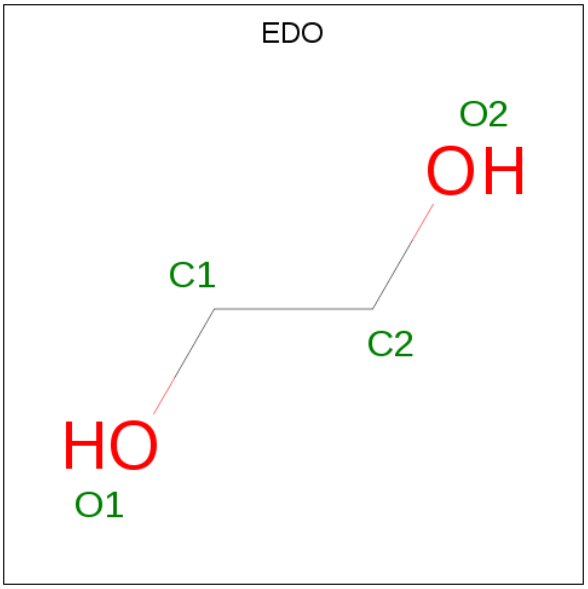
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C H O 13 3 7 3	0	0
3	I	1	Total C H O 13 3 7 3	0	0
3	O	1	Total C H O 11 3 5 3	0	0
3	O	1	Total C H O 13 3 7 3	0	0
3	O	1	Total C H O 11 3 5 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	107	Total O 107 107	0	0
5	A	142	Total O 142 142	0	0
5	F	95	Total O 95 95	0	0

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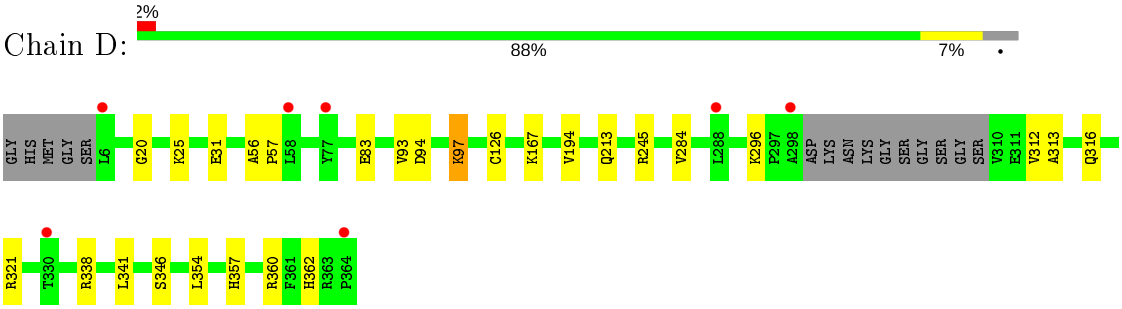
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	94	Total O 94 94	0	0
5	L	102	Total O 102 102	0	0
5	O	134	Total O 134 134	0	0

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.

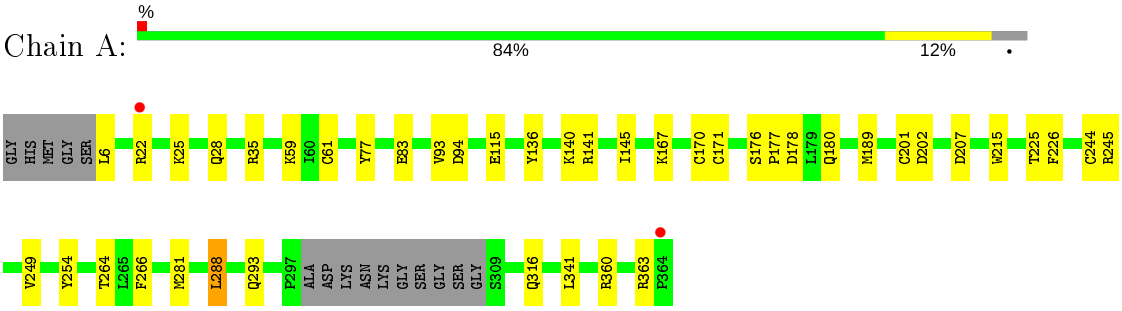
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain D:



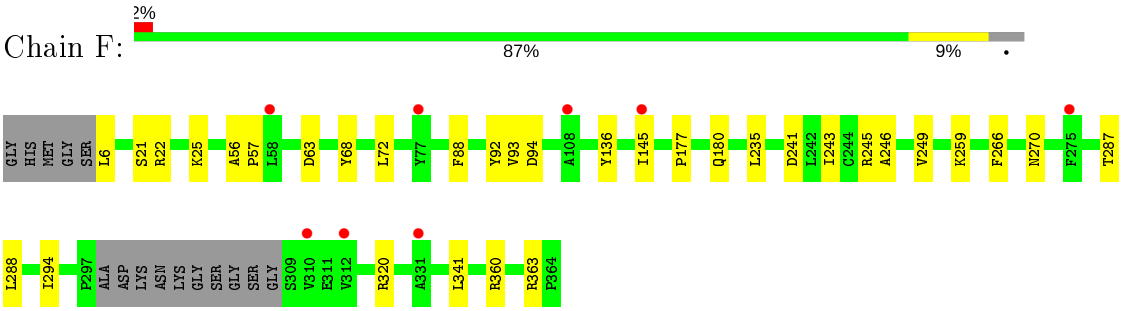
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain A:



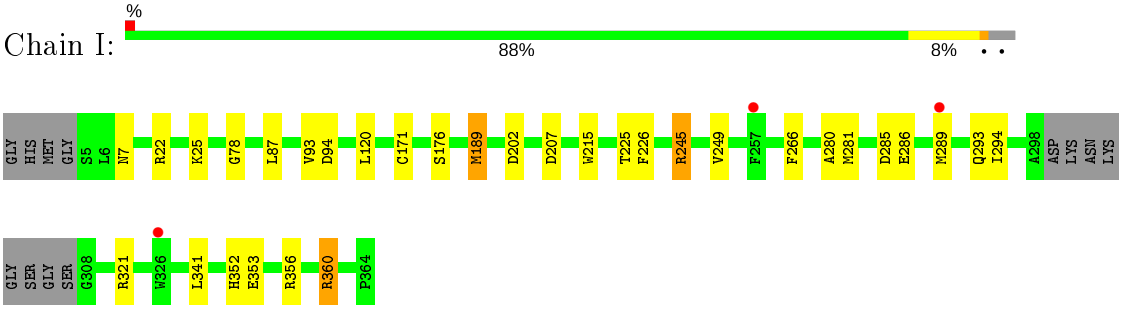
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain F:



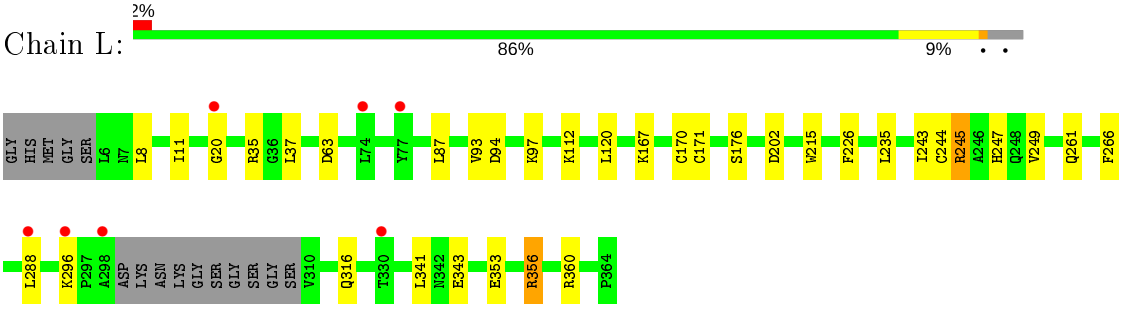
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain I:



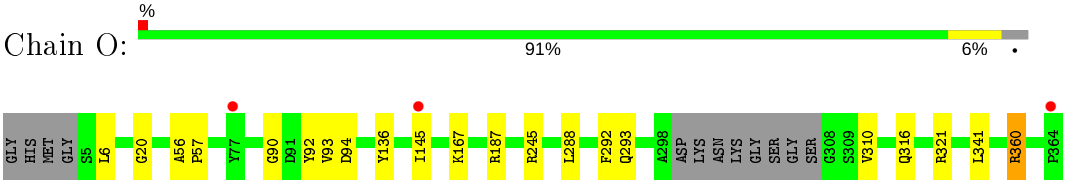
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain L:



• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit,Phosphatase and actin regulator

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	137.37Å 137.37Å 238.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.68 – 1.78 68.69 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (68.68-1.78) 99.7 (68.69-1.78)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.18_3845, PHENIX 1.18_3845	Depositor
R, R_{free}	0.242 , 0.271 0.242 , 0.272	Depositor DCC
R_{free} test set	12173 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	33602	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 62.07 % 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 1.1918e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, 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	0.60	2/2860 (0.1%)	0.60	0/3865
1	D	0.56	0/2836	0.55	0/3835
1	F	0.52	0/2835	0.54	0/3836
1	I	0.50	0/2842	0.53	0/3846
1	L	0.49	0/2828	0.53	0/3826
1	O	0.62	0/2871	0.59	0/3882
All	All	0.55	2/17072 (0.0%)	0.56	0/23090

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	CYS	CB-SG	-5.71	1.72	1.81
1	A	171	CYS	CB-SG	-5.71	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

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	2794	2724	2722	18	2
1	D	2770	2686	2686	13	1
1	F	2769	2674	2674	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2779	2669	2669	14	1
1	L	2765	2668	2668	16	2
1	O	2805	2717	2717	12	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
2	F	2	0	0	0	0
2	I	2	0	0	0	0
2	L	2	0	0	0	0
2	O	2	0	0	0	0
3	A	12	13	16	0	0
3	F	6	7	8	0	0
3	I	6	7	8	1	0
3	O	18	17	23	2	0
4	A	4	6	6	1	0
5	A	142	0	0	3	0
5	D	107	0	0	4	1
5	F	95	0	0	1	0
5	I	94	0	0	0	0
5	L	102	0	0	1	1
5	O	134	0	0	1	0
All	All	17414	16188	16197	83	4

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.

The worst 5 of 83 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:L:353:GLU:OE2	1:L:356:ARG:NH1	2.07	0.88
1:D:97:LYS:NZ	1:D:321:ARG:O	2.12	0.82
1:A:115:GLU:OE2	5:A:501:HOH:O	2.02	0.78
1:F:241:ASP:OD2	5:F:501:HOH:O	2.04	0.74
1:F:22:ARG:N	1:O:20:GLY:O	2.23	0.72

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:537:HOH:O	5:L:583:HOH:O[6_554]	2.04	0.16
1:A:22:ARG:N	1:L:20:GLY:O[6_554]	2.10	0.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLY:O	1:I:22:ARG:H[6_554]	1.55	0.05
1:A:22:ARG:H	1:L:20:GLY:O[6_554]	1.58	0.02

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	345/363 (95%)	330 (96%)	15 (4%)	0	100	100
1	D	345/363 (95%)	329 (95%)	16 (5%)	0	100	100
1	F	345/363 (95%)	331 (96%)	14 (4%)	0	100	100
1	I	347/363 (96%)	331 (95%)	16 (5%)	0	100	100
1	L	344/363 (95%)	329 (96%)	15 (4%)	0	100	100
1	O	348/363 (96%)	338 (97%)	10 (3%)	0	100	100
All	All	2074/2178 (95%)	1988 (96%)	86 (4%)	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	299/316 (95%)	288 (96%)	11 (4%)	34	17
1	D	294/316 (93%)	286 (97%)	8 (3%)	44	28
1	F	295/316 (93%)	286 (97%)	9 (3%)	40	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	295/316 (93%)	287 (97%)	8 (3%)	44 28
1	L	293/316 (93%)	284 (97%)	9 (3%)	40 22
1	O	299/316 (95%)	292 (98%)	7 (2%)	50 34
All	All	1775/1896 (94%)	1723 (97%)	52 (3%)	42 25

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	288	LEU
1	I	189	MET
1	O	316	GLN
1	F	294	ILE
1	F	360	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.18	0
3	GOL	A	402	-	5,5,5	0.52	0	5,5,5	1.21	1 (20%)
3	GOL	O	403	-	5,5,5	1.34	1 (20%)	5,5,5	1.12	0
3	GOL	A	401	-	5,5,5	0.86	0	5,5,5	1.08	0
3	GOL	F	401	-	5,5,5	0.47	0	5,5,5	0.72	0
3	GOL	O	402	-	5,5,5	0.43	0	5,5,5	1.03	0
3	GOL	I	401	-	5,5,5	0.81	0	5,5,5	0.83	0
3	GOL	O	401	-	5,5,5	0.96	0	5,5,5	1.00	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	EDO	A	403	-	-	1/1/1/1	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	O	403	-	-	2/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	F	401	-	-	2/4/4/4	-
3	GOL	O	402	-	-	1/4/4/4	-
3	GOL	I	401	-	-	2/4/4/4	-
3	GOL	O	401	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	403	GOL	O2-C2	-2.58	1.35	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	GOL	C3-C2-C1	-2.05	103.74	111.70

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	403	GOL	O1-C1-C2-C3
3	I	401	GOL	O1-C1-C2-C3
3	I	401	GOL	O1-C1-C2-O2
3	O	401	GOL	C1-C2-C3-O3
3	F	401	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	EDO	1	0
3	O	403	GOL	2	0
3	I	401	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, 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	348/363 (95%)	0.03	2 (0%)	89	89	19, 33, 50, 75	0
1	D	348/363 (95%)	0.14	7 (2%)	65	65	30, 39, 61, 89	0
1	F	348/363 (95%)	0.24	8 (2%)	60	60	29, 44, 65, 81	0
1	I	351/363 (96%)	0.26	3 (0%)	84	84	33, 44, 65, 93	0
1	L	348/363 (95%)	0.20	7 (2%)	65	65	32, 42, 60, 74	0
1	O	351/363 (96%)	0.07	3 (0%)	84	84	19, 32, 55, 74	0
All	All	2094/2178 (96%)	0.16	30 (1%)	75	75	19, 40, 61, 93	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	TYR	4.4
1	L	77	TYR	4.2
1	I	326	TRP	3.5
1	A	364	PRO	3.5
1	F	312	VAL	3.5

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^{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	GOL	O	402	6/6	0.87	0.10	38,46,56,57	0
3	GOL	F	401	6/6	0.89	0.14	45,54,58,62	0
3	GOL	A	401	6/6	0.91	0.12	34,42,47,47	0
2	MN	L	402	1/1	0.91	0.07	81,81,81,81	0
2	MN	A	404	1/1	0.92	0.18	48,48,48,48	0
3	GOL	I	401	6/6	0.92	0.07	41,54,56,67	0
2	MN	D	402	1/1	0.92	0.10	78,78,78,78	0
4	EDO	A	403	4/4	0.94	0.09	47,56,61,61	0
3	GOL	O	401	6/6	0.94	0.11	34,43,56,56	0
2	MN	I	403	1/1	0.95	0.09	79,79,79,79	0
3	GOL	O	403	6/6	0.95	0.17	33,40,48,48	0
2	MN	O	405	1/1	0.96	0.09	63,63,63,63	0
2	MN	O	404	1/1	0.96	0.13	27,27,27,27	0
2	MN	A	405	1/1	0.96	0.08	65,65,65,65	0
2	MN	F	403	1/1	0.97	0.07	77,77,77,77	0
3	GOL	A	402	6/6	0.97	0.08	26,32,36,41	0
2	MN	I	402	1/1	0.97	0.17	32,32,32,32	0
2	MN	D	401	1/1	0.99	0.15	33,33,33,33	0
2	MN	L	401	1/1	0.99	0.19	33,33,33,33	0
2	MN	F	402	1/1	0.99	0.15	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.