



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:37 am BST

PDB ID : 4YOS
Title : p107 pocket domain complexed with LIN52 peptide
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Deposited on : 2015-03-12
Resolution : 2.30 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

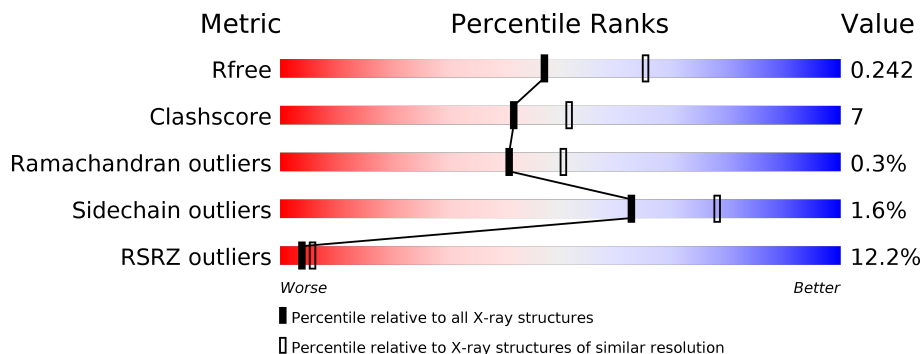
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	369	<p>9% 77% 14% • 8%</p>
2	E	20	<p>50% 45% 10% 10% 35%</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2970 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 Retinoblastoma-like protein 1, Retinoblastoma-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2743	1764	462	499	18	0	0	0

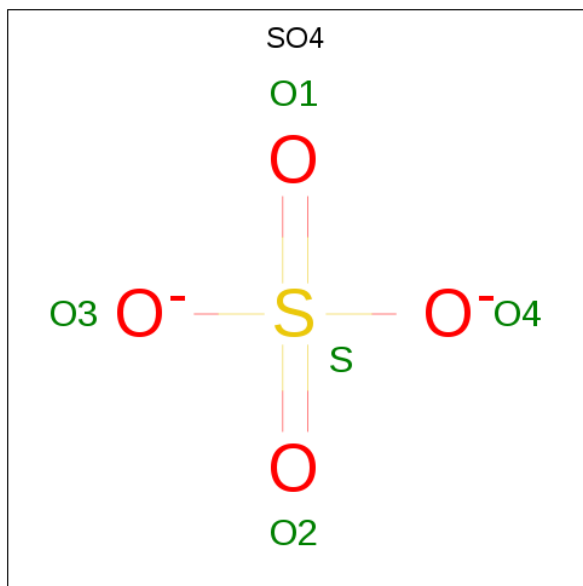
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	GLY	-	expression tag	UNP P28749
A	389	GLU	-	expression tag	UNP P28749
A	390	PHE	-	expression tag	UNP P28749
A	780	GLY	GLY	linker	UNP P28749
A	?	-	PRO	deletion	UNP L5LUA8
A	?	-	ARG	deletion	UNP L5LUA8
A	?	-	GLU	deletion	UNP L5LUA8
A	?	-	ILE	deletion	UNP L5LUA8
A	?	-	VAL	deletion	UNP L5LUA8
A	?	-	ALA	deletion	UNP L5LUA8
A	?	-	TYR	deletion	UNP L5LUA8
A	?	-	ASN	deletion	UNP L5LUA8
A	?	-	LYS	deletion	UNP L5LUA8
A	?	-	LYS	deletion	UNP L5LUA8
A	?	-	VAL	deletion	UNP L5LUA8
A	?	-	ASN	deletion	UNP L5LUA8
A	?	-	GLY	deletion	UNP L5LUA8
A	?	-	ASP	deletion	UNP L5LUA8
A	?	-	PHE	deletion	UNP L5LUA8
A	?	-	GLU	deletion	UNP L5LUA8
A	?	-	MET	deletion	UNP L5LUA8
A	?	-	THR	deletion	UNP L5LUA8
A	?	-	ASP	deletion	UNP L5LUA8
A	?	-	CYS	deletion	UNP L5LUA8
A	?	-	VAL	deletion	UNP L5LUA8
A	924	LYS	ARG	conflict	UNP L5LUA8

- Molecule 2 is a protein called Protein lin-52 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
2	E	13	106	65	17	23	1	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

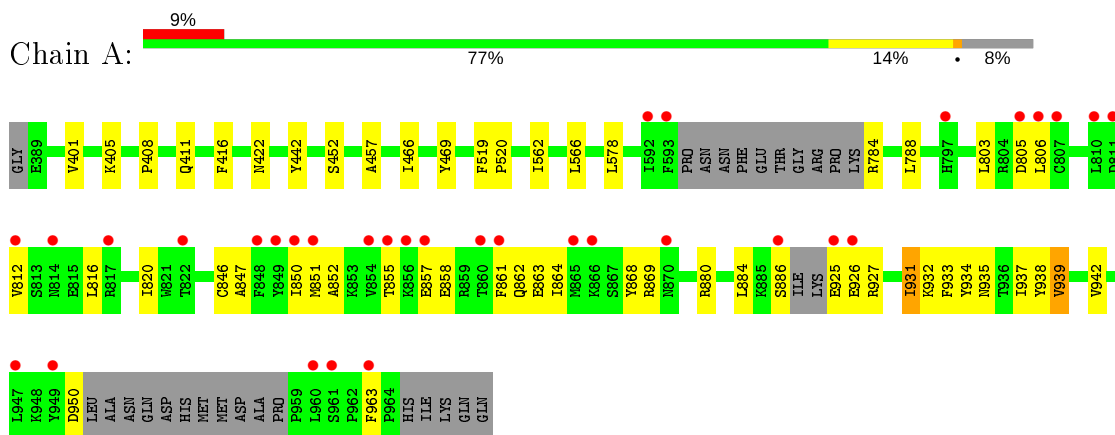
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	95	Total O 95 95	0	0

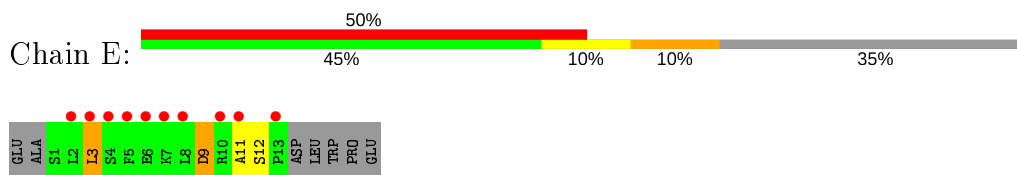
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Retinoblastoma-like protein 1,Retinoblastoma-like protein 1



- Molecule 2: Protein lin-52 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.43Å 101.06Å 140.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.45 – 2.30 60.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (60.45-2.30) 99.4 (60.45-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.242 0.202 , 0.242	Depositor DCC
R_{free} test set	2469 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.653	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2970	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: SEP, EDO, 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	0.28	0/2800	0.43	0/3790
2	E	0.40	0/96	0.97	1/125 (0.8%)
All	All	0.29	0/2896	0.46	1/3915 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	3	LEU	CA-CB-CG	6.82	130.98	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	2743	0	2716	37	0
2	E	106	0	105	6	0
3	A	10	0	0	0	0
4	A	16	0	24	0	0
5	A	95	0	0	1	0
All	All	2970	0	2845	40	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 7.

All (40) 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:850:ILE:HD11	1:A:934:TYR:CZ	2.24	0.73
1:A:935:ASN:HB3	2:E:3:LEU:HD23	1.79	0.63
1:A:562:ILE:HA	1:A:566:LEU:HB2	1.79	0.63
1:A:846:CYS:O	1:A:850:ILE:HD13	1.98	0.63
1:A:850:ILE:HD11	1:A:934:TYR:CE1	2.36	0.61
1:A:803:LEU:HD21	1:A:820:ILE:HG23	1.81	0.61
1:A:934:TYR:CE1	1:A:939:VAL:HG13	2.40	0.57
1:A:862:GLN:N	1:A:862:GLN:OE1	2.39	0.56
1:A:805:ASP:OD1	1:A:806:LEU:N	2.39	0.55
1:A:884:LEU:HD11	1:A:932:LYS:HE3	1.89	0.53
2:E:12:SEP:N	2:E:12:SEP:O1P	2.43	0.52
1:A:884:LEU:HA	1:A:937:ILE:HD11	1.92	0.50
1:A:846:CYS:HG	1:A:933:PHE:HE2	1.60	0.50
1:A:820:ILE:HD13	1:A:851:MET:HB2	1.95	0.48
2:E:9:ASP:OD1	2:E:9:ASP:N	2.44	0.48
1:A:938:TYR:CZ	1:A:942:VAL:HG21	2.48	0.48
1:A:851:MET:O	1:A:855:THR:OG1	2.15	0.47
1:A:816:LEU:HD13	1:A:857:GLU:HB2	1.96	0.47
1:A:864:ILE:O	1:A:868:TYR:N	2.48	0.47
2:E:11:ALA:HB1	2:E:12:SEP:HA	1.96	0.46
1:A:869:ARG:NH2	2:E:12:SEP:O3P	2.49	0.46
1:A:405:LYS:HA	1:A:405:LYS:HD2	1.32	0.46
1:A:442:TYR:CD1	1:A:457:ALA:HB2	2.50	0.46
1:A:401:VAL:HB	1:A:466:ILE:HG21	1.98	0.46
1:A:442:TYR:CE1	1:A:452:SER:HB2	2.50	0.46
1:A:886:SER:HA	1:A:925:GLU:HB2	1.98	0.45
1:A:820:ILE:HD11	1:A:847:ALA:C	2.37	0.45
1:A:411:GLN:OE1	5:A:1101:HOH:O	2.20	0.45
1:A:880:ARG:NH2	2:E:11:ALA:HB3	2.32	0.45
1:A:519:PHE:CG	1:A:520:PRO:HA	2.52	0.44
1:A:408:PRO:HD3	1:A:469:TYR:CZ	2.53	0.44
1:A:852:ALA:O	1:A:858:GLU:HA	2.16	0.44
1:A:803:LEU:HD23	1:A:963:PHE:CE1	2.54	0.42
1:A:861:PHE:O	1:A:864:ILE:HG13	2.20	0.42
1:A:931:ILE:HA	1:A:931:ILE:HD12	1.83	0.41
1:A:933:PHE:CD1	1:A:937:ILE:HD12	2.56	0.41
1:A:578:LEU:HA	1:A:788:LEU:HD11	2.02	0.41
1:A:784:ARG:HA	1:A:784:ARG:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PHE:HB3	1:A:422:ASN:OD1	2.21	0.40
1:A:926:GLU:HG2	1:A:927:ARG:H	1.86	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	332/369 (90%)	322 (97%)	9 (3%)	1 (0%)	41 50
2	E	10/20 (50%)	7 (70%)	3 (30%)	0	100 100
All	All	342/389 (88%)	329 (96%)	12 (4%)	1 (0%)	41 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	VAL

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	303/340 (89%)	299 (99%)	4 (1%)	69 82
2	E	11/17 (65%)	10 (91%)	1 (9%)	9 11
All	All	314/357 (88%)	309 (98%)	5 (2%)	62 78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	863	GLU
1	A	931	ILE
1	A	939	VAL
1	A	950	ASP
2	E	9	ASP

Some 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](#)

1 non-standard protein/DNA/RNA residue is 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	SEP	E	12	2	8,9,10	1.58	1 (12%)	8,12,14	1.63	2 (25%)

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	SEP	E	12	2	-	5/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	12	SEP	P-O1P	3.50	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	12	SEP	OG-CB-CA	3.16	111.22	108.14
2	E	12	SEP	OG-P-O1P	2.37	113.11	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	12	SEP	N-CA-CB-OG
2	E	12	SEP	CB-OG-P-O1P
2	E	12	SEP	CB-OG-P-O2P
2	E	12	SEP	CB-OG-P-O3P
2	E	12	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	12	SEP	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	EDO	A	1005	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	A	1004	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	A	1003	-	3,3,3	0.45	0	2,2,2	0.27	0
3	SO4	A	1001	-	4,4,4	0.16	0	6,6,6	0.10	0
4	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.35	0
3	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.06	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	1003	-	-	1/1/1/1	-
4	EDO	A	1005	-	-	0/1/1/1	-
4	EDO	A	1004	-	-	0/1/1/1	-
4	EDO	A	1006	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	EDO	O1-C1-C2-O2
4	A	1006	EDO	O1-C1-C2-O2

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

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	340/369 (92%)	0.66	33 (9%) 7 10	28, 50, 113, 145	0
2	E	12/20 (60%)	4.16	10 (83%) 0 0	106, 126, 145, 147	0
All	All	352/389 (90%)	0.78	43 (12%) 4 6	28, 51, 121, 147	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	5	PHE	12.8
1	A	856	LYS	6.6
2	E	7	LYS	6.6
1	A	812	VAL	5.7
2	E	3	LEU	4.8
1	A	805	ASP	4.3
1	A	861	PHE	4.3
1	A	593	PHE	4.3
1	A	947	LEU	4.3
1	A	592	ILE	4.2
1	A	960	LEU	4.1
1	A	886	SER	4.1
2	E	11	ALA	4.0
1	A	961	SER	3.9
2	E	8	LEU	3.9
1	A	854	VAL	3.7
2	E	2	LEU	3.5
1	A	857	GLU	3.4
1	A	817	ARG	3.4
1	A	963	PHE	3.3
1	A	851	MET	3.2
1	A	949	TYR	3.1
2	E	13	PRO	3.0
1	A	855	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	926	GLU	2.9
2	E	6	GLU	2.9
2	E	10	ARG	2.8
1	A	849	TYR	2.7
1	A	806	LEU	2.6
1	A	807	CYS	2.5
1	A	810	LEU	2.5
1	A	814	ASN	2.5
1	A	848	PHE	2.5
1	A	860	THR	2.5
1	A	925	GLU	2.4
1	A	870	ASN	2.4
2	E	4	SER	2.3
1	A	797	HIS	2.3
1	A	811	ASP	2.3
1	A	822	THR	2.1
1	A	865	MET	2.1
1	A	866	LYS	2.1
1	A	850	ILE	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, 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
2	SEP	E	12	10/11	0.79	0.31	88,128,137,151	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(\AA^2)	Q<0.9
4	EDO	A	1004	4/4	0.71	0.33	65,69,74,75	0
4	EDO	A	1005	4/4	0.86	0.14	63,67,69,70	0
4	EDO	A	1006	4/4	0.89	0.35	53,66,73,74	0
4	EDO	A	1003	4/4	0.92	0.29	46,55,55,69	0
3	SO4	A	1002	5/5	0.94	0.15	85,90,95,98	0
3	SO4	A	1001	5/5	0.98	0.18	31,36,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.