wwPDB X-ray Structure Validation Summary Report (i)

Jul 11, 2016 – 03:56 PM EDT

PDB ID	:	5L3R
Title	:	Structure of the GTPase heterodimer of chloroplast SRP54 and FtsY from Arabidopsis thaliana
Authors	:	Bange, G.; Kribelbauer, J.; Wild, K.; Sinning, I.
Deposited on	:	2016-05-24
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/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:

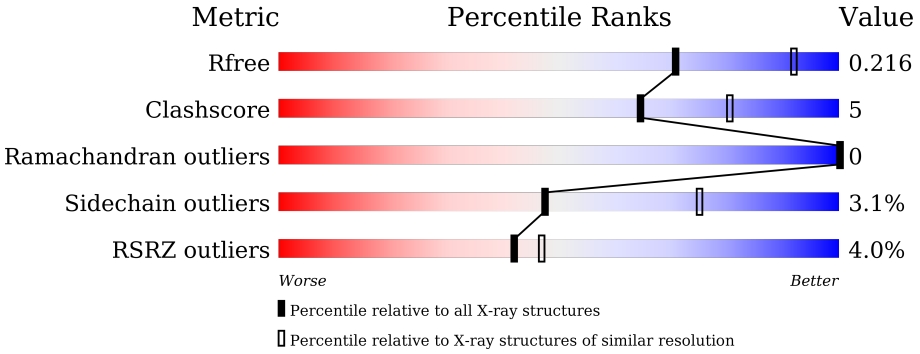
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	301	6% 75% 13% • 11%
1	C	301	8% 77% 12% • 11%
2	B	293	% 88% 11% ••
2	D	293	% 84% 13% ••

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	403	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8672 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 Signal recognition particle 54 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	1997	1260	345	379	13	0	0	0
1	C	269	2015	1273	347	382	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	HIS	-	expression tag	UNP P37107
A	72	HIS	-	expression tag	UNP P37107
A	73	HIS	-	expression tag	UNP P37107
A	74	HIS	-	expression tag	UNP P37107
A	75	HIS	-	expression tag	UNP P37107
A	76	HIS	-	expression tag	UNP P37107
C	71	HIS	-	expression tag	UNP P37107
C	72	HIS	-	expression tag	UNP P37107
C	73	HIS	-	expression tag	UNP P37107
C	74	HIS	-	expression tag	UNP P37107
C	75	HIS	-	expression tag	UNP P37107
C	76	HIS	-	expression tag	UNP P37107

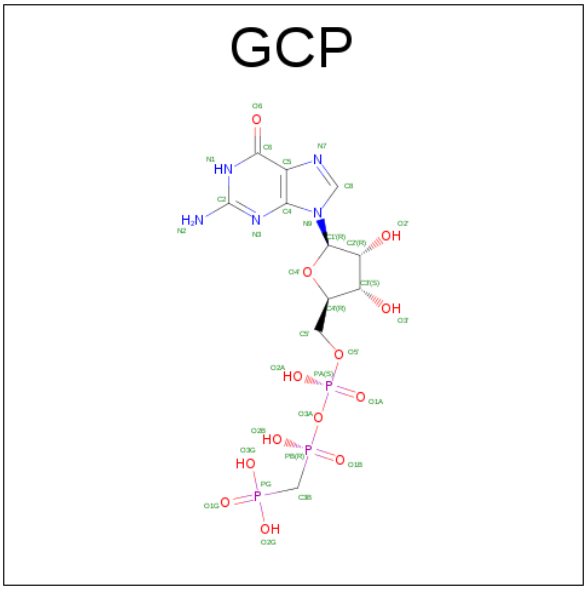
- Molecule 2 is a protein called Cell division protein FtsY homolog, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	290	2193	1387	375	421	10	0	0	0
2	D	289	2183	1381	372	420	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	HIS	-	expression tag	UNP O80842
B	75	HIS	-	expression tag	UNP O80842
B	76	HIS	-	expression tag	UNP O80842
B	77	HIS	-	expression tag	UNP O80842
B	78	HIS	-	expression tag	UNP O80842
B	79	HIS	-	expression tag	UNP O80842
D	74	HIS	-	expression tag	UNP O80842
D	75	HIS	-	expression tag	UNP O80842
D	76	HIS	-	expression tag	UNP O80842
D	77	HIS	-	expression tag	UNP O80842
D	78	HIS	-	expression tag	UNP O80842
D	79	HIS	-	expression tag	UNP O80842

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

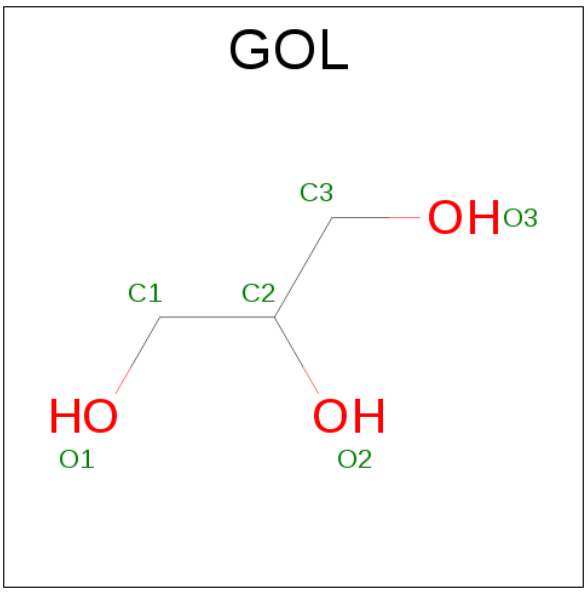


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

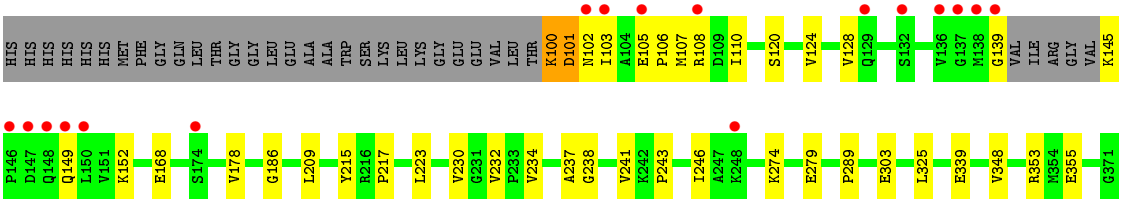
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	42	Total O 42 42	0	0
6	B	38	Total O 38 38	0	0
6	C	13	Total O 13 13	0	0
6	D	47	Total O 47 47	0	0

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 errors 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.

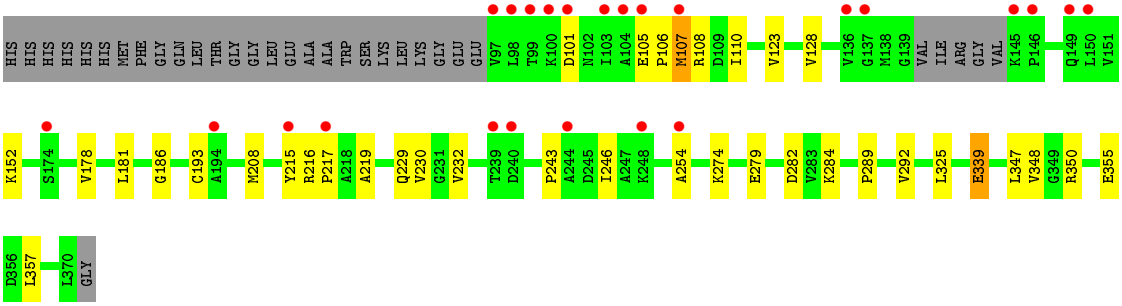
- Molecule 1: Signal recognition particle 54 kDa protein, chloroplastic

Chain A:



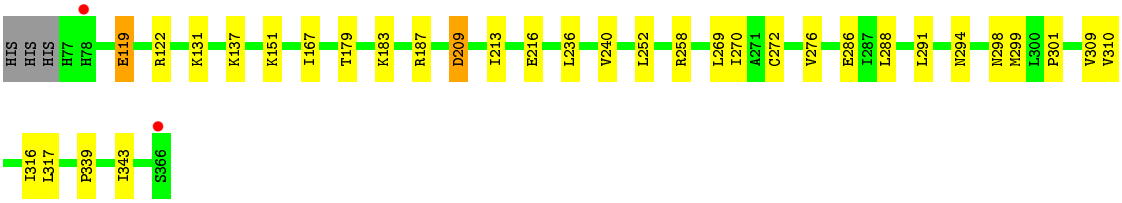
- Molecule 1: Signal recognition particle 54 kDa protein, chloroplastic

Chain C:



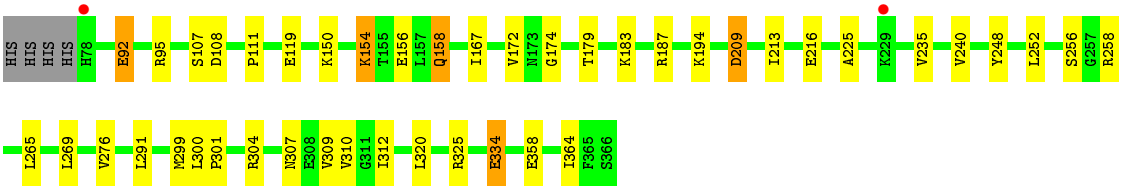
- Molecule 2: Cell division protein FtsY homolog, chloroplastic

Chain B:



- Molecule 2: Cell division protein FtsY homolog, chloroplastic

Chain D:


HIS
HIS
HIS
HIS
H78
E92
R95
S107
D108
P111
E119
K150
K154
T155
E156
L157
Q158
I167
V172
N173
G174
T179
K183
R187
K194
D209
I213
E216
A225
K229
V235
V240
Y248
L252
S256
G257
R258
L265
L269
V276
L291
M299
L300
P301
R304
N307
E308
V309
V310
G311
I312
L320
R325
E334
E358
I364
F365
S366

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.79Å 74.75Å 107.21Å 90.00° 91.14° 90.00°	Depositor
Resolution (Å)	44.89 – 2.50 57.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.89-2.50) 96.5 (57.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.173 , 0.218 0.170 , 0.216	Depositor DCC
R_{free} test set	2410 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8672	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, GCP

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	0.42	0/2016	0.61	0/2715
1	C	0.35	0/2034	0.52	0/2741
2	B	0.44	0/2219	0.60	0/2991
2	D	0.42	0/2208	0.58	0/2976
All	All	0.41	0/8477	0.58	0/11423

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ASP	Peptide

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	1997	0	2101	26	0
1	C	2015	0	2125	20	0
2	B	2193	0	2265	20	0
2	D	2183	0	2258	27	0
3	A	32	0	13	2	0
3	B	32	0	13	0	0
3	C	32	0	14	1	0
3	D	32	0	14	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	6	0	8	1	0
5	D	6	0	8	1	0
6	A	42	0	0	1	0
6	B	38	0	0	0	0
6	C	13	0	0	1	0
6	D	47	0	0	2	0
All	All	8672	0	8819	89	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 5.

The worst 5 of 89 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:100:LYS:O	1:A:103:ILE:N	1.95	0.98
2:D:92:GLU:OE2	2:D:95:ARG:NH1	2.13	0.81
2:D:187:ARG:NE	5:D:403:GOL:O1	2.13	0.78
2:D:291:LEU:HD13	2:D:299:MET:HE3	1.75	0.67
1:C:215:TYR:OH	1:C:279:GLU:OE2	2.14	0.66

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	263/301 (87%)	259 (98%)	4 (2%)	0	100	100
1	C	265/301 (88%)	261 (98%)	4 (2%)	0	100	100
2	B	288/293 (98%)	283 (98%)	5 (2%)	0	100	100
2	D	287/293 (98%)	278 (97%)	9 (3%)	0	100	100
All	All	1103/1188 (93%)	1081 (98%)	22 (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	216/243 (89%)	209 (97%)	7 (3%)	46	74
1	C	219/243 (90%)	211 (96%)	8 (4%)	41	68
2	B	237/240 (99%)	233 (98%)	4 (2%)	68	89
2	D	236/240 (98%)	227 (96%)	9 (4%)	40	67
All	All	908/966 (94%)	880 (97%)	28 (3%)	47	75

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	107	MET
1	C	274	LYS
2	D	256	SER
1	C	152	LYS
1	C	229	GLN

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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	GCP	A	401	4	29,34,34	3.86	13 (44%)	31,54,54	1.35	4 (12%)
3	GCP	B	401	4	29,34,34	3.98	13 (44%)	31,54,54	1.32	4 (12%)
5	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.46	0
3	GCP	C	402	4	29,34,34	4.08	15 (51%)	31,54,54	1.25	4 (12%)
3	GCP	D	402	4	29,34,34	3.98	14 (48%)	31,54,54	1.30	4 (12%)
5	GOL	D	403	-	5,5,5	0.33	0	5,5,5	0.56	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
3	GCP	A	401	4	-	0/18/38/38	0/3/3/3
3	GCP	B	401	4	-	0/18/38/38	0/3/3/3
5	GOL	B	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCP	C	402	4	-	0/18/38/38	0/3/3/3
3	GCP	D	402	4	-	0/18/38/38	0/3/3/3
5	GOL	D	403	-	-	0/4/4/4	0/0/0/0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	GCP	C4-N9	-10.27	1.34	1.47
3	B	401	GCP	C4-N9	-10.11	1.34	1.47
3	D	402	GCP	C4-N9	-9.33	1.35	1.47
3	A	401	GCP	C4-N9	-9.22	1.35	1.47
3	C	402	GCP	C5-C6	-7.35	1.39	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	GCP	O6-C6-N1	-2.61	119.37	122.80
3	B	401	GCP	O6-C6-N1	-2.58	119.41	122.80
3	D	402	GCP	O6-C6-N1	-2.51	119.50	122.80
3	B	401	GCP	C5'-C4'-C3'	-2.28	106.39	115.20
3	C	402	GCP	O6-C6-N1	-2.26	119.83	122.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GCP	2	0
5	B	403	GOL	1	0
3	C	402	GCP	1	0
3	D	402	GCP	1	0
5	D	403	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 (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	267/301 (88%)	0.08	17 (6%)	23	25	17, 37, 92, 144	0
1	C	269/301 (89%)	0.41	24 (8%)	12	13	35, 60, 96, 125	0
2	B	290/293 (98%)	-0.17	2 (0%)	89	90	16, 31, 50, 94	0
2	D	289/293 (98%)	-0.20	2 (0%)	89	90	17, 33, 56, 119	0
All	All	1115/1188 (93%)	0.02	45 (4%)	42	47	16, 38, 88, 144	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	VAL	5.5
1	A	103	ILE	5.4
1	C	239	THR	4.8
1	A	136	VAL	4.7
1	A	146	PRO	4.5

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	D	403	6/6	0.91	0.20	3.64	56,59,66,68	0
5	GOL	B	403	6/6	0.87	0.16	1.94	45,57,59,61	0
3	GCP	D	402	32/32	0.99	0.15	0.11	20,29,37,43	0
3	GCP	A	401	32/32	0.99	0.15	-0.02	16,23,29,31	0
3	GCP	B	401	32/32	0.99	0.15	-0.17	12,22,29,32	0
3	GCP	C	402	32/32	0.99	0.14	-0.42	24,34,44,48	0
4	MG	B	402	1/1	0.99	0.11	-1.30	20,20,20,20	0
4	MG	A	402	1/1	0.99	0.12	-1.88	31,31,31,31	0
4	MG	C	401	1/1	0.94	0.07	-2.78	42,42,42,42	0
4	MG	D	401	1/1	0.99	0.10	-3.18	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.