wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 05:04 PM JST

PDB ID	:	5XN6
Title	:	Heterodimer crystal structure of geranylgeranyl diphosphate synthases 1 with GGPPS Recruiting Protein(OsGRP) from Oryza sativa
Authors	:	Wang, C.; Zhou, F.; Lu, S.; Zhang, P.
Deposited on	:	2017-05-18
Resolution	:	3.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

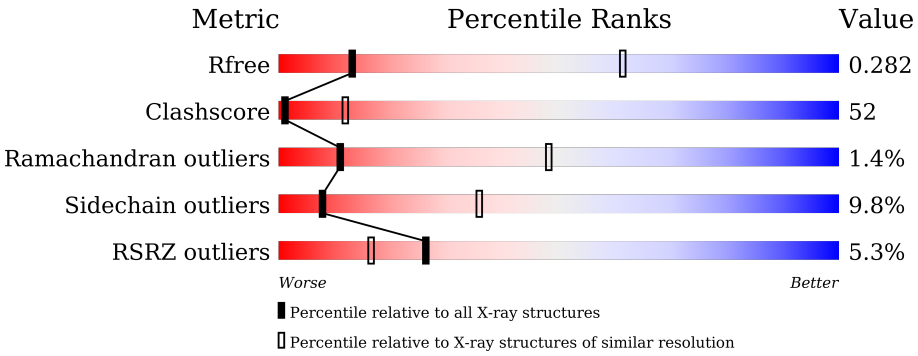
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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 <=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	305	5% 56% 33% • 8%
1	B	305	5% 60% 27% • 9%
1	E	305	4% 60% 29% • 9%
2	C	304	7% 35% 39% 12% • 14%
2	D	304	5% 32% 44% 11% • 12%
2	F	304	3% 28% 45% 12% • 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12244 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 Os07g0580900 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2142	1353	373	402	14			
1	B	277	Total	C	N	O	S	0	0	0
			2105	1331	368	392	14			
1	E	278	Total	C	N	O	S	0	0	0
			2117	1337	367	399	14			

- Molecule 2 is a protein called Os02g0668100 protein.

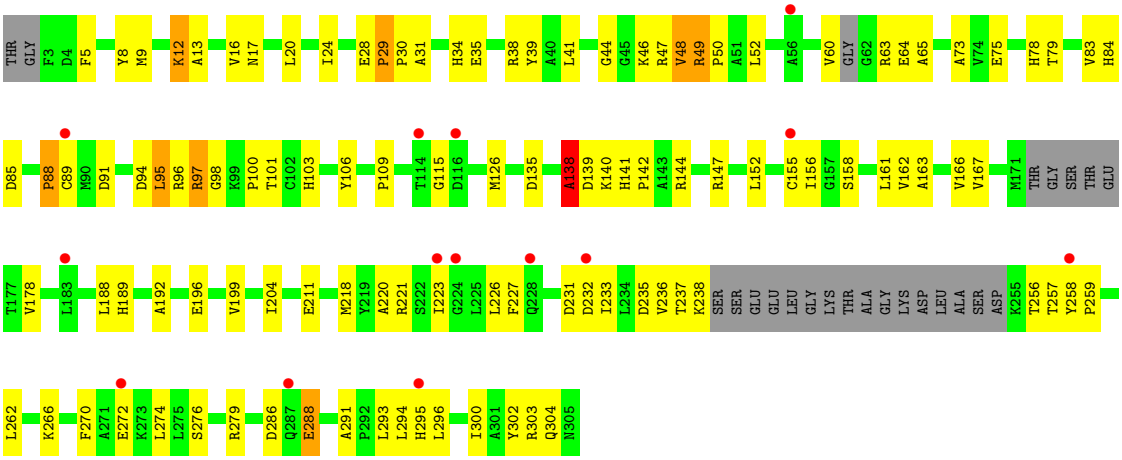
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	262	Total	C	N	O	S	0	0	0
			1941	1232	334	359	16			
2	D	266	Total	C	N	O	S	0	0	0
			1973	1250	344	363	16			
2	F	263	Total	C	N	O	S	0	0	0
			1966	1245	344	361	16			

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.

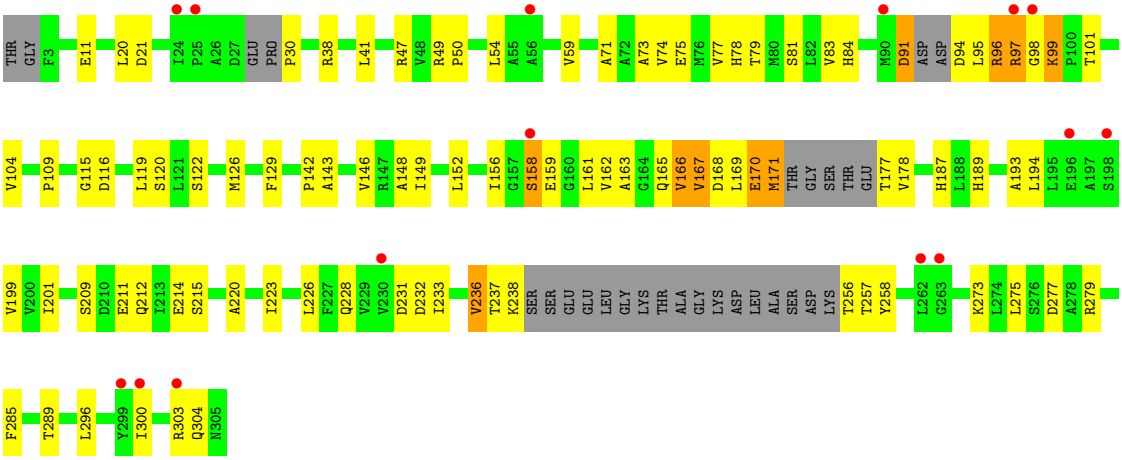
• Molecule 1: Os07g0580900 protein

Chain A:



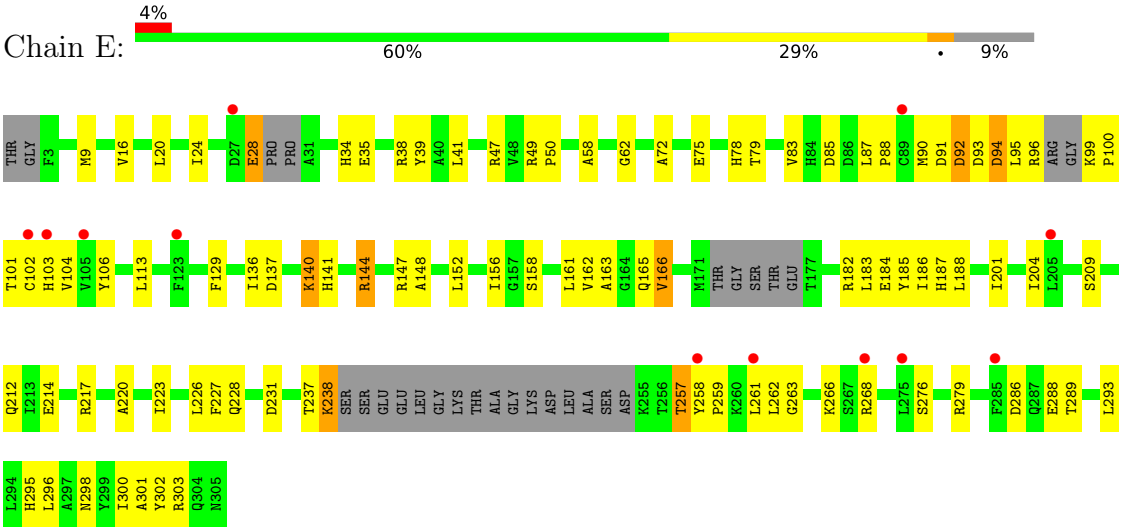
• Molecule 1: Os07g0580900 protein

Chain B:



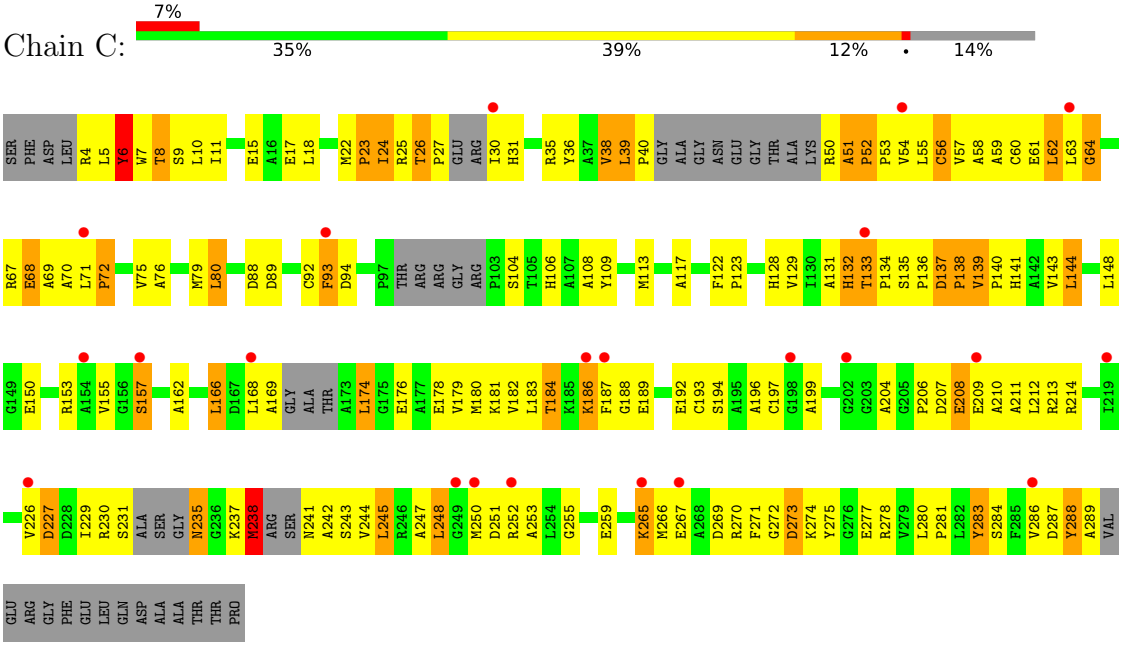
• Molecule 1: Os07g0580900 protein

Chain E:



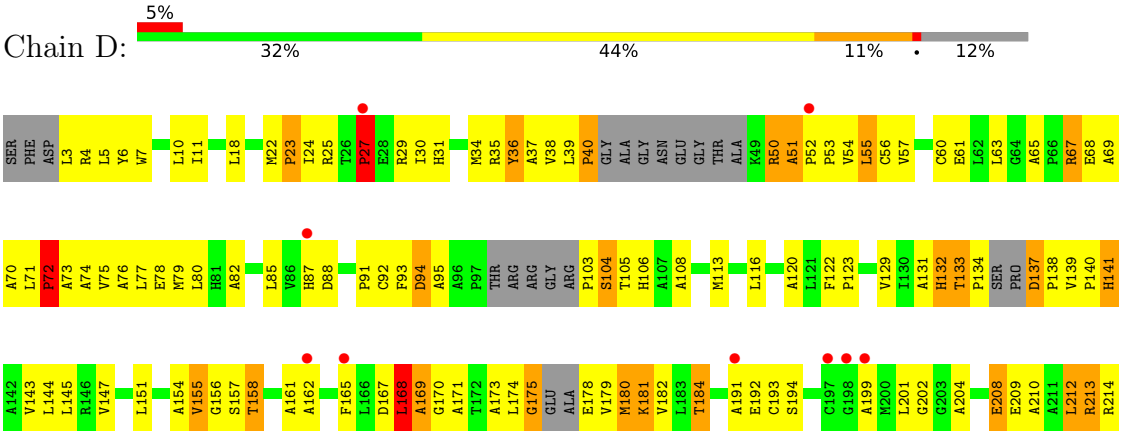
• Molecule 2: Os02g0668100 protein

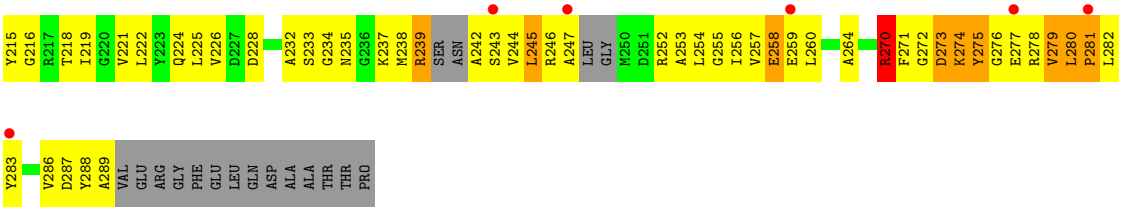
Chain C:



• Molecule 2: Os02g0668100 protein

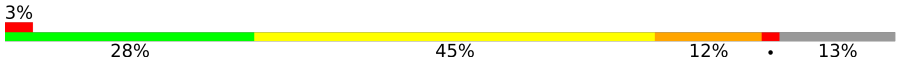
Chain D:

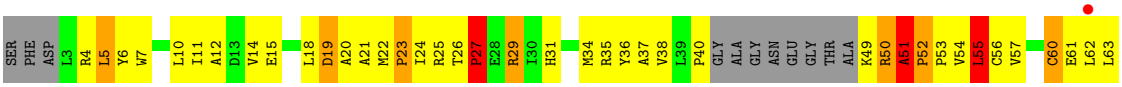


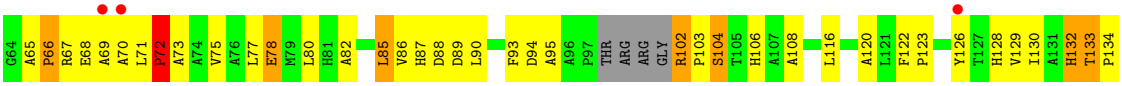


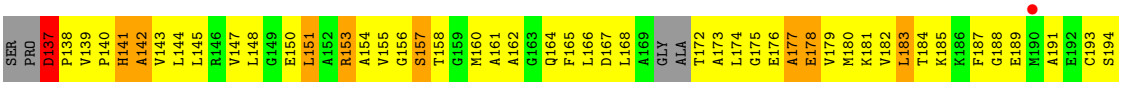
• Molecule 2: Os02g0668100 protein

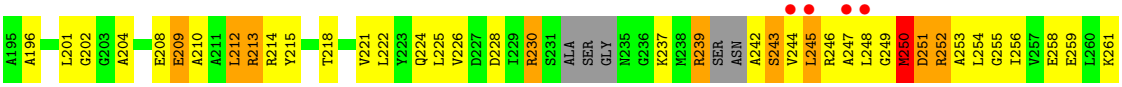
Chain F:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	103.06Å 102.98Å 103.49Å 109.39° 109.59° 109.13°	Depositor
Resolution (Å)	37.76 – 3.60 37.75 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (37.76-3.60) 95.5 (37.75-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.263 0.271 , 0.282	Depositor DCC
R_{free} test set	1845 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	107.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage

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[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.

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Property	Value	Source
Estimated twinning fraction	0.016 for h+k+l,-l,-h 0.016 for -l,h+k+l,-k 0.014 for -k,h+k+l,-h 0.014 for -l,-h,h+k+l 0.015 for -k,-l,h+k+l 0.015 for h+k+l,-h,-k 0.270 for l,k,-h-k-l 0.270 for -h-k-l,k,h 0.015 for h,-h-k-l,k 0.015 for h,l,-h-k-l 0.013 for -h-k-l,h,l 0.013 for k,-h-k-l,l 0.013 for l,h,k 0.013 for k,l,h 0.015 for k,h,-h-k-l 0.017 for -k,-h,-l 0.016 for -h-k-l,l,k 0.016 for -h,-l,-k 0.015 for l,-h-k-l,h 0.035 for -l,-k,-h 0.039 for -h,-k,h+k+l 0.030 for h+k+l,-k,-l 0.014 for -h,h+k+l,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12244	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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	0.49	0/2180	0.77	10/2954 (0.3%)
1	B	0.42	0/2141	0.62	1/2898 (0.0%)
1	E	0.38	0/2152	0.68	6/2913 (0.2%)
2	C	0.82	0/1975	1.05	10/2677 (0.4%)
2	D	0.80	0/2006	1.10	14/2715 (0.5%)
2	F	0.83	0/1997	1.12	24/2702 (0.9%)
All	All	0.65	0/12451	0.90	65/16859 (0.4%)

There are no bond length outliers.

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	230	ARG	N-CA-C	-9.53	85.27	111.00
2	F	27	PRO	CA-N-CD	-9.49	98.21	111.50
2	D	40	PRO	N-CA-C	-9.49	87.43	112.10
2	F	250	MET	CB-CA-C	-9.45	91.51	110.40
2	F	66	PRO	CB-CA-C	-8.50	90.75	112.00

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	2142	0	2138	127	0
1	B	2105	0	2107	111	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2117	0	2110	74	0
2	C	1941	0	1943	285	0
2	D	1973	0	1984	357	0
2	F	1966	0	1977	377	2
All	All	12244	0	12259	1281	2

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 52.

The worst 5 of 1281 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:49:ARG:HH12	1:A:78:HIS:CD2	1.08	1.62
2:D:264:ALA:CB	2:D:283:TYR:CE1	1.81	1.59
1:A:49:ARG:NH1	1:A:78:HIS:CD2	1.74	1.51
2:D:264:ALA:HB1	2:D:283:TYR:CZ	1.45	1.51
1:A:49:ARG:NH1	1:A:78:HIS:CG	1.78	1.51

All (2) 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)
1:B:304:GLN:NE2	2:F:29:ARG:NH2[1_545]	1.64	0.56
1:B:279:ARG:NH2	2:F:108:ALA:O[1_545]	2.04	0.16

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	273/305 (90%)	258 (94%)	14 (5%)	1 (0%)	34 71
1	B	267/305 (88%)	252 (94%)	14 (5%)	1 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	268/305 (88%)	239 (89%)	28 (10%)	1 (0%)	34 71
2	C	248/304 (82%)	223 (90%)	20 (8%)	5 (2%)	7 41
2	D	252/304 (83%)	221 (88%)	25 (10%)	6 (2%)	6 37
2	F	247/304 (81%)	220 (89%)	19 (8%)	8 (3%)	4 31
All	All	1555/1827 (85%)	1413 (91%)	120 (8%)	22 (1%)	11 48

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	137	ASP
2	F	27	PRO
2	F	51	ALA
2	C	68	GLU
2	F	142	ALA

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	222/239 (93%)	216 (97%)	6 (3%)	44 73
1	B	217/239 (91%)	207 (95%)	10 (5%)	27 61
1	E	219/239 (92%)	211 (96%)	8 (4%)	34 66
2	C	194/223 (87%)	160 (82%)	34 (18%)	2 12
2	D	196/223 (88%)	168 (86%)	28 (14%)	3 21
2	F	197/223 (88%)	161 (82%)	36 (18%)	1 10
All	All	1245/1386 (90%)	1123 (90%)	122 (10%)	8 36

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	104	SER
2	F	213	ARG

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Mol	Chain	Res	Type
2	D	218	THR
2	F	212	LEU
2	F	265	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	224	GLN
1	E	228	GLN
2	F	235	ASN
2	F	128	HIS
2	F	164	GLN

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)

There are no ligands in this entry.

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	281/305 (92%)	0.20	14 (4%)	28	18	30, 84, 108, 141	0
1	B	277/305 (90%)	0.26	15 (5%)	25	16	68, 86, 112, 129	0
1	E	278/305 (91%)	0.42	12 (4%)	35	22	55, 84, 110, 142	0
2	C	262/304 (86%)	0.26	22 (8%)	11	7	50, 91, 119, 135	0
2	D	266/304 (87%)	0.21	15 (5%)	24	14	51, 90, 125, 138	0
2	F	263/304 (86%)	0.33	9 (3%)	45	30	53, 90, 119, 141	0
All	All	1627/1827 (89%)	0.28	87 (5%)	26	16	30, 88, 118, 142	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	ILE	9.1
2	F	247	ALA	7.6
2	C	202	GLY	6.3
1	A	228	GLN	5.4
2	C	265	LYS	5.2

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

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.