



Full wwPDB X-ray Structure Validation Report i

Apr 29, 2024 – 03:57 pm BST

PDB ID : 2WAS
Title : Structure of the fungal type I FAS PPT domain
Authors : Johansson, P.; Mulincacci, B.; Koestler, C.; Grininger, M.
Deposited on : 2009-02-15
Resolution : 1.90 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 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 : 2.36.2
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) : 2.36.2

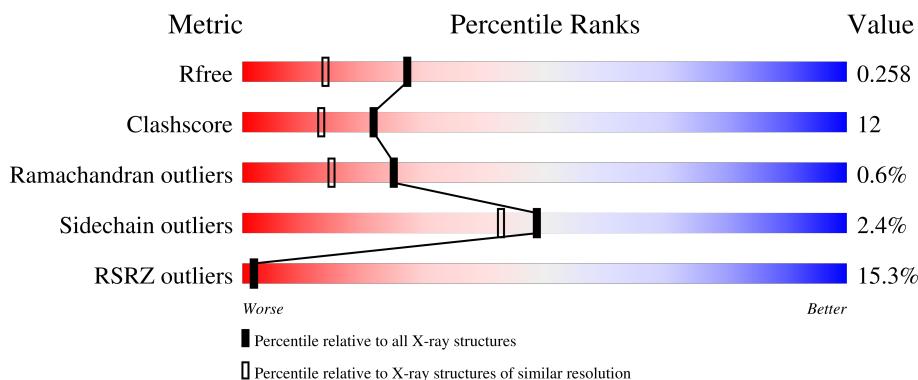
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



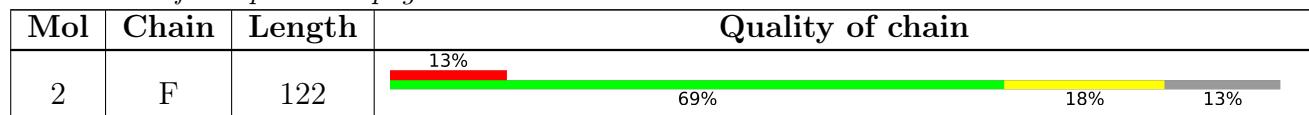
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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.



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2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 5154 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 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	1	0
			846	530	143	172	1			
1	D	107	Total	C	N	O	S	0	1	0
			801	502	133	165	1			
1	E	106	Total	C	N	O	S	0	1	0
			800	502	133	164	1			

- Molecule 2 is a protein called 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	S	0	1	0
			871	544	147	179	1			
2	C	111	Total	C	N	O	S	0	1	0
			839	525	141	172	1			
2	F	106	Total	C	N	O	S	0	1	0
			803	504	133	165	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1842	THR	VAL	conflict	UNP P19097
C	1842	THR	VAL	conflict	UNP P19097
F	1842	THR	VAL	conflict	UNP P19097

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	31	Total O 31 31	0	0
3	B	46	Total O 46 46	0	0

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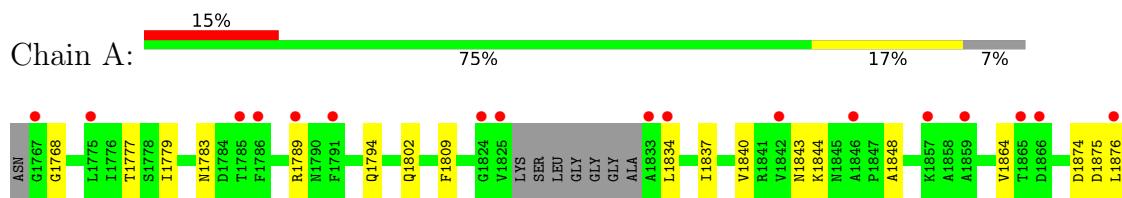
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	36	Total O 36 36	0	0
3	D	22	Total O 22 22	0	0
3	E	31	Total O 31 31	0	0
3	F	28	Total O 28 28	0	0

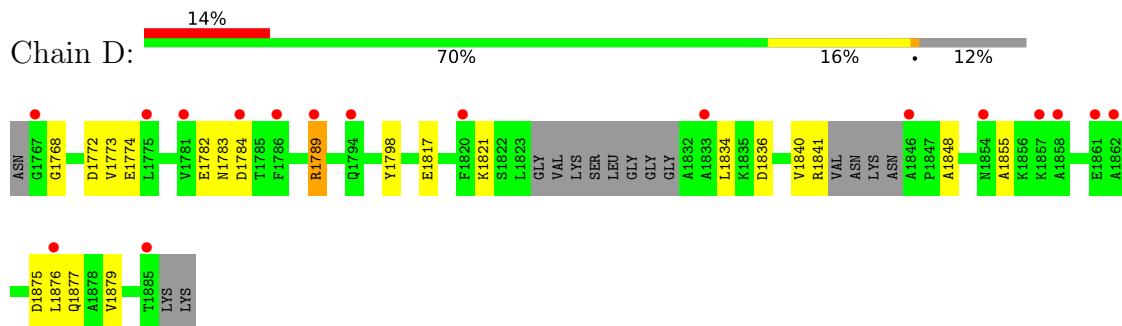
3 Residue-property plots

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.

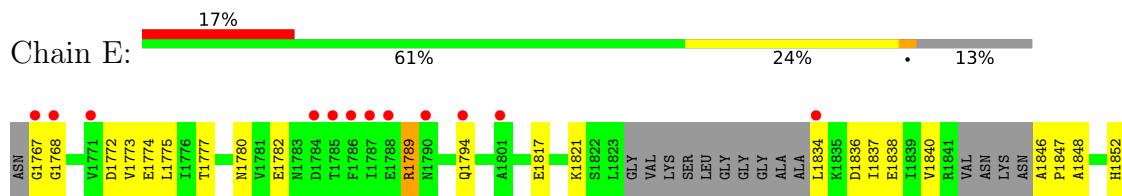
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE



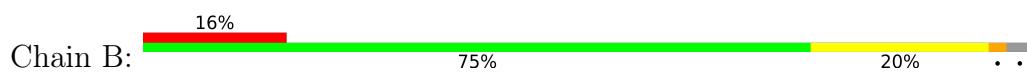
- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

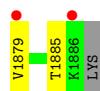


- Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

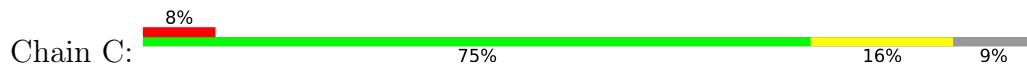


- Molecule 2: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE

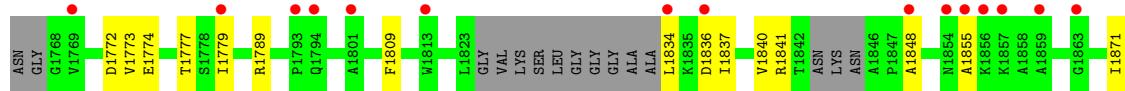




- Molecule 2: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE



- Molecule 2: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] SYNTHASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.12Å 55.76Å 81.00Å 90.00° 111.43° 90.00°	Depositor
Resolution (Å)	31.26 – 1.90 31.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.26-1.90) 98.3 (31.26-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.65 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R , R_{free}	0.218 , 0.254 0.221 , 0.258	Depositor DCC
R_{free} test set	1989 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$< L > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.256 for l,-k,h	Xtriage
Reported twinning fraction	0.303 for L,-K,H	Depositor
Outliers	0 of 52729 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.48	0/856	0.56	0/1161
1	D	0.46	0/810	0.62	0/1099
1	E	0.45	0/809	0.54	0/1096
2	B	0.48	0/881	0.62	0/1194
2	C	0.48	0/849	0.56	0/1152
2	F	0.47	0/812	0.54	0/1101
All	All	0.47	0/5017	0.57	0/6803

There are no bond length outliers.

There are no bond angle outliers.

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	846	0	837	18	0
1	D	801	0	787	22	0
1	E	800	0	790	28	0
2	B	871	0	864	25	0
2	C	839	0	832	22	0
2	F	803	0	794	22	0
3	A	31	0	0	1	0
3	B	46	0	0	4	0
3	C	36	0	0	0	0
3	D	22	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	0	4	0
3	F	28	0	0	2	0
All	All	5154	0	4904	117	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 12.

All (117) 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)
2:B:1840:VAL:HG22	2:B:1848:ALA:HB3	1.36	1.07
1:A:1843:ASN:O	1:A:1844:LYS:HG2	1.59	1.02
2:C:1875:ASP:OD2	1:D:1875:ASP:OD2	1.84	0.94
1:D:1836:ASP:HB3	1:D:1855:ALA:HB2	1.63	0.80
2:B:1875:ASP:OD2	1:E:1875:ASP:OD2	2.00	0.79
1:A:1875:ASP:OD2	2:F:1875:ASP:OD2	2.01	0.78
2:B:1794:GLN:NE2	2:B:1840:VAL:HA	1.99	0.77
1:A:1876:LEU:HD21	2:F:1876:LEU:HD11	1.67	0.75
1:A:1840:VAL:CG2	1:A:1848:ALA:HB3	2.18	0.74
2:B:1789:ARG:NH1	3:B:2008:HOH:O	2.20	0.73
2:C:1876:LEU:HD11	1:D:1876:LEU:HD21	1.70	0.73
1:A:1876:LEU:HD11	2:F:1876:LEU:HD21	1.69	0.73
1:E:1836:ASP:HB3	1:E:1855:ALA:HB2	1.75	0.68
2:B:1876:LEU:HD21	1:E:1876:LEU:HD11	1.75	0.67
1:E:1775:LEU:HG	3:E:2025:HOH:O	1.94	0.67
2:C:1876:LEU:HD21	1:D:1876:LEU:HD11	1.76	0.67
2:C:1773:VAL:HG23	2:C:1879[A]:VAL:HG12	1.76	0.67
2:B:1819:VAL:HG13	2:B:1867:VAL:HG11	1.77	0.67
2:B:1876:LEU:HD11	1:E:1876:LEU:HD21	1.77	0.66
2:C:1773:VAL:HG23	2:C:1879[B]:VAL:HG22	1.77	0.66
1:E:1840:VAL:HG22	1:E:1848:ALA:HB3	1.78	0.66
1:D:1836:ASP:HB3	1:D:1855:ALA:CB	2.26	0.65
2:C:1840:VAL:CG2	2:C:1848:ALA:HB3	2.28	0.64
2:B:1845:ASN:HB2	3:B:2031:HOH:O	1.99	0.63
1:E:1864:VAL:HA	1:E:1886:LYS:HG2	1.81	0.63
2:B:1820:PHE:CZ	2:B:1828:LEU:HG	2.34	0.62
2:F:1840:VAL:HG22	2:F:1848:ALA:HB3	1.81	0.62
1:D:1782:GLU:N	1:D:1782:GLU:OE2	2.34	0.61
2:B:1789:ARG:HD3	3:B:2012:HOH:O	2.01	0.61
2:B:1782:GLU:HG3	1:D:1782:GLU:OE1	2.01	0.60
1:E:1864:VAL:CG2	1:E:1886:LYS:HE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1840:VAL:CG2	1:E:1848:ALA:HB3	2.32	0.60
1:A:1840:VAL:HG22	1:A:1848:ALA:HB3	1.83	0.60
1:A:1794:GLN:HE22	1:A:1840:VAL:HA	1.67	0.59
1:A:1874:ASP:HB2	3:A:2029:HOH:O	2.02	0.59
1:E:1789:ARG:O	1:E:1789:ARG:HG2	2.01	0.59
1:E:1773:VAL:HG23	1:E:1879[A]:VAL:HG12	1.85	0.59
1:E:1864:VAL:HG22	1:E:1886:LYS:HE2	1.85	0.59
1:A:1864:VAL:HG22	1:A:1886:LYS:HE2	1.86	0.58
1:E:1780:ASN:HB2	3:E:2010:HOH:O	2.04	0.58
2:B:1860:GLU:HG3	3:B:2035:HOH:O	2.04	0.57
2:C:1840:VAL:HG22	2:C:1848:ALA:HB3	1.87	0.57
1:D:1773:VAL:HG23	1:D:1879[A]:VAL:HG12	1.86	0.57
1:D:1773:VAL:HG23	1:D:1879[B]:VAL:HG22	1.87	0.56
2:B:1773:VAL:HG23	2:B:1879[A]:VAL:HG12	1.86	0.56
1:E:1836:ASP:HB3	1:E:1855:ALA:CB	2.35	0.56
1:E:1773:VAL:HG23	1:E:1879[B]:VAL:HG22	1.86	0.56
1:D:1840:VAL:HG23	1:D:1848:ALA:HB3	1.87	0.56
2:B:1834:LEU:HD22	2:B:1837:ILE:HD12	1.88	0.55
1:D:1789:ARG:HG2	1:D:1789:ARG:O	2.07	0.55
2:B:1773:VAL:HG23	2:B:1879[B]:VAL:HG22	1.89	0.54
1:D:1840:VAL:CG2	1:D:1848:ALA:HB3	2.38	0.54
2:F:1773:VAL:HG23	2:F:1879[B]:VAL:HG22	1.91	0.53
2:B:1794:GLN:HE22	2:B:1840:VAL:HA	1.70	0.53
2:B:1782:GLU:CG	1:D:1782:GLU:OE1	2.57	0.53
2:C:1834:LEU:HD22	2:C:1837:ILE:HD12	1.91	0.53
1:A:1834:LEU:HD22	1:A:1837:ILE:HD12	1.90	0.53
1:D:1773:VAL:HG21	1:D:1877:GLN:NE2	2.23	0.52
1:D:1773:VAL:CG2	1:D:1877:GLN:NE2	2.72	0.52
1:E:1834:LEU:HD22	1:E:1837:ILE:HD12	1.91	0.52
1:E:1767:GLY:N	3:E:2004:HOH:O	2.43	0.52
1:A:1840:VAL:HG23	1:A:1840:VAL:O	2.10	0.51
1:E:1817:GLU:O	1:E:1821:LYS:HG3	2.09	0.51
1:E:1834:LEU:N	3:E:2014:HOH:O	2.44	0.51
2:B:1794:GLN:NE2	2:B:1839:ILE:O	2.44	0.50
2:B:1825:VAL:O	2:B:1826:LYS:C	2.51	0.50
1:D:1774:GLU:O	1:D:1877:GLN:HB2	2.12	0.49
1:A:1802:GLN:HE22	1:A:1843:ASN:HD21	1.60	0.49
2:F:1834:LEU:HD22	2:F:1837:ILE:HD12	1.93	0.49
2:F:1873:HIS:HE1	3:F:2023:HOH:O	1.95	0.49
2:F:1885:THR:CG2	2:F:1886:LYS:N	2.76	0.49
1:D:1782:GLU:O	1:D:1784:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1773:VAL:HG23	2:F:1879[A]:VAL:HG12	1.94	0.48
1:A:1843:ASN:O	1:A:1844:LYS:CG	2.47	0.48
2:B:1876:LEU:CD2	1:D:1876:LEU:CD2	2.92	0.48
2:C:1774:GLU:O	2:C:1877:GLN:HB2	2.13	0.47
2:C:1777:THR:CG2	2:F:1777:THR:CG2	2.92	0.47
2:C:1840:VAL:O	2:C:1840:VAL:HG23	2.14	0.47
1:A:1877:GLN:NE2	2:C:1877:GLN:HE22	2.13	0.46
2:C:1836:ASP:HB3	2:C:1855:ALA:HB2	1.97	0.46
1:E:1773:VAL:HG21	1:E:1877:GLN:NE2	2.31	0.46
2:F:1779:ILE:HG21	2:F:1809:PHE:CB	2.46	0.46
2:B:1773:VAL:HA	2:B:1878:ALA:O	2.16	0.46
1:D:1817:GLU:O	1:D:1821:LYS:HG3	2.17	0.46
2:F:1874:ASP:HB2	3:F:2025:HOH:O	2.15	0.46
2:B:1877:GLN:HE22	2:C:1877:GLN:NE2	2.15	0.45
2:C:1844:LYS:HE2	2:C:1844:LYS:HB3	1.69	0.45
2:C:1777:THR:HG22	2:F:1777:THR:HG22	1.99	0.44
2:F:1836:ASP:HB3	2:F:1855:ALA:HB2	2.00	0.44
1:A:1779:ILE:HG21	1:A:1809:PHE:CB	2.47	0.43
1:A:1768:GLY:HA3	1:A:1884:SER:OG	2.18	0.43
2:B:1840:VAL:O	2:B:1840:VAL:CG2	2.65	0.43
2:B:1794:GLN:HG3	2:B:1838:GLU:OE2	2.18	0.43
2:F:1840:VAL:O	2:F:1840:VAL:CG2	2.67	0.43
1:E:1821:LYS:NZ	2:F:1871:ILE:O	2.52	0.43
2:F:1836:ASP:HB3	2:F:1855:ALA:CB	2.49	0.43
2:C:1772:ASP:OD2	2:C:1774:GLU:OE2	2.37	0.42
2:C:1773:VAL:HG21	2:C:1877:GLN:NE2	2.34	0.42
2:C:1777:THR:HG23	2:F:1777:THR:CG2	2.49	0.42
2:C:1777:THR:CG2	2:F:1777:THR:HG23	2.49	0.42
1:E:1838:GLU:OE1	1:E:1852:HIS:HE1	2.03	0.42
1:E:1768:GLY:HA3	1:E:1884:SER:OG	2.19	0.42
2:F:1885:THR:HG22	2:F:1886:LYS:N	2.35	0.42
1:A:1777:THR:CG2	1:E:1777:THR:CG2	2.98	0.42
1:D:1798:TYR:OH	3:D:2006:HOH:O	2.20	0.42
1:E:1865:THR:HG23	1:E:1886:LYS:HA	2.01	0.41
1:A:1789:ARG:O	1:A:1789:ARG:HG2	2.20	0.41
1:D:1768:GLY:HA2	3:D:2002:HOH:O	2.20	0.41
2:B:1865:THR:OG1	2:B:1885:THR:HG22	2.21	0.41
2:F:1772:ASP:OD2	2:F:1774:GLU:OE2	2.38	0.41
1:E:1772:ASP:OD2	1:E:1774:GLU:OE2	2.39	0.41
1:E:1780:ASN:OD1	1:E:1782:GLU:HB2	2.21	0.41
2:C:1836:ASP:HB3	2:C:1855:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1846:ALA:HA	1:E:1847:PRO:HD3	1.96	0.40
1:D:1772:ASP:OD2	1:D:1774:GLU:OE2	2.39	0.40
2:C:1771:VAL:HG23	2:C:1881:VAL:HG22	2.03	0.40
2:F:1840:VAL:HG22	2:F:1840:VAL:O	2.21	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	110/122 (90%)	104 (94%)	5 (4%)	1 (1%)	17 7
1	D	102/122 (84%)	100 (98%)	1 (1%)	1 (1%)	15 6
1	E	101/122 (83%)	97 (96%)	4 (4%)	0	100 100
2	B	115/122 (94%)	108 (94%)	5 (4%)	2 (2%)	9 2
2	C	108/122 (88%)	106 (98%)	2 (2%)	0	100 100
2	F	101/122 (83%)	98 (97%)	3 (3%)	0	100 100
All	All	637/732 (87%)	613 (96%)	20 (3%)	4 (1%)	25 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1783	ASN
2	B	1827	SER
1	D	1783	ASN
1	A	1783	ASN

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	92/97 (95%)	92 (100%)	0	100 100
1	D	87/97 (90%)	84 (97%)	3 (3%)	37 28
1	E	88/97 (91%)	85 (97%)	3 (3%)	37 28
2	B	94/97 (97%)	91 (97%)	3 (3%)	39 30
2	C	93/97 (96%)	91 (98%)	2 (2%)	52 47
2	F	89/97 (92%)	87 (98%)	2 (2%)	52 47
All	All	543/582 (93%)	530 (98%)	13 (2%)	49 43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1825	VAL
2	B	1827	SER
2	B	1840	VAL
2	C	1789	ARG
2	C	1825	VAL
1	D	1789	ARG
1	D	1834	LEU
1	D	1841	ARG
1	E	1789	ARG
1	E	1794	GLN
1	E	1865	THR
2	F	1789	ARG
2	F	1841	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1794	GLN
1	A	1802	GLN
1	A	1852	HIS
1	A	1873	HIS

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Mol	Chain	Res	Type
1	A	1877	GLN
2	B	1794	GLN
2	B	1852	HIS
2	B	1877	GLN
2	C	1852	HIS
2	C	1877	GLN
1	D	1852	HIS
1	D	1877	GLN
1	E	1802	GLN
1	E	1852	HIS
1	E	1877	GLN
2	F	1852	HIS
2	F	1877	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 (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	113/122 (92%)	0.94	18 (15%)	1 2	21, 40, 71, 86
1	D	107/122 (87%)	0.90	17 (15%)	1 2	23, 41, 70, 77
1	E	106/122 (86%)	1.08	21 (19%)	1 1	23, 41, 73, 83
2	B	118/122 (96%)	1.07	19 (16%)	1 2	22, 40, 64, 78
2	C	111/122 (90%)	0.81	10 (9%)	9 10	21, 38, 66, 79
2	F	106/122 (86%)	0.98	16 (15%)	2 2	23, 41, 63, 79
All	All	661/732 (90%)	0.96	101 (15%)	2 2	21, 40, 70, 86

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1858	ALA	7.9
1	E	1834	LEU	6.5
1	D	1767	GLY	6.0
1	E	1801	ALA	5.9
2	B	1876	LEU	5.9
1	A	1842	VAL	5.9
2	F	1857	LYS	5.7
2	F	1854	ASN	5.4
1	A	1824	GLY	5.4
2	B	1829	GLY	5.2
1	E	1785	THR	4.8
1	E	1786	PHE	4.7
1	E	1858	ALA	4.7
2	B	1857	LYS	4.7
1	D	1857	LYS	4.4
1	A	1857	LYS	4.3
1	A	1876	LEU	4.2
1	E	1857	LYS	4.1
1	D	1854	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	1863	GLY	4.0
1	D	1833	ALA	3.9
2	C	1784	ASP	3.9
1	A	1833	ALA	3.8
2	F	1848	ALA	3.8
1	D	1862	ALA	3.7
2	F	1859	ALA	3.7
1	A	1786	PHE	3.6
2	B	1826	LYS	3.5
1	D	1846	ALA	3.5
2	F	1801	ALA	3.5
2	C	1857	LYS	3.5
1	A	1866	ASP	3.4
2	F	1793	PRO	3.4
1	A	1825	VAL	3.4
1	E	1863	GLY	3.4
1	A	1789	ARG	3.4
2	C	1836	ASP	3.4
2	C	1854	ASN	3.2
1	A	1886	LYS	3.2
2	B	1842	THR	3.2
1	A	1859	ALA	3.2
2	F	1794	GLN	3.1
2	B	1767	GLY	3.1
1	E	1787	ILE	3.1
2	C	1789	ARG	3.0
1	E	1788	GLU	3.0
2	B	1854	ASN	3.0
2	C	1861	GLU	2.9
1	A	1846	ALA	2.9
1	E	1784	ASP	2.9
2	B	1828	LEU	2.9
1	E	1855	ALA	2.8
1	D	1781	VAL	2.8
1	E	1876	LEU	2.7
1	E	1790	ASN	2.7
2	C	1788	GLU	2.7
1	D	1789	ARG	2.7
1	D	1861	GLU	2.7
2	F	1813	TRP	2.6
2	B	1836	ASP	2.6
1	A	1865	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1861	GLU	2.6
1	D	1786	PHE	2.6
1	D	1784	ASP	2.6
1	D	1876	LEU	2.5
2	B	1831	GLY	2.5
2	F	1856	LYS	2.5
1	A	1775	LEU	2.5
2	F	1779	ILE	2.5
1	E	1767	GLY	2.5
1	E	1794	GLN	2.4
2	B	1777	THR	2.4
2	B	1865	THR	2.4
1	E	1771	VAL	2.4
1	E	1859	ALA	2.4
1	E	1856	LYS	2.3
1	E	1862	ALA	2.3
1	A	1785	THR	2.3
2	C	1844	LYS	2.3
2	F	1769	VAL	2.3
1	A	1834	LEU	2.2
2	F	1886	LYS	2.2
2	B	1859	ALA	2.1
2	F	1855	ALA	2.1
1	A	1767	GLY	2.1
1	E	1768	GLY	2.1
2	B	1863	GLY	2.1
1	D	1820	PHE	2.1
2	B	1860	GLU	2.1
2	C	1886	LYS	2.1
1	E	1854	ASN	2.1
1	D	1794	GLN	2.1
2	F	1834	LEU	2.1
2	B	1785	THR	2.0
2	B	1879[A]	VAL	2.0
1	D	1885	THR	2.0
2	B	1886	LYS	2.0
1	A	1791	PHE	2.0
2	F	1836	ASP	2.0
1	D	1775	LEU	2.0
2	C	1779	ILE	2.0

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 [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.