



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 10:29 AM EDT

PDB ID : 1XJ5
Title : X-RAY STRUCTURE OF SPERMIDINE SYNTHASE FROM ARABIDOPSIS THALIANA GENE AT1G23820
Authors : Wesenberg, G.E.; Smith, D.W.; Phillips Jr., G.N.; Bitto, E.; Bingman, C.A.; Allard, S.T.M.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2004-09-22
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

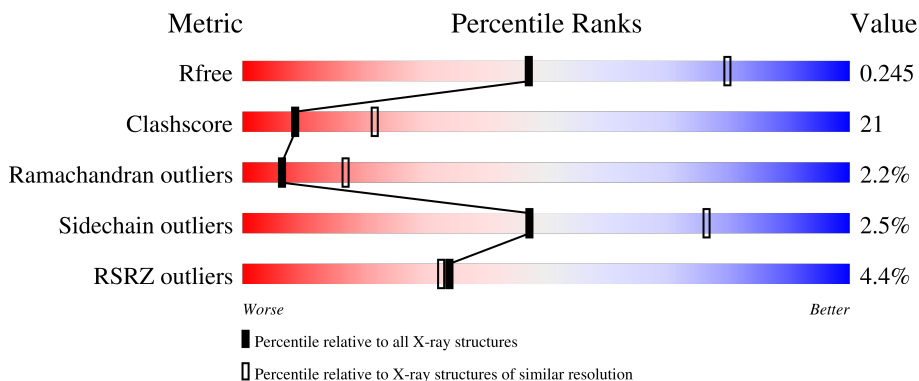
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	334	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 40px;">4% 48% 37% • 13%</p>
1	B	334	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 40px;">2% 60% 24% • 15%</p>
1	C	334	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 40px;">6% 54% 30% • 13%</p>
1	D	334	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 40px;">2% 56% 27% • 15%</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 9440 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 Spermidine synthase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	290	2234	1433	361	426	7	7	0	0	0
1	B	285	2198	1417	354	412	8	7	0	0	0
1	C	290	2234	1433	361	426	7	7	0	0	0
1	D	285	2198	1417	354	412	8	7	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q9ZUB3
A	26	MSE	MET	modified residue	UNP Q9ZUB3
A	51	MSE	MET	modified residue	UNP Q9ZUB3
A	54	MSE	MET	modified residue	UNP Q9ZUB3
A	109	MSE	MET	modified residue	UNP Q9ZUB3
A	149	MSE	MET	modified residue	UNP Q9ZUB3
A	155	MSE	MET	modified residue	UNP Q9ZUB3
A	242	MSE	MET	modified residue	UNP Q9ZUB3
A	278	MSE	MET	modified residue	UNP Q9ZUB3
B	1	SER	-	cloning artifact	UNP Q9ZUB3
B	26	MSE	MET	modified residue	UNP Q9ZUB3
B	51	MSE	MET	modified residue	UNP Q9ZUB3
B	54	MSE	MET	modified residue	UNP Q9ZUB3
B	109	MSE	MET	modified residue	UNP Q9ZUB3
B	149	MSE	MET	modified residue	UNP Q9ZUB3
B	155	MSE	MET	modified residue	UNP Q9ZUB3
B	242	MSE	MET	modified residue	UNP Q9ZUB3
B	278	MSE	MET	modified residue	UNP Q9ZUB3
C	1	SER	-	cloning artifact	UNP Q9ZUB3
C	26	MSE	MET	modified residue	UNP Q9ZUB3
C	51	MSE	MET	modified residue	UNP Q9ZUB3

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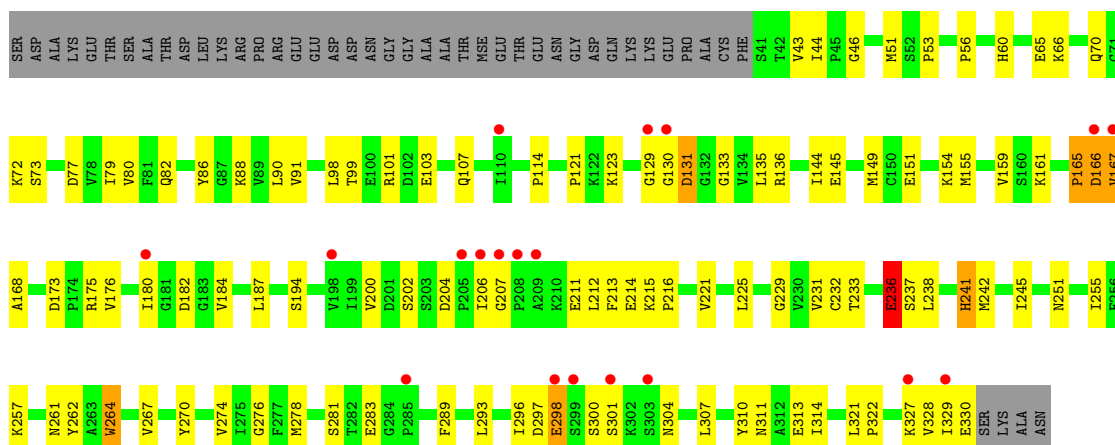
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Chain	Residue	Modelled	Actual	Comment	Reference
C	54	MSE	MET	modified residue	UNP Q9ZUB3
C	109	MSE	MET	modified residue	UNP Q9ZUB3
C	149	MSE	MET	modified residue	UNP Q9ZUB3
C	155	MSE	MET	modified residue	UNP Q9ZUB3
C	242	MSE	MET	modified residue	UNP Q9ZUB3
C	278	MSE	MET	modified residue	UNP Q9ZUB3
D	1	SER	-	cloning artifact	UNP Q9ZUB3
D	26	MSE	MET	modified residue	UNP Q9ZUB3
D	51	MSE	MET	modified residue	UNP Q9ZUB3
D	54	MSE	MET	modified residue	UNP Q9ZUB3
D	109	MSE	MET	modified residue	UNP Q9ZUB3
D	149	MSE	MET	modified residue	UNP Q9ZUB3
D	155	MSE	MET	modified residue	UNP Q9ZUB3
D	242	MSE	MET	modified residue	UNP Q9ZUB3
D	278	MSE	MET	modified residue	UNP Q9ZUB3

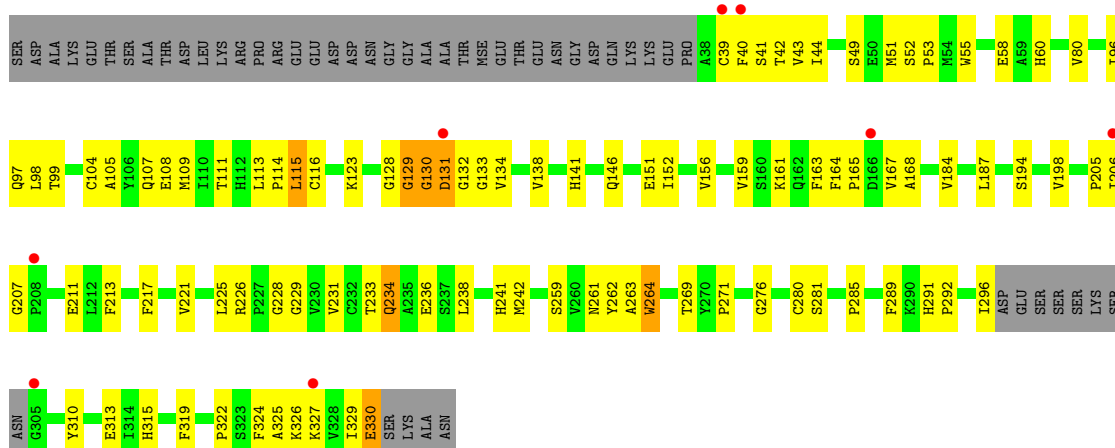
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 132 132	0	0
2	B	173	Total O 173 173	0	0
2	C	135	Total O 135 135	0	0
2	D	136	Total O 136 136	0	0

- Molecule 1: Spermidine synthase 1



- Molecule 1: Spermidine synthase 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.81Å 95.21Å 89.16Å 90.00° 104.96° 90.00°	Depositor
Resolution (Å)	26.29 – 2.70 26.28 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.6 (26.29-2.70) 94.0 (26.28-2.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.64Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.245 0.188 , 0.245	Depositor DCC
R_{free} test set	3788 reflections (9.55%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtrriage
Anisotropy	0.700	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9440	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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](#)

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	0.36	0/2282	0.62	0/3089
1	B	0.42	0/2246	0.64	0/3040
1	C	0.37	0/2282	0.62	0/3089
1	D	0.39	0/2246	0.63	0/3040
All	All	0.38	0/9056	0.63	0/12258

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	2234	0	2199	117	0
1	B	2198	0	2168	71	0
1	C	2234	0	2199	110	0
1	D	2198	0	2168	71	0
2	A	132	0	0	5	0
2	B	173	0	0	9	0
2	C	135	0	0	7	0
2	D	136	0	0	8	0
All	All	9440	0	8734	362	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 21.

All (362) 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:C:135:LEU:HD22	1:C:149:MSE:HE2	1.45	0.98
1:A:238:LEU:HA	1:A:242:MSE:HE3	1.48	0.96
1:C:238:LEU:HA	1:C:242:MSE:HE3	1.50	0.94
1:A:236:GLU:HB3	1:A:241:HIS:CD2	2.11	0.84
1:A:135:LEU:HD22	1:A:149:MSE:HE2	1.61	0.82
1:C:242:MSE:HA	1:C:242:MSE:HE2	1.60	0.81
1:B:187:LEU:HD21	1:B:221:VAL:HG22	1.64	0.79
1:B:238:LEU:O	1:B:242:MSE:HE2	1.82	0.78
1:A:109:MSE:HE3	1:A:309:PHE:HD1	1.49	0.78
1:C:301:SER:HB3	1:C:304:ASN:HD22	1.49	0.77
1:D:187:LEU:HD21	1:D:221:VAL:HG22	1.66	0.77
1:B:135:LEU:HD11	1:B:149:MSE:HG3	1.66	0.75
1:A:223:ARG:HD2	2:A:444:HOH:O	1.85	0.75
1:C:131:ASP:O	1:C:167:VAL:HG12	1.87	0.74
1:C:107:GLN:NE2	1:C:133:GLY:HA3	2.02	0.74
1:A:242:MSE:HE2	1:A:242:MSE:HA	1.70	0.74
1:D:238:LEU:O	1:D:242:MSE:HE2	1.87	0.74
1:B:292:PRO:HD3	1:B:315:HIS:CD2	2.22	0.73
1:A:161:LYS:HA	1:A:168:ALA:CB	2.19	0.73
1:A:242:MSE:HE2	1:A:245:ILE:HD12	1.70	0.72
1:B:136:ARG:HH21	1:B:167:VAL:HG12	1.54	0.72
1:C:161:LYS:HA	1:C:168:ALA:CB	2.19	0.72
1:C:238:LEU:HD21	1:C:262:TYR:CE2	2.24	0.72
1:A:215:LYS:HG2	1:A:255:ILE:HD11	1.71	0.71
1:A:236:GLU:HB3	1:A:241:HIS:HD2	1.56	0.70
1:A:173:ASP:HB3	1:A:176:VAL:HG23	1.72	0.70
1:D:242:MSE:HE3	1:D:324:PHE:CE1	2.27	0.70
1:C:200:VAL:HB	1:C:233:THR:HG22	1.73	0.69
1:C:257:LYS:HE2	2:C:367:HOH:O	1.91	0.69
1:B:173:ASP:HB3	1:B:176:VAL:HG23	1.74	0.68
1:C:257:LYS:HB3	1:C:283:GLU:HB3	1.74	0.68
1:A:109:MSE:CE	1:A:310:TYR:HB2	2.24	0.67
1:A:161:LYS:HA	1:A:168:ALA:HB2	1.77	0.67
1:C:155:MSE:O	1:C:159:VAL:HG23	1.95	0.66
1:D:327:LYS:O	1:D:330:GLU:HG2	1.95	0.66
1:D:123:LYS:HE3	1:D:146:GLN:OE1	1.95	0.66
1:A:66:LYS:HG2	1:A:82:GLN:HB3	1.77	0.66
1:A:123:LYS:HD3	1:A:194:SER:O	1.96	0.66
1:A:252:CYS:SG	1:A:278:MSE:HE2	2.35	0.66
1:B:104:CYS:O	1:B:108:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LYS:HB2	1:C:180:ILE:HD13	1.79	0.65
1:C:215:LYS:HG2	1:C:255:ILE:HD11	1.77	0.65
1:D:164:PHE:HB3	1:D:167:VAL:HG22	1.77	0.64
1:D:58:GLU:O	2:D:353:HOH:O	2.15	0.64
1:B:96:ILE:HG21	1:B:269:THR:CG2	2.28	0.64
1:A:121:PRO:O	1:A:144:ILE:HD13	1.98	0.64
1:C:53:PRO:O	1:C:56:PRO:HD3	1.98	0.64
1:D:99:THR:CG2	1:D:269:THR:HG21	2.28	0.64
1:C:99:THR:HG22	1:C:101:ARG:H	1.63	0.63
1:A:53:PRO:O	1:A:56:PRO:HD3	1.98	0.63
1:A:131:ASP:O	1:A:167:VAL:HG12	1.97	0.63
1:D:96:ILE:HG21	1:D:269:THR:CG2	2.28	0.63
1:A:187:LEU:HD21	1:A:221:VAL:HG22	1.79	0.63
1:C:66:LYS:HD3	2:C:411:HOH:O	1.99	0.63
1:C:86:TYR:HB3	1:C:99:THR:CG2	2.28	0.63
1:A:257:LYS:HB2	1:A:283:GLU:HB2	1.81	0.62
1:C:161:LYS:HA	1:C:168:ALA:HB2	1.80	0.62
1:C:242:MSE:HE2	1:C:245:ILE:HD12	1.82	0.62
1:B:99:THR:O	1:B:103:GLU:HG3	2.00	0.61
1:B:269:THR:HB	2:B:392:HOH:O	2.00	0.61
1:B:223:ARG:HD2	2:B:409:HOH:O	2.00	0.61
1:A:109:MSE:HE1	1:A:310:TYR:HA	1.83	0.60
1:C:187:LEU:HD21	1:C:221:VAL:HG22	1.80	0.60
1:A:329:ILE:O	1:A:330:GLU:HB2	2.01	0.60
1:B:242:MSE:HE3	1:B:324:PHE:CE1	2.37	0.60
1:C:73:SER:HB2	2:C:339:HOH:O	2.01	0.60
1:C:72:LYS:HE2	1:C:77:ASP:OD1	2.01	0.60
1:C:123:LYS:HD3	1:C:194:SER:O	2.01	0.60
1:C:129:GLY:HA3	1:C:151:GLU:HB2	1.84	0.60
1:C:238:LEU:HD23	1:C:242:MSE:HE1	1.83	0.60
1:A:214:GLU:HB3	1:A:216:PRO:HD2	1.83	0.59
1:A:54:MSE:HE2	1:A:54:MSE:HA	1.85	0.59
1:C:86:TYR:HB3	1:C:99:THR:HG21	1.85	0.59
1:A:109:MSE:HE3	1:A:309:PHE:CD1	2.35	0.59
1:D:99:THR:HG23	1:D:269:THR:HG21	1.84	0.59
1:D:132:GLY:HA3	1:D:167:VAL:O	2.03	0.58
1:D:238:LEU:HB3	1:D:242:MSE:HE1	1.84	0.58
1:A:267:VAL:HG11	1:A:270:TYR:CD2	2.38	0.58
1:C:161:LYS:HA	1:C:168:ALA:HB1	1.85	0.58
1:D:43:VAL:HG23	1:D:44:ILE:HG13	1.84	0.58
1:A:257:LYS:NZ	2:A:465:HOH:O	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:PRO:HG2	1:C:166:ASP:H	1.69	0.58
1:D:111:THR:O	1:D:115:LEU:HB2	2.03	0.58
1:D:261:ASN:HD22	1:D:289:PHE:HD2	1.51	0.58
1:A:166:ASP:O	1:A:169:ILE:HG22	2.03	0.57
1:B:241:HIS:HD2	2:B:373:HOH:O	1.85	0.57
1:A:238:LEU:CA	1:A:242:MSE:HE3	2.27	0.57
1:A:129:GLY:HA3	1:A:149:MSE:SE	2.55	0.57
1:B:238:LEU:HB3	1:B:242:MSE:HE1	1.87	0.57
1:D:187:LEU:HD23	1:D:217:PHE:CE1	2.40	0.56
1:A:238:LEU:HD21	1:A:262:TYR:CE1	2.40	0.56
1:C:221:VAL:HG11	1:C:231:VAL:HG21	1.85	0.56
1:C:329:ILE:O	1:C:329:ILE:HG22	2.04	0.56
1:A:80:VAL:HG21	1:A:159:VAL:HG12	1.87	0.56
1:D:292:PRO:HD3	1:D:315:HIS:CD2	2.39	0.56
1:C:329:ILE:O	1:C:330:GLU:HB2	2.06	0.56
1:B:242:MSE:HE3	1:B:324:PHE:HE1	1.71	0.55
1:A:253:ARG:HG3	1:A:260:VAL:HG21	1.89	0.55
1:B:60:HIS:CE1	2:B:488:HOH:O	2.60	0.55
1:B:130:GLY:O	1:B:131:ASP:HB2	2.05	0.55
1:D:269:THR:O	1:D:269:THR:HG22	2.07	0.55
1:B:96:ILE:HG21	1:B:269:THR:HG22	1.88	0.55
1:A:86:TYR:HD2	1:A:99:THR:HG21	1.71	0.55
1:A:161:LYS:HA	1:A:168:ALA:HB1	1.88	0.55
1:A:244:ILE:O	1:A:248:ILE:HG13	2.07	0.55
1:C:173:ASP:HB3	1:C:176:VAL:HG23	1.89	0.55
1:C:225:LEU:HD11	1:C:231:VAL:CG2	2.37	0.55
1:A:109:MSE:HE1	1:A:310:TYR:CB	2.36	0.54
1:A:206:ILE:HG23	1:A:207:GLY:N	2.22	0.54
1:C:261:ASN:HD22	1:C:289:PHE:HD2	1.55	0.54
1:D:115:LEU:HD23	1:D:141:HIS:CD2	2.42	0.54
1:C:182:ASP:OD2	1:C:184:VAL:HG22	2.08	0.54
1:A:109:MSE:HE1	1:A:310:TYR:CA	2.37	0.54
1:C:238:LEU:CA	1:C:242:MSE:HE3	2.32	0.54
1:A:99:THR:HG22	1:A:101:ARG:H	1.71	0.54
1:D:151:GLU:OE1	1:D:152:ILE:N	2.41	0.54
1:C:80:VAL:HG21	1:C:159:VAL:CG1	2.37	0.54
1:A:52:SER:HB3	1:A:55:TRP:CE2	2.43	0.53
1:A:165:PRO:HG2	1:A:166:ASP:H	1.72	0.53
1:B:173:ASP:HB2	2:B:360:HOH:O	2.08	0.53
1:C:66:LYS:HG2	1:C:82:GLN:HB3	1.91	0.53
1:B:166:ASP:O	1:B:167:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HB2	1:A:180:ILE:HD13	1.90	0.53
1:D:242:MSE:HE3	1:D:324:PHE:HE1	1.69	0.53
1:B:242:MSE:CE	1:B:324:PHE:HE1	2.21	0.53
1:C:121:PRO:O	1:C:144:ILE:HD13	2.08	0.53
1:D:40:PHE:O	1:D:42:THR:N	2.42	0.53
1:A:109:MSE:HE2	1:A:310:TYR:HB2	1.88	0.53
1:A:109:MSE:HE1	1:A:310:TYR:HB2	1.90	0.53
1:A:182:ASP:OD2	1:A:184:VAL:HG22	2.09	0.53
1:D:98:LEU:HD12	1:D:98:LEU:C	2.28	0.53
1:A:107:GLN:OE1	1:A:136:ARG:NH2	2.42	0.53
1:B:130:GLY:O	1:B:131:ASP:CB	2.57	0.52
1:A:283:GLU:CB	2:A:466:HOH:O	2.57	0.52
1:A:329:ILE:O	1:A:329:ILE:HG22	2.09	0.52
1:C:129:GLY:CA	1:C:151:GLU:HB2	2.38	0.52
1:D:134:VAL:O	1:D:138:VAL:HG23	2.09	0.52
1:C:236:GLU:HB3	1:C:241:HIS:CD2	2.43	0.52
1:C:236:GLU:HG3	1:C:241:HIS:CD2	2.45	0.52
1:C:80:VAL:HG21	1:C:159:VAL:HG12	1.92	0.51
1:C:82:GLN:NE2	1:C:88:LYS:HG2	2.24	0.51
1:C:221:VAL:HG11	1:C:231:VAL:CG2	2.40	0.51
1:D:329:ILE:C	1:D:330:GLU:HG3	2.28	0.51
1:C:86:TYR:HD2	1:C:99:THR:HG21	1.74	0.51
1:A:265:THR:HG22	1:A:275:ILE:HG22	1.93	0.51
1:A:296:ILE:HG23	1:A:300:SER:HB2	1.92	0.51
1:C:129:GLY:HA2	1:C:149:MSE:SE	2.60	0.51
1:A:237:SER:H	1:A:241:HIS:HD2	1.57	0.51
1:B:233:THR:HG23	2:B:401:HOH:O	2.09	0.51
1:C:129:GLY:H	1:C:151:GLU:HB2	1.75	0.51
1:D:225:LEU:HD11	1:D:231:VAL:HG22	1.91	0.51
1:A:104:CYS:O	1:A:108:GLU:HG3	2.10	0.51
1:A:135:LEU:HD13	1:A:149:MSE:HE2	1.93	0.51
1:A:72:LYS:H	1:C:51:MSE:SE	2.43	0.51
1:C:238:LEU:CD2	1:C:242:MSE:HE1	2.41	0.51
1:D:116:CYS:SG	1:D:296:ILE:HG13	2.51	0.51
1:C:206:ILE:HG23	1:C:207:GLY:N	2.26	0.51
1:C:301:SER:HB3	1:C:304:ASN:HB2	1.92	0.51
1:C:313:GLU:HB2	2:C:407:HOH:O	2.10	0.51
1:D:184:VAL:HG21	1:D:211:GLU:OE1	2.11	0.51
1:D:123:LYS:HD3	1:D:194:SER:O	2.11	0.50
1:D:259:SER:O	1:D:280:CYS:HA	2.11	0.50
1:A:292:PRO:HB3	1:A:315:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLY:O	1:B:131:ASP:N	2.44	0.50
1:C:242:MSE:HA	1:C:242:MSE:CE	2.35	0.50
1:D:262:TYR:OH	1:D:276:GLY:HA3	2.12	0.50
1:B:228:GLY:HA3	1:B:285:PRO:HD2	1.92	0.50
1:C:214:GLU:HB3	1:C:216:PRO:HD2	1.93	0.50
1:C:297:ASP:OD1	1:C:298:GLU:N	2.41	0.50
1:D:107:GLN:HB2	2:D:436:HOH:O	2.11	0.50
1:D:206:ILE:HG23	1:D:207:GLY:N	2.27	0.50
1:C:262:TYR:OH	1:C:276:GLY:HA3	2.12	0.49
1:A:68:LEU:HB2	1:A:80:VAL:HG12	1.94	0.49
1:A:86:TYR:HB3	1:A:99:THR:CG2	2.41	0.49
1:A:238:LEU:HA	1:A:242:MSE:CE	2.31	0.49
1:A:130:GLY:HA2	1:A:151:GLU:OE2	2.12	0.49
1:A:220:SER:O	1:A:223:ARG:HG2	2.12	0.49
1:C:238:LEU:HD11	1:C:321:LEU:HD22	1.94	0.49
1:D:205:PRO:HB3	1:D:213:PHE:CD1	2.48	0.49
1:C:145:GLU:O	1:C:175:ARG:HG2	2.12	0.49
1:C:165:PRO:C	1:C:167:VAL:H	2.16	0.49
1:B:163:PHE:O	1:B:165:PRO:HD3	2.12	0.49
1:A:263:ALA:HB2	1:A:319:PHE:CE1	2.48	0.49
1:B:206:ILE:HG23	1:B:207:GLY:N	2.27	0.49
1:C:293:LEU:HD23	1:C:293:LEU:O	2.13	0.49
1:C:99:THR:O	1:C:103:GLU:HB3	2.11	0.49
1:B:99:THR:CG2	1:B:269:THR:HG21	2.43	0.49
1:B:112:HIS:ND1	1:B:296:ILE:HD11	2.28	0.49
1:A:131:ASP:HB2	1:A:167:VAL:HG11	1.94	0.49
1:A:242:MSE:CE	1:A:245:ILE:HD12	2.39	0.49
1:D:228:GLY:HA3	1:D:285:PRO:HD2	1.95	0.49
1:A:145:GLU:O	1:A:175:ARG:HG2	2.12	0.48
1:B:43:VAL:HA	1:C:43:VAL:HG13	1.95	0.48
1:B:263:ALA:HB2	1:B:319:PHE:CE1	2.48	0.48
1:C:237:SER:H	1:C:241:HIS:HD2	1.61	0.48
1:D:80:VAL:HG21	1:D:159:VAL:CG1	2.43	0.48
1:C:267:VAL:HG11	1:C:270:TYR:CD2	2.49	0.48
1:D:161:LYS:HA	1:D:168:ALA:HB2	1.96	0.48
1:B:134:VAL:O	1:B:138:VAL:HG23	2.14	0.48
1:C:264:TRP:CZ2	1:C:322:PRO:HD3	2.48	0.48
1:A:283:GLU:HB3	2:A:466:HOH:O	2.14	0.48
1:A:99:THR:HG22	1:A:101:ARG:N	2.28	0.47
1:C:215:LYS:HE2	1:C:251:ASN:OD1	2.14	0.47
1:B:127:ILE:HD11	1:B:187:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:HD11	1:C:231:VAL:HG23	1.97	0.47
1:D:238:LEU:HD22	1:D:242:MSE:HE1	1.96	0.47
1:D:263:ALA:HB2	1:D:319:PHE:CE1	2.49	0.47
1:B:98:LEU:C	1:B:98:LEU:HD12	2.35	0.47
1:B:98:LEU:HD13	1:B:103:GLU:OE2	2.14	0.47
1:C:296:ILE:HG23	1:C:300:SER:HB2	1.96	0.47
1:B:99:THR:HG23	1:B:269:THR:HG21	1.96	0.47
1:D:313:GLU:CD	1:D:313:GLU:H	2.18	0.47
1:C:107:GLN:OE1	1:C:136:ARG:NH2	2.48	0.47
1:B:123:LYS:HE3	1:B:146:GLN:NE2	2.30	0.47
1:A:44:ILE:HD12	1:D:51:MSE:HE1	1.97	0.47
1:B:96:ILE:HG21	1:B:269:THR:HG21	1.96	0.47
1:C:154:LYS:CB	1:C:180:ILE:HD13	2.44	0.47
1:A:261:ASN:HD22	1:A:289:PHE:HD2	1.62	0.47
1:D:60:HIS:CE1	1:D:271:PRO:HA	2.50	0.47
1:A:169:ILE:O	1:A:172:GLU:HB2	2.16	0.46
1:B:149:MSE:HE3	1:B:171:TYR:HE1	1.79	0.46
1:D:113:LEU:N	1:D:114:PRO:HD2	2.31	0.46
1:A:151:GLU:O	1:A:180:ILE:HA	2.14	0.46
1:C:129:GLY:O	1:C:131:ASP:N	2.41	0.46
1:A:237:SER:HA	2:A:387:HOH:O	2.15	0.46
1:B:205:PRO:HB3	1:B:213:PHE:CD1	2.50	0.46
1:C:215:LYS:N	1:C:216:PRO:CD	2.78	0.46
1:A:238:LEU:HD23	1:A:242:MSE:HE1	1.96	0.46
1:A:229:GLY:O	1:A:281:SER:HA	2.16	0.46
1:B:111:THR:O	1:B:114:PRO:HG2	2.16	0.46
1:B:291:HIS:HA	1:B:292:PRO:HD2	1.78	0.46
1:A:311:ASN:O	1:A:314:ILE:HG22	2.16	0.46
1:B:66:LYS:HE3	1:B:68:LEU:HD23	1.98	0.46
1:C:251:ASN:O	1:C:255:ILE:HG12	2.16	0.46
1:D:161:LYS:HA	1:D:168:ALA:CB	2.46	0.46
1:C:221:VAL:CG1	1:C:231:VAL:HG21	2.45	0.46
1:C:238:LEU:HD23	1:C:242:MSE:CE	2.46	0.46
1:A:86:TYR:HB3	1:A:99:THR:HG21	1.97	0.45
1:A:301:SER:HB3	1:A:304:ASN:HB2	1.98	0.45
1:B:49:SER:HB2	1:B:51:MSE:HE2	1.97	0.45
1:D:96:ILE:HG21	1:D:269:THR:HG21	1.98	0.45
1:A:124:VAL:HG23	1:A:144:ILE:HD12	1.98	0.45
1:A:130:GLY:O	1:A:156:VAL:HG12	2.17	0.45
1:B:252:CYS:SG	1:B:278:MSE:HE2	2.55	0.45
1:D:128:GLY:HA2	2:D:463:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG23	1:B:225:LEU:HD21	1.99	0.45
1:A:86:TYR:O	1:A:99:THR:HG23	2.17	0.45
1:A:232:CYS:HA	1:A:278:MSE:O	2.17	0.45
1:B:43:VAL:HG23	1:B:44:ILE:HG13	1.98	0.45
1:D:52:SER:HB3	1:D:55:TRP:CE2	2.52	0.45
1:C:79:ILE:HB	1:C:91:VAL:HB	1.98	0.45
1:C:136:ARG:NH1	1:C:166:ASP:O	2.49	0.45
1:A:215:LYS:N	1:A:216:PRO:CD	2.80	0.45
1:D:49:SER:HB2	1:D:51:MSE:HE2	1.98	0.45
1:B:288:ASP:HB3	2:B:434:HOH:O	2.17	0.45
1:C:151:GLU:O	1:C:180:ILE:HA	2.16	0.45
1:D:128:GLY:O	1:D:130:GLY:N	2.50	0.45
1:C:236:GLU:HB3	1:C:241:HIS:HD2	1.83	0.44
1:D:326:LYS:NZ	2:D:351:HOH:O	2.49	0.44
1:A:115:LEU:HD23	1:A:141:HIS:CD2	2.52	0.44
1:A:228:GLY:HA3	1:A:285:PRO:HD2	1.98	0.44
1:C:202:SER:HB3	1:C:212:LEU:HD13	1.99	0.44
1:B:135:LEU:HD21	1:B:149:MSE:HG2	1.98	0.44
1:C:86:TYR:CD2	1:C:99:THR:HG21	2.52	0.44
1:A:50:GLU:OE2	1:A:96:ILE:N	2.47	0.44
1:D:104:CYS:O	1:D:108:GLU:HB2	2.16	0.44
1:B:163:PHE:C	1:B:165:PRO:HD3	2.38	0.44
1:C:90:LEU:HB3	1:C:98:LEU:HG	2.00	0.44
1:C:200:VAL:CB	1:C:233:THR:HG22	2.45	0.44
1:D:163:PHE:C	1:D:165:PRO:HD3	2.38	0.44
1:A:80:VAL:HG21	1:A:159:VAL:CG1	2.47	0.44
1:C:297:ASP:O	1:C:298:GLU:HB2	2.17	0.44
1:A:135:LEU:HD22	1:A:149:MSE:CE	2.41	0.44
1:B:40:PHE:O	1:B:42:THR:N	2.50	0.44
1:A:202:SER:HB3	1:A:212:LEU:HD13	2.00	0.43
1:B:48:PHE:O	1:B:61:SER:HA	2.18	0.43
1:A:310:TYR:HA	1:A:314:ILE:HG21	2.00	0.43
1:B:105:ALA:O	1:B:109:MSE:HG2	2.18	0.43
1:C:274:VAL:HG13	2:C:396:HOH:O	2.18	0.43
1:C:297:ASP:HB3	2:C:351:HOH:O	2.18	0.43
1:D:198:VAL:HG23	1:D:225:LEU:HD21	1.99	0.43
1:C:161:LYS:NZ	2:C:386:HOH:O	2.50	0.43
1:A:297:ASP:O	1:A:298:GLU:HB2	2.17	0.43
1:B:60:HIS:CE1	2:B:487:HOH:O	2.71	0.43
1:B:217:PHE:O	1:B:220:SER:HB3	2.17	0.43
1:C:129:GLY:N	1:C:151:GLU:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:PRO:HB3	1:D:213:PHE:CE1	2.54	0.43
1:A:262:TYR:OH	1:A:276:GLY:HA3	2.18	0.43
1:A:292:PRO:HB3	1:A:315:HIS:CE1	2.52	0.43
1:D:39:CYS:SG	1:D:39:CYS:O	2.76	0.43
1:B:267:VAL:HG11	1:B:270:TYR:CD2	2.52	0.43
1:D:60:HIS:CD2	2:D:363:HOH:O	2.71	0.43
1:A:329:ILE:O	1:A:329:ILE:CG2	2.67	0.43
1:B:80:VAL:HG21	1:B:159:VAL:CG1	2.49	0.43
1:C:131:ASP:HB2	1:C:167:VAL:HG11	2.00	0.43
1:A:301:SER:HB3	1:A:304:ASN:OD1	2.18	0.43
1:D:129:GLY:O	1:D:156:VAL:HG11	2.18	0.43
1:D:130:GLY:HA2	2:D:465:HOH:O	2.19	0.43
1:C:257:LYS:HA	1:C:257:LYS:HD2	1.86	0.42
1:A:90:LEU:HB3	1:A:98:LEU:HG	2.00	0.42
1:A:313:GLU:HG3	2:D:351:HOH:O	2.18	0.42
1:A:264:TRP:CZ2	1:A:322:PRO:HD3	2.54	0.42
1:A:308:LYS:O	1:D:324:PHE:HB3	2.20	0.42
1:C:242:MSE:CE	1:C:245:ILE:HD12	2.48	0.42
1:D:233:THR:HG22	1:D:234:GLN:O	2.19	0.42
1:B:125:LEU:HB2	1:B:195:TYR:CE1	2.55	0.42
1:B:169:ILE:HA	1:B:169:ILE:HD12	1.81	0.42
1:C:129:GLY:N	1:C:151:GLU:OE1	2.52	0.42
1:B:113:LEU:N	1:B:114:PRO:HD2	2.34	0.42
1:A:237:SER:H	1:A:241:HIS:CD2	2.35	0.42
1:B:187:LEU:HD23	1:B:217:PHE:CE1	2.54	0.42
1:C:232:CYS:HA	1:C:278:MSE:O	2.20	0.42
1:D:107:GLN:NE2	1:D:133:GLY:HA3	2.34	0.42
1:C:135:LEU:HD12	1:C:135:LEU:HA	1.87	0.42
1:A:164:PHE:HA	1:A:165:PRO:HD2	1.94	0.42
1:A:242:MSE:HA	1:A:242:MSE:CE	2.45	0.42
1:A:321:LEU:HD13	1:A:329:ILE:HD12	2.02	0.41
1:B:51:MSE:HE1	1:C:44:ILE:HD12	2.01	0.41
1:C:70:GLN:HG3	1:C:79:ILE:HG12	2.02	0.41
1:A:43:VAL:HG13	1:D:43:VAL:HA	2.02	0.41
1:A:125:LEU:HD23	1:A:198:VAL:HG22	2.02	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.92	0.41
1:C:86:TYR:HB3	1:C:99:THR:HG23	2.00	0.41
1:B:269:THR:HG22	1:B:269:THR:O	2.19	0.41
1:A:244:ILE:HG22	1:A:248:ILE:HD11	2.02	0.41
1:B:165:PRO:C	1:B:167:VAL:H	2.23	0.41
1:C:225:LEU:HD11	1:C:231:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LEU:HD22	1:D:325:ALA:HB1	2.03	0.41
1:B:227:PRO:HG2	2:B:399:HOH:O	2.20	0.41
1:C:327:LYS:HG3	1:C:328:VAL:N	2.35	0.41
1:D:111:THR:HG22	1:D:134:VAL:HG13	2.03	0.41
1:A:197:ALA:HA	1:A:230:VAL:O	2.20	0.41
1:C:310:TYR:HA	1:C:314:ILE:HG21	2.02	0.41
1:A:204:ASP:C	1:A:206:ILE:H	2.24	0.41
1:D:52:SER:HA	1:D:53:PRO:HD3	1.94	0.41
1:D:310:TYR:CD1	1:D:310:TYR:C	2.93	0.41
1:A:55:TRP:HB3	1:A:240:LEU:HD13	2.01	0.41
1:C:221:VAL:CG1	1:C:231:VAL:CG2	2.98	0.41
1:D:229:GLY:O	1:D:281:SER:HA	2.21	0.41
1:A:231:VAL:CG1	1:A:280:CYS:HB2	2.50	0.41
1:A:251:ASN:O	1:A:255:ILE:HG12	2.21	0.41
1:C:296:ILE:HB	1:C:307:LEU:HD11	2.03	0.41
1:C:310:TYR:CD1	1:C:311:ASN:N	2.89	0.41
1:D:241:HIS:ND1	2:D:411:HOH:O	2.37	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.90	0.41
1:B:149:MSE:CE	1:B:171:TYR:HE1	2.34	0.41
1:B:248:ILE:CG2	1:B:278:MSE:HG3	2.51	0.41
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.21	0.41
1:A:238:LEU:CD2	1:A:242:MSE:HE1	2.52	0.40
1:B:238:LEU:HD22	1:B:242:MSE:HE1	2.03	0.40
1:A:206:ILE:HG23	1:A:207:GLY:H	1.86	0.40
1:A:253:ARG:CG	1:A:260:VAL:HG21	2.50	0.40
1:A:310:TYR:CD1	1:A:310:TYR:C	2.95	0.40
1:B:229:GLY:O	1:B:281:SER:HA	2.22	0.40
1:D:264:TRP:CZ2	1:D:322:PRO:HD3	2.56	0.40
1:D:291:HIS:HA	1:D:292:PRO:HD2	1.77	0.40
1:C:229:GLY:O	1:C:281:SER:HA	2.21	0.40
1:A:67:VAL:O	1:C:46:GLY:HA2	2.21	0.40
1:A:310:TYR:CD1	1:A:311:ASN:N	2.89	0.40
1:C:200:VAL:CG2	1:C:233:THR:HG22	2.52	0.40
1:D:105:ALA:O	1:D:109:MSE:HG2	2.22	0.40
1:C:211:GLU:C	1:C:213:PHE:H	2.24	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	288/334 (86%)	268 (93%)	14 (5%)	6 (2%)	7	18
1	B	281/334 (84%)	264 (94%)	11 (4%)	6 (2%)	7	18
1	C	288/334 (86%)	264 (92%)	16 (6%)	8 (3%)	5	11
1	D	281/334 (84%)	261 (93%)	15 (5%)	5 (2%)	8	21
All	All	1138/1336 (85%)	1057 (93%)	56 (5%)	25 (2%)	6	17

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	ASP
1	B	236	GLU
1	C	131	ASP
1	D	131	ASP
1	A	130	GLY
1	A	298	GLU
1	B	130	GLY
1	C	236	GLU
1	C	298	GLU
1	B	166	ASP
1	C	130	GLY
1	D	41	SER
1	D	130	GLY
1	D	236	GLU
1	A	236	GLU
1	A	302	LYS
1	B	167	VAL
1	C	165	PRO
1	D	129	GLY
1	B	41	SER
1	C	166	ASP
1	A	114	PRO

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Mol	Chain	Res	Type
1	A	165	PRO
1	C	167	VAL
1	C	114	PRO

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	249/276 (90%)	243 (98%)	6 (2%)	49	77
1	B	243/276 (88%)	236 (97%)	7 (3%)	42	71
1	C	249/276 (90%)	244 (98%)	5 (2%)	55	81
1	D	243/276 (88%)	236 (97%)	7 (3%)	42	71
All	All	984/1104 (89%)	959 (98%)	25 (2%)	47	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	115	LEU
1	A	226	ARG
1	A	234	GLN
1	A	241	HIS
1	A	264	TRP
1	B	97	GLN
1	B	149	MSE
1	B	187	LEU
1	B	226	ARG
1	B	233	THR
1	B	234	GLN
1	B	264	TRP
1	C	60	HIS
1	C	204	ASP
1	C	236	GLU
1	C	241	HIS
1	C	264	TRP

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Mol	Chain	Res	Type
1	D	97	GLN
1	D	115	LEU
1	D	131	ASP
1	D	226	ARG
1	D	234	GLN
1	D	264	TRP
1	D	330	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	97	GLN
1	A	261	ASN
1	B	97	GLN
1	B	120	ASN
1	B	146	GLN
1	B	162	GLN
1	B	241	HIS
1	C	82	GLN
1	C	261	ASN
1	C	294	ASN
1	C	304	ASN
1	D	60	HIS
1	D	97	GLN
1	D	120	ASN
1	D	162	GLN
1	D	234	GLN
1	D	261	ASN

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, 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	283/334 (84%)	0.09	14 (4%) 29 28	20, 40, 97, 124	0
1	B	278/334 (83%)	-0.12	8 (2%) 51 52	15, 36, 79, 123	0
1	C	283/334 (84%)	0.17	19 (6%) 17 16	18, 40, 93, 133	0
1	D	278/334 (83%)	-0.03	8 (2%) 51 52	14, 36, 81, 114	0
All	All	1122/1336 (83%)	0.03	49 (4%) 34 33	14, 38, 85, 133	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	ILE	6.3
1	C	208	PRO	6.2
1	A	206	ILE	5.8
1	C	166	ASP	5.3
1	C	301	SER	4.5
1	D	39	CYS	4.5
1	C	207	GLY	4.5
1	A	208	PRO	3.9
1	A	166	ASP	3.8
1	A	207	GLY	3.8
1	D	40	PHE	3.7
1	D	206	ILE	3.7
1	C	327	LYS	3.6
1	C	299	SER	3.6
1	C	298	GLU	3.5
1	D	327	LYS	3.5
1	C	129	GLY	3.4
1	D	131	ASP	3.3
1	A	130	GLY	3.2
1	A	298	GLU	2.8
1	B	330	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	2.8
1	C	329	ILE	2.8
1	B	39	CYS	2.6
1	D	166	ASP	2.5
1	A	169	ILE	2.5
1	C	167	VAL	2.5
1	C	205	PRO	2.5
1	A	301	SER	2.5
1	D	208	PRO	2.4
1	C	130	GLY	2.4
1	A	205	PRO	2.4
1	A	303	SER	2.4
1	D	305	GLY	2.3
1	B	40	PHE	2.3
1	C	180	ILE	2.2
1	A	327	LYS	2.2
1	A	167	VAL	2.1
1	B	131	ASP	2.1
1	B	327	LYS	2.1
1	C	209	ALA	2.1
1	C	110	ILE	2.1
1	B	74	ASP	2.1
1	B	128	GLY	2.1
1	C	285	PRO	2.1
1	C	303	SER	2.1
1	C	198	VAL	2.0
1	A	129	GLY	2.0
1	A	211	GLU	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.