Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:33 AM GMT

PDB ID	:	3MDN
Title	:	Structure of glutamine aminotransferase class-II domain protein (SPO2029) from silicibacter pomeroyi
Authors	:	Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-03-30
Resolution	:	2.09 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

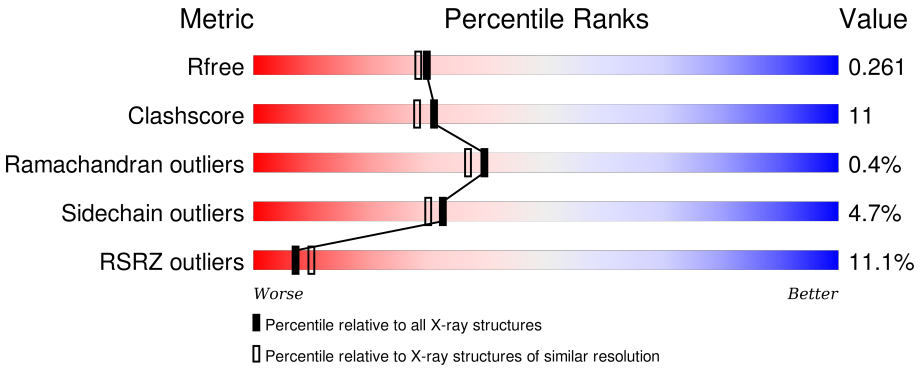
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.09 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	274	6% 65% 14% • 20%
1	B	274	9% 59% 16% • 22%
1	C	274	10% 62% 15% • 21%
1	D	274	9% 66% 12% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6847 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 Glutamine aminotransferase class-II domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	Se	0	0	0
			1711	1087	310	307	3	4			
1	B	214	Total	C	N	O	S	Se	0	0	0
			1677	1066	307	297	3	4			
1	C	216	Total	C	N	O	S	Se	0	0	0
			1692	1075	309	301	3	4			
1	D	223	Total	C	N	O	S	Se	0	0	0
			1731	1095	316	313	3	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q5LRU5
A	0	SER	-	expression tag	UNP Q5LRU5
A	1	LEU	-	expression tag	UNP Q5LRU5
A	265	GLU	-	expression tag	UNP Q5LRU5
A	266	GLY	-	expression tag	UNP Q5LRU5
A	267	HIS	-	expression tag	UNP Q5LRU5
A	268	HIS	-	expression tag	UNP Q5LRU5
A	269	HIS	-	expression tag	UNP Q5LRU5
A	270	HIS	-	expression tag	UNP Q5LRU5
A	271	HIS	-	expression tag	UNP Q5LRU5
A	272	HIS	-	expression tag	UNP Q5LRU5
B	-1	MSE	-	expression tag	UNP Q5LRU5
B	0	SER	-	expression tag	UNP Q5LRU5
B	1	LEU	-	expression tag	UNP Q5LRU5
B	265	GLU	-	expression tag	UNP Q5LRU5
B	266	GLY	-	expression tag	UNP Q5LRU5
B	267	HIS	-	expression tag	UNP Q5LRU5
B	268	HIS	-	expression tag	UNP Q5LRU5
B	269	HIS	-	expression tag	UNP Q5LRU5
B	270	HIS	-	expression tag	UNP Q5LRU5
B	271	HIS	-	expression tag	UNP Q5LRU5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	272	HIS	-	expression tag	UNP Q5LRU5
C	-1	MSE	-	expression tag	UNP Q5LRU5
C	0	SER	-	expression tag	UNP Q5LRU5
C	1	LEU	-	expression tag	UNP Q5LRU5
C	265	GLU	-	expression tag	UNP Q5LRU5
C	266	GLY	-	expression tag	UNP Q5LRU5
C	267	HIS	-	expression tag	UNP Q5LRU5
C	268	HIS	-	expression tag	UNP Q5LRU5
C	269	HIS	-	expression tag	UNP Q5LRU5
C	270	HIS	-	expression tag	UNP Q5LRU5
C	271	HIS	-	expression tag	UNP Q5LRU5
C	272	HIS	-	expression tag	UNP Q5LRU5
D	-1	MSE	-	expression tag	UNP Q5LRU5
D	0	SER	-	expression tag	UNP Q5LRU5
D	1	LEU	-	expression tag	UNP Q5LRU5
D	265	GLU	-	expression tag	UNP Q5LRU5
D	266	GLY	-	expression tag	UNP Q5LRU5
D	267	HIS	-	expression tag	UNP Q5LRU5
D	268	HIS	-	expression tag	UNP Q5LRU5
D	269	HIS	-	expression tag	UNP Q5LRU5
D	270	HIS	-	expression tag	UNP Q5LRU5
D	271	HIS	-	expression tag	UNP Q5LRU5
D	272	HIS	-	expression tag	UNP Q5LRU5

- Molecule 2 is water.

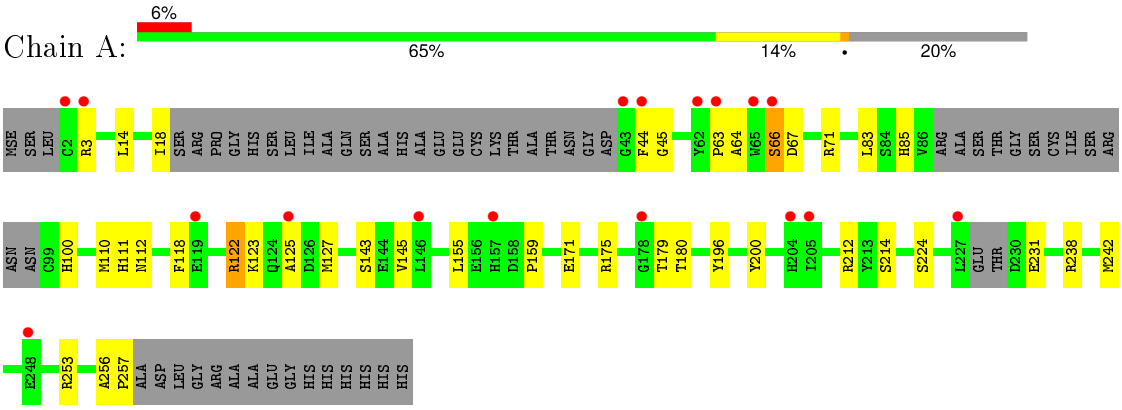
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	6	Total O 6 6	0	0
2	C	11	Total O 11 11	0	0
2	D	8	Total O 8 8	0	0

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.

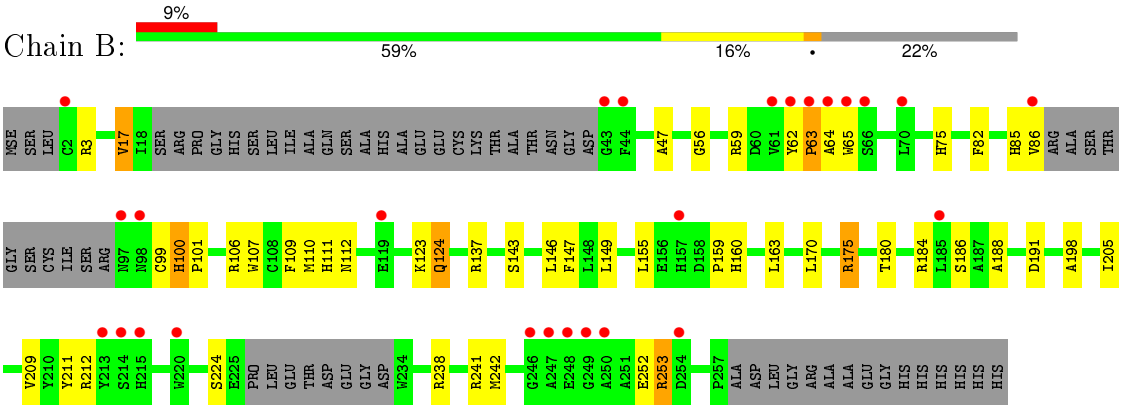
- Molecule 1: Glutamine aminotransferase class-II domain protein

Chain A:



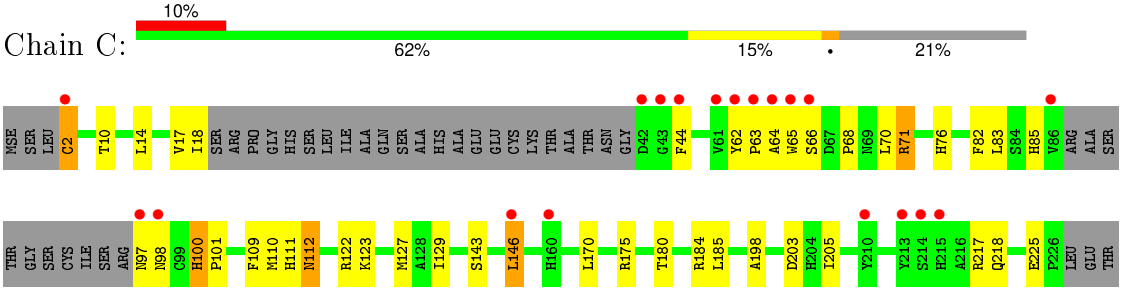
- Molecule 1: Glutamine aminotransferase class-II domain protein

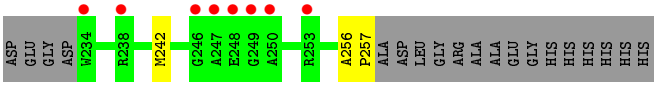
Chain B:



- Molecule 1: Glutamine aminotransferase class-II domain protein

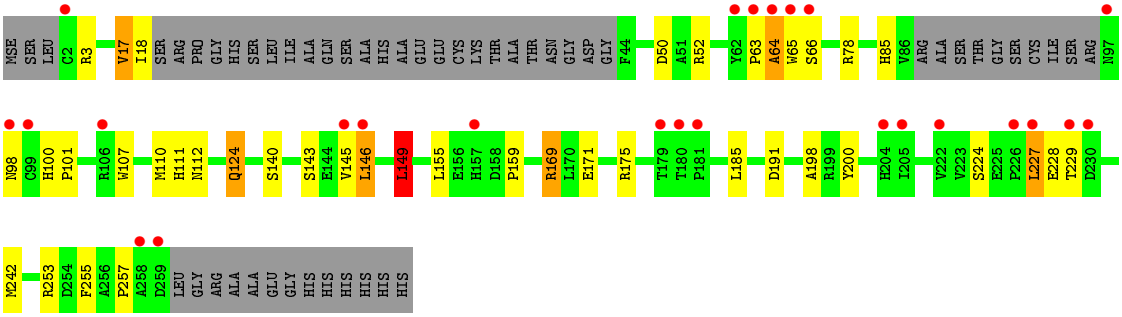
Chain C:





- Molecule 1: Glutamine aminotransferase class-II domain protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.37Å 72.96Å 106.72Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	40.00 – 2.09 35.71 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.09) 98.9 (35.71-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.253 0.214 , 0.261	Depositor DCC
R_{free} test set	3004 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.2	EDS
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 59478 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6847	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4428e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.68	0/1759	0.75	1/2380 (0.0%)
1	B	0.69	0/1724	0.74	1/2333 (0.0%)
1	C	0.71	0/1740	0.71	1/2356 (0.0%)
1	D	0.64	0/1779	0.69	1/2413 (0.0%)
All	All	0.68	0/7002	0.72	4/9482 (0.0%)

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	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	224	SER	CB-CA-C	-5.60	99.46	110.10
1	D	149	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	203	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	185	LEU	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	1711	0	1601	40	0
1	B	1677	0	1570	40	0
1	C	1692	0	1581	32	0
1	D	1731	0	1608	34	0
2	A	11	0	0	0	0
2	B	6	0	0	0	0
2	C	11	0	0	1	0
2	D	8	0	0	1	0
All	All	6847	0	6360	143	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 11.

All (143) 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:83:LEU:HB3	1:A:110:MSE:CE	1.39	1.53
1:A:83:LEU:HB3	1:A:110:MSE:HE2	1.29	1.12
1:A:83:LEU:CB	1:A:110:MSE:CE	2.30	1.09
1:B:175:ARG:HH11	1:B:175:ARG:HG3	1.15	1.05
1:A:83:LEU:HB3	1:A:110:MSE:HE1	1.12	1.04
1:D:169:ARG:CG	1:D:169:ARG:HH11	1.72	1.03
1:A:83:LEU:CB	1:A:110:MSE:HE1	1.89	1.02
1:D:169:ARG:NH1	1:D:169:ARG:HG3	1.61	0.93
1:D:169:ARG:HG3	1:D:169:ARG:HH11	0.80	0.92
1:A:85:HIS:HB2	1:A:110:MSE:SE	2.20	0.91
1:D:124:GLN:H	1:D:124:GLN:HE21	1.18	0.90
1:B:146:LEU:HD12	1:B:170:LEU:HD12	1.53	0.90
1:B:17:VAL:HG23	1:B:17:VAL:O	1.70	0.90
1:D:85:HIS:HB2	1:D:110:MSE:SE	2.25	0.86
1:B:175:ARG:CG	1:B:175:ARG:HH11	1.90	0.85
1:C:62:TYR:HB2	1:C:63:PRO:HD2	1.61	0.82
1:B:175:ARG:NH1	1:B:175:ARG:HG3	1.89	0.82
1:C:111:HIS:HD2	1:C:143:SER:OG	1.67	0.78
1:B:175:ARG:NH1	1:B:175:ARG:CG	2.44	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:O	1:C:122:ARG:NH2	2.17	0.77
1:B:160:HIS:CD2	1:B:253:ARG:HD3	2.20	0.76
1:A:179:THR:HG22	1:A:180:THR:H	1.53	0.74
1:A:111:HIS:HD2	1:A:143:SER:OG	1.70	0.73
1:A:123:LYS:HE2	1:A:127:MSE:CE	2.21	0.70
1:C:146:LEU:HD12	1:C:170:LEU:HD12	1.73	0.70
1:C:44:PHE:CD2	1:C:70:LEU:HD21	2.29	0.68
1:B:155:LEU:HD12	1:B:159:PRO:HA	1.76	0.67
1:A:63:PRO:HG2	1:A:66:SER:HB2	1.77	0.66
1:A:83:LEU:CA	1:A:110:MSE:HE1	2.25	0.66
1:C:184:ARG:HD3	1:C:205:ILE:O	1.95	0.66
1:B:111:HIS:HD2	1:B:143:SER:OG	1.78	0.65
1:A:14:LEU:O	1:A:18:ILE:HG13	1.97	0.65
1:A:100:HIS:HD2	1:A:111:HIS:H	1.45	0.64
1:B:124:GLN:HE21	1:B:124:GLN:H	1.45	0.64
1:A:155:LEU:HD12	1:A:159:PRO:HA	1.80	0.63
1:D:146:LEU:HD11	1:D:185:LEU:CD1	2.29	0.63
1:A:44:PHE:CD2	1:A:45:GLY:N	2.67	0.63
1:B:238:ARG:HG3	1:B:241:ARG:HG3	1.79	0.62
1:D:111:HIS:HD2	1:D:143:SER:OG	1.82	0.62
1:C:68:PRO:HA	1:C:71:ARG:HD3	1.81	0.61
1:D:85:HIS:CD2	1:D:100:HIS:HB2	2.35	0.61
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.15	0.61
1:A:212:ARG:HH12	1:A:231:GLU:HB2	1.65	0.60
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.65	0.60
1:D:229:THR:HG22	1:D:229:THR:O	2.02	0.59
1:B:100:HIS:HB3	1:B:101:PRO:HA	1.85	0.58
1:B:17:VAL:CG2	1:B:17:VAL:O	2.43	0.57
1:A:123:LYS:HE2	1:A:127:MSE:HE3	1.87	0.57
1:B:64:ALA:O	1:B:65:TRP:C	2.43	0.57
1:D:124:GLN:HE21	1:D:124:GLN:N	1.98	0.56
1:A:123:LYS:HE2	1:A:127:MSE:HE1	1.86	0.56
1:A:83:LEU:CB	1:A:110:MSE:HE2	2.18	0.56
1:C:146:LEU:HD12	1:C:170:LEU:CD1	2.35	0.55
1:A:83:LEU:C	1:A:110:MSE:HE1	2.27	0.55
1:A:44:PHE:CD1	1:A:64:ALA:HB2	2.42	0.55
1:C:198:ALA:HB2	1:C:242:MSE:HE2	1.88	0.55
1:A:100:HIS:CD2	1:A:111:HIS:H	2.24	0.54
1:C:2:CYS:HA	1:C:112:ASN:ND2	2.23	0.54
1:D:242:MSE:HE3	1:D:255:PHE:CD1	2.42	0.54
1:A:179:THR:HG22	1:A:180:THR:N	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:CZ	1:C:146:LEU:HD23	2.44	0.53
1:C:109:PHE:HZ	1:C:146:LEU:HD23	1.72	0.53
1:D:18:ILE:HG22	1:D:18:ILE:O	2.08	0.53
1:D:124:GLN:H	1:D:124:GLN:NE2	1.99	0.53
1:B:59:ARG:NH1	1:B:99:CYS:O	2.40	0.53
1:C:63:PRO:O	1:C:66:SER:HB3	2.09	0.52
1:C:62:TYR:CB	1:C:63:PRO:HD2	2.37	0.52
1:A:123:LYS:HG2	1:A:127:MSE:HE2	1.90	0.52
1:B:146:LEU:CD1	1:B:170:LEU:HD12	2.32	0.52
1:D:171:GLU:OE2	1:D:175:ARG:NH2	2.41	0.52
1:D:229:THR:CG2	1:D:229:THR:O	2.57	0.51
1:D:198:ALA:HB2	1:D:242:MSE:HE2	1.91	0.51
1:C:18:ILE:HG22	1:C:18:ILE:O	2.09	0.51
1:D:155:LEU:HD12	1:D:159:PRO:HA	1.92	0.51
1:A:83:LEU:HD23	1:A:110:MSE:CE	2.41	0.51
1:C:17:VAL:HG22	1:C:217:ARG:NH1	2.25	0.51
1:B:17:VAL:HG22	1:B:82:PHE:CE1	2.46	0.50
1:D:50:ASP:HB3	2:D:280:HOH:O	2.11	0.50
1:B:186:SER:HB2	1:B:209:VAL:CG2	2.40	0.50
1:C:82:PHE:C	1:C:83:LEU:HD12	2.32	0.50
1:B:123:LYS:NZ	1:C:129:ILE:O	2.30	0.50
1:C:97:ASN:ND2	1:C:98:ASN:H	2.09	0.49
1:B:110:MSE:HE2	1:B:188:ALA:HB3	1.94	0.49
1:A:171:GLU:OE2	1:A:175:ARG:NH2	2.44	0.49
1:D:227:LEU:HD12	1:D:228:GLU:H	1.77	0.49
1:A:83:LEU:HD23	1:A:110:MSE:HE2	1.95	0.48
1:C:100:HIS:HB3	1:C:101:PRO:HA	1.95	0.48
1:C:85:HIS:HB2	1:C:110:MSE:SE	2.63	0.48
1:A:196:TYR:CD2	1:A:242:MSE:HE3	2.49	0.48
1:B:3:ARG:O	1:B:86:VAL:N	2.47	0.48
1:B:160:HIS:HB2	1:B:253:ARG:NH1	2.29	0.47
1:D:169:ARG:NH1	1:D:169:ARG:CG	2.45	0.47
1:C:2:CYS:HA	1:C:112:ASN:HD21	1.79	0.47
1:B:160:HIS:HD2	1:B:253:ARG:HD3	1.77	0.47
1:B:184:ARG:HD3	1:B:205:ILE:O	2.14	0.47
1:D:100:HIS:CD2	1:D:111:HIS:H	2.32	0.47
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.28	0.47
1:C:175:ARG:HG2	1:C:175:ARG:HH11	1.80	0.47
1:B:75:HIS:CD2	1:D:52:ARG:HE	2.32	0.47
1:D:63:PRO:HG2	1:D:66:SER:OG	2.15	0.47
1:B:85:HIS:HB2	1:B:110:MSE:SE	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:HIS:HD2	1:C:111:HIS:H	1.62	0.46
1:A:83:LEU:CG	1:A:110:MSE:CE	2.93	0.46
1:C:111:HIS:CD2	1:C:143:SER:OG	2.58	0.46
1:C:217:ARG:O	1:C:218:GLN:HB2	2.16	0.46
1:A:123:LYS:HG2	1:A:127:MSE:CE	2.46	0.46
1:B:47:ALA:HA	1:B:56:GLY:O	2.15	0.45
1:D:3:ARG:HA	1:D:224:SER:OG	2.16	0.45
1:A:118:PHE:CE2	1:A:122:ARG:HG3	2.52	0.45
1:C:198:ALA:HB2	1:C:242:MSE:CE	2.45	0.44
1:B:211:TYR:OH	1:B:252:GLU:OE2	2.23	0.44
1:B:100:HIS:N	1:B:100:HIS:ND1	2.65	0.44
1:B:163:LEU:HD23	1:B:242:MSE:CE	2.46	0.44
1:A:3:ARG:HA	1:A:224:SER:OG	2.18	0.44
1:B:163:LEU:HD23	1:B:242:MSE:HE1	2.00	0.44
1:D:63:PRO:O	1:D:65:TRP:N	2.51	0.44
1:C:256:ALA:O	1:C:257:PRO:C	2.56	0.44
1:D:98:ASN:HD21	1:D:140:SER:H	1.65	0.43
1:B:109:PHE:CD1	1:B:147:PHE:HB2	2.54	0.43
1:C:14:LEU:O	1:C:18:ILE:HD13	2.19	0.43
1:B:198:ALA:HB2	1:B:242:MSE:HE3	1.99	0.43
1:D:200:TYR:CE1	1:D:257:PRO:HD3	2.54	0.43
1:C:65:TRP:O	1:C:71:ARG:NH1	2.51	0.42
1:C:123:LYS:O	1:C:127:MSE:HG2	2.19	0.42
1:A:85:HIS:CD2	1:A:100:HIS:HB2	2.54	0.42
1:D:145:VAL:HG12	1:D:149:LEU:HG	2.02	0.42
1:A:200:TYR:CZ	1:A:257:PRO:HG3	2.54	0.42
1:B:198:ALA:HB2	1:B:242:MSE:CE	2.49	0.42
1:C:76:HIS:HD2	2:C:283:HOH:O	2.01	0.42
1:B:107:TRP:CZ2	1:B:191:ASP:HB3	2.55	0.42
1:A:67:ASP:C	1:A:67:ASP:OD1	2.59	0.42
1:D:78:ARG:HE	1:D:78:ARG:HB2	1.59	0.42
1:D:107:TRP:CZ2	1:D:191:ASP:HB3	2.55	0.41
1:A:256:ALA:HA	1:A:257:PRO:HD2	1.77	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.93	0.41
1:D:100:HIS:HD2	1:D:111:HIS:H	1.67	0.41
1:B:62:TYR:O	1:B:63:PRO:C	2.60	0.41
1:A:125:ALA:HB1	1:A:145:VAL:HG11	2.02	0.41
1:D:17:VAL:HG12	1:D:18:ILE:N	2.35	0.40
1:B:109:PHE:HZ	1:B:146:LEU:HD23	1.86	0.40
1:B:100:HIS:HD2	1:B:111:HIS:H	1.68	0.40
1:D:100:HIS:HB3	1:D:101:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:PRO:O	1:D:64:ALA:C	2.59	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	210/274 (77%)	207 (99%)	3 (1%)	0	100	100
1	B	206/274 (75%)	197 (96%)	8 (4%)	1 (0%)	34	30
1	C	208/274 (76%)	199 (96%)	8 (4%)	1 (0%)	34	30
1	D	217/274 (79%)	210 (97%)	6 (3%)	1 (0%)	34	30
All	All	841/1096 (77%)	813 (97%)	25 (3%)	3 (0%)	39	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	PRO
1	D	64	ALA
1	C	64	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	166/207 (80%)	161 (97%)	5 (3%)	48	51
1	B	162/207 (78%)	152 (94%)	10 (6%)	23	19
1	C	164/207 (79%)	156 (95%)	8 (5%)	31	28
1	D	167/207 (81%)	159 (95%)	8 (5%)	31	29
All	All	659/828 (80%)	628 (95%)	31 (5%)	32	30

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	112	ASN
1	A	214	SER
1	A	238	ARG
1	A	253	ARG
1	B	17	VAL
1	B	100	HIS
1	B	106	ARG
1	B	112	ASN
1	B	124	GLN
1	B	149	LEU
1	B	175	ARG
1	B	180	THR
1	B	212	ARG
1	B	253	ARG
1	C	2	CYS
1	C	10	THR
1	C	71	ARG
1	C	100	HIS
1	C	112	ASN
1	C	146	LEU
1	C	180	THR
1	C	225	GLU
1	D	17	VAL
1	D	112	ASN
1	D	124	GLN
1	D	146	LEU
1	D	149	LEU
1	D	169	ARG
1	D	227	LEU
1	D	253	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	85	HIS
1	A	111	HIS
1	A	112	ASN
1	B	76	HIS
1	B	111	HIS
1	B	112	ASN
1	B	124	GLN
1	B	218	GLN
1	C	76	HIS
1	C	111	HIS
1	C	112	ASN
1	D	85	HIS
1	D	98	ASN
1	D	111	HIS
1	D	112	ASN
1	D	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	214/274 (78%)	0.68	17 (7%) 15 21	19, 29, 49, 56	0
1	B	210/274 (76%)	0.85	26 (12%) 5 7	19, 29, 47, 55	0
1	C	212/274 (77%)	0.72	27 (12%) 5 6	18, 29, 47, 58	0
1	D	219/274 (79%)	0.84	25 (11%) 7 9	19, 28, 51, 57	0
All	All	855/1096 (78%)	0.77	95 (11%) 7 10	18, 29, 49, 58	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	42	ASP	9.4
1	B	43	GLY	7.0
1	C	247	ALA	6.7
1	A	62	TYR	6.4
1	D	258	ALA	6.2
1	D	205	ILE	6.2
1	D	230	ASP	6.1
1	A	65	TRP	6.1
1	B	64	ALA	5.7
1	D	62	TYR	5.7
1	C	62	TYR	5.6
1	B	247	ALA	5.2
1	B	44	PHE	5.2
1	C	65	TRP	5.2
1	B	98	ASN	5.1
1	D	227	LEU	5.1
1	C	98	ASN	5.0
1	C	43	GLY	5.0
1	B	62	TYR	4.8
1	B	2	CYS	4.6
1	B	65	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	249	GLY	4.4
1	B	63	PRO	4.4
1	C	63	PRO	4.4
1	C	2	CYS	4.3
1	B	246	GLY	4.2
1	D	63	PRO	4.1
1	D	229	THR	4.0
1	A	66	SER	3.9
1	B	97	ASN	3.9
1	D	97	ASN	3.9
1	C	248	GLU	3.9
1	A	44	PHE	3.8
1	D	66	SER	3.6
1	D	204	HIS	3.6
1	D	226	PRO	3.6
1	D	179	THR	3.6
1	B	213	TYR	3.6
1	D	157	HIS	3.6
1	A	248	GLU	3.5
1	D	64	ALA	3.5
1	C	44	PHE	3.5
1	D	65	TRP	3.5
1	B	248	GLU	3.4
1	C	66	SER	3.4
1	D	99	CYS	3.4
1	B	250	ALA	3.3
1	B	249	GLY	3.3
1	C	64	ALA	3.3
1	D	98	ASN	3.1
1	B	86	VAL	3.1
1	A	2	CYS	3.1
1	C	250	ALA	3.0
1	B	61	VAL	3.0
1	C	253	ARG	3.0
1	C	213	TYR	3.0
1	B	185	LEU	2.9
1	D	259	ASP	2.9
1	C	215	HIS	2.8
1	A	204	HIS	2.8
1	A	227	LEU	2.8
1	D	146	LEU	2.8
1	D	180	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	146	LEU	2.7
1	A	157	HIS	2.7
1	B	220	TRP	2.7
1	D	222	VAL	2.7
1	B	66	SER	2.7
1	A	3	ARG	2.6
1	A	63	PRO	2.6
1	A	43	GLY	2.6
1	C	160	HIS	2.6
1	D	2	CYS	2.5
1	D	181	PRO	2.5
1	C	97	ASN	2.5
1	A	178	GLY	2.4
1	B	157	HIS	2.4
1	A	119	GLU	2.3
1	A	125	ALA	2.3
1	C	146	LEU	2.3
1	B	215	HIS	2.3
1	C	86	VAL	2.3
1	B	254	ASP	2.2
1	C	214	SER	2.2
1	C	246	GLY	2.2
1	D	106	ARG	2.2
1	C	238	ARG	2.2
1	C	234	TRP	2.2
1	D	145	VAL	2.1
1	A	205	ILE	2.1
1	C	210	TYR	2.1
1	B	119	GLU	2.1
1	C	61	VAL	2.1
1	B	70	LEU	2.0
1	B	214	SER	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.