Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:50 PM GMT

PDB ID	:	4ANF
Title	:	Structure of the ornithine carbamoyltransferase from Mycoplasma penetrans with a P23 Space group
Authors	:	Gallego, P.; Benach, J.; Planell, R.; Querol, E.; Perez-Pons, J.A.; Reverter, D.
Deposited on	:	2012-03-16
Resolution	:	2.60 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 (i) symbol.

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

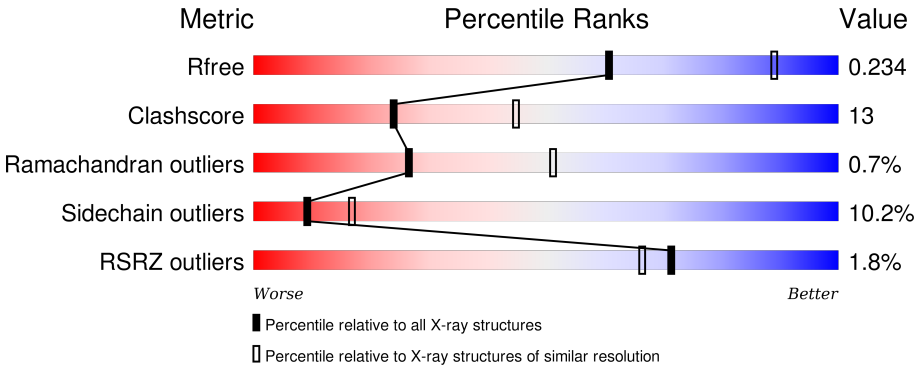
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	365	2% 68% 21% 5% 6%
1	B	365	2% 68% 22% • 6%
1	C	365	% 68% 23% • 6%
1	D	365	3% 63% 25% 6% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10953 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 ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2674	1701	452	506	15			
1	B	342	Total	C	N	O	S	0	0	0
			2674	1701	452	506	15			
1	C	342	Total	C	N	O	S	0	0	0
			2674	1701	452	506	15			
1	D	342	Total	C	N	O	S	0	0	0
			2674	1701	452	506	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
A	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
A	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
A	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
A	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
A	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
A	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
A	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
B	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
B	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
B	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
B	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
B	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
B	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
B	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
C	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
C	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
C	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
C	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
C	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
C	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
D	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
D	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
D	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
D	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
D	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
D	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
D	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5

- Molecule 2 is water.

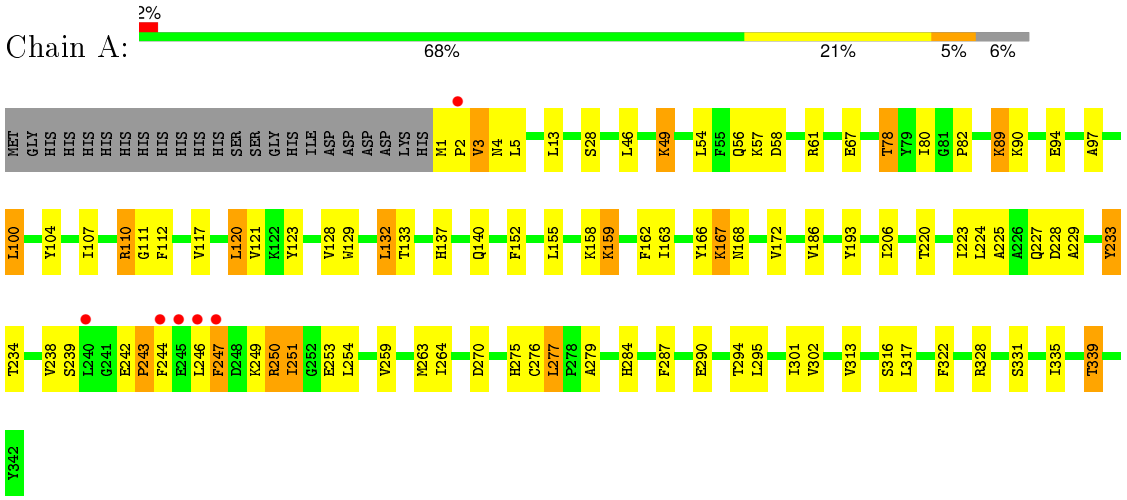
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	72	Total O 72 72	0	0
2	B	54	Total O 54 54	0	0
2	C	73	Total O 73 73	0	0
2	D	58	Total O 58 58	0	0

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.

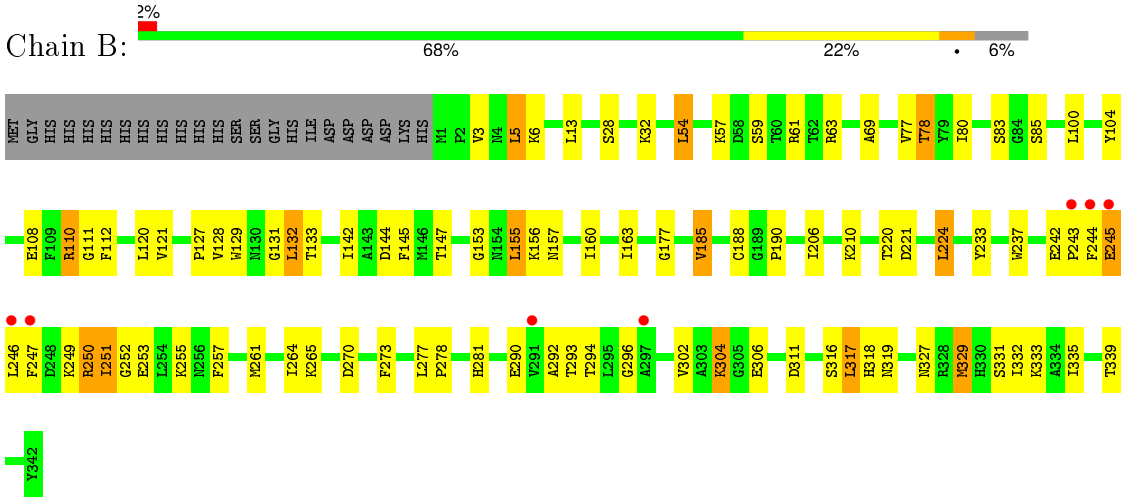
• Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC

Chain A:



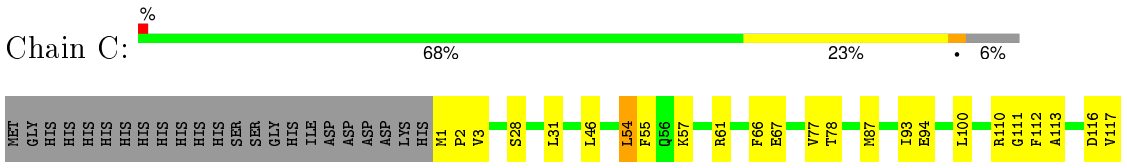
• Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC

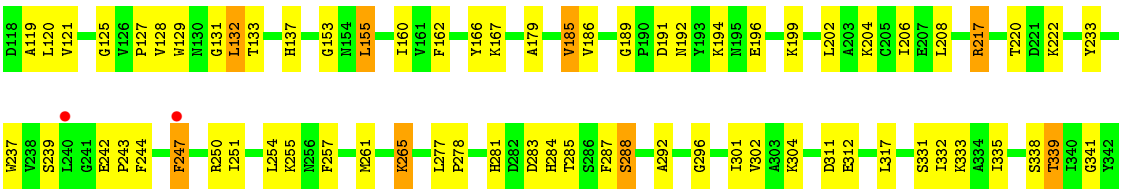
Chain B:



• Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC

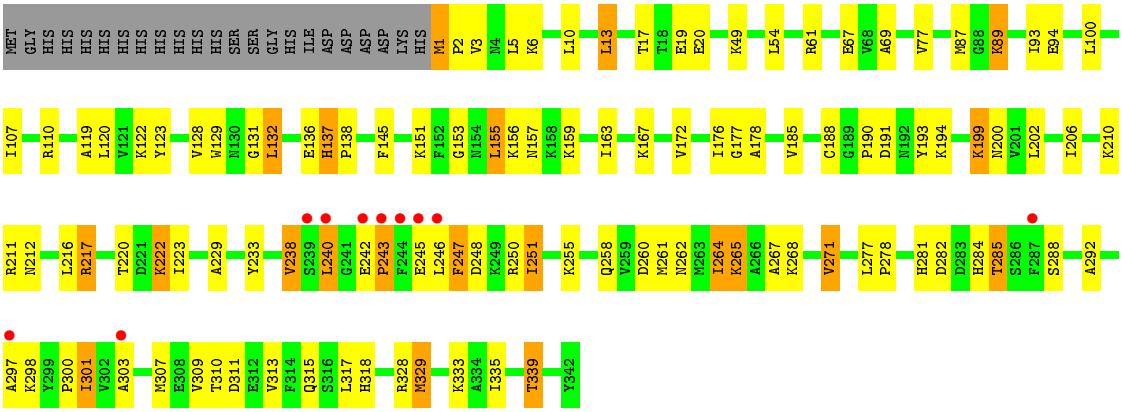
Chain C:





• Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	167.91Å 167.91Å 167.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.60 48.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.6 (48.47-2.60) 98.2 (48.47-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.237 0.169 , 0.234	Depositor DCC
R_{free} test set	2415 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 47859 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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	0.45	0/2724	0.61	0/3670
1	B	0.44	0/2724	0.60	1/3670 (0.0%)
1	C	0.45	0/2724	0.58	0/3670
1	D	0.44	0/2724	0.64	1/3670 (0.0%)
All	All	0.45	0/10896	0.61	2/14680 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	267	ALA	CB-CA-C	-7.20	99.31	110.10
1	B	317	LEU	CA-CB-CG	6.28	129.74	115.30

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	2674	0	2672	58	0
1	B	2674	0	2672	58	0
1	C	2674	0	2672	66	0
1	D	2674	0	2672	99	0
2	A	72	0	0	2	0
2	B	54	0	0	0	0
2	C	73	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	58	0	0	2	0
All	All	10953	0	10688	279	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 13.

All (279) 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:B:129:TRP:HE1	1:B:339:THR:HG21	1.16	1.06
1:A:129:TRP:HE1	1:A:339:THR:HG21	1.20	1.02
1:D:129:TRP:HE1	1:D:339:THR:HG21	1.26	1.00
1:D:242:GLU:HB2	1:D:243:PRO:HD3	1.40	1.00
1:B:129:TRP:NE1	1:B:339:THR:HG21	1.89	0.88
1:D:329:MET:CE	1:D:333:LYS:HE3	2.05	0.87
1:D:329:MET:HE3	1:D:333:LYS:HE3	1.57	0.87
1:A:129:TRP:NE1	1:A:339:THR:HG21	1.90	0.85
1:D:247:PHE:O	1:D:251:ILE:HG22	1.76	0.85
1:D:297:ALA:HA	1:D:298:LYS:C	1.98	0.81
1:D:129:TRP:NE1	1:D:339:THR:HG21	1.95	0.80
1:B:329:MET:HE3	1:B:333:LYS:HE3	1.63	0.80
1:D:285:THR:HG23	1:D:288:SER:HB2	1.63	0.80
1:D:243:PRO:HG2	1:D:246:LEU:H	1.48	0.79
1:C:129:TRP:HE1	1:C:339:THR:HG21	1.46	0.79
1:C:244:PHE:HA	1:C:247:PHE:CD1	2.19	0.78
1:A:335:ILE:O	1:A:339:THR:HB	1.84	0.78
1:D:89:LYS:H	1:D:89:LYS:HD2	1.49	0.77
1:C:285:THR:OG1	1:C:288:SER:HB2	1.84	0.76
1:B:329:MET:CE	1:B:333:LYS:HE3	2.15	0.76
1:B:145:PHE:CE1	1:B:177:GLY:HA3	2.23	0.74
1:A:246:LEU:O	1:A:250:ARG:HG3	1.88	0.73
1:D:19:GLU:OE2	1:D:211:ARG:NH2	2.21	0.73
1:A:239:SER:O	1:A:242:GLU:HB3	1.89	0.72
1:A:159:LYS:HG2	1:A:229:ALA:HA	1.71	0.72
1:C:247:PHE:HE2	1:C:287:PHE:CE1	2.08	0.72
1:D:206:ILE:O	1:D:210:LYS:HG3	1.90	0.71
1:D:258:GLN:HG3	1:D:307:MET:O	1.91	0.70
1:D:281:HIS:O	1:D:311:ASP:HB2	1.91	0.70
1:D:285:THR:HG23	1:D:288:SER:CB	2.23	0.69
1:A:290:GLU:O	1:A:294:THR:HG23	1.93	0.69
1:B:335:ILE:O	1:B:339:THR:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:PRO:HG3	1:D:246:LEU:HD13	1.77	0.67
1:C:1:MET:HG3	1:C:2:PRO:HD2	1.77	0.67
1:B:153:GLY:O	1:B:155:LEU:HD13	1.95	0.66
1:D:240:LEU:HD12	1:D:240:LEU:C	2.15	0.66
1:D:298:LYS:O	1:D:300:PRO:HD3	1.95	0.65
1:B:252:GLY:O	1:B:255:LYS:HG2	1.96	0.65
1:D:178:ALA:HB1	1:D:185:VAL:HG22	1.79	0.65
1:D:238:VAL:HG11	1:D:247:PHE:CD2	2.32	0.65
1:A:251:ILE:HD12	1:A:302:VAL:HG11	1.80	0.64
1:C:167:LYS:HD2	1:C:196:GLU:HG3	1.80	0.63
1:C:191:ASP:O	1:C:194:LYS:HG2	1.98	0.63
1:B:242:GLU:HB2	1:B:243:PRO:HD2	1.81	0.63
1:C:167:LYS:NZ	1:C:250:ARG:HH12	1.98	0.62
1:D:268:LYS:O	1:D:271:VAL:HG12	1.98	0.61
1:C:335:ILE:O	1:C:339:THR:HB	2.01	0.61
1:A:238:VAL:HB	1:A:247:PHE:CE1	2.36	0.61
1:B:243:PRO:HB2	1:B:245:GLU:HG3	1.83	0.61
1:D:255:LYS:HE3	2:D:2053:HOH:O	2.01	0.60
1:D:191:ASP:O	1:D:194:LYS:HE2	2.01	0.60
1:D:89:LYS:N	1:D:89:LYS:HD2	2.16	0.60
1:C:261:MET:HE1	1:C:265:LYS:HD3	1.83	0.60
1:D:190:PRO:HG2	1:D:193:TYR:CE2	2.36	0.60
1:D:238:VAL:HG11	1:D:247:PHE:CE2	2.36	0.60
1:C:129:TRP:NE1	1:C:339:THR:HG21	2.16	0.60
1:C:28:SER:OG	1:C:331:SER:HA	2.02	0.60
1:D:159:LYS:HB3	1:D:229:ALA:HA	1.84	0.60
1:D:335:ILE:O	1:D:339:THR:HB	2.01	0.60
1:D:178:ALA:CB	1:D:185:VAL:HG22	2.32	0.60
1:C:189:GLY:HA2	1:C:257:PHE:CE1	2.36	0.60
1:C:66:PHE:CE2	1:C:332:ILE:HD13	2.37	0.60
1:B:249:LYS:O	1:B:253:GLU:HG2	2.01	0.59
1:A:264:ILE:HD11	1:A:313:VAL:HG13	1.84	0.59
1:A:78:THR:HG21	1:A:104:TYR:OH	2.02	0.59
1:D:329:MET:HE1	1:D:333:LYS:HE3	1.84	0.59
1:A:168:ASN:O	1:A:172:VAL:HG23	2.03	0.58
1:D:247:PHE:H	1:D:247:PHE:HD1	1.50	0.58
1:D:271:VAL:O	1:D:318:HIS:HD2	1.86	0.58
1:B:221:ASP:OD2	1:B:224:LEU:HB2	2.04	0.57
1:D:145:PHE:CE2	1:D:177:GLY:HA3	2.39	0.57
1:D:49:LYS:HE3	2:D:2020:HOH:O	2.03	0.57
1:D:242:GLU:HB2	1:D:243:PRO:CD	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:PRO:CG	1:D:246:LEU:HD13	2.35	0.57
1:B:163:ILE:HA	1:B:188:CYS:O	2.05	0.56
1:C:31:LEU:HD13	1:C:333:LYS:HG2	1.86	0.56
1:B:3:VAL:O	1:B:3:VAL:HG23	2.05	0.56
1:A:97:ALA:HB2	1:A:120:LEU:HD12	1.87	0.56
1:B:54:LEU:HD22	1:B:80:ILE:HD12	1.86	0.56
1:C:202:LEU:O	1:C:206:ILE:HG12	2.04	0.56
1:A:301:ILE:HG13	1:A:302:VAL:HG13	1.86	0.56
1:B:28:SER:OG	1:B:331:SER:HA	2.06	0.56
1:D:242:GLU:HB2	1:D:246:LEU:HD22	1.87	0.56
1:D:1:MET:HG2	1:D:2:PRO:HD3	1.88	0.55
1:A:242:GLU:HG3	1:A:243:PRO:HD2	1.87	0.55
1:A:4:ASN:ND2	1:C:125:GLY:O	2.39	0.55
1:D:247:PHE:CD1	1:D:247:PHE:N	2.75	0.55
1:A:322:PHE:HB2	2:A:2071:HOH:O	2.05	0.55
1:A:186:VAL:HG11	1:A:225:ALA:HB1	1.88	0.54
1:A:89:LYS:HA	1:A:89:LYS:HE3	1.88	0.54
1:D:247:PHE:HD1	1:D:247:PHE:N	2.05	0.54
1:D:156:LYS:HE3	1:D:212:ASN:O	2.08	0.54
1:D:172:VAL:O	1:D:176:ILE:HG13	2.09	0.53
1:D:255:LYS:HB2	1:D:301:ILE:HD11	1.90	0.53
1:B:290:GLU:O	1:B:294:THR:HG23	2.09	0.53
1:C:247:PHE:HE2	1:C:287:PHE:CZ	2.26	0.53
1:A:247:PHE:O	1:A:251:ILE:HG22	2.08	0.53
1:C:66:PHE:CD2	1:C:332:ILE:HD13	2.44	0.53
1:B:32:LYS:NZ	1:B:327:ASN:OD1	2.41	0.53
1:A:159:LYS:CG	1:A:229:ALA:HA	2.37	0.53
1:B:304:LYS:HB2	1:B:304:LYS:NZ	2.24	0.53
1:B:281:HIS:O	1:B:311:ASP:HB2	2.08	0.53
1:A:247:PHE:CE2	1:A:287:PHE:HZ	2.27	0.52
1:D:216:LEU:HD12	1:D:217:ARG:H	1.74	0.52
1:B:265:LYS:NZ	1:B:318:HIS:NE2	2.48	0.52
1:C:111:GLY:O	1:C:133:THR:HA	2.09	0.52
1:C:167:LYS:HD2	1:C:196:GLU:CB	2.39	0.52
1:B:5:LEU:HD12	1:B:5:LEU:N	2.25	0.52
1:A:276:CYS:O	1:A:277:LEU:HB2	2.10	0.52
1:C:237:TRP:O	1:C:250:ARG:HD2	2.10	0.51
1:B:292:ALA:O	1:B:296:GLY:HA3	2.10	0.51
1:C:292:ALA:O	1:C:296:GLY:HA3	2.10	0.51
1:D:281:HIS:O	1:D:282:ASP:HB3	2.10	0.51
1:D:94:GLU:HG3	1:D:123:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:A:132:LEU:HD23	2.25	0.51
1:A:54:LEU:CD2	1:A:80:ILE:HD12	2.40	0.51
1:C:242:GLU:HG3	1:C:247:PHE:CE1	2.45	0.51
1:B:244:PHE:HE2	1:B:294:THR:HG1	1.56	0.51
1:B:302:VAL:HA	1:B:306:GLU:O	2.11	0.51
1:B:247:PHE:O	1:B:251:ILE:HG23	2.10	0.51
1:D:247:PHE:O	1:D:251:ILE:CG2	2.55	0.50
1:C:153:GLY:O	1:C:155:LEU:HD13	2.10	0.50
1:C:247:PHE:HE2	1:C:287:PHE:HE1	1.58	0.50
1:D:156:LYS:O	1:D:157:ASN:HB2	2.10	0.50
1:B:110:ARG:CZ	1:B:132:LEU:HD23	2.42	0.50
1:A:264:ILE:HD12	1:A:313:VAL:HG22	1.93	0.50
1:B:69:ALA:HB2	1:B:329:MET:HE2	1.93	0.50
1:C:261:MET:CE	1:C:265:LYS:HD3	2.41	0.50
1:A:275:HIS:CD2	1:A:279:ALA:HB2	2.46	0.50
1:C:167:LYS:HZ1	1:C:250:ARG:HH12	1.58	0.49
1:C:179:ALA:HB1	1:C:208:LEU:HB2	1.94	0.49
1:D:167:LYS:HB3	1:D:193:TYR:HB3	1.93	0.49
1:D:285:THR:CG2	1:D:288:SER:HB2	2.37	0.49
1:B:277:LEU:HB3	1:B:278:PRO:HA	1.94	0.49
1:B:206:ILE:O	1:B:210:LYS:HG3	2.12	0.49
1:A:238:VAL:HB	1:A:247:PHE:CZ	2.46	0.49
1:D:245:GLU:O	1:D:248:ASP:HB3	2.12	0.49
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.59	0.49
1:A:117:VAL:O	1:A:121:VAL:HG23	2.12	0.49
1:D:243:PRO:HG2	1:D:245:GLU:H	1.78	0.49
1:D:251:ILE:O	1:D:255:LYS:HB3	2.12	0.49
1:B:277:LEU:HA	1:B:278:PRO:C	2.33	0.49
1:D:265:LYS:HA	1:D:265:LYS:HE2	1.94	0.48
1:A:56:GLN:NE2	2:A:2030:HOH:O	2.47	0.48
1:A:264:ILE:CD1	1:A:313:VAL:HG13	2.43	0.48
1:A:56:GLN:HA	1:A:82:PRO:HA	1.95	0.48
1:B:190:PRO:HD3	1:B:257:PHE:CE2	2.48	0.48
1:D:87:MET:SD	1:D:93:ILE:HD12	2.53	0.48
1:D:310:THR:OG1	1:D:313:VAL:HG23	2.12	0.48
1:D:311:ASP:O	1:D:315:GLN:HG2	2.13	0.48
1:A:152:PHE:HB3	1:A:158:LYS:HE2	1.94	0.48
1:A:46:LEU:O	1:A:49:LYS:HB2	2.14	0.48
1:C:87:MET:SD	1:C:93:ILE:HG13	2.53	0.48
1:C:127:PRO:HB3	1:C:339:THR:HG23	1.94	0.48
1:C:167:LYS:HD2	1:C:196:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ASP:OD1	1:D:298:LYS:HE3	2.13	0.48
1:B:332:ILE:HA	1:B:335:ILE:HD12	1.96	0.47
1:A:247:PHE:CE2	1:A:287:PHE:CZ	3.02	0.47
1:A:28:SER:OG	1:A:331:SER:HA	2.14	0.47
1:B:111:GLY:O	1:B:133:THR:HA	2.14	0.47
1:B:57:LYS:HD3	1:B:112:PHE:HZ	1.79	0.47
1:C:131:GLY:O	1:C:132:LEU:CB	2.62	0.47
1:A:112:PHE:CD1	1:A:112:PHE:N	2.82	0.47
1:B:127:PRO:HB3	1:B:339:THR:OG1	2.14	0.47
1:A:111:GLY:O	1:A:133:THR:HA	2.15	0.47
1:C:265:LYS:HA	1:C:265:LYS:HD2	1.62	0.47
1:D:277:LEU:HA	1:D:278:PRO:C	2.35	0.47
1:C:160:ILE:HG23	1:C:185:VAL:HG13	1.96	0.47
1:A:249:LYS:O	1:A:253:GLU:HG3	2.15	0.47
1:A:247:PHE:HE2	1:A:287:PHE:CZ	2.32	0.47
1:A:140:GLN:NE2	1:A:328:ARG:HD3	2.30	0.47
1:D:199:LYS:HA	1:D:202:LEU:HD12	1.96	0.47
1:C:167:LYS:HD2	1:C:196:GLU:CG	2.44	0.47
1:B:160:ILE:HG23	1:B:185:VAL:HG13	1.98	0.46
1:A:163:ILE:HG21	1:A:259:VAL:HG22	1.96	0.46
1:C:202:LEU:HA	1:C:202:LEU:HD23	1.81	0.46
1:D:5:LEU:HD12	1:D:5:LEU:N	2.30	0.46
1:D:297:ALA:CA	1:D:298:LYS:C	2.80	0.46
1:A:223:ILE:HD13	1:A:263:MET:HA	1.98	0.46
1:D:242:GLU:CB	1:D:243:PRO:HD3	2.28	0.46
1:D:264:ILE:CD1	1:D:264:ILE:N	2.77	0.46
1:D:292:ALA:HB1	1:D:303:ALA:O	2.15	0.46
1:D:153:GLY:O	1:D:155:LEU:HD13	2.16	0.46
1:B:54:LEU:N	1:B:54:LEU:HD23	2.30	0.46
1:A:233:TYR:HD1	1:A:234:THR:N	2.13	0.46
1:A:250:ARG:HG2	1:A:250:ARG:NH1	2.32	0.45
1:C:261:MET:HG3	1:C:312:GLU:OE2	2.16	0.45
1:C:93:ILE:HD13	1:C:119:ALA:HB3	1.97	0.45
1:C:186:VAL:HG22	1:C:217:ARG:HD2	1.98	0.45
1:D:222:LYS:HG2	1:D:223:ILE:N	2.31	0.45
1:B:108:GLU:OE2	1:B:131:GLY:HA3	2.16	0.45
1:D:13:LEU:HD23	1:D:13:LEU:HA	1.77	0.45
1:C:239:SER:O	1:C:242:GLU:HG2	2.17	0.45
1:B:131:GLY:O	1:B:132:LEU:CB	2.64	0.45
1:C:281:HIS:O	1:C:311:ASP:HB2	2.17	0.45
1:C:55:PHE:C	1:C:57:LYS:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:MET:HE3	1:D:333:LYS:CE	2.37	0.44
1:B:243:PRO:HB2	1:B:245:GLU:CG	2.46	0.44
1:D:297:ALA:HA	1:D:298:LYS:O	2.15	0.44
1:D:122:LYS:HD3	1:D:123:TYR:CE2	2.53	0.44
1:D:265:LYS:HA	1:D:265:LYS:CE	2.48	0.44
1:A:129:TRP:CE2	1:A:339:THR:HG21	2.51	0.44
1:D:243:PRO:HG2	1:D:246:LEU:N	2.25	0.44
1:A:251:ILE:CD1	1:A:302:VAL:HG11	2.46	0.44
1:A:3:VAL:HG23	1:A:3:VAL:O	2.18	0.44
1:B:78:THR:HG21	1:B:104:TYR:OH	2.17	0.44
1:D:329:MET:HE2	1:D:329:MET:O	2.18	0.44
1:B:145:PHE:CZ	1:B:177:GLY:HA3	2.51	0.44
1:D:93:ILE:HG12	1:D:119:ALA:HB3	2.00	0.44
1:C:167:LYS:CD	1:C:196:GLU:HG3	2.46	0.43
1:B:250:ARG:HB2	1:B:250:ARG:HH11	1.83	0.43
1:D:167:LYS:HD3	1:D:193:TYR:CD1	2.53	0.43
1:D:151:LYS:HD2	1:D:151:LYS:O	2.19	0.43
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.72	0.43
1:D:17:THR:OG1	1:D:20:GLU:HG3	2.17	0.43
1:B:59:SER:OG	1:B:110:ARG:HD2	2.19	0.43
1:D:107:ILE:O	1:D:128:VAL:HA	2.19	0.43
1:C:332:ILE:HG13	2:C:2044:HOH:O	2.18	0.43
1:C:189:GLY:HA2	1:C:257:PHE:CZ	2.53	0.43
1:D:10:LEU:HD21	1:D:138:PRO:HB2	2.01	0.43
1:D:129:TRP:CE2	1:D:339:THR:HG21	2.53	0.43
1:C:247:PHE:CE2	1:C:287:PHE:CZ	3.06	0.43
1:B:242:GLU:HB2	1:B:243:PRO:CD	2.46	0.43
1:C:247:PHE:HD1	1:C:247:PHE:H	1.67	0.43
1:A:244:PHE:HZ	1:A:295:LEU:HD21	1.84	0.43
1:A:250:ARG:HH11	1:A:250:ARG:CG	2.31	0.42
1:C:251:ILE:HD11	1:C:302:VAL:HG11	2.01	0.42
1:B:121:VAL:HG22	1:B:128:VAL:HB	2.01	0.42
1:C:121:VAL:HG22	1:C:128:VAL:HB	2.02	0.42
1:C:54:LEU:HD23	1:C:54:LEU:N	2.34	0.42
1:C:113:ALA:O	1:C:116:ASP:HB2	2.19	0.42
1:C:242:GLU:HB2	1:C:243:PRO:HD2	2.00	0.42
1:A:107:ILE:O	1:A:128:VAL:HA	2.20	0.42
1:D:328:ARG:HD2	1:D:328:ARG:HA	1.87	0.42
1:D:136:GLU:HG2	1:D:137:HIS:N	2.35	0.42
1:C:127:PRO:CB	1:C:339:THR:HG23	2.49	0.42
1:D:240:LEU:O	1:D:240:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HB3	1:D:2:PRO:CD	2.48	0.42
1:B:144:ASP:O	1:B:147:THR:HB	2.20	0.42
1:A:162:PHE:CE1	1:A:166:TYR:HA	2.55	0.42
1:C:1:MET:HA	1:C:2:PRO:HD3	1.92	0.42
1:C:189:GLY:HA2	1:C:257:PHE:CD1	2.55	0.42
1:D:132:LEU:HD13	1:D:137:HIS:CG	2.55	0.42
1:C:341:GLY:HA2	2:C:2072:HOH:O	2.20	0.42
1:D:310:THR:O	1:D:313:VAL:N	2.53	0.41
1:A:57:LYS:O	1:A:58:ASP:C	2.56	0.41
1:D:281:HIS:H	1:D:281:HIS:CD2	2.38	0.41
1:B:142:ILE:CG2	1:B:331:SER:HB2	2.50	0.41
1:B:54:LEU:HB3	1:B:85:SER:OG	2.21	0.41
1:D:1:MET:CB	1:D:2:PRO:CD	2.98	0.41
1:B:244:PHE:HE2	1:B:294:THR:OG1	2.04	0.41
1:C:191:ASP:O	1:C:194:LYS:HE2	2.19	0.41
1:C:117:VAL:O	1:C:121:VAL:HG23	2.21	0.41
1:D:199:LYS:H	1:D:199:LYS:HD2	1.85	0.41
1:A:1:MET:HA	1:A:2:PRO:HD3	1.69	0.41
1:D:240:LEU:CD1	1:D:240:LEU:C	2.86	0.41
1:D:260:ASP:OD1	1:D:262:ASN:HB2	2.21	0.41
1:D:281:HIS:O	1:D:311:ASP:CB	2.67	0.41
1:B:190:PRO:HG3	1:B:253:GLU:O	2.19	0.41
1:C:57:LYS:HD2	1:C:112:PHE:CZ	2.55	0.41
1:B:6:LYS:HE2	1:D:6:LYS:HE2	2.01	0.41
1:A:227:GLN:O	1:A:228:ASP:HB2	2.20	0.41
1:A:94:GLU:HG3	1:A:123:TYR:CZ	2.55	0.41
1:D:69:ALA:HA	1:D:329:MET:HE3	2.02	0.41
1:B:273:PHE:HB3	1:B:319:ASN:HA	2.03	0.41
1:D:245:GLU:HA	1:D:248:ASP:HB2	2.03	0.41
1:C:283:ASP:OD1	1:C:283:ASP:N	2.54	0.41
1:D:309:VAL:HG22	1:D:310:THR:N	2.36	0.40
1:B:237:TRP:O	1:B:250:ARG:HG2	2.21	0.40
1:C:162:PHE:CE1	1:C:166:TYR:HA	2.56	0.40
1:B:156:LYS:O	1:B:157:ASN:HB2	2.21	0.40
1:C:242:GLU:O	1:C:247:PHE:HE1	2.04	0.40
1:B:264:ILE:HG22	1:B:265:LYS:N	2.36	0.40
1:B:78:THR:HG23	1:B:104:TYR:CE1	2.56	0.40
1:C:1:MET:N	2:C:2001:HOH:O	2.54	0.40
1:D:163:ILE:HA	1:D:188:CYS:O	2.21	0.40
1:A:167:LYS:HD3	1:A:193:TYR:CG	2.56	0.40
1:D:131:GLY:O	1:D:132:LEU:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:HB3	1:C:278:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	340/365 (93%)	325 (96%)	12 (4%)	3 (1%)	21	42
1	B	340/365 (93%)	319 (94%)	20 (6%)	1 (0%)	46	72
1	C	340/365 (93%)	327 (96%)	12 (4%)	1 (0%)	46	72
1	D	340/365 (93%)	313 (92%)	23 (7%)	4 (1%)	16	33
All	All	1360/1460 (93%)	1284 (94%)	67 (5%)	9 (1%)	26	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	B	132	LEU
1	C	132	LEU
1	D	132	LEU
1	D	243	PRO
1	A	243	PRO
1	D	3	VAL
1	D	271	VAL
1	A	3	VAL

5.3.2 Protein sidechains

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	291/312 (93%)	262 (90%)	29 (10%)	9 18
1	B	291/312 (93%)	264 (91%)	27 (9%)	11 21
1	C	291/312 (93%)	260 (89%)	31 (11%)	8 15
1	D	291/312 (93%)	259 (89%)	32 (11%)	8 14
All	All	1164/1248 (93%)	1045 (90%)	119 (10%)	9 17

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	13	LEU
1	A	49	LYS
1	A	61	ARG
1	A	67	GLU
1	A	78	THR
1	A	89	LYS
1	A	90	LYS
1	A	100	LEU
1	A	110	ARG
1	A	120	LEU
1	A	137	HIS
1	A	155	LEU
1	A	159	LYS
1	A	167	LYS
1	A	206	ILE
1	A	220	THR
1	A	224	LEU
1	A	233	TYR
1	A	247	PHE
1	A	250	ARG
1	A	251	ILE
1	A	254	LEU
1	A	270	ASP
1	A	277	LEU
1	A	284	HIS
1	A	316	SER
1	A	317	LEU

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Mol	Chain	Res	Type
1	A	339	THR
1	B	5	LEU
1	B	13	LEU
1	B	54	LEU
1	B	61	ARG
1	B	63	ARG
1	B	77	VAL
1	B	78	THR
1	B	83	SER
1	B	100	LEU
1	B	110	ARG
1	B	120	LEU
1	B	155	LEU
1	B	185	VAL
1	B	220	THR
1	B	224	LEU
1	B	233	TYR
1	B	245	GLU
1	B	246	LEU
1	B	250	ARG
1	B	251	ILE
1	B	261	MET
1	B	270	ASP
1	B	293	THR
1	B	304	LYS
1	B	316	SER
1	B	317	LEU
1	B	329	MET
1	C	3	VAL
1	C	46	LEU
1	C	54	LEU
1	C	61	ARG
1	C	67	GLU
1	C	77	VAL
1	C	78	THR
1	C	94	GLU
1	C	100	LEU
1	C	110	ARG
1	C	120	LEU
1	C	137	HIS
1	C	155	LEU
1	C	185	VAL

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Mol	Chain	Res	Type
1	C	192	ASN
1	C	199	LYS
1	C	204	LYS
1	C	217	ARG
1	C	220	THR
1	C	222	LYS
1	C	233	TYR
1	C	247	PHE
1	C	254	LEU
1	C	255	LYS
1	C	265	LYS
1	C	284	HIS
1	C	288	SER
1	C	301	ILE
1	C	317	LEU
1	C	338	SER
1	C	339	THR
1	D	1	MET
1	D	13	LEU
1	D	54	LEU
1	D	61	ARG
1	D	67	GLU
1	D	77	VAL
1	D	89	LYS
1	D	100	LEU
1	D	110	ARG
1	D	120	LEU
1	D	137	HIS
1	D	155	LEU
1	D	199	LYS
1	D	200	ASN
1	D	217	ARG
1	D	220	THR
1	D	222	LYS
1	D	233	TYR
1	D	238	VAL
1	D	240	LEU
1	D	247	PHE
1	D	250	ARG
1	D	251	ILE
1	D	261	MET
1	D	264	ILE

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Mol	Chain	Res	Type
1	D	265	LYS
1	D	284	HIS
1	D	285	THR
1	D	301	ILE
1	D	317	LEU
1	D	329	MET
1	D	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	140	GLN
1	C	37	GLN
1	D	318	HIS

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	342/365 (93%)	-0.54	6 (1%)	71	66	13, 28, 53, 97	0
1	B	342/365 (93%)	-0.33	7 (2%)	68	63	14, 31, 68, 113	0
1	C	342/365 (93%)	-0.59	2 (0%)	90	88	14, 25, 45, 77	0
1	D	342/365 (93%)	-0.38	10 (2%)	55	48	14, 33, 72, 115	0
All	All	1368/1460 (93%)	-0.46	25 (1%)	71	66	13, 29, 63, 115	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	PHE	4.9
1	A	245	GLU	4.3
1	B	245	GLU	4.0
1	A	246	LEU	4.0
1	D	243	PRO	3.9
1	D	244	PHE	3.7
1	D	242	GLU	3.7
1	B	244	PHE	3.3
1	A	244	PHE	3.2
1	D	303	ALA	3.1
1	B	246	LEU	3.1
1	B	243	PRO	3.0
1	D	245	GLU	3.0
1	B	247	PHE	2.9
1	D	239	SER	2.9
1	C	240	LEU	2.8
1	D	297	ALA	2.6
1	A	2	PRO	2.5
1	D	240	LEU	2.5
1	A	240	LEU	2.4
1	A	247	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	287	PHE	2.3
1	B	297	ALA	2.2
1	B	291	VAL	2.0
1	D	246	LEU	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.