Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:30 PM GMT

PDB ID	:	1TZ9
Title	:	Crystal Structure of the Putative Mannonate Dehydratase from Enterococcus faecalis, Northeast Structural Genomics Target EfR41
Authors	:	Forouhar, F.; Chen, Y.; Xiao, R.; Cooper, B.; Shastry, R.; Acton, T.A.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-07-09
Resolution	:	2.90 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
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:

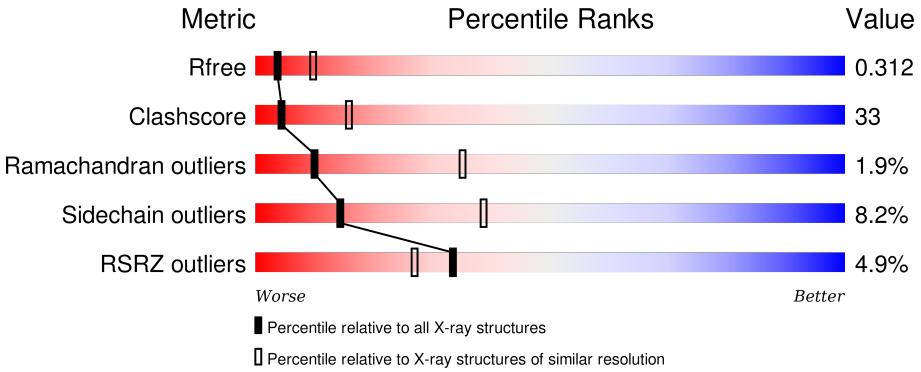
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 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	367	3% 46% 42% 6% 6%
1	B	367	6% 47% 42% 5% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5495 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 Mannonate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	Se	0	0	0
			2731	1742	464	511	4	10			
1	B	344	Total	C	N	O	S	Se	0	0	0
			2731	1742	464	511	4	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	CLONING ARTIFACT	UNP Q82ZC9
A	-8	GLY	-	CLONING ARTIFACT	UNP Q82ZC9
A	-7	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-6	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-5	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-4	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-3	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-2	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	-1	SER	-	CLONING ARTIFACT	UNP Q82ZC9
A	0	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	143	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	173	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	204	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	260	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	298	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	302	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	328	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
A	338	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	-9	MET	-	CLONING ARTIFACT	UNP Q82ZC9
B	-8	GLY	-	CLONING ARTIFACT	UNP Q82ZC9
B	-7	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	-6	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	-5	HIS	-	CLONING ARTIFACT	UNP Q82ZC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	-3	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	-2	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	-1	SER	-	CLONING ARTIFACT	UNP Q82ZC9
B	0	HIS	-	CLONING ARTIFACT	UNP Q82ZC9
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	143	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	173	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	204	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	260	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	298	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	302	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	328	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9
B	338	MSE	MET	MODIFIED RESIDUE	UNP Q82ZC9

- Molecule 2 is water.

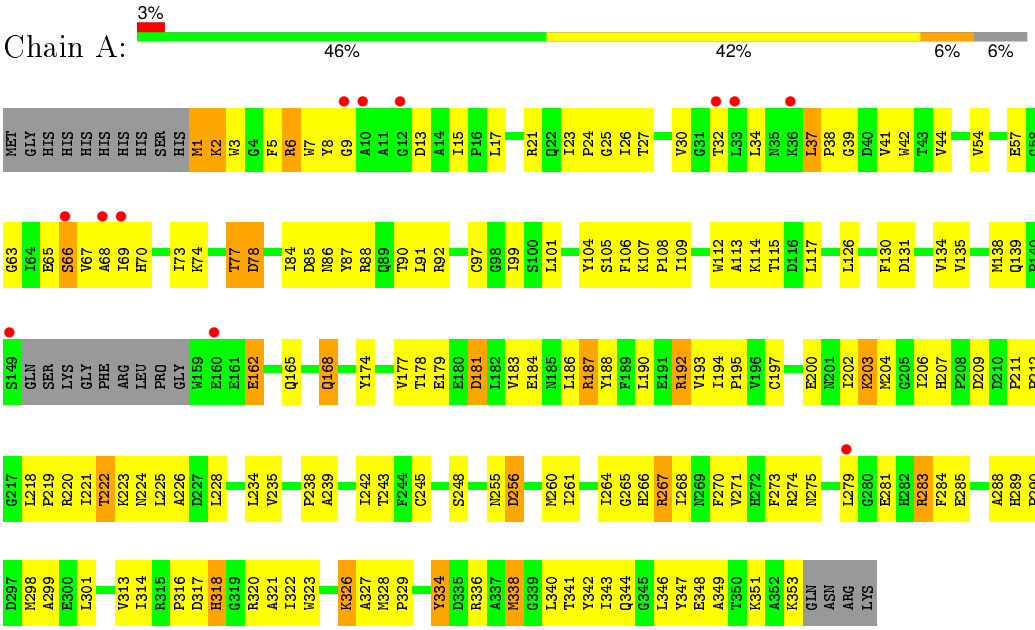
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	16	Total O 16 16	0	0

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.

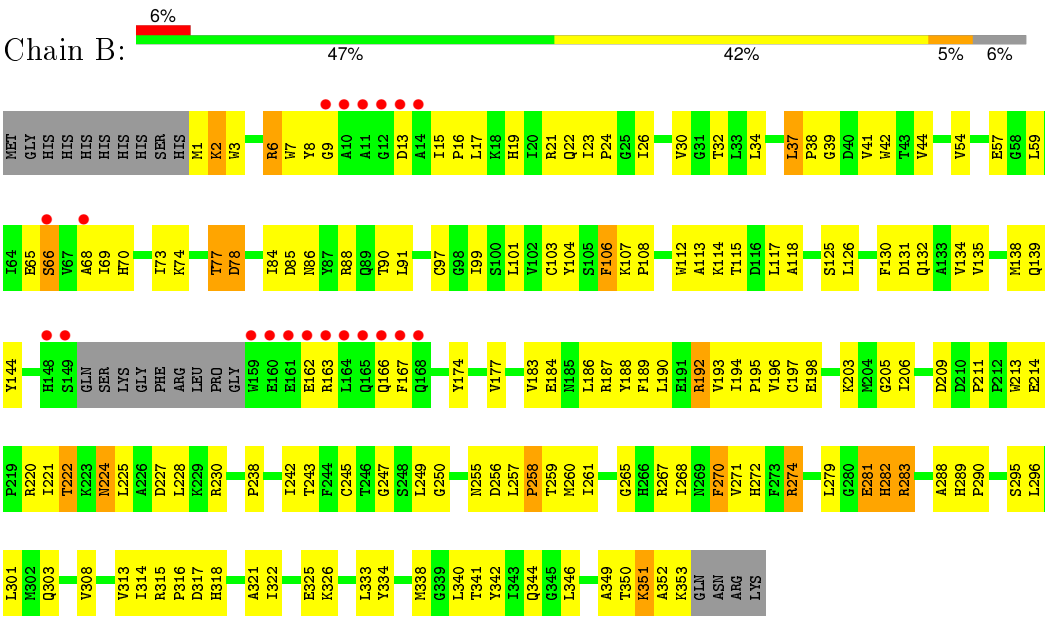
- Molecule 1: Mannonate dehydratase

Chain A:



- Molecule 1: Mannonate dehydratase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.34Å 89.94Å 156.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.90 29.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.61-2.90) 98.2 (29.60-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.292 0.240 , 0.312	Depositor DCC
R_{free} test set	1539 reflections (10.96%)	DCC
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29345 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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	0/2785	0.62	0/3760
1	B	0.42	0/2785	0.60	0/3760
All	All	0.44	0/5570	0.61	0/7520

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

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	2731	0	2682	190	0
1	B	2731	0	2682	177	0
2	A	17	0	0	3	0
2	B	16	0	0	5	0
All	All	5495	0	5364	354	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 33.

All (354) 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:39:GLY:H	1:A:68:ALA:HB1	1.13	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLY:H	1:B:68:ALA:HB1	1.13	1.08
1:B:326:LYS:NZ	1:B:326:LYS:H	1.73	0.86
1:B:296:LEU:HB3	1:B:298:MSE:HE3	1.56	0.85
1:A:206:ILE:HG12	1:A:222:THR:HG21	1.60	0.84
1:A:206:ILE:HG22	1:A:242:ILE:HG22	1.62	0.82
1:A:296:LEU:HB2	1:A:298:MSE:HE3	1.63	0.80
1:A:255:ASN:HD22	1:A:260:MSE:HE1	1.47	0.80
1:B:61:LEU:HD23	1:B:99:ILE:HD11	1.64	0.80
1:A:316:PRO:HD3	1:A:340:LEU:HD13	1.65	0.79
1:A:101:LEU:HD22	1:A:313:VAL:HG11	1.64	0.78
1:A:77:THR:HG22	1:A:78:ASP:H	1.48	0.77
1:A:61:LEU:HD23	1:A:99:ILE:HD11	1.66	0.77
1:A:283:ARG:HB2	1:A:283:ARG:HH21	1.51	0.76
1:A:326:LYS:HD3	1:A:327:ALA:H	1.50	0.76
1:B:77:THR:HG22	1:B:78:ASP:H	1.50	0.75
1:A:225:LEU:HD13	1:A:260:MSE:HB3	1.69	0.74
1:B:117:LEU:HD23	1:B:117:LEU:H	1.53	0.73
1:B:206:ILE:HG22	1:B:242:ILE:HG22	1.70	0.73
1:B:274:ARG:HG2	1:B:317:ASP:HB3	1.71	0.73
1:A:117:LEU:H	1:A:117:LEU:HD23	1.53	0.73
1:B:101:LEU:HD22	1:B:313:VAL:HG11	1.71	0.72
1:A:255:ASN:ND2	1:A:260:MSE:HE1	2.04	0.72
1:A:107:LYS:HG2	1:A:209:ASP:OD2	1.90	0.72
1:B:39:GLY:N	1:B:68:ALA:HB1	1.98	0.70
1:A:25:GLY:HA3	1:A:344:GLN:HE22	1.57	0.70
1:B:296:LEU:HB3	1:B:298:MSE:CE	2.21	0.69
1:A:206:ILE:CG2	1:A:242:ILE:HG22	2.22	0.69
1:A:174:TYR:O	1:A:177:VAL:HG22	1.93	0.69
1:B:221:ILE:HG13	1:B:222:THR:H	1.58	0.69
1:A:39:GLY:N	1:A:68:ALA:HB1	1.98	0.69
1:B:326:LYS:HZ3	1:B:326:LYS:H	1.39	0.69
1:A:283:ARG:HB2	1:A:283:ARG:NH2	2.07	0.69
1:B:70:HIS:O	1:B:73:ILE:HG12	1.93	0.69
1:A:104:TYR:CE1	1:A:206:ILE:HD12	2.29	0.68
1:A:70:HIS:O	1:A:73:ILE:HG12	1.93	0.68
1:B:249:LEU:HD13	1:B:260:MSE:HE1	1.76	0.68
1:A:349:ALA:HB3	1:B:349:ALA:HB3	1.76	0.67
1:B:290:PRO:HA	1:B:342:TYR:CZ	2.29	0.67
1:B:194:ILE:N	1:B:195:PRO:HD2	2.10	0.67
1:B:250:GLY:HA2	1:B:257:LEU:HD21	1.77	0.67
1:A:65:GLU:O	1:A:66:SER:C	2.34	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLY:HA3	1:B:274:ARG:NE	2.10	0.66
1:B:139:GLN:HA	2:B:365:HOH:O	1.96	0.66
1:A:274:ARG:HG3	1:A:317:ASP:HB3	1.78	0.66
1:A:228:LEU:HD23	1:A:264:ILE:HG12	1.78	0.65
1:A:107:LYS:HE2	1:A:209:ASP:HA	1.79	0.65
1:A:187:ARG:NH2	1:A:234:LEU:HD23	2.11	0.65
1:B:42:TRP:H	1:B:90:THR:CG2	2.10	0.64
1:B:65:GLU:O	1:B:66:SER:C	2.36	0.64
1:B:114:LYS:H	1:B:143:MSE:HE1	1.61	0.64
1:B:274:ARG:HH11	1:B:274:ARG:HG2	1.63	0.64
1:A:283:ARG:HH21	1:A:283:ARG:CB	2.10	0.64
1:B:198:GLU:HA	2:B:367:HOH:O	1.98	0.64
1:A:289:HIS:N	1:A:290:PRO:HD2	2.13	0.64
1:B:42:TRP:H	1:B:90:THR:HG22	1.63	0.64
1:A:271:VAL:HG23	1:A:314:ILE:HG13	1.79	0.64
1:B:247:GLY:HA3	1:B:274:ARG:HE	1.63	0.63
1:A:178:THR:H	1:A:181:ASP:HB2	1.63	0.63
1:B:296:LEU:CB	1:B:298:MSE:HE3	2.28	0.63
1:B:61:LEU:HD23	1:B:99:ILE:CD1	2.28	0.63
1:B:73:ILE:HG13	1:B:74:LYS:N	2.13	0.63
1:A:224:ASN:ND2	1:A:226:ALA:HB3	2.14	0.62
1:A:61:LEU:HD23	1:A:99:ILE:CD1	2.29	0.62
1:A:126:LEU:HB2	1:A:321:ALA:HB3	1.82	0.62
1:A:114:LYS:H	1:A:143:MSE:HE1	1.65	0.62
1:A:194:ILE:N	1:A:195:PRO:HD2	2.15	0.62
1:A:42:TRP:H	1:A:90:THR:CG2	2.13	0.61
1:A:270:PHE:CD2	1:A:313:VAL:HG13	2.35	0.61
1:A:187:ARG:HH21	1:A:234:LEU:HD23	1.66	0.61
1:A:326:LYS:HD3	1:A:327:ALA:N	2.14	0.61
1:A:73:ILE:HG13	1:A:74:LYS:N	2.14	0.61
1:A:221:ILE:HG13	1:A:222:THR:H	1.66	0.61
1:A:91:LEU:HD11	1:A:204:MSE:HE3	1.82	0.61
1:A:224:ASN:HD21	1:A:226:ALA:HB3	1.66	0.60
1:B:326:LYS:CE	1:B:326:LYS:H	2.13	0.60
1:A:87:TYR:HE1	1:A:204:MSE:HE1	1.65	0.60
1:B:3:TRP:CE2	1:B:344:GLN:HG2	2.36	0.60
1:B:32:THR:OG1	1:B:66:SER:HB3	2.02	0.60
1:B:114:LYS:N	1:B:143:MSE:HE1	2.17	0.60
1:B:44:VAL:HG13	1:B:97:CYS:SG	2.42	0.60
1:A:32:THR:OG1	1:A:66:SER:HB3	2.02	0.59
1:A:348:GLU:HG2	1:B:299:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:HD2	1:B:57:GLU:HB3	1.83	0.59
1:A:298:MSE:HE2	1:A:301:LEU:HD12	1.85	0.58
1:A:21:ARG:HD2	1:A:57:GLU:HB3	1.85	0.58
1:A:44:VAL:HG13	1:A:97:CYS:SG	2.43	0.58
1:B:221:ILE:HB	1:B:227:ASP:OD1	2.03	0.58
1:B:130:PHE:CZ	1:B:211:PRO:HG3	2.39	0.58
1:B:274:ARG:HG2	1:B:274:ARG:NH1	2.18	0.58
1:A:114:LYS:N	1:A:143:MSE:HE1	2.18	0.58
1:B:86:ASN:O	1:B:90:THR:HG23	2.04	0.57
1:A:228:LEU:HG	1:A:242:ILE:HD12	1.86	0.57
1:A:261:ILE:O	1:A:265:GLY:HA3	2.03	0.57
1:B:115:THR:HG21	1:B:134:VAL:HB	1.84	0.57
1:A:296:LEU:CB	1:A:298:MSE:HE3	2.35	0.57
1:B:144:TYR:CD2	1:B:167:PHE:HB2	2.40	0.57
1:A:219:PRO:O	1:A:220:ARG:HG3	2.05	0.57
1:A:42:TRP:H	1:A:90:THR:HG22	1.69	0.57
1:A:115:THR:HG21	1:A:134:VAL:HB	1.86	0.57
1:A:187:ARG:HB2	1:A:234:LEU:HD22	1.87	0.57
1:B:257:LEU:N	1:B:258:PRO:HD2	2.20	0.57
1:B:107:LYS:HG2	1:B:209:ASP:OD2	2.04	0.57
1:B:298:MSE:HE2	1:B:298:MSE:HA	1.86	0.56
1:B:189:PHE:O	1:B:193:VAL:HG12	2.05	0.56
1:B:206:ILE:CG2	1:B:242:ILE:HG22	2.35	0.56
1:A:349:ALA:HB2	1:B:346:LEU:HA	1.87	0.56
1:B:91:LEU:HD21	1:B:197:CYS:SG	2.46	0.56
1:B:218:LEU:HG	2:B:369:HOH:O	2.05	0.56
1:A:349:ALA:CB	1:B:349:ALA:HB3	2.36	0.56
1:A:86:ASN:O	1:A:90:THR:HG23	2.05	0.56
1:B:2:LYS:N	1:B:2:LYS:HD3	2.21	0.56
1:B:188:TYR:CZ	1:B:192:ARG:NH1	2.73	0.56
1:A:54:VAL:HG21	1:A:61:LEU:HD13	1.88	0.56
1:A:353:LYS:HD3	1:B:353:LYS:NZ	2.20	0.56
1:B:215:ILE:HG13	1:B:215:ILE:O	2.04	0.56
1:B:41:VAL:HG22	1:B:86:ASN:HB3	1.87	0.55
1:B:140:PRO:HG3	1:B:216:PHE:CD1	2.42	0.55
1:B:54:VAL:HG21	1:B:61:LEU:HD13	1.89	0.55
1:A:178:THR:H	1:A:181:ASP:CB	2.20	0.55
1:B:224:ASN:N	1:B:224:ASN:HD22	2.05	0.55
1:A:41:VAL:HG22	1:A:86:ASN:HB3	1.89	0.55
1:B:8:TYR:HB2	1:B:13:ASP:HB2	1.88	0.55
1:B:352:ALA:O	1:B:353:LYS:HD2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HD12	1:B:260:MSE:HG2	1.89	0.54
1:A:266:HIS:CD2	1:A:267:ARG:HG2	2.43	0.54
1:B:26:ILE:O	1:B:26:ILE:HD12	2.07	0.54
1:A:77:THR:HG22	1:A:78:ASP:N	2.20	0.54
1:A:91:LEU:HD21	1:A:197:CYS:SG	2.47	0.54
1:B:326:LYS:N	1:B:326:LYS:HZ3	2.04	0.54
1:B:117:LEU:H	1:B:117:LEU:CD2	2.20	0.54
1:A:8:TYR:HB2	1:A:13:ASP:HB2	1.90	0.54
1:A:26:ILE:O	1:A:26:ILE:HD12	2.08	0.54
1:B:84:ILE:O	1:B:88:ARG:HG2	2.08	0.53
1:B:272:HIS:CE1	1:B:315:ARG:HH11	2.26	0.53
1:B:245:CYS:HA	1:B:272:HIS:HB2	1.89	0.53
1:A:245:CYS:SG	1:A:274:ARG:NH2	2.81	0.53
1:B:211:PRO:HB2	1:B:213:TRP:CE2	2.44	0.53
1:A:215:ILE:HG13	1:A:215:ILE:O	2.08	0.53
1:A:221:ILE:O	1:A:223:LYS:N	2.41	0.53
1:A:299:ALA:HA	1:A:346:LEU:HD22	1.91	0.53
1:B:91:LEU:HD23	1:B:196:VAL:HG13	1.91	0.53
1:A:190:LEU:HA	1:A:193:VAL:HG12	1.91	0.52
1:B:7:TRP:CZ3	1:B:9:GLY:HA2	2.44	0.52
1:A:6:ARG:NH1	1:A:6:ARG:HG2	2.24	0.52
1:A:32:THR:HG23	1:A:32:THR:O	2.10	0.52
1:A:2:LYS:N	1:A:2:LYS:HD3	2.24	0.52
1:A:117:LEU:H	1:A:117:LEU:CD2	2.21	0.52
1:A:188:TYR:CE1	1:A:192:ARG:NH2	2.78	0.52
1:A:7:TRP:CH2	1:A:17:LEU:HD22	2.44	0.52
1:A:92:ARG:HA	1:A:200:GLU:HG3	1.91	0.52
1:B:17:LEU:HD21	1:B:54:VAL:HA	1.92	0.52
1:B:23:ILE:O	1:B:26:ILE:HG13	2.10	0.52
1:A:323:TRP:CZ2	1:A:338:MSE:HE1	2.45	0.52
1:B:227:ASP:O	1:B:230:ARG:N	2.43	0.52
1:A:264:ILE:C	1:A:264:ILE:HD12	2.30	0.52
1:B:351:LYS:C	1:B:353:LYS:H	2.12	0.52
1:A:290:PRO:HA	1:A:342:TYR:CZ	2.44	0.51
1:A:139:GLN:HB2	1:A:142:ASP:OD2	2.10	0.51
1:A:322:ILE:HD12	1:A:323:TRP:CE2	2.45	0.51
1:A:202:ILE:O	1:A:203:LYS:HE3	2.10	0.51
1:A:353:LYS:HD3	1:B:353:LYS:HZ3	1.75	0.51
1:B:6:ARG:NH1	1:B:6:ARG:HG2	2.25	0.51
1:A:322:ILE:HD11	1:A:334:TYR:HB3	1.92	0.51
1:A:316:PRO:HG3	1:A:340:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:O	1:A:88:ARG:HG2	2.11	0.51
1:A:32:THR:HG21	2:A:364:HOH:O	2.10	0.51
1:A:23:ILE:O	1:A:26:ILE:HG13	2.11	0.51
1:A:87:TYR:CE1	1:A:204:MSE:HE1	2.46	0.51
1:A:338:MSE:HG3	1:B:341:THR:HG21	1.93	0.51
1:A:298:MSE:CE	1:A:301:LEU:HD12	2.41	0.50
1:A:30:VAL:HG13	1:A:63:GLY:O	2.10	0.50
1:A:41:VAL:HG13	1:A:90:THR:HG22	1.94	0.50
1:B:85:ASP:HA	1:B:88:ARG:HG2	1.93	0.50
1:B:321:ALA:HA	1:B:325:GLU:OE1	2.11	0.50
1:B:139:GLN:HB2	1:B:142:ASP:OD2	2.11	0.50
1:B:41:VAL:HA	1:B:90:THR:CG2	2.42	0.50
1:A:84:ILE:HD13	1:A:192:ARG:HD2	1.93	0.50
1:A:256:ASP:N	1:A:260:MSE:HE3	2.27	0.50
1:B:222:THR:N	1:B:227:ASP:OD1	2.45	0.50
1:A:194:ILE:HG21	1:A:235:VAL:HG11	1.94	0.50
1:A:85:ASP:HA	1:A:88:ARG:HG2	1.94	0.50
1:A:338:MSE:CG	1:B:341:THR:HG21	2.41	0.50
1:B:289:HIS:N	1:B:290:PRO:HD2	2.27	0.50
1:A:54:VAL:HG12	1:A:59:LEU:O	2.12	0.49
1:A:270:PHE:HD2	1:A:313:VAL:HG13	1.75	0.49
1:B:326:LYS:NZ	1:B:326:LYS:N	2.53	0.49
1:B:74:LYS:HE3	1:B:174:TYR:OH	2.12	0.49
1:B:30:VAL:HG13	1:B:63:GLY:O	2.13	0.49
1:B:243:THR:HB	1:B:270:PHE:HB3	1.94	0.49
1:B:325:GLU:HA	1:B:326:LYS:NZ	2.27	0.49
1:A:184:GLU:HA	1:A:184:GLU:OE1	2.11	0.49
1:A:342:TYR:CZ	1:A:346:LEU:HD11	2.48	0.49
1:A:101:LEU:HD22	1:A:313:VAL:CG1	2.40	0.49
1:B:205:GLY:C	1:B:243:THR:HG23	2.32	0.49
1:A:288:ALA:CB	1:B:24:PRO:HB3	2.43	0.49
1:A:225:LEU:HD13	1:A:260:MSE:CB	2.42	0.48
1:B:243:THR:HG22	1:B:270:PHE:HB3	1.94	0.48
1:B:113:ALA:O	1:B:114:LYS:HG2	2.13	0.48
1:A:113:ALA:O	1:A:114:LYS:HG2	2.13	0.48
1:A:279:LEU:HD11	1:A:285:GLU:OE2	2.13	0.48
1:A:275:ASN:ND2	1:A:294:GLY:HA3	2.28	0.48
1:B:54:VAL:HG12	1:B:59:LEU:O	2.13	0.48
1:A:323:TRP:CH2	1:A:338:MSE:HE1	2.49	0.48
1:A:41:VAL:HA	1:A:90:THR:CG2	2.43	0.48
1:A:206:ILE:O	1:A:243:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD21	1:A:54:VAL:HA	1.95	0.48
1:B:247:GLY:HA3	1:B:274:ARG:CD	2.43	0.48
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.79	0.48
1:A:74:LYS:HE3	1:A:174:TYR:OH	2.13	0.48
1:A:130:PHE:CZ	1:A:211:PRO:HG3	2.48	0.48
1:A:209:ASP:O	1:A:248:SER:HB3	2.14	0.48
1:B:42:TRP:N	1:B:90:THR:HG22	2.28	0.48
1:B:91:LEU:HD22	1:B:193:VAL:HG23	1.95	0.48
1:A:340:LEU:O	1:A:344:GLN:HG3	2.14	0.47
1:A:105:SER:HB3	1:A:207:HIS:HB3	1.96	0.47
1:B:104:TYR:O	1:B:206:ILE:HA	2.14	0.47
1:B:193:VAL:O	1:B:196:VAL:HG13	2.14	0.47
1:B:132:GLN:HB2	1:B:282:HIS:HB3	1.96	0.47
1:B:250:GLY:HA3	1:B:296:LEU:HD11	1.95	0.47
1:B:139:GLN:HB3	1:B:141:GLU:OE1	2.14	0.47
1:A:243:THR:HA	1:A:270:PHE:O	2.14	0.47
1:A:341:THR:O	1:B:342:TYR:HA	2.14	0.47
1:A:37:LEU:HB2	1:A:38:PRO:HD2	1.97	0.47
1:A:26:ILE:HD13	1:A:59:LEU:HD21	1.96	0.47
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.78	0.47
1:B:77:THR:HG22	1:B:78:ASP:N	2.23	0.47
1:B:227:ASP:O	1:B:228:LEU:C	2.51	0.47
1:A:221:ILE:O	1:A:223:LYS:HG2	2.15	0.46
1:A:225:LEU:HB2	1:A:260:MSE:HE2	1.96	0.46
1:B:214:GLU:HG2	1:B:218:LEU:O	2.15	0.46
1:A:139:GLN:HB3	1:A:141:GLU:OE1	2.15	0.46
1:B:26:ILE:HD13	1:B:59:LEU:HD21	1.97	0.46
1:A:6:ARG:NH2	2:A:364:HOH:O	2.48	0.46
1:B:271:VAL:HG13	1:B:314:ILE:HA	1.97	0.46
1:B:8:TYR:HB2	1:B:13:ASP:OD1	2.15	0.46
1:B:243:THR:CB	1:B:270:PHE:HB3	2.46	0.46
1:A:338:MSE:HE2	1:A:338:MSE:HB2	1.86	0.46
1:B:271:VAL:HG13	1:B:314:ILE:HG13	1.96	0.46
1:B:163:ARG:HG3	1:B:166:GLN:OE1	2.16	0.46
1:A:130:PHE:CZ	1:A:135:VAL:HG21	2.51	0.46
1:A:203:LYS:HG3	1:A:239:ALA:HA	1.97	0.46
1:B:41:VAL:HG13	1:B:90:THR:HG22	1.97	0.46
1:B:32:THR:O	1:B:32:THR:HG23	2.16	0.46
1:A:42:TRP:N	1:A:90:THR:HG22	2.32	0.45
1:B:272:HIS:CE1	1:B:315:ARG:NH1	2.84	0.45
1:A:320:ARG:NH1	1:B:22:GLN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASP:OD2	1:B:15:ILE:HB	2.17	0.45
1:B:303:GLN:NE2	1:B:350:THR:HG23	2.31	0.45
1:B:258:PRO:HG3	2:B:370:HOH:O	2.17	0.45
1:A:109:ILE:HD12	1:A:218:LEU:HD21	1.98	0.45
1:B:221:ILE:HG13	1:B:222:THR:N	2.27	0.45
1:A:221:ILE:HG13	1:A:222:THR:N	2.32	0.45
1:B:131:ASP:OD2	1:B:283:ARG:HB3	2.16	0.45
1:A:194:ILE:N	1:A:195:PRO:CD	2.78	0.45
1:A:8:TYR:HB2	1:A:13:ASP:OD1	2.16	0.45
1:B:256:ASP:OD2	1:B:258:PRO:HG2	2.17	0.45
1:A:7:TRP:CZ3	1:A:9:GLY:HA2	2.52	0.45
1:B:85:ASP:O	1:B:88:ARG:HG3	2.17	0.45
1:B:265:GLY:HA3	1:B:308:VAL:HG11	1.98	0.45
1:B:130:PHE:CZ	1:B:135:VAL:HG21	2.52	0.44
1:A:7:TRP:CD2	1:A:17:LEU:HD13	2.52	0.44
1:B:238:PRO:HA	1:B:267:ARG:NE	2.32	0.44
1:A:85:ASP:O	1:A:88:ARG:HG3	2.17	0.44
1:B:316:PRO:HD3	1:B:340:LEU:HD13	1.98	0.44
1:A:228:LEU:HA	1:A:228:LEU:HD12	1.87	0.44
1:A:242:ILE:HD11	1:A:264:ILE:HB	1.99	0.44
1:A:211:PRO:HB2	1:A:213:TRP:CE2	2.52	0.44
1:A:131:ASP:HB2	1:A:283:ARG:NH2	2.32	0.44
1:A:265:GLY:HA2	1:A:268:ILE:CD1	2.48	0.44
1:B:322:ILE:HD11	1:B:338:MSE:HE1	1.99	0.44
1:B:37:LEU:HB2	1:B:38:PRO:HD2	1.99	0.44
1:A:238:PRO:HA	1:A:267:ARG:NE	2.31	0.44
1:A:13:ASP:OD2	1:A:15:ILE:HB	2.18	0.44
1:B:68:ALA:HB2	2:B:371:HOH:O	2.18	0.44
1:B:281:GLU:HG2	1:B:282:HIS:N	2.32	0.44
1:A:6:ARG:HH11	1:A:6:ARG:CG	2.31	0.44
1:A:162:GLU:H	1:A:162:GLU:CD	2.21	0.44
1:A:91:LEU:HD22	1:A:193:VAL:HG23	2.00	0.43
1:B:7:TRP:CD2	1:B:17:LEU:HD13	2.54	0.43
1:A:5:PHE:HD2	1:A:340:LEU:HD22	1.83	0.43
1:B:183:VAL:HG11	1:B:230:ARG:HD2	1.99	0.43
1:B:194:ILE:N	1:B:195:PRO:CD	2.79	0.43
1:B:7:TRP:CH2	1:B:17:LEU:HD22	2.53	0.43
1:A:347:TYR:CZ	1:A:351:LYS:HG3	2.53	0.43
1:B:192:ARG:HB2	1:B:192:ARG:HE	1.59	0.43
1:A:317:ASP:CG	1:A:318:HIS:H	2.20	0.43
1:A:275:ASN:HD21	1:A:294:GLY:HA3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HG	1:A:190:LEU:HD12	1.99	0.43
1:B:6:ARG:CG	1:B:6:ARG:HH11	2.31	0.43
1:B:242:ILE:O	1:B:268:ILE:HA	2.18	0.43
1:B:69:ILE:O	1:B:74:LYS:HE2	2.19	0.43
1:A:113:ALA:HB1	1:A:143:MSE:HE3	2.00	0.43
1:B:184:GLU:O	1:B:187:ARG:HB3	2.18	0.43
1:B:224:ASN:ND2	1:B:227:ASP:H	2.17	0.43
1:A:178:THR:OG1	1:A:181:ASP:HB2	2.19	0.43
1:A:323:TRP:CE2	1:B:333:LEU:HD21	2.53	0.43
1:A:179:GLU:O	1:A:183:VAL:HG23	2.18	0.43
1:B:352:ALA:C	1:B:353:LYS:HD2	2.39	0.43
1:A:168:GLN:HB2	1:A:168:GLN:HE21	1.62	0.43
1:B:255:ASN:O	1:B:257:LEU:HD22	2.18	0.42
1:A:135:VAL:HA	1:A:138:MSE:HG2	2.01	0.42
1:A:207:HIS:HA	1:A:243:THR:HG23	2.01	0.42
1:A:206:ILE:C	1:A:243:THR:HG22	2.39	0.42
1:A:130:PHE:O	1:A:283:ARG:HA	2.19	0.42
1:B:221:ILE:C	1:B:227:ASP:OD1	2.57	0.42
1:A:328:MSE:HG3	1:A:329:PRO:HD2	2.01	0.42
1:B:243:THR:CG2	1:B:270:PHE:HB3	2.49	0.42
1:B:224:ASN:ND2	1:B:224:ASN:N	2.68	0.42
1:A:1:MSE:HE3	1:A:314:ILE:HD13	2.02	0.42
1:A:130:PHE:CE2	1:A:211:PRO:HG3	2.55	0.42
1:B:135:VAL:HA	1:B:138:MSE:HG2	2.02	0.42
1:B:126:LEU:HB2	1:B:321:ALA:HB3	2.01	0.42
1:A:342:TYR:CE2	1:A:346:LEU:HD11	2.54	0.42
1:B:315:ARG:HG3	1:B:315:ARG:HH21	1.85	0.42
1:A:69:ILE:O	1:A:74:LYS:HE2	2.19	0.42
1:A:42:TRP:HB2	1:A:90:THR:HB	2.02	0.42
1:B:125:SER:HB2	1:B:322:ILE:HG22	2.02	0.42
1:A:67:VAL:HG22	1:A:68:ALA:H	1.85	0.41
1:B:258:PRO:HG2	1:B:259:THR:H	1.84	0.41
1:B:317:ASP:O	1:B:318:HIS:C	2.58	0.41
1:B:74:LYS:HA	1:B:106:PHE:CZ	2.55	0.41
1:B:188:TYR:CE1	1:B:192:ARG:NH2	2.87	0.41
1:B:117:LEU:N	1:B:117:LEU:HD23	2.29	0.41
1:B:218:LEU:HA	1:B:218:LEU:HD12	1.95	0.41
1:A:223:LYS:HG3	1:A:224:ASN:N	2.35	0.41
1:B:174:TYR:O	1:B:177:VAL:HG23	2.20	0.41
1:A:134:VAL:HG21	2:A:362:HOH:O	2.20	0.41
1:A:284:PHE:CD1	1:A:284:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PHE:HB2	1:A:218:LEU:HD13	2.02	0.41
1:B:270:PHE:CD2	1:B:313:VAL:HG13	2.55	0.41
1:A:114:LYS:C	1:A:143:MSE:HE1	2.41	0.41
1:B:107:LYS:HE2	1:B:209:ASP:HA	2.02	0.41
1:B:84:ILE:HD13	1:B:192:ARG:HD2	2.03	0.41
1:A:322:ILE:HD12	1:A:323:TRP:CD2	2.56	0.41
1:B:242:ILE:HG12	1:B:267:ARG:O	2.21	0.41
1:B:163:ARG:O	1:B:166:GLN:HB3	2.20	0.41
1:A:165:GLN:HA	1:A:168:GLN:HE21	1.86	0.41
1:A:212:PRO:O	1:A:223:LYS:HB2	2.21	0.40
1:A:7:TRP:CE2	1:A:17:LEU:HD13	2.56	0.40
1:B:261:ILE:O	1:B:308:VAL:HG11	2.22	0.40
1:A:343:ILE:HA	1:A:346:LEU:HD12	2.03	0.40
1:A:221:ILE:H	1:A:221:ILE:HG12	1.63	0.40
1:B:103:CYS:HA	1:B:205:GLY:O	2.22	0.40
1:B:41:VAL:HA	1:B:90:THR:HG22	2.04	0.40
1:B:279:LEU:O	1:B:283:ARG:HG3	2.21	0.40
1:B:322:ILE:CD1	1:B:338:MSE:HE1	2.51	0.40
1:A:24:PRO:HB3	1:B:288:ALA:CB	2.52	0.40
1:B:186:LEU:HG	1:B:190:LEU:CD1	2.51	0.40
1:A:3:TRP:CE2	1:A:344:GLN:HG2	2.57	0.40
1:B:104:TYR:CZ	1:B:206:ILE:HB	2.56	0.40
1:A:271:VAL:HG21	1:A:314:ILE:HD12	2.03	0.40
1:B:186:LEU:HG	1:B:190:LEU:HD12	2.03	0.40
1:B:16:PRO:HG2	1:B:19:HIS:CG	2.56	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	340/367 (93%)	294 (86%)	40 (12%)	6 (2%)	11 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	340/367 (93%)	290 (85%)	43 (13%)	7 (2%)	9 32
All	All	680/734 (93%)	584 (86%)	83 (12%)	13 (2%)	10 35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	108	PRO
1	A	222	THR
1	B	77	THR
1	B	108	PRO
1	B	281	GLU
1	A	281	GLU
1	B	334	TYR
1	A	66	SER
1	A	334	TYR
1	B	66	SER
1	B	118	ALA
1	B	258	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	288/298 (97%)	264 (92%)	24 (8%)	14 38
1	B	288/298 (97%)	265 (92%)	23 (8%)	15 40
All	All	576/596 (97%)	529 (92%)	47 (8%)	14 39

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	LYS
1	A	6	ARG

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Mol	Chain	Res	Type
1	A	27	THR
1	A	34	LEU
1	A	37	LEU
1	A	78	ASP
1	A	106	PHE
1	A	112	TRP
1	A	143	MSE
1	A	162	GLU
1	A	168	GLN
1	A	181	ASP
1	A	187	ARG
1	A	192	ARG
1	A	203	LYS
1	A	256	ASP
1	A	267	ARG
1	A	273	PHE
1	A	283	ARG
1	A	318	HIS
1	A	326	LYS
1	A	336	ARG
1	A	338	MSE
1	B	1	MSE
1	B	2	LYS
1	B	6	ARG
1	B	34	LEU
1	B	37	LEU
1	B	78	ASP
1	B	106	PHE
1	B	112	TRP
1	B	143	MSE
1	B	162	GLU
1	B	192	ARG
1	B	203	LYS
1	B	220	ARG
1	B	222	THR
1	B	224	ASN
1	B	270	PHE
1	B	274	ARG
1	B	282	HIS
1	B	283	ARG
1	B	295	SER
1	B	300	GLU

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Mol	Chain	Res	Type
1	B	301	LEU
1	B	351	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	121	ASN
1	A	165	GLN
1	A	168	GLN
1	A	207	HIS
1	A	224	ASN
1	A	240	ASN
1	A	255	ASN
1	A	266	HIS
1	A	269	ASN
1	A	289	HIS
1	A	344	GLN
1	B	86	ASN
1	B	168	GLN
1	B	207	HIS
1	B	224	ASN
1	B	272	HIS
1	B	289	HIS
1	B	303	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	334/367 (91%)	0.09	12 (3%)	46 38	6, 26, 52, 64	0
1	B	334/367 (91%)	0.33	21 (6%)	23 17	6, 28, 58, 91	0
All	All	668/734 (91%)	0.21	33 (4%)	33 27	6, 27, 55, 91	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	TRP	8.1
1	B	12	GLY	5.8
1	B	162	GLU	5.4
1	B	13	ASP	5.1
1	B	161	GLU	4.9
1	B	149	SER	4.6
1	B	160	GLU	4.0
1	B	68	ALA	3.9
1	B	165	GLN	3.8
1	A	9	GLY	3.7
1	B	163	ARG	3.2
1	A	10	ALA	2.9
1	A	68	ALA	2.9
1	B	166	GLN	2.9
1	B	66	SER	2.8
1	A	160	GLU	2.8
1	A	33	LEU	2.7
1	B	148	HIS	2.6
1	B	9	GLY	2.6
1	A	149	SER	2.6
1	A	69	ILE	2.5
1	A	279	LEU	2.4
1	A	32	THR	2.4
1	B	14	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	LYS	2.2
1	B	164	LEU	2.2
1	B	10	ALA	2.2
1	B	168	GLN	2.2
1	B	11	ALA	2.1
1	A	66	SER	2.0
1	B	140	PRO	2.0
1	B	167	PHE	2.0
1	A	12	GLY	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.