Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:13 AM GMT

PDB ID	:	2G6T
Title	:	Crystal structure of an uncharacterized protein from Clostridium acetobutylicum
Authors	:	Rao, K.N.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-02-25
Resolution	:	3.00 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:

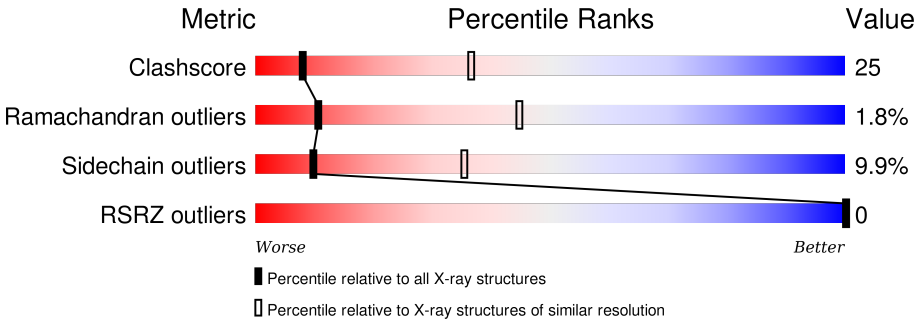
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	306	56% 38% 5%
1	B	306	62% 32% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5056 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 Uncharacterized protein, homolog HI1244 from Haemophilus influenzae.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	Se	0	0	0
			2490	1612	396	466	8	8			
1	B	306	Total	C	N	O	S	Se	0	0	0
			2515	1629	404	466	8	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	153	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	174	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	219	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	248	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	280	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	282	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	294	MSE	MET	MODIFIED RESIDUE	GB 15025180
A	306	UNK	-	SEE REMARK 999	GB 15025180
B	1	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	153	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	174	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	219	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	248	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	280	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	282	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	294	MSE	MET	MODIFIED RESIDUE	GB 15025180
B	306	UNK	-	SEE REMARK 999	GB 15025180

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		

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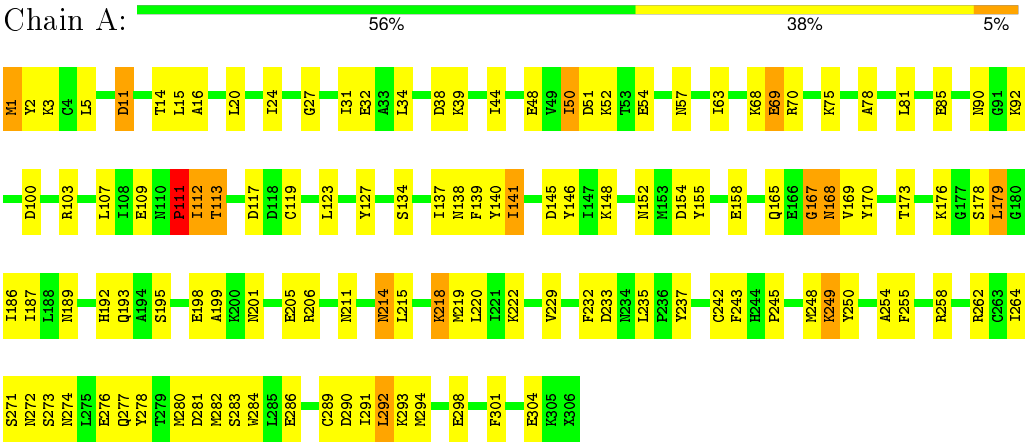
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	29	Total O 29 29	0	0

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.

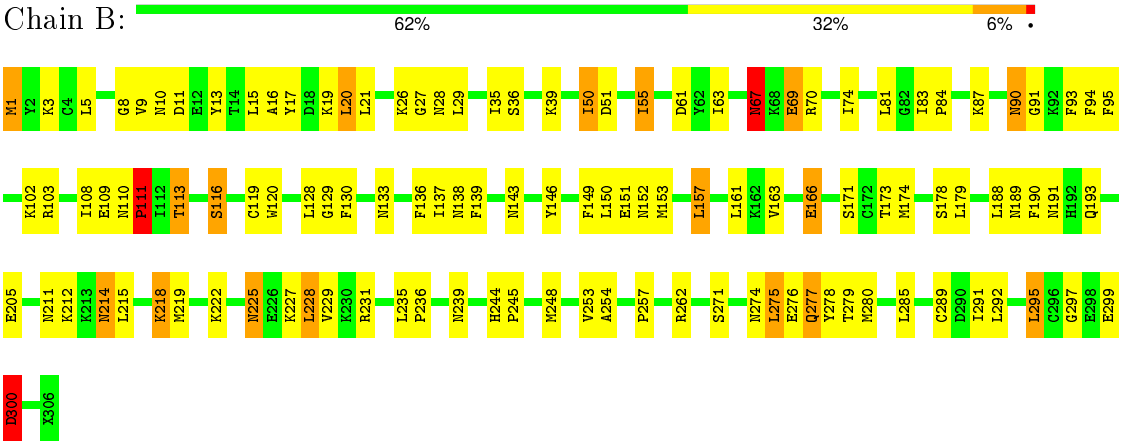
- Molecule 1: Uncharacterized protein, homolog HI1244 from Haemophilus influenzae

Chain A:



- Molecule 1: Uncharacterized protein, homolog HI1244 from Haemophilus influenzae

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.97Å 123.97Å 254.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 3.00 46.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.00-3.00) 96.6 (46.00-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	5.69 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.257 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.1	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 23919 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5056	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.39	0/2538	0.62	0/3419
1	B	0.41	0/2563	0.62	0/3445
All	All	0.40	0/5101	0.62	0/6864

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	2490	0	2363	138	0
1	B	2515	0	2427	105	0
2	A	22	0	0	2	0
2	B	29	0	0	1	0
All	All	5056	0	4790	242	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 25.

All (242) 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:50:ILE:HB	1:A:54:GLU:HG3	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HB3	1:A:112:ILE:HD11	1.50	0.94
1:B:113:THR:HG21	1:B:211:ASN:H	1.29	0.93
1:A:249:LYS:HD2	1:A:249:LYS:H	1.43	0.83
1:A:198:GLU:HA	1:A:201:ASN:HD22	1.44	0.81
1:A:176:LYS:HE3	1:A:189:ASN:HD22	1.45	0.80
1:A:249:LYS:H	1:A:249:LYS:CD	1.95	0.79
1:A:168:ASN:HD22	1:A:169:VAL:N	1.80	0.78
1:A:1:MSE:HG3	1:A:27:GLY:O	1.84	0.78
1:B:212:LYS:HA	1:B:215:LEU:HD13	1.66	0.77
1:A:198:GLU:HA	1:A:201:ASN:ND2	1.99	0.77
1:A:290:ASP:OD2	1:A:293:LYS:HB2	1.84	0.77
1:B:69:GLU:H	1:B:69:GLU:CD	1.88	0.77
1:B:113:THR:HG21	1:B:211:ASN:N	2.00	0.76
1:A:168:ASN:ND2	1:A:170:TYR:H	1.84	0.75
1:B:153:MSE:HE2	1:B:212:LYS:NZ	2.04	0.73
1:A:16:ALA:HB2	1:A:95:PHE:CZ	2.23	0.73
1:A:107:LEU:HB3	1:A:112:ILE:CD1	2.19	0.73
1:B:1:MSE:HG2	1:B:27:GLY:O	1.90	0.72
1:B:110:ASN:ND2	1:B:214:ASN:HB2	2.05	0.72
1:A:266:TYR:O	1:A:269:ARG:HB3	1.90	0.71
1:A:113:THR:HG23	1:A:215:LEU:HD23	1.71	0.71
1:A:127:TYR:CD1	1:A:282:MSE:HE2	2.26	0.70
1:A:182:GLY:C	1:A:184:ASN:H	1.92	0.70
1:A:148:LYS:HE3	1:A:186:ILE:HD11	1.75	0.67
1:B:227:LYS:O	1:B:231:ARG:HG3	1.95	0.67
1:A:113:THR:HG21	1:A:211:ASN:H	1.60	0.67
1:B:113:THR:CG2	1:B:211:ASN:HB3	2.25	0.67
1:B:116:SER:HB2	1:B:218:LYS:HG3	1.77	0.66
1:A:75:LYS:NZ	1:A:85:GLU:HG3	2.11	0.66
1:B:276:GLU:HG2	1:B:277:GLN:N	2.10	0.66
1:B:193:GLN:NE2	1:B:193:GLN:HA	2.11	0.66
1:A:184:ASN:H	1:A:184:ASN:HD22	1.44	0.65
1:A:195:SER:OG	1:A:198:GLU:HG3	1.97	0.65
1:B:5:LEU:HB2	1:B:63:ILE:HD13	1.77	0.65
1:B:67:ASN:HD22	1:B:67:ASN:C	2.00	0.64
1:B:35:ILE:HG12	1:B:50:ILE:HD11	1.79	0.64
1:B:225:ASN:HD22	1:B:225:ASN:C	2.00	0.63
1:A:97:SER:HB2	1:A:286:GLU:OE2	1.98	0.63
1:B:262:ARG:HH12	1:B:277:GLN:NE2	1.96	0.62
1:A:249:LYS:HD2	1:A:249:LYS:N	2.15	0.62
1:A:176:LYS:HE3	1:A:189:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASP:O	1:A:140:TYR:HA	1.99	0.62
1:A:214:ASN:HD22	1:A:214:ASN:C	2.03	0.62
1:A:107:LEU:HD13	1:A:112:ILE:HD11	1.82	0.61
1:A:123:LEU:HD12	1:A:280:MSE:HG2	1.83	0.61
1:A:254:ALA:O	1:A:255:PHE:HB3	2.00	0.61
1:A:69:GLU:OE1	1:A:69:GLU:N	2.31	0.61
1:A:145:ASP:HB3	1:A:186:ILE:HD12	1.81	0.61
1:A:220:LEU:HD23	1:A:243:PHE:HB2	1.82	0.60
1:B:262:ARG:HH12	1:B:277:GLN:HE21	1.49	0.60
1:B:143:ASN:HB3	1:B:228:LEU:HD11	1.84	0.60
1:A:146:TYR:HD2	1:A:219:MSE:HE3	1.66	0.59
1:A:39:LYS:HD2	1:A:39:LYS:N	2.18	0.59
1:B:102:LYS:C	1:B:102:LYS:HD3	2.22	0.59
1:B:70:ARG:O	1:B:74:ILE:HG12	2.02	0.59
1:A:107:LEU:CB	1:A:112:ILE:HD11	2.31	0.58
1:B:229:VAL:HG11	1:B:248:MSE:HE2	1.83	0.58
1:B:16:ALA:HB2	1:B:95:PHE:CZ	2.38	0.58
1:A:294:MSE:HE2	1:A:301:PHE:CE2	2.38	0.58
1:A:138:ASN:HB3	1:A:192:HIS:HB3	1.86	0.58
1:A:229:VAL:HG11	1:A:248:MSE:HE3	1.84	0.58
1:A:258:ARG:NH1	1:A:304:GLU:OE1	2.36	0.58
1:A:182:GLY:C	1:A:184:ASN:N	2.57	0.58
1:A:222:LYS:O	1:A:245:PRO:HG2	2.04	0.57
1:B:113:THR:HB	1:B:133:ASN:O	2.05	0.57
1:A:187:ILE:HD12	1:A:187:ILE:N	2.18	0.57
1:A:24:ILE:HD11	1:A:31:ILE:HD13	1.87	0.57
1:A:168:ASN:HD22	1:A:168:ASN:C	2.07	0.57
1:A:294:MSE:HE2	1:A:301:PHE:HE2	1.69	0.57
1:A:282:MSE:O	1:A:286:GLU:HG2	2.05	0.56
1:B:110:ASN:HD21	1:B:214:ASN:HB2	1.71	0.56
1:A:34:LEU:CD1	1:A:44:ILE:HB	2.35	0.56
1:B:193:GLN:HE21	1:B:193:GLN:HA	1.69	0.56
1:B:113:THR:HG22	1:B:211:ASN:HB3	1.87	0.56
1:B:35:ILE:CG1	1:B:50:ILE:HD11	2.35	0.56
1:B:193:GLN:HE21	1:B:193:GLN:CA	2.18	0.56
1:A:178:SER:OG	1:A:185:LYS:HD2	2.07	0.55
1:A:235:LEU:HB3	1:A:237:TYR:HD1	1.72	0.55
1:B:171:SER:OG	1:B:173:THR:HG23	2.06	0.55
1:B:113:THR:HG21	1:B:211:ASN:HB3	1.88	0.55
1:A:52:LYS:HB2	1:A:81:LEU:HD11	1.88	0.54
1:A:107:LEU:HB3	1:A:112:ILE:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:HB2	1:B:218:LYS:CG	2.37	0.54
1:A:57:ASN:HD22	1:A:57:ASN:N	2.04	0.54
1:A:184:ASN:ND2	1:A:184:ASN:H	2.06	0.54
1:A:50:ILE:HB	1:A:54:GLU:CG	2.30	0.54
1:A:168:ASN:HD21	1:A:170:TYR:HD1	1.54	0.54
1:A:113:THR:CG2	1:A:215:LEU:HD23	2.37	0.53
1:B:143:ASN:HB3	1:B:228:LEU:CD1	2.38	0.53
1:A:90:ASN:HB3	1:A:93:PHE:CD1	2.43	0.53
1:A:249:LYS:H	1:A:249:LYS:CE	2.20	0.53
1:A:220:LEU:HD11	1:A:222:LYS:HG2	1.91	0.53
1:B:274:ASN:ND2	1:B:277:GLN:HG2	2.24	0.53
1:B:9:VAL:HA	1:B:13:TYR:CG	2.44	0.52
1:A:270:THR:HG22	2:A:328:HOH:O	2.09	0.52
1:B:212:LYS:HA	1:B:215:LEU:CD1	2.37	0.52
1:B:153:MSE:HG2	1:B:157:LEU:HD22	1.91	0.52
1:B:222:LYS:O	1:B:245:PRO:HG2	2.09	0.52
1:A:139:PHE:CD1	1:A:139:PHE:C	2.83	0.52
1:B:90:ASN:HD22	1:B:90:ASN:C	2.13	0.52
1:A:186:ILE:C	1:A:187:ILE:HD12	2.31	0.51
1:A:75:LYS:HZ1	1:A:85:GLU:HG3	1.75	0.51
1:B:225:ASN:ND2	1:B:228:LEU:H	2.09	0.51
1:A:134:SER:O	1:A:206:ARG:HG2	2.10	0.51
1:A:304:GLU:HB2	2:A:311:HOH:O	2.11	0.50
1:B:69:GLU:N	1:B:69:GLU:CD	2.61	0.50
1:B:299:GLU:O	1:B:300:ASP:CB	2.60	0.50
1:A:167:GLY:HA2	1:A:173:THR:HG22	1.92	0.50
1:A:168:ASN:C	1:A:168:ASN:ND2	2.65	0.50
1:A:154:ASP:O	1:A:158:GLU:HG3	2.10	0.50
1:B:299:GLU:O	1:B:300:ASP:CG	2.50	0.50
1:B:193:GLN:NE2	1:B:193:GLN:CA	2.73	0.49
1:A:39:LYS:CD	1:A:39:LYS:N	2.75	0.49
1:A:165:GLN:HB3	1:A:176:LYS:HB2	1.93	0.49
1:A:123:LEU:HD11	1:A:280:MSE:HE3	1.94	0.49
1:B:225:ASN:ND2	1:B:228:LEU:HB2	2.27	0.49
1:B:139:PHE:C	1:B:139:PHE:CD1	2.85	0.49
1:A:123:LEU:HD11	1:A:280:MSE:CE	2.42	0.49
1:B:239:ASN:ND2	1:B:297:GLY:HA3	2.27	0.49
1:B:26:LYS:HE2	1:B:28:ASN:ND2	2.27	0.49
1:A:109:GLU:HA	1:A:109:GLU:OE1	2.12	0.49
1:B:277:GLN:HG3	1:B:278:TYR:N	2.28	0.49
1:A:184:ASN:N	1:A:184:ASN:HD22	2.06	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD12	1:B:179:LEU:CD1	2.43	0.48
1:A:183:ASP:N	1:A:183:ASP:OD2	2.46	0.48
1:B:188:LEU:HD23	1:B:188:LEU:N	2.28	0.48
1:A:181:THR:HG23	1:A:182:GLY:N	2.28	0.48
1:B:139:PHE:HB2	1:B:189:ASN:O	2.13	0.48
1:A:107:LEU:HD22	1:A:112:ILE:HD13	1.96	0.48
1:B:102:LYS:HD3	1:B:103:ARG:N	2.29	0.48
1:A:15:LEU:HD23	1:A:15:LEU:O	2.14	0.48
1:A:220:LEU:CD1	1:A:222:LYS:HG2	2.44	0.48
1:A:103:ARG:NE	1:A:298:GLU:OE2	2.36	0.48
1:A:282:MSE:HE3	1:A:291:ILE:HD13	1.95	0.48
1:A:294:MSE:HG3	1:A:301:PHE:CE2	2.49	0.47
1:A:90:ASN:O	1:A:90:ASN:OD1	2.32	0.47
1:B:218:LYS:HD2	1:B:219:MSE:N	2.29	0.47
1:A:69:GLU:CD	1:A:69:GLU:H	2.03	0.47
1:A:119:CYS:HB2	1:A:280:MSE:HE3	1.97	0.47
1:B:271:SER:HB3	1:B:274:ASN:CG	2.34	0.47
1:A:11:ASP:O	1:A:15:LEU:HB2	2.14	0.47
1:B:136:PHE:O	1:B:137:ILE:HD13	2.15	0.47
1:B:119:CYS:SG	1:B:138:ASN:HA	2.54	0.47
1:A:232:PHE:CE2	1:A:242:CYS:HB2	2.49	0.47
1:B:276:GLU:HB2	1:B:280:MSE:CE	2.45	0.47
1:A:117:ASP:OD2	1:A:117:ASP:N	2.48	0.47
1:B:276:GLU:HG2	1:B:277:GLN:H	1.79	0.46
1:A:278:TYR:CZ	1:A:284:TRP:HB3	2.51	0.46
1:B:275:LEU:HD22	1:B:279:THR:HG23	1.96	0.46
1:B:300:ASP:C	1:B:300:ASP:OD1	2.54	0.46
1:B:178:SER:O	1:B:179:LEU:HD12	2.15	0.46
1:A:168:ASN:H	1:A:173:THR:HB	1.81	0.46
1:A:289:CYS:SG	1:A:294:MSE:HE3	2.55	0.46
1:B:257:PRO:HD2	2:B:322:HOH:O	2.15	0.46
1:A:5:LEU:HB2	1:A:63:ILE:HD13	1.97	0.46
1:B:9:VAL:HA	1:B:13:TYR:CD2	2.51	0.46
1:B:153:MSE:HE1	1:B:215:LEU:HD21	1.98	0.46
1:A:168:ASN:ND2	1:A:169:VAL:N	2.59	0.45
1:A:262:ARG:HG3	1:A:266:TYR:CB	2.46	0.45
1:B:149:PHE:CZ	1:B:153:MSE:HG3	2.52	0.45
1:A:127:TYR:CD1	1:A:282:MSE:CE	2.99	0.45
1:A:235:LEU:HD22	1:A:237:TYR:HE1	1.82	0.45
1:A:107:LEU:HD13	1:A:112:ILE:CD1	2.46	0.45
1:A:145:ASP:O	1:A:148:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HG12	1:B:51:ASP:N	2.32	0.45
1:B:225:ASN:ND2	1:B:225:ASN:C	2.70	0.45
1:A:31:ILE:N	1:A:31:ILE:HD12	2.32	0.45
1:B:84:PRO:HD2	1:B:87:LYS:HD3	1.98	0.45
1:B:17:TYR:O	1:B:20:LEU:HB2	2.17	0.45
1:A:141:ILE:HD11	1:A:145:ASP:C	2.38	0.45
1:B:108:ILE:HD11	1:B:130:PHE:CE2	2.52	0.45
1:B:29:LEU:C	1:B:29:LEU:HD12	2.37	0.44
1:A:75:LYS:O	1:A:78:ALA:HB3	2.17	0.44
1:A:137:ILE:HG22	1:A:138:ASN:ND2	2.32	0.44
1:B:26:LYS:HE2	1:B:28:ASN:HD21	1.82	0.44
1:B:113:THR:HG21	1:B:211:ASN:CA	2.47	0.44
1:A:146:TYR:CD2	1:A:219:MSE:HE3	2.52	0.44
1:B:151:GLU:OE1	1:B:231:ARG:NH2	2.49	0.44
1:B:146:TYR:CE2	1:B:150:LEU:HD11	2.52	0.44
1:A:181:THR:HG23	1:A:182:GLY:H	1.82	0.44
1:B:109:GLU:O	1:B:111:PRO:HD3	2.17	0.44
1:B:111:PRO:O	1:B:211:ASN:ND2	2.51	0.44
1:B:166:GLU:HA	1:B:166:GLU:OE1	2.17	0.44
1:B:67:ASN:ND2	1:B:69:GLU:OE1	2.51	0.43
1:A:272:ASN:HB3	1:B:191:ASN:O	2.18	0.43
1:B:291:ILE:HG22	1:B:295:LEU:HD22	1.99	0.43
1:A:148:LYS:HE3	1:A:186:ILE:CD1	2.44	0.43
1:A:294:MSE:CE	1:A:301:PHE:CE2	3.01	0.43
1:B:153:MSE:HE2	1:B:212:LYS:CE	2.49	0.43
1:A:50:ILE:CB	1:A:54:GLU:HG3	2.33	0.43
1:B:253:VAL:HG12	1:B:254:ALA:N	2.33	0.43
1:B:300:ASP:O	1:B:300:ASP:OD1	2.37	0.43
1:A:262:ARG:NH2	1:A:277:GLN:OE1	2.49	0.43
1:B:120:TRP:CB	1:B:218:LYS:HE2	2.49	0.43
1:A:233:ASP:OD1	1:A:250:TYR:HB3	2.19	0.43
1:A:235:LEU:HB3	1:A:237:TYR:CD1	2.52	0.42
1:A:51:ASP:H	1:A:54:GLU:CG	2.32	0.42
1:B:153:MSE:HE2	1:B:212:LYS:HZ3	1.79	0.42
1:A:96:ILE:HG13	1:A:127:TYR:CZ	2.54	0.42
1:A:57:ASN:N	1:A:57:ASN:ND2	2.68	0.42
1:A:281:ASP:OD1	1:A:283:SER:HB2	2.18	0.42
1:A:100:ASP:OD1	1:A:103:ARG:HG3	2.19	0.42
1:A:127:TYR:CG	1:A:282:MSE:HE2	2.53	0.42
1:B:244:HIS:HA	1:B:245:PRO:HD3	1.86	0.42
1:A:113:THR:HG21	1:A:211:ASN:N	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CZ	1:B:129:GLY:HA3	2.55	0.42
1:A:1:MSE:HE2	1:A:2:TYR:O	2.20	0.42
1:B:84:PRO:HB2	1:B:87:LYS:HG3	2.01	0.42
1:A:107:LEU:HD22	1:A:112:ILE:CD1	2.49	0.42
1:A:214:ASN:ND2	1:A:214:ASN:C	2.71	0.42
1:B:55:ILE:HD11	1:B:83:ILE:CD1	2.50	0.42
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.84	0.42
1:A:111:PRO:O	1:A:211:ASN:ND2	2.53	0.41
1:B:28:ASN:OD1	1:B:102:LYS:HB2	2.20	0.41
1:A:278:TYR:CE1	1:A:284:TRP:HB3	2.55	0.41
1:B:67:ASN:ND2	1:B:67:ASN:C	2.70	0.41
1:A:90:ASN:O	1:A:92:LYS:N	2.53	0.41
1:B:128:LEU:HD23	1:B:130:PHE:CE1	2.55	0.41
1:A:182:GLY:O	1:A:184:ASN:N	2.54	0.41
1:A:3:LYS:HD2	1:A:32:GLU:CD	2.40	0.41
1:B:174:MSE:HB2	1:B:190:PHE:O	2.19	0.41
1:B:36:SER:O	1:B:39:LYS:NZ	2.52	0.41
1:B:163:VAL:HG13	1:B:163:VAL:O	2.20	0.41
1:A:127:TYR:CD2	1:A:282:MSE:HG3	2.55	0.41
1:B:153:MSE:HE2	1:B:212:LYS:HZ1	1.83	0.41
1:B:3:LYS:HE3	1:B:3:LYS:HB2	1.91	0.41
1:B:153:MSE:HG2	1:B:157:LEU:CD2	2.50	0.41
1:B:235:LEU:HA	1:B:236:PRO:HD3	1.86	0.41
1:A:271:SER:HB3	1:A:274:ASN:CG	2.41	0.41
1:B:278:TYR:CD2	1:B:278:TYR:C	2.94	0.40
1:A:141:ILE:HD13	1:A:146:TYR:HA	2.03	0.40
1:A:69:GLU:N	1:A:69:GLU:CD	2.71	0.40
1:B:91:GLY:O	1:B:94:PHE:HB2	2.22	0.40
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.87	0.40
1:A:48:GLU:HG2	1:A:50:ILE:HG22	2.03	0.40
1:A:282:MSE:CE	1:A:291:ILE:HD13	2.51	0.40
1:A:179:LEU:O	1:A:186:ILE:HB	2.20	0.40
1:A:117:ASP:OD2	1:A:218:LYS:HE3	2.21	0.40
1:A:193:GLN:HG3	1:A:199:ALA:HA	2.04	0.40
1:A:75:LYS:HZ2	1:A:85:GLU:HG3	1.85	0.40
1:B:276:GLU:CG	1:B:277:GLN:N	2.83	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	304/306 (99%)	256 (84%)	41 (14%)	7 (2%)	8 36
1	B	304/306 (99%)	278 (91%)	22 (7%)	4 (1%)	15 53
All	All	608/612 (99%)	534 (88%)	63 (10%)	11 (2%)	11 45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	ASP
1	A	68	LYS
1	A	273	SER
1	A	111	PRO
1	A	205	GLU
1	B	67	ASN
1	A	70	ARG
1	A	155	TYR
1	A	167	GLY
1	B	8	GLY
1	B	111	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	265/274 (97%)	243 (92%)	22 (8%)	14 46
1	B	271/274 (99%)	240 (89%)	31 (11%)	7 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	536/548 (98%)	483 (90%)	53 (10%)	10 35

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	11	ASP
1	A	14	THR
1	A	20	LEU
1	A	38	ASP
1	A	50	ILE
1	A	69	GLU
1	A	96	ILE
1	A	111	PRO
1	A	112	ILE
1	A	113	THR
1	A	141	ILE
1	A	152	ASN
1	A	168	ASN
1	A	179	LEU
1	A	184	ASN
1	A	214	ASN
1	A	218	LYS
1	A	249	LYS
1	A	264	ILE
1	A	276	GLU
1	A	292	LEU
1	B	1	MSE
1	B	10	ASN
1	B	11	ASP
1	B	15	LEU
1	B	19	LYS
1	B	20	LEU
1	B	50	ILE
1	B	55	ILE
1	B	61	ASP
1	B	67	ASN
1	B	69	GLU
1	B	81	LEU
1	B	90	ASN
1	B	111	PRO
1	B	113	THR

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Mol	Chain	Res	Type
1	B	116	SER
1	B	152	ASN
1	B	157	LEU
1	B	166	GLU
1	B	205	GLU
1	B	214	ASN
1	B	218	LYS
1	B	225	ASN
1	B	228	LEU
1	B	275	LEU
1	B	277	GLN
1	B	285	LEU
1	B	289	CYS
1	B	292	LEU
1	B	295	LEU
1	B	300	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	57	ASN
1	A	90	ASN
1	A	138	ASN
1	A	143	ASN
1	A	152	ASN
1	A	165	GLN
1	A	168	ASN
1	A	184	ASN
1	A	189	ASN
1	A	201	ASN
1	A	214	ASN
1	B	67	ASN
1	B	76	ASN
1	B	90	ASN
1	B	138	ASN
1	B	143	ASN
1	B	152	ASN
1	B	192	HIS
1	B	193	GLN
1	B	201	ASN
1	B	214	ASN

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Mol	Chain	Res	Type
1	B	225	ASN
1	B	234	ASN
1	B	239	ASN
1	B	265	ASN
1	B	277	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	297/306 (97%)	-0.48	0	100	100	20, 39, 60, 70	0
1	B	297/306 (97%)	-0.55	0	100	100	16, 34, 52, 60	0
All	All	594/612 (97%)	-0.52	0	100	100	16, 36, 57, 70	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

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.