Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:08 AM GMT

PDB ID	:	3HB7
Title	:	The Crystal Structure of an Isochorismatase-like Hydrolase from Alkaliphilus metalliredigens to 2.3A
Authors	:	Stein, A.J.; Xu, X.; Cui, H.; Ng, J.; Edwards, A.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-05-04
Resolution	:	2.30 Å(reported)

The following versions of software and data (see references (i)) 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 2.30 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.
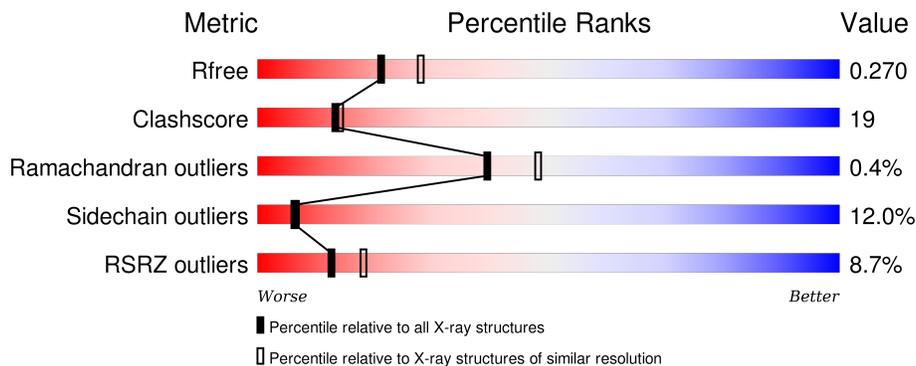
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	204	
1	B	204	
1	C	204	
1	D	204	
1	E	204	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	204	5% ... 64% ... 24% ... 10%
1	G	204	4% ... 60% ... 24% ... 5% ... 11%
1	H	204	19% ... 39% ... 34% ... 11% ... 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NH4	C	201	-	-	-	X
3	NA	A	202	-	-	-	X
3	NA	B	202	-	-	-	X
3	NA	E	202	-	-	-	X
3	NA	F	201	-	-	-	X
3	NA	G	201	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11682 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 Isochorismatase hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total 1478	C 945	N 254	O 274	S 2	Se 3	0	2	0
1	C	178	Total 1396	C 887	N 240	O 264	S 2	Se 3	0	0	0
1	B	179	Total 1419	C 908	N 239	O 267	S 2	Se 3	0	1	0
1	D	179	Total 1398	C 890	N 241	O 262	S 2	Se 3	0	0	0
1	E	189	Total 1474	C 935	N 253	O 281	S 2	Se 3	0	0	0
1	F	183	Total 1437	C 914	N 246	O 272	S 2	Se 3	0	0	0
1	G	182	Total 1423	C 907	N 242	O 269	S 2	Se 3	0	0	0
1	H	171	Total 1309	C 835	N 226	O 243	S 2	Se 3	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP A6TWT6
A	-2	PHE	-	expression tag	UNP A6TWT6
A	-1	GLN	-	expression tag	UNP A6TWT6
A	0	GLY	-	expression tag	UNP A6TWT6
C	-3	TYR	-	expression tag	UNP A6TWT6
C	-2	PHE	-	expression tag	UNP A6TWT6
C	-1	GLN	-	expression tag	UNP A6TWT6
C	0	GLY	-	expression tag	UNP A6TWT6
B	-3	TYR	-	expression tag	UNP A6TWT6
B	-2	PHE	-	expression tag	UNP A6TWT6
B	-1	GLN	-	expression tag	UNP A6TWT6
B	0	GLY	-	expression tag	UNP A6TWT6
D	-3	TYR	-	expression tag	UNP A6TWT6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PHE	-	expression tag	UNP A6TWT6
D	-1	GLN	-	expression tag	UNP A6TWT6
D	0	GLY	-	expression tag	UNP A6TWT6
E	-3	TYR	-	expression tag	UNP A6TWT6
E	-2	PHE	-	expression tag	UNP A6TWT6
E	-1	GLN	-	expression tag	UNP A6TWT6
E	0	GLY	-	expression tag	UNP A6TWT6
F	-3	TYR	-	expression tag	UNP A6TWT6
F	-2	PHE	-	expression tag	UNP A6TWT6
F	-1	GLN	-	expression tag	UNP A6TWT6
F	0	GLY	-	expression tag	UNP A6TWT6
G	-3	TYR	-	expression tag	UNP A6TWT6
G	-2	PHE	-	expression tag	UNP A6TWT6
G	-1	GLN	-	expression tag	UNP A6TWT6
G	0	GLY	-	expression tag	UNP A6TWT6
H	-3	TYR	-	expression tag	UNP A6TWT6
H	-2	PHE	-	expression tag	UNP A6TWT6
H	-1	GLN	-	expression tag	UNP A6TWT6
H	0	GLY	-	expression tag	UNP A6TWT6

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).
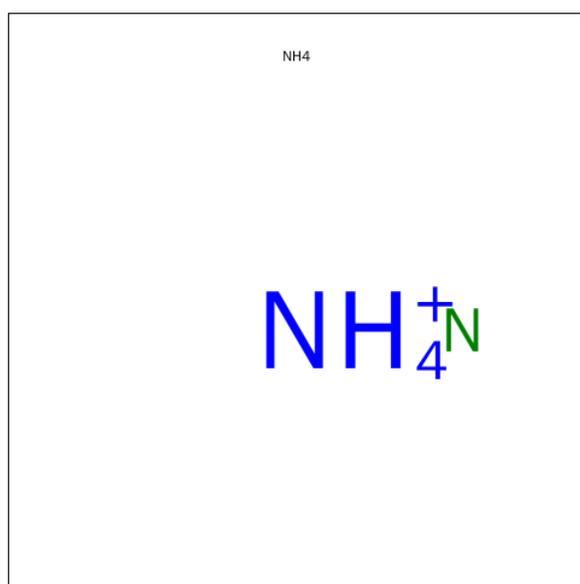
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	N 1	0	0
2	C	1	Total 1	N 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	N 1	0	0
2	D	1	Total 1	N 1	0	0
2	E	1	Total 1	N 1	0	0
2	H	1	Total 1	N 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	C	52	Total 52	O 52	0	0
4	B	67	Total 67	O 67	0	0
4	D	38	Total 38	O 38	0	0
4	E	19	Total 19	O 19	0	0
4	F	44	Total 44	O 44	0	0
4	G	35	Total 35	O 35	0	0
4	H	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

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: Isochorismatase hydrolase
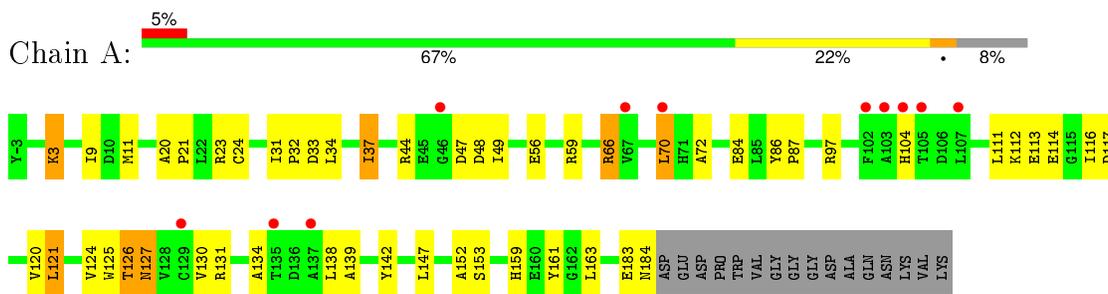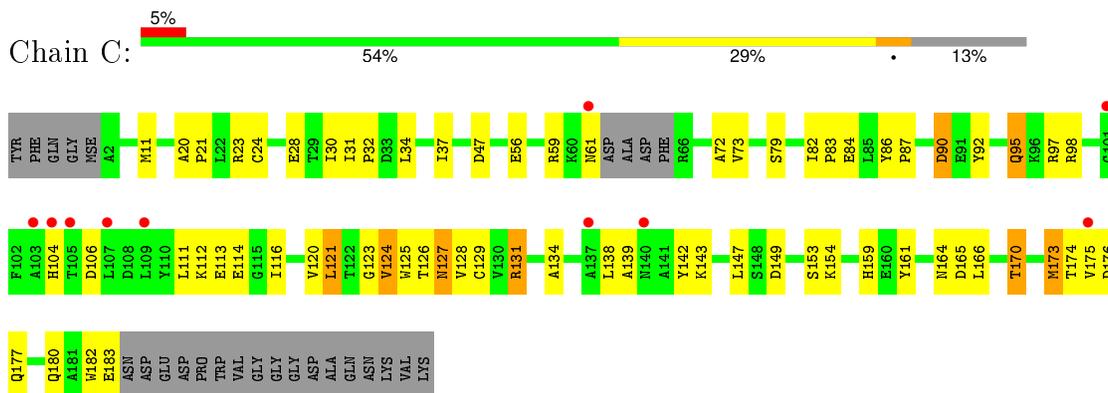
- Molecule 1: Isochorismatase hydrolase

- Molecule 1: Isochorismatase hydrolase

- Molecule 1: Isochorismatase hydrolase

• Molecule 1: Isochorismatase hydrolase

Chain E:

• Molecule 1: Isochorismatase hydrolase

Chain F:

• Molecule 1: Isochorismatase hydrolase

Chain G:

• Molecule 1: Isochorismatase hydrolase

Chain H:
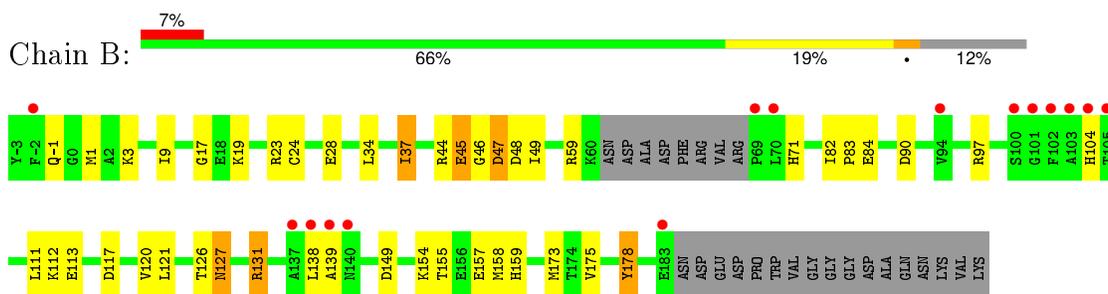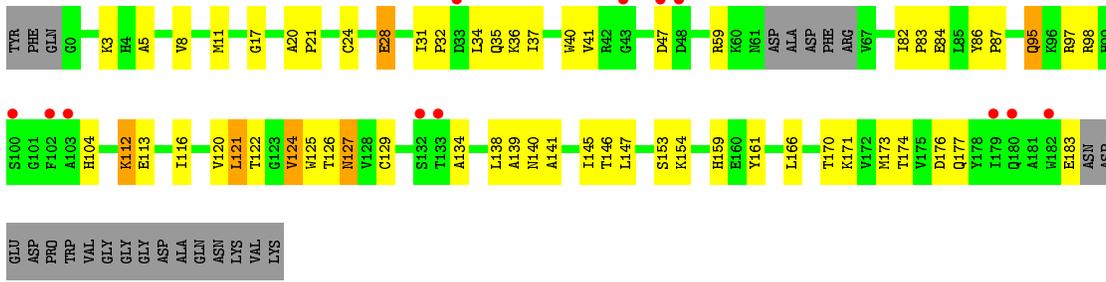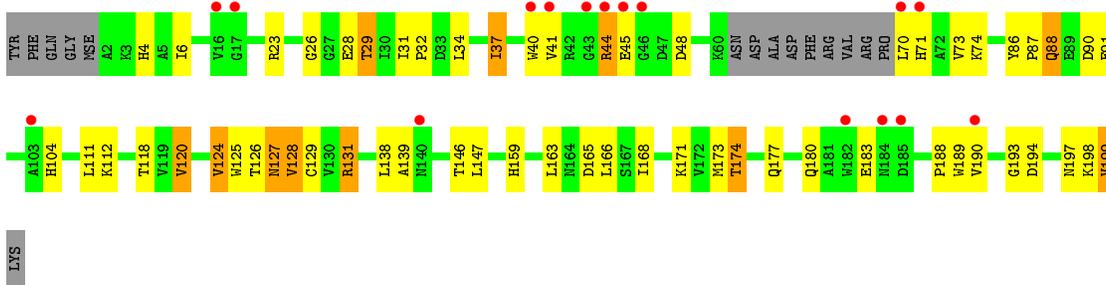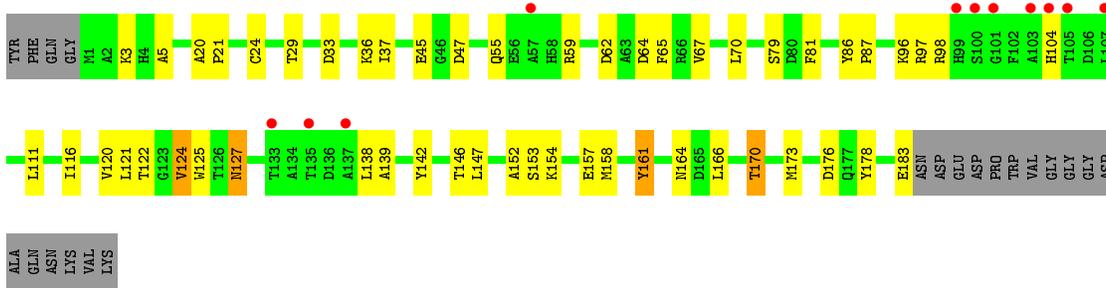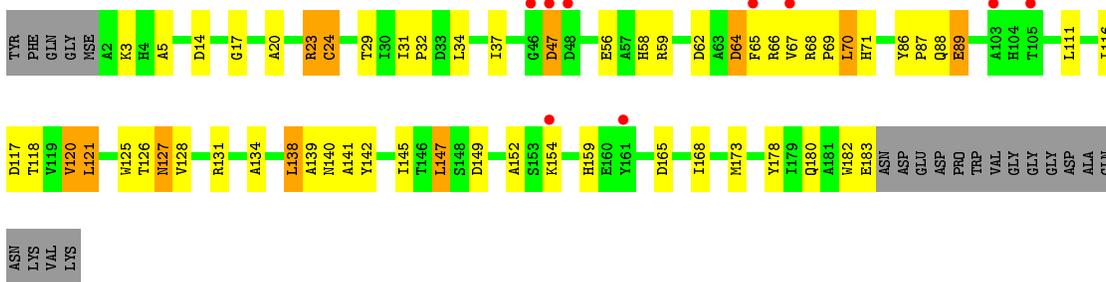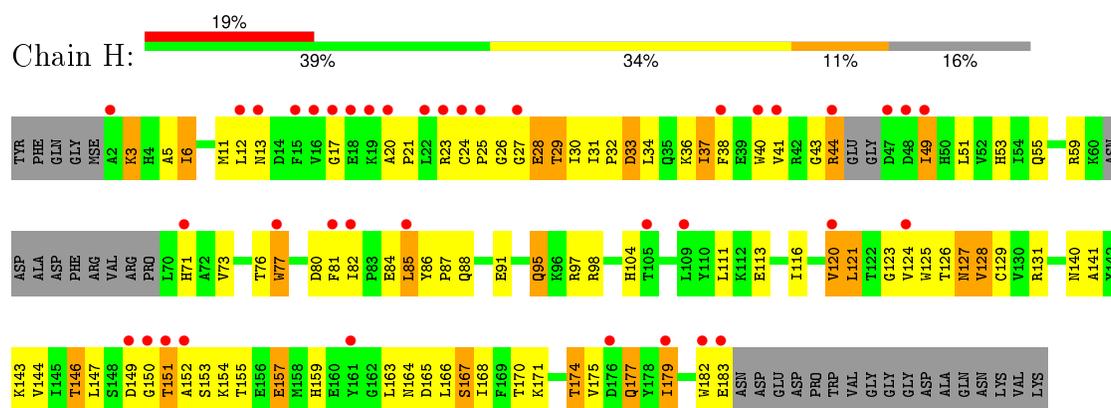
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.65Å 105.42Å 106.27Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	46.32 – 2.30 46.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.32-2.30) 99.5 (46.33-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.196 , 0.238 0.227 , 0.270	Depositor DCC
R_{free} test set	4050 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.1	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 80857 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11682	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, NA

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	1.56	4/1515 (0.3%)	0.78	0/2057
1	B	1.58	3/1451 (0.2%)	0.81	2/1965 (0.1%)
1	C	1.45	3/1424 (0.2%)	0.73	0/1934
1	D	1.45	2/1425 (0.1%)	0.70	0/1932
1	E	1.33	0/1504	0.70	0/2042
1	F	1.49	2/1467 (0.1%)	0.72	0/1992
1	G	1.44	2/1453 (0.1%)	0.72	0/1974
1	H	1.23	1/1334 (0.1%)	0.75	0/1813
All	All	1.45	17/11573 (0.1%)	0.74	2/15709 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9[A]	ILE	N-CA	-12.13	1.22	1.46
1	B	9[B]	ILE	N-CA	-12.13	1.22	1.46
1	A	9[A]	ILE	N-CA	-10.13	1.26	1.46
1	A	9[B]	ILE	N-CA	-10.13	1.26	1.46
1	C	24	CYS	CB-SG	-7.41	1.69	1.82
1	A	24	CYS	CB-SG	-6.80	1.70	1.82
1	G	24	CYS	CB-SG	-6.17	1.71	1.82
1	F	24	CYS	CB-SG	-5.91	1.72	1.81
1	C	129	CYS	CB-SG	-5.80	1.72	1.81
1	C	142	TYR	CD1-CE1	-5.61	1.30	1.39
1	D	24	CYS	CB-SG	-5.59	1.72	1.81
1	A	142	TYR	CD1-CE1	-5.54	1.31	1.39
1	F	142	TYR	CD1-CE1	-5.53	1.31	1.39
1	H	24	CYS	CB-SG	-5.26	1.73	1.81
1	G	142	TYR	CD1-CE1	-5.24	1.31	1.39
1	D	129	CYS	CB-SG	-5.23	1.73	1.81
1	B	178	TYR	CD1-CE1	-5.17	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9[A]	ILE	CA-C-O	5.75	132.18	120.10
1	B	9[B]	ILE	CA-C-O	5.75	132.18	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1478	0	1424	41	0
1	B	1419	0	1377	38	0
1	C	1396	0	1341	58	0
1	D	1398	0	1352	57	0
1	E	1474	0	1409	61	0
1	F	1437	0	1385	32	1
1	G	1423	0	1367	46	0
1	H	1309	0	1242	115	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	69	0	0	0	0
4	B	67	0	0	1	0
4	C	52	0	0	3	0
4	D	38	0	0	2	0
4	E	19	0	0	0	0
4	F	44	0	0	2	0
4	G	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	13	0	0	2	0
All	All	11682	0	10897	417	1

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 19.

All (417) 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:H:13:ASN:ND2	1:H:77:TRP:CE3	1.68	1.55
1:E:174:THR:CG2	1:E:177:GLN:HG3	1.34	1.53
1:H:82:ILE:HD11	1:H:85:LEU:CD1	1.53	1.35
1:H:146:THR:OG1	1:H:170:THR:HG21	1.26	1.32
1:H:13:ASN:ND2	1:H:77:TRP:CZ3	1.95	1.31
1:H:49:ILE:HD11	1:H:182:TRP:CZ2	1.67	1.27
1:E:174:THR:CG2	1:E:177:GLN:CG	2.25	1.14
1:A:126:THR:HG21	1:A:159:HIS:HD2	1.05	1.14
1:A:126:THR:HG21	1:A:159:HIS:CD2	1.83	1.13
1:C:11:MSE:HE1	1:C:30:ILE:HD11	1.26	1.12
1:H:11:MSE:HE2	1:H:123:GLY:HA2	1.17	1.12
1:B:154:LYS:HB3	1:B:158:MSE:CE	1.78	1.12
1:B:154:LYS:HB3	1:B:158:MSE:HE1	1.19	1.11
1:E:171:LYS:NZ	1:E:190:VAL:O	1.83	1.10
1:E:193:GLY:HA3	1:F:67:VAL:CG2	1.82	1.10
1:H:146:THR:OG1	1:H:170:THR:CG2	2.01	1.09
1:A:112:LYS:HE2	1:D:112:LYS:HE3	1.33	1.09
1:B:131:ARG:NH2	1:D:127:ASN:O	1.85	1.09
1:C:23:ARG:NH1	1:C:28:GLU:OE1	1.86	1.09
1:H:13:ASN:CG	1:H:77:TRP:CZ3	2.26	1.07
1:E:174:THR:HG23	1:E:177:GLN:HG3	1.10	1.05
1:C:11:MSE:CE	1:C:123:GLY:HA2	1.87	1.04
1:C:11:MSE:HE2	1:C:123:GLY:CA	1.89	1.02
1:H:149:ASP:OD1	1:H:175:VAL:HG23	1.61	1.01
1:H:82:ILE:HD11	1:H:85:LEU:HD12	1.41	1.00
1:E:171:LYS:CG	1:E:173:MSE:CE	2.40	1.00
1:H:82:ILE:CD1	1:H:85:LEU:CD1	2.40	1.00
1:E:171:LYS:HG2	1:E:173:MSE:CE	1.91	0.99
1:G:70:LEU:C	1:G:70:LEU:CD1	2.30	0.99
1:E:174:THR:HG22	1:E:177:GLN:HG3	1.45	0.99
1:B:127:ASN:H	1:B:127:ASN:HD22	1.05	0.99
1:E:193:GLY:HA3	1:F:67:VAL:HG23	1.41	0.98

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:LEU:O	1:D:170:THR:HB	1.64	0.98
1:G:70:LEU:HD13	1:G:70:LEU:C	1.83	0.97
1:H:11:MSE:HE1	1:H:30:ILE:CD1	1.95	0.96
1:F:127:ASN:H	1:F:127:ASN:HD22	1.01	0.95
1:H:82:ILE:CD1	1:H:85:LEU:HD12	1.97	0.95
1:H:146:THR:HG1	1:H:170:THR:HG21	1.31	0.95
1:H:13:ASN:ND2	1:H:77:TRP:HE3	1.59	0.94
1:D:127:ASN:HD22	1:D:127:ASN:H	1.10	0.94
1:H:124:VAL:HG13	1:H:125:TRP:CD1	2.04	0.93
1:C:11:MSE:HE2	1:C:123:GLY:HA2	0.95	0.93
1:E:127:ASN:H	1:E:127:ASN:HD22	1.18	0.92
1:H:163:LEU:O	1:H:167:SER:OG	1.87	0.92
1:G:70:LEU:HD12	1:G:70:LEU:O	1.69	0.91
1:H:127:ASN:H	1:H:127:ASN:HD22	1.14	0.91
1:H:88:GLN:N	1:H:91:GLU:OE1	2.04	0.90
1:E:171:LYS:HG2	1:E:173:MSE:HE1	1.52	0.90
1:C:127:ASN:HD22	1:C:127:ASN:H	0.92	0.90
1:C:11:MSE:CE	1:C:30:ILE:HD11	2.01	0.89
1:H:88:GLN:O	1:H:91:GLU:HG3	1.72	0.89
1:H:11:MSE:HE1	1:H:30:ILE:HD11	1.53	0.88
1:E:174:THR:HG21	1:E:177:GLN:HG3	1.55	0.88
1:H:82:ILE:HD11	1:H:85:LEU:HD13	1.55	0.88
1:E:174:THR:HG23	1:E:177:GLN:CG	1.96	0.88
1:C:127:ASN:H	1:C:127:ASN:ND2	1.65	0.88
1:H:124:VAL:HG13	1:H:125:TRP:HD1	1.40	0.86
1:F:124:VAL:HG13	1:F:125:TRP:HD1	1.38	0.86
1:C:127:ASN:N	1:C:127:ASN:HD22	1.73	0.86
1:H:166:LEU:O	1:H:170:THR:HB	1.76	0.86
1:H:53:HIS:CD2	1:H:87:PRO:HB3	2.11	0.86
1:C:83:PRO:HD2	1:C:84:GLU:OE1	1.76	0.85
1:A:121:LEU:HD21	1:A:134:ALA:HB2	1.58	0.85
1:H:82:ILE:CG1	1:H:85:LEU:HD12	2.07	0.85
1:E:171:LYS:HG3	1:E:173:MSE:CE	2.06	0.85
1:G:56:GLU:OE1	1:G:58:HIS:NE2	2.10	0.84
1:H:11:MSE:CE	1:H:123:GLY:HA2	2.05	0.83
1:A:112:LYS:CE	1:D:112:LYS:HE3	2.09	0.83
1:H:124:VAL:CG1	1:H:125:TRP:HD1	1.92	0.83
1:H:82:ILE:HD11	1:H:85:LEU:HD11	1.59	0.82
1:H:13:ASN:HB3	1:H:77:TRP:CH2	2.16	0.81
1:E:23:ARG:HH12	1:E:28:GLU:CD	1.84	0.81
1:H:11:MSE:HE3	1:H:34:LEU:HD11	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:ILE:HD11	1:H:182:TRP:CE2	2.16	0.80
1:F:166:LEU:O	1:F:170:THR:HB	1.81	0.80
1:B:154:LYS:CB	1:B:158:MSE:HE1	2.09	0.80
1:D:127:ASN:ND2	1:D:127:ASN:H	1.80	0.80
1:A:126:THR:CG2	1:A:159:HIS:HD2	1.92	0.79
1:B:126:THR:OG1	1:B:159:HIS:HD2	1.66	0.79
1:G:70:LEU:CD1	1:G:70:LEU:O	2.30	0.78
1:C:112:LYS:HE3	1:B:112:LYS:HE3	1.65	0.78
1:H:40:TRP:HH2	1:H:182:TRP:CD1	2.01	0.78
1:F:127:ASN:H	1:F:127:ASN:ND2	1.79	0.78
1:G:127:ASN:HD22	1:G:127:ASN:H	1.31	0.77
1:A:104:HIS:HE1	1:C:139:ALA:O	1.67	0.76
1:F:33:ASP:OD2	4:F:219:HOH:O	2.03	0.76
1:H:49:ILE:CD1	1:H:182:TRP:CZ2	2.60	0.76
1:G:17:GLY:O	1:G:23:ARG:HD2	1.87	0.75
1:E:23:ARG:NH1	1:E:28:GLU:OE2	2.19	0.75
1:E:174:THR:HG22	1:E:177:GLN:CG	2.05	0.74
1:H:26:GLY:HA3	1:H:152:ALA:HB1	1.70	0.73
1:F:124:VAL:HG13	1:F:125:TRP:CD1	2.23	0.73
1:A:127:ASN:H	1:A:127:ASN:HD22	1.36	0.73
1:H:127:ASN:ND2	1:H:127:ASN:H	1.85	0.73
1:B:104:HIS:HE1	1:D:139:ALA:O	1.74	0.71
1:F:36:LYS:NZ	1:F:176:ASP:OD1	2.23	0.71
1:E:173:MSE:HE1	1:E:188:PRO:O	1.91	0.71
1:H:124:VAL:CG1	1:H:125:TRP:CD1	2.72	0.71
1:D:3:LYS:NZ	1:D:47:ASP:O	2.24	0.71
1:H:6:ILE:HG13	1:H:120:VAL:HG13	1.72	0.71
1:H:17:GLY:O	1:H:23:ARG:HD3	1.91	0.70
1:H:43:GLY:O	1:H:44:ARG:CB	2.38	0.70
1:C:182:TRP:C	1:C:183:GLU:OE2	2.30	0.70
1:A:183:GLU:O	1:A:184:ASN:C	2.30	0.70
1:H:13:ASN:HB3	1:H:77:TRP:CZ2	2.27	0.70
1:G:182:TRP:C	1:G:183:GLU:OE1	2.31	0.69
1:E:127:ASN:H	1:E:127:ASN:ND2	1.91	0.69
1:A:112:LYS:HE2	1:D:112:LYS:CE	2.16	0.69
1:G:70:LEU:HD13	1:G:71:HIS:N	2.08	0.69
1:D:126:THR:OG1	1:D:159:HIS:HD2	1.73	0.69
1:H:11:MSE:HE1	1:H:30:ILE:HD12	1.72	0.69
1:E:171:LYS:CG	1:E:173:MSE:HE2	2.24	0.68
1:H:40:TRP:CE2	1:H:179:ILE:HG23	2.29	0.68
1:F:127:ASN:N	1:F:127:ASN:HD22	1.83	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ASP:OD1	1:H:81:PHE:N	2.27	0.67
1:C:166:LEU:O	1:C:170:THR:HB	1.93	0.67
1:E:174:THR:HG22	1:E:177:GLN:CD	2.13	0.67
1:H:49:ILE:HD11	1:H:182:TRP:HZ2	1.52	0.67
1:D:124:VAL:HG13	1:D:125:TRP:HD1	1.60	0.67
1:H:40:TRP:CH2	1:H:182:TRP:CD1	2.82	0.67
1:B:127:ASN:ND2	1:B:127:ASN:H	1.82	0.67
1:H:175:VAL:O	1:H:179:ILE:HG13	1.95	0.67
1:C:113:GLU:OE2	1:D:97:ARG:NH2	2.26	0.67
1:E:171:LYS:HG3	1:E:173:MSE:HE2	1.76	0.67
1:E:44:ARG:NH1	1:E:48:ASP:HB2	2.10	0.67
1:H:82:ILE:HG13	1:H:85:LEU:HD12	1.75	0.66
1:E:171:LYS:CG	1:E:173:MSE:HE3	2.24	0.66
1:A:121:LEU:CD2	1:A:134:ALA:HB2	2.23	0.66
1:H:43:GLY:O	1:H:44:ARG:HB3	1.95	0.66
1:H:127:ASN:HD22	1:H:127:ASN:N	1.91	0.66
1:G:126:THR:OG1	1:G:159:HIS:HD2	1.78	0.66
1:D:84:GLU:H	1:D:84:GLU:CD	1.92	0.66
1:D:183:GLU:OE2	1:D:183:GLU:N	2.30	0.65
1:B:154:LYS:HB3	1:B:158:MSE:HE3	1.74	0.65
1:C:97:ARG:NH2	1:D:113:GLU:OE2	2.26	0.64
1:E:171:LYS:HG3	1:E:173:MSE:HE3	1.79	0.64
1:H:11:MSE:CE	1:H:30:ILE:HD12	2.27	0.64
1:G:183:GLU:N	1:G:183:GLU:OE1	2.30	0.64
1:D:127:ASN:N	1:D:127:ASN:HD22	1.90	0.64
1:H:40:TRP:CD2	1:H:179:ILE:HG23	2.32	0.64
1:E:174:THR:HG23	1:E:177:GLN:H	1.62	0.63
1:E:124:VAL:HG13	1:E:125:TRP:HD1	1.64	0.63
1:C:86:TYR:CD1	1:C:87:PRO:HD2	2.34	0.63
1:C:84:GLU:N	1:C:84:GLU:OE1	2.29	0.63
1:D:174:THR:OG1	1:D:177:GLN:HG3	1.98	0.63
1:G:3:LYS:HE3	1:G:47:ASP:O	1.99	0.63
1:E:139:ALA:O	1:F:104:HIS:HE1	1.81	0.63
1:C:83:PRO:CD	1:C:84:GLU:OE1	2.46	0.62
1:A:124:VAL:HG13	1:A:125:TRP:HD1	1.63	0.62
1:F:146:THR:OG1	1:F:170:THR:HG21	1.98	0.62
1:B:17:GLY:O	1:B:23:ARG:CD	2.47	0.62
1:H:53:HIS:HD2	1:H:87:PRO:HB3	1.61	0.62
1:C:11:MSE:HE3	1:C:34:LEU:HD11	1.81	0.62
1:E:126:THR:OG1	1:E:159:HIS:HD2	1.83	0.62
1:H:33:ASP:N	1:H:33:ASP:OD2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:GLY:HA3	1:F:67:VAL:HG22	1.81	0.62
1:B:37:ILE:HD12	1:B:175:VAL:HG13	1.82	0.61
1:G:5:ALA:HB2	1:G:116:ILE:HD13	1.82	0.61
1:E:171:LYS:HE2	1:E:173:MSE:HE2	1.83	0.61
1:A:124:VAL:HG13	1:A:125:TRP:CD1	2.35	0.61
1:C:28:GLU:HG3	4:C:272:HOH:O	2.00	0.61
1:E:159:HIS:CE1	1:E:163:LEU:HD11	2.35	0.61
1:C:90:ASP:OD2	1:C:90:ASP:N	2.29	0.61
1:D:36:LYS:NZ	1:D:176:ASP:OD1	2.33	0.60
1:A:84:GLU:OE1	1:A:84:GLU:N	2.30	0.60
1:D:59:ARG:HD2	4:D:229:HOH:O	2.01	0.60
1:D:82:ILE:HD12	1:D:84:GLU:HG2	1.82	0.60
1:H:121:LEU:CD2	1:H:144:VAL:CG1	2.79	0.60
1:H:38:PHE:CE1	1:H:85:LEU:HB3	2.37	0.60
1:A:124:VAL:CG1	1:A:125:TRP:HD1	2.15	0.60
1:G:126:THR:OG1	1:G:159:HIS:CD2	2.55	0.59
1:E:86:TYR:CD1	1:E:87:PRO:HD2	2.37	0.59
1:B:127:ASN:N	1:B:127:ASN:HD22	1.86	0.59
1:G:56:GLU:OE1	1:G:58:HIS:CD2	2.56	0.59
1:A:114:GLU:HB2	1:A:116:ILE:HD12	1.85	0.59
1:G:64:ASP:O	1:G:67:VAL:N	2.34	0.59
1:G:139:ALA:HA	1:H:98:ARG:HG3	1.84	0.59
1:H:37:ILE:HG22	1:H:38:PHE:N	2.17	0.58
1:H:40:TRP:CE2	1:H:179:ILE:CG2	2.86	0.58
1:H:182:TRP:HB2	1:H:183:GLU:OE2	2.04	0.58
1:C:23:ARG:HH12	1:C:28:GLU:CD	2.07	0.58
1:F:173:MSE:HE2	1:F:178:TYR:HA	1.86	0.58
1:H:123:GLY:O	1:H:151:THR:HG22	2.04	0.58
1:A:139:ALA:HA	1:C:98:ARG:HG3	1.86	0.58
1:H:170:THR:HG22	1:H:171:LYS:N	2.17	0.58
1:D:40:TRP:CE3	1:D:41:VAL:HG23	2.38	0.58
1:H:13:ASN:CB	1:H:77:TRP:CZ3	2.86	0.58
1:B:154:LYS:HD3	1:B:158:MSE:HE1	1.85	0.57
1:G:127:ASN:ND2	1:G:127:ASN:H	2.01	0.57
1:E:104:HIS:HE1	1:F:139:ALA:O	1.86	0.57
1:D:146:THR:OG1	1:D:170:THR:HG21	2.03	0.57
1:D:84:GLU:N	1:D:84:GLU:OE1	2.30	0.57
1:B:155:THR:H	1:B:158:MSE:HE3	1.69	0.57
1:C:23:ARG:NH1	1:C:28:GLU:CD	2.58	0.57
1:C:92:TYR:CE1	1:D:59:ARG:HD3	2.39	0.57
1:G:139:ALA:O	1:H:104:HIS:HE1	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:OE1	1:B:84:GLU:N	2.30	0.57
1:E:199:VAL:HB	1:F:158:MSE:HE1	1.85	0.57
1:A:139:ALA:O	1:C:104:HIS:HE1	1.88	0.57
1:E:159:HIS:NE2	1:E:163:LEU:HD11	2.20	0.56
1:H:11:MSE:CE	1:H:30:ILE:CD1	2.78	0.56
1:H:6:ILE:HG13	1:H:120:VAL:CG1	2.35	0.56
1:F:96:LYS:HD2	1:F:98:ARG:O	2.05	0.56
1:C:124:VAL:HG13	1:C:125:TRP:CD1	2.41	0.56
1:E:44:ARG:HH12	1:E:48:ASP:HB2	1.70	0.56
1:H:95:GLN:HG2	4:H:323:HOH:O	2.06	0.56
1:E:168:ILE:HG12	1:E:199:VAL:HG11	1.88	0.56
1:F:55:GLN:HB3	1:F:81:PHE:CZ	2.41	0.56
1:H:126:THR:OG1	1:H:159:HIS:HD2	1.89	0.56
1:C:124:VAL:HG13	1:C:125:TRP:HD1	1.70	0.55
1:D:84:GLU:N	1:D:84:GLU:CD	2.60	0.55
1:A:97:ARG:NH2	1:B:113:GLU:OE2	2.38	0.55
1:H:153:SER:OG	1:H:154:LYS:N	2.35	0.55
1:E:174:THR:HG22	1:E:177:GLN:OE1	2.06	0.55
1:A:121:LEU:HD21	1:A:134:ALA:CB	2.33	0.55
1:D:5:ALA:HB2	1:D:116:ILE:HD13	1.89	0.55
1:A:126:THR:HG22	1:A:152:ALA:C	2.26	0.55
1:D:170:THR:CG2	1:D:171:LYS:N	2.67	0.55
1:C:59:ARG:HD2	4:C:228:HOH:O	2.05	0.55
1:B:139:ALA:O	1:D:104:HIS:HE1	1.90	0.55
1:D:86:TYR:CD1	1:D:87:PRO:HD2	2.42	0.55
1:A:20:ALA:HB3	1:A:23:ARG:HB2	1.90	0.54
1:C:121:LEU:HD21	1:C:134:ALA:HB2	1.90	0.54
1:B:45:GLU:HG2	1:B:46:GLY:N	2.21	0.53
1:A:113:GLU:OE1	1:B:97:ARG:NH2	2.41	0.53
1:B:155:THR:HG23	1:B:158:MSE:HE2	1.89	0.53
1:E:31:ILE:N	1:E:32:PRO:CD	2.72	0.53
1:C:149:ASP:OD1	1:C:175:VAL:HG23	2.08	0.53
1:H:128:VAL:HG12	1:H:129:CYS:N	2.23	0.53
1:B:23:ARG:NH1	1:B:28:GLU:OE1	2.41	0.53
1:H:40:TRP:O	1:H:43:GLY:O	2.26	0.52
1:F:5:ALA:HB2	1:F:116:ILE:HD13	1.91	0.52
1:G:140:ASN:O	1:G:141:ALA:HB3	2.09	0.52
1:H:53:HIS:CD2	1:H:87:PRO:CB	2.90	0.52
1:C:126:THR:OG1	1:C:159:HIS:HD2	1.93	0.52
1:H:84:GLU:C	1:H:85:LEU:HG	2.29	0.52
1:A:113:GLU:CD	1:B:97:ARG:HH22	2.12	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LEU:CD2	1:C:134:ALA:HB2	2.41	0.51
1:H:164:ASN:HA	1:H:167:SER:OG	2.10	0.51
1:D:171:LYS:HD3	1:D:173:MSE:CE	2.40	0.51
1:C:56:GLU:HG2	1:C:72:ALA:HB3	1.91	0.51
1:G:120:VAL:HA	1:G:145:ILE:O	2.10	0.51
1:A:127:ASN:H	1:A:127:ASN:ND2	2.07	0.51
1:F:158:MSE:HA	1:F:161:TYR:CE2	2.46	0.51
1:C:131:ARG:NH2	1:C:165:ASP:OD2	2.44	0.51
1:H:174:THR:HG23	1:H:177:GLN:H	1.75	0.51
1:G:121:LEU:CD2	1:G:134:ALA:HB2	2.41	0.51
1:A:126:THR:HA	1:A:130:VAL:HB	1.92	0.51
1:D:140:ASN:O	1:D:141:ALA:HB3	2.10	0.50
1:G:59:ARG:O	1:G:62:ASP:HB2	2.10	0.50
1:E:127:ASN:N	1:E:127:ASN:HD22	1.96	0.50
1:A:31:ILE:N	1:A:32:PRO:CD	2.73	0.50
1:H:175:VAL:O	1:H:179:ILE:CG1	2.60	0.50
1:H:146:THR:HG21	1:H:166:LEU:HD13	1.93	0.50
1:G:65:PHE:CD1	1:G:70:LEU:HA	2.47	0.50
1:E:131:ARG:NH2	1:F:127:ASN:O	2.43	0.50
1:A:183:GLU:O	1:A:184:ASN:O	2.30	0.50
1:E:194:ASP:OD2	1:E:199:VAL:HG22	2.12	0.50
1:H:31:ILE:N	1:H:32:PRO:CD	2.75	0.50
1:C:61:ASN:OD1	1:C:61:ASN:O	2.30	0.50
1:B:157:GLU:H	1:B:157:GLU:CD	2.15	0.50
1:E:34:LEU:O	1:E:37:ILE:HG22	2.12	0.50
1:E:171:LYS:HE2	1:E:173:MSE:CE	2.42	0.49
1:B:17:GLY:O	1:B:23:ARG:HD2	2.11	0.49
1:H:26:GLY:O	1:H:29:THR:HG23	2.12	0.49
1:G:120:VAL:HB	1:G:145:ILE:HB	1.93	0.49
1:H:147:LEU:HB3	1:H:150:GLY:HA3	1.93	0.49
1:C:97:ARG:HH22	1:D:113:GLU:CD	2.13	0.49
1:E:40:TRP:CE3	1:E:41:VAL:HG23	2.48	0.48
1:H:13:ASN:CB	1:H:77:TRP:CH2	2.90	0.48
1:H:40:TRP:HH2	1:H:182:TRP:NE1	2.10	0.48
1:E:131:ARG:NH2	1:E:165:ASP:OD2	2.45	0.48
1:C:31:ILE:N	1:C:32:PRO:CD	2.76	0.48
1:D:82:ILE:HD12	1:D:84:GLU:CG	2.43	0.48
1:C:113:GLU:OE1	1:D:97:ARG:NH2	2.47	0.48
1:G:152:ALA:HA	1:G:159:HIS:CD2	2.49	0.48
1:G:88:GLN:O	1:G:89:GLU:C	2.50	0.48
1:D:17:GLY:HA2	1:D:28:GLU:OE2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLU:CD	1:D:97:ARG:NH2	2.67	0.48
1:D:28:GLU:H	1:D:28:GLU:HG2	1.50	0.48
1:H:121:LEU:HD22	1:H:144:VAL:CG1	2.44	0.47
1:F:96:LYS:HB2	4:F:328:HOH:O	2.12	0.47
1:H:73:VAL:O	1:H:76:THR:HG23	2.14	0.47
1:C:106:ASP:OD1	1:D:97:ARG:NH1	2.40	0.47
1:D:31:ILE:O	1:D:35:GLN:HG3	2.14	0.47
1:C:20:ALA:HA	1:C:21:PRO:HD3	1.77	0.47
1:H:140:ASN:O	1:H:141:ALA:HB3	2.15	0.47
1:H:86:TYR:CD1	1:H:87:PRO:HD2	2.49	0.47
1:B:173:MSE:CE	1:B:178:TYR:HA	2.45	0.47
1:D:170:THR:HG22	1:D:171:LYS:N	2.30	0.47
1:D:82:ILE:CD1	1:D:84:GLU:HG2	2.44	0.47
1:E:6:ILE:HG12	1:E:120:VAL:HG22	1.96	0.47
1:G:149:ASP:OD1	1:G:149:ASP:N	2.40	0.47
1:E:180:GLN:HG3	1:E:180:GLN:O	2.13	0.47
1:B:126:THR:OG1	1:B:159:HIS:CD2	2.58	0.46
1:H:26:GLY:CA	1:H:152:ALA:HB1	2.42	0.46
1:E:194:ASP:OD2	1:E:197:ASN:HA	2.15	0.46
1:B:173:MSE:HE1	1:B:178:TYR:HA	1.96	0.46
1:C:97:ARG:NH2	1:D:113:GLU:CD	2.69	0.46
1:A:31:ILE:N	1:A:32:PRO:HD3	2.29	0.46
1:A:56:GLU:HG2	1:A:72:ALA:HB3	1.97	0.46
1:B:3:LYS:NZ	1:B:47:ASP:O	2.48	0.46
1:E:88:GLN:O	1:E:91:GLU:HG3	2.14	0.46
1:G:173:MSE:HE2	1:G:178:TYR:HA	1.97	0.46
1:E:31:ILE:HB	1:E:32:PRO:HD3	1.96	0.46
1:G:121:LEU:HD21	1:G:134:ALA:HB2	1.98	0.46
1:C:182:TRP:O	1:C:183:GLU:OE2	2.34	0.46
1:A:11:MSE:HE2	1:A:34:LEU:HD12	1.96	0.46
1:E:146:THR:HG21	1:E:166:LEU:HD13	1.97	0.46
1:E:128:VAL:HG12	1:E:129:CYS:N	2.31	0.45
1:A:47:ASP:OD1	1:A:47:ASP:O	2.35	0.45
1:H:31:ILE:HB	1:H:32:PRO:HD3	1.98	0.45
1:H:170:THR:CG2	1:H:171:LYS:N	2.78	0.45
1:D:20:ALA:HA	1:D:21:PRO:HD3	1.76	0.45
1:G:14:ASP:O	1:G:20:ALA:HB1	2.17	0.45
4:C:202:HOH:O	1:D:104:HIS:CD2	2.69	0.45
1:D:153:SER:OG	1:D:154:LYS:N	2.50	0.45
1:B:155:THR:N	1:B:158:MSE:HE3	2.31	0.45
1:B:17:GLY:O	1:B:23:ARG:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LEU:O	1:H:37:ILE:HB	2.17	0.45
1:H:97:ARG:HG3	4:H:212:HOH:O	2.16	0.45
1:H:20:ALA:HA	1:H:21:PRO:HD3	1.90	0.45
1:H:41:VAL:HG22	1:H:49:ILE:HG21	1.98	0.45
1:B:155:THR:HG23	1:B:158:MSE:CE	2.46	0.45
1:H:155:THR:OG1	1:H:157:GLU:HG2	2.16	0.44
1:A:127:ASN:ND2	1:A:153:SER:OG	2.50	0.44
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.84	0.44
1:G:65:PHE:CE1	1:G:70:LEU:HA	2.52	0.44
1:D:86:TYR:HA	1:D:87:PRO:HD3	1.89	0.44
1:A:20:ALA:HA	1:A:21:PRO:HD3	1.82	0.44
1:F:153:SER:OG	1:F:154:LYS:N	2.51	0.44
1:C:113:GLU:CD	1:D:97:ARG:HH22	2.17	0.44
1:C:95:GLN:HG2	1:C:95:GLN:H	1.56	0.44
1:E:4:HIS:CD2	1:E:118:THR:HB	2.53	0.44
1:D:40:TRP:CZ3	1:D:41:VAL:HG23	2.53	0.44
1:C:31:ILE:HB	1:C:32:PRO:HD3	2.00	0.44
1:C:153:SER:OG	1:C:154:LYS:N	2.50	0.44
1:C:176:ASP:O	1:C:180:GLN:HB3	2.18	0.44
1:G:125:TRP:CH2	1:G:154:LYS:HD2	2.53	0.44
1:G:117:ASP:OD2	1:G:118:THR:OG1	2.32	0.44
1:D:82:ILE:HA	1:D:83:PRO:HD3	1.81	0.43
1:D:8:VAL:HA	1:D:122:THR:OG1	2.18	0.43
1:H:146:THR:OG1	1:H:170:THR:HG22	2.06	0.43
1:H:25:PRO:C	1:H:27:GLY:N	2.72	0.43
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.81	0.43
1:G:64:ASP:C	1:G:66:ARG:N	2.72	0.43
1:D:86:TYR:CG	1:D:87:PRO:HD2	2.52	0.43
1:D:121:LEU:HD21	1:D:134:ALA:HB2	2.00	0.43
1:D:95:GLN:H	1:D:95:GLN:HG2	1.67	0.43
1:A:66:ARG:H	1:A:66:ARG:HG2	1.09	0.43
1:F:98:ARG:HA	1:F:98:ARG:HD3	1.85	0.43
1:A:48:ASP:C	1:A:49:ILE:HG13	2.37	0.43
1:E:174:THR:HG23	1:E:177:GLN:CB	2.46	0.43
1:H:163:LEU:HA	1:H:163:LEU:HD23	1.68	0.43
1:H:30:ILE:HG22	1:H:149:ASP:O	2.19	0.43
1:D:95:GLN:HG2	4:D:209:HOH:O	2.19	0.43
1:H:174:THR:H	1:H:177:GLN:CD	2.22	0.42
1:H:165:ASP:O	1:H:168:ILE:HG13	2.20	0.42
1:E:26:GLY:O	1:E:29:THR:HG23	2.18	0.42
1:G:31:ILE:HB	1:G:32:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.71	0.42
1:G:127:ASN:HD22	1:G:127:ASN:N	2.08	0.42
1:A:34:LEU:O	1:A:37:ILE:HG22	2.19	0.42
1:F:70:LEU:C	1:F:70:LEU:HD23	2.40	0.42
1:G:86:TYR:HA	1:G:87:PRO:HD3	1.78	0.42
1:A:86:TYR:HA	1:A:87:PRO:HD3	1.91	0.42
1:C:82:ILE:HA	1:C:83:PRO:HD3	1.87	0.42
1:G:31:ILE:N	1:G:32:PRO:CD	2.82	0.42
1:G:138:LEU:HA	1:G:138:LEU:HD23	1.84	0.42
1:G:34:LEU:O	1:G:37:ILE:HG22	2.20	0.42
1:E:73:VAL:HG12	1:E:74:LYS:N	2.35	0.42
1:B:59:ARG:HD2	4:B:252:HOH:O	2.19	0.42
1:C:73:VAL:O	1:C:79:SER:HB2	2.19	0.42
1:G:165:ASP:O	1:G:168:ILE:HB	2.20	0.42
1:H:125:TRP:CD1	1:H:125:TRP:N	2.88	0.42
1:F:124:VAL:CG1	1:F:125:TRP:HD1	2.20	0.42
1:H:86:TYR:HA	1:H:87:PRO:HD3	1.78	0.42
1:H:95:GLN:H	1:H:95:GLN:HG2	1.39	0.41
1:F:124:VAL:HG22	1:F:152:ALA:O	2.21	0.41
1:F:20:ALA:HA	1:F:21:PRO:HD3	1.81	0.41
1:G:59:ARG:HD2	1:G:59:ARG:HH11	1.73	0.41
1:C:174:THR:HG23	1:C:177:GLN:OE1	2.20	0.41
1:F:86:TYR:HA	1:F:87:PRO:HD3	1.90	0.41
1:C:173:MSE:HB3	1:C:173:MSE:HE3	1.96	0.41
1:B:-1:GLN:O	1:B:1:MSE:N	2.50	0.41
1:C:114:GLU:HB2	1:C:116:ILE:HD12	2.02	0.41
1:H:147:LEU:O	1:H:150:GLY:CA	2.68	0.41
1:H:147:LEU:O	1:H:150:GLY:HA3	2.20	0.41
1:C:183:GLU:N	1:C:183:GLU:OE2	2.52	0.41
1:F:59:ARG:O	1:F:62:ASP:HB2	2.21	0.41
1:G:65:PHE:O	1:G:68:ARG:O	2.38	0.41
1:H:73:VAL:HB	1:H:76:THR:HG21	2.02	0.41
1:G:147:LEU:HA	1:G:173:MSE:O	2.20	0.41
1:F:122:THR:HG22	1:F:147:LEU:HD12	2.03	0.41
1:H:41:VAL:CG2	1:H:49:ILE:HG21	2.51	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.87	0.41
1:H:13:ASN:HB3	1:H:77:TRP:CZ3	2.49	0.41
1:H:182:TRP:CB	1:H:183:GLU:OE2	2.69	0.41
1:G:68:ARG:CB	1:G:69:PRO:CD	2.99	0.41
1:H:124:VAL:HG12	1:H:125:TRP:HD1	1.79	0.41
1:E:126:THR:OG1	1:E:159:HIS:CD2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:GLU:O	1:H:31:ILE:HG13	2.21	0.41
1:B:82:ILE:HA	1:B:83:PRO:HD3	1.90	0.41
1:D:120:VAL:HA	1:D:145:ILE:O	2.21	0.41
1:H:149:ASP:CG	1:H:175:VAL:HG23	2.37	0.41
1:D:11:MSE:HE2	1:D:34:LEU:HD12	2.02	0.40
1:D:31:ILE:N	1:D:32:PRO:CD	2.84	0.40
1:A:3:LYS:HE3	1:A:114:GLU:O	2.21	0.40
1:F:65:PHE:CE1	1:F:70:LEU:HA	2.56	0.40
1:B:48:ASP:C	1:B:49:ILE:HG13	2.41	0.40
1:H:97:ARG:O	1:H:98:ARG:HD3	2.21	0.40
1:H:5:ALA:HB2	1:H:116:ILE:HD12	2.02	0.40
1:B:149:ASP:OD1	1:B:149:ASP:N	2.50	0.40
1:C:11:MSE:HE3	1:C:34:LEU:CD1	2.49	0.40
1:B:34:LEU:O	1:B:37:ILE:HG22	2.22	0.40
1:H:3:LYS:HB3	1:H:116:ILE:HA	2.04	0.40
1:E:189:TRP:O	1:E:189:TRP:CG	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ARG:NH2	1:H:113:GLU:OE1[1_655]	2.15	0.05

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	188/204 (92%)	185 (98%)	3 (2%)	0	100	100
1	B	176/204 (86%)	172 (98%)	4 (2%)	0	100	100
1	C	174/204 (85%)	170 (98%)	3 (2%)	1 (1%)	30	36
1	D	175/204 (86%)	171 (98%)	4 (2%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	185/204 (91%)	179 (97%)	5 (3%)	1 (0%)	34	41
1	F	181/204 (89%)	178 (98%)	3 (2%)	0	100	100
1	G	180/204 (88%)	176 (98%)	2 (1%)	2 (1%)	17	18
1	H	165/204 (81%)	160 (97%)	4 (2%)	1 (1%)	30	36
All	All	1424/1632 (87%)	1391 (98%)	28 (2%)	5 (0%)	39	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	89	GLU
1	E	128	VAL
1	H	128	VAL
1	C	128	VAL
1	G	128	VAL

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	153/170 (90%)	136 (89%)	17 (11%)	8	8
1	B	150/170 (88%)	135 (90%)	15 (10%)	9	11
1	C	147/170 (86%)	130 (88%)	17 (12%)	7	7
1	D	146/170 (86%)	135 (92%)	11 (8%)	17	21
1	E	154/170 (91%)	134 (87%)	20 (13%)	5	5
1	F	151/170 (89%)	133 (88%)	18 (12%)	6	7
1	G	149/170 (88%)	135 (91%)	14 (9%)	11	12
1	H	133/170 (78%)	103 (77%)	30 (23%)	1	1
All	All	1183/1360 (87%)	1041 (88%)	142 (12%)	6	6

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	33	ASP
1	A	37	ILE
1	A	44	ARG
1	A	59	ARG
1	A	66	ARG
1	A	70	LEU
1	A	111	LEU
1	A	117	ASP
1	A	120	VAL
1	A	121	LEU
1	A	126	THR
1	A	127	ASN
1	A	131	ARG
1	A	138	LEU
1	A	147	LEU
1	A	161	TYR
1	C	37	ILE
1	C	47	ASP
1	C	90	ASP
1	C	95	GLN
1	C	111	LEU
1	C	120	VAL
1	C	121	LEU
1	C	124	VAL
1	C	127	ASN
1	C	131	ARG
1	C	138	LEU
1	C	143	LYS
1	C	147	LEU
1	C	161	TYR
1	C	164	ASN
1	C	170	THR
1	C	173	MSE
1	B	19	LYS
1	B	24	CYS
1	B	37	ILE
1	B	44	ARG
1	B	45	GLU
1	B	47	ASP
1	B	71	HIS
1	B	90	ASP
1	B	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	ASP
1	B	120	VAL
1	B	121	LEU
1	B	127	ASN
1	B	131	ARG
1	B	138	LEU
1	D	28	GLU
1	D	37	ILE
1	D	95	GLN
1	D	98	ARG
1	D	112	LYS
1	D	121	LEU
1	D	124	VAL
1	D	127	ASN
1	D	138	LEU
1	D	147	LEU
1	D	161	TYR
1	E	29	THR
1	E	37	ILE
1	E	44	ARG
1	E	45	GLU
1	E	70	LEU
1	E	71	HIS
1	E	88	GLN
1	E	90	ASP
1	E	111	LEU
1	E	112	LYS
1	E	120	VAL
1	E	124	VAL
1	E	127	ASN
1	E	131	ARG
1	E	138	LEU
1	E	147	LEU
1	E	174	THR
1	E	183	GLU
1	E	198	LYS
1	E	199	VAL
1	F	3	LYS
1	F	29	THR
1	F	37	ILE
1	F	45	GLU
1	F	47	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	64	ASP
1	F	79	SER
1	F	111	LEU
1	F	120	VAL
1	F	121	LEU
1	F	124	VAL
1	F	127	ASN
1	F	138	LEU
1	F	157	GLU
1	F	161	TYR
1	F	164	ASN
1	F	170	THR
1	F	183	GLU
1	G	23	ARG
1	G	24	CYS
1	G	29	THR
1	G	47	ASP
1	G	64	ASP
1	G	70	LEU
1	G	111	LEU
1	G	120	VAL
1	G	121	LEU
1	G	127	ASN
1	G	131	ARG
1	G	138	LEU
1	G	147	LEU
1	G	180	GLN
1	H	3	LYS
1	H	6	ILE
1	H	12	LEU
1	H	28	GLU
1	H	29	THR
1	H	33	ASP
1	H	36	LYS
1	H	37	ILE
1	H	44	ARG
1	H	49	ILE
1	H	51	LEU
1	H	55	GLN
1	H	59	ARG
1	H	71	HIS
1	H	77	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	85	LEU
1	H	95	GLN
1	H	111	LEU
1	H	120	VAL
1	H	121	LEU
1	H	127	ASN
1	H	131	ARG
1	H	143	LYS
1	H	146	THR
1	H	151	THR
1	H	157	GLU
1	H	167	SER
1	H	174	THR
1	H	177	GLN
1	H	179	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	104	HIS
1	A	127	ASN
1	A	159	HIS
1	C	61	ASN
1	C	104	HIS
1	C	127	ASN
1	C	159	HIS
1	B	55	GLN
1	B	104	HIS
1	B	127	ASN
1	B	159	HIS
1	D	55	GLN
1	D	104	HIS
1	D	127	ASN
1	D	159	HIS
1	E	104	HIS
1	E	127	ASN
1	E	159	HIS
1	E	196	GLN
1	E	197	ASN
1	F	58	HIS
1	F	71	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	104	HIS
1	F	127	ASN
1	G	55	GLN
1	G	127	ASN
1	G	159	HIS
1	H	53	HIS
1	H	55	GLN
1	H	104	HIS
1	H	127	ASN
1	H	159	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 are modelled with single atom and 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	184/204 (90%)	0.28	11 (5%)	25	33	13, 21, 30, 56	0
1	B	175/204 (85%)	0.51	15 (8%)	13	18	8, 23, 32, 64	0
1	C	175/204 (85%)	0.35	10 (5%)	27	36	14, 24, 30, 36	0
1	D	175/204 (85%)	0.52	12 (6%)	20	27	15, 24, 31, 55	0
1	E	186/204 (91%)	0.63	16 (8%)	13	18	19, 28, 49, 66	0
1	F	179/204 (87%)	0.35	11 (6%)	25	33	14, 23, 29, 38	0
1	G	179/204 (87%)	0.30	9 (5%)	32	41	11, 24, 39, 63	0
1	H	168/204 (82%)	1.17	39 (23%)	1	1	17, 30, 38, 40	0
All	All	1421/1632 (87%)	0.51	123 (8%)	13	18	8, 24, 36, 66	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	182	TRP	5.4
1	H	77	TRP	4.5
1	H	16	VAL	4.5
1	H	22	LEU	4.5
1	H	17	GLY	4.5
1	H	161	TYR	4.3
1	H	19	LYS	4.3
1	H	85	LEU	4.0
1	E	45	GLU	4.0
1	D	182	TRP	4.0
1	E	70	LEU	3.8
1	H	124	VAL	3.6
1	H	15	PHE	3.6
1	H	150	GLY	3.6
1	E	46	GLY	3.5
1	F	104	HIS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	40	TRP	3.5
1	H	41	VAL	3.4
1	H	27	GLY	3.3
1	F	103	ALA	3.2
1	F	100	SER	3.2
1	H	49	ILE	3.2
1	B	100	SER	3.1
1	H	2	ALA	3.1
1	G	154	LYS	3.1
1	H	71	HIS	3.0
1	B	70	LEU	3.0
1	G	65	PHE	3.0
1	C	103	ALA	2.9
1	B	103	ALA	2.9
1	C	105	THR	2.9
1	E	40	TRP	2.9
1	E	103	ALA	2.9
1	H	81	PHE	2.9
1	A	46	GLY	2.9
1	B	139	ALA	2.9
1	B	102	PHE	2.9
1	H	48	ASP	2.9
1	H	149	ASP	2.8
1	H	24	CYS	2.8
1	B	101	GLY	2.8
1	G	67	VAL	2.8
1	G	46	GLY	2.8
1	H	18	GLU	2.8
1	E	41	VAL	2.7
1	B	69	PRO	2.7
1	F	105	THR	2.7
1	B	137	ALA	2.6
1	H	20	ALA	2.6
1	C	104	HIS	2.6
1	C	107	LEU	2.6
1	E	190	VAL	2.6
1	G	103	ALA	2.6
1	H	38	PHE	2.5
1	D	43	GLY	2.5
1	H	23	ARG	2.5
1	H	152	ALA	2.5
1	H	120	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	104	HIS	2.5
1	F	107	LEU	2.5
1	D	100	SER	2.5
1	A	137	ALA	2.5
1	E	185	ASP	2.5
1	A	103	ALA	2.5
1	A	105	THR	2.5
1	B	138	LEU	2.5
1	H	151	THR	2.4
1	A	104	HIS	2.4
1	A	107	LEU	2.4
1	D	48	ASP	2.4
1	G	161	TYR	2.4
1	C	175	VAL	2.4
1	H	179	ILE	2.4
1	D	102	PHE	2.4
1	C	61	ASN	2.4
1	F	133	THR	2.4
1	H	105	THR	2.4
1	H	25	PRO	2.4
1	G	105	THR	2.4
1	C	101	GLY	2.4
1	D	103	ALA	2.4
1	E	43	GLY	2.4
1	A	102	PHE	2.4
1	B	105	THR	2.4
1	A	135[A]	THR	2.4
1	B	94	VAL	2.3
1	E	16	VAL	2.3
1	F	101	GLY	2.3
1	E	44	ARG	2.3
1	F	57	ALA	2.3
1	G	47	ASP	2.3
1	G	48	ASP	2.3
1	H	176	ASP	2.3
1	H	12	LEU	2.3
1	F	135	THR	2.2
1	H	82	ILE	2.2
1	B	140	ASN	2.2
1	F	137	ALA	2.2
1	H	109	LEU	2.2
1	E	184	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	47	ASP	2.1
1	D	179	ILE	2.1
1	H	47	ASP	2.1
1	A	129	CYS	2.1
1	C	137	ALA	2.1
1	C	140	ASN	2.1
1	E	140	ASN	2.1
1	B	-2	PHE	2.1
1	C	109	LEU	2.1
1	H	183	GLU	2.1
1	E	182	TRP	2.1
1	D	133	THR	2.1
1	E	17	GLY	2.1
1	H	13	ASN	2.1
1	F	99	HIS	2.1
1	A	67	VAL	2.1
1	E	71	HIS	2.1
1	H	44	ARG	2.0
1	D	180	GLN	2.0
1	B	183	GLU	2.0
1	D	33	ASP	2.0
1	A	70	LEU	2.0
1	D	132	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	E	202	1/1	0.96	0.60	11.65	41,41,41,41	0
2	NH4	C	201	1/1	0.86	0.73	11.62	28,28,28,28	0
3	NA	B	202	1/1	0.98	0.52	11.47	31,31,31,31	0
3	NA	F	201	1/1	0.96	0.35	10.71	29,29,29,29	0
3	NA	G	201	1/1	0.88	0.44	10.20	49,49,49,49	0
3	NA	A	202	1/1	0.98	0.41	6.87	27,27,27,27	0
2	NH4	B	201	1/1	0.82	0.72	-	26,26,26,26	0
2	NH4	A	201	1/1	0.96	0.50	-	20,20,20,20	0
2	NH4	D	201	1/1	0.96	0.88	-	25,25,25,25	0
2	NH4	H	201	1/1	0.83	0.45	-	27,27,27,27	0
2	NH4	E	201	1/1	0.86	0.53	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.