Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 02:24 am BST

PDB ID	:	2EPG
Title	:	Crystal structure of TTHA1785
Authors	:	Sekine, S.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-30
Resolution	:	2.10 Å(reported)

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

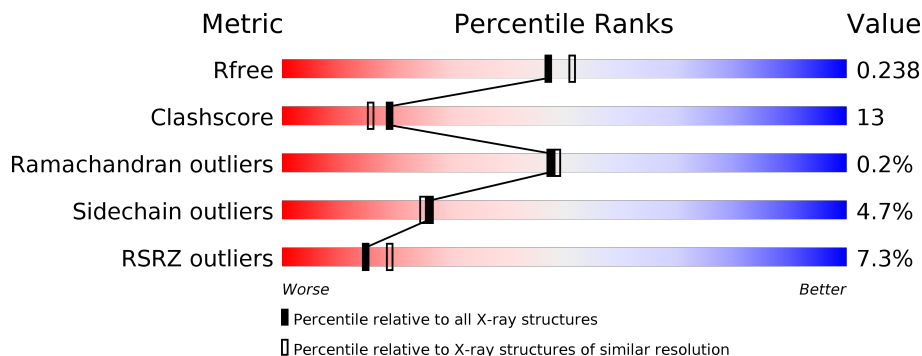|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
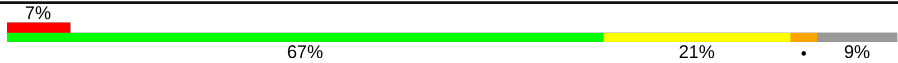*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		4.7%
RSRZ outliers		7.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	487	7% 67% 21% • 9%
1	B	487	6% 68% 21% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7188 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 Hypothetical protein TTHA1785.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	Se	0	0	0
			3440	2197	617	616	3	7			
1	B	444	Total	C	N	O	S	Se	0	0	0
			3459	2207	620	622	3	7			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	EXPRESSION TAG	UNP Q5SHE5
A	-9	ALA	-	EXPRESSION TAG	UNP Q5SHE5
A	-8	ARG	-	EXPRESSION TAG	UNP Q5SHE5
A	-7	THR	-	EXPRESSION TAG	UNP Q5SHE5
A	-6	LEU	-	EXPRESSION TAG	UNP Q5SHE5
A	-5	PHE	-	EXPRESSION TAG	UNP Q5SHE5
A	-4	LEU	-	EXPRESSION TAG	UNP Q5SHE5
A	-3	GLU	-	EXPRESSION TAG	UNP Q5SHE5
A	-2	GLU	-	EXPRESSION TAG	UNP Q5SHE5
A	-1	GLY	-	EXPRESSION TAG	UNP Q5SHE5
A	0	PRO	-	EXPRESSION TAG	UNP Q5SHE5
B	-10	MSE	-	EXPRESSION TAG	UNP Q5SHE5
B	-9	ALA	-	EXPRESSION TAG	UNP Q5SHE5
B	-8	ARG	-	EXPRESSION TAG	UNP Q5SHE5
B	-7	THR	-	EXPRESSION TAG	UNP Q5SHE5
B	-6	LEU	-	EXPRESSION TAG	UNP Q5SHE5
B	-5	PHE	-	EXPRESSION TAG	UNP Q5SHE5
B	-4	LEU	-	EXPRESSION TAG	UNP Q5SHE5
B	-3	GLU	-	EXPRESSION TAG	UNP Q5SHE5
B	-2	GLU	-	EXPRESSION TAG	UNP Q5SHE5
B	-1	GLY	-	EXPRESSION TAG	UNP Q5SHE5
B	0	PRO	-	EXPRESSION TAG	UNP Q5SHE5

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total 148	O 148	0	0
2	B	141	Total 141	O 141	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 the various outlier classes 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: Hypothetical protein TTHA1785
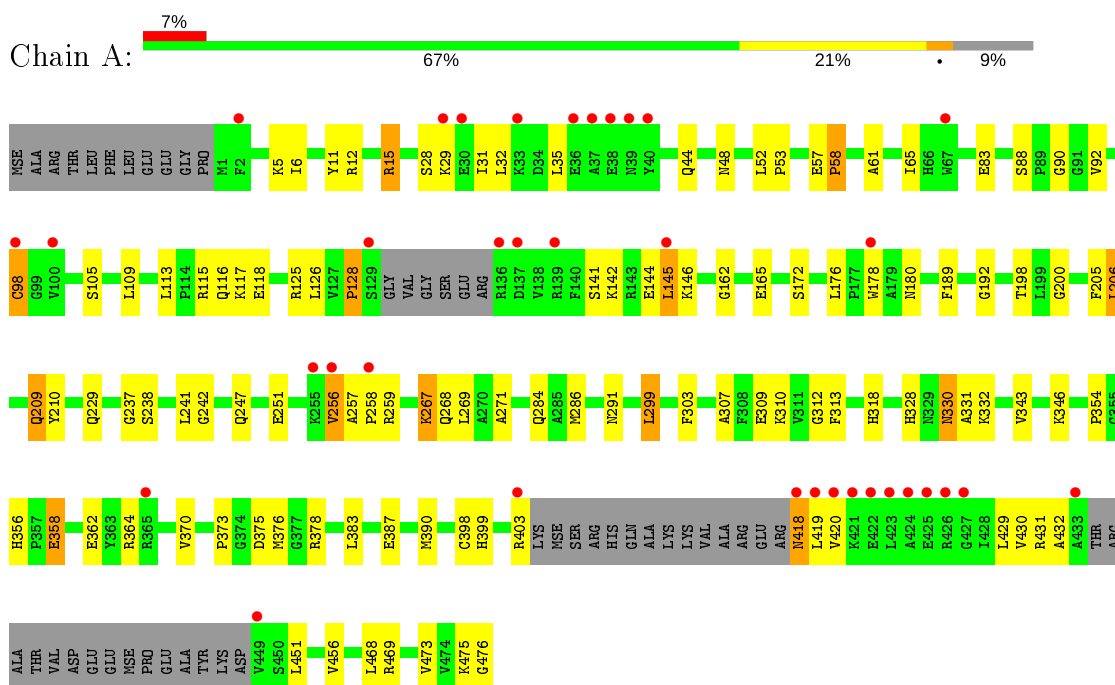
- Molecule 1: Hypothetical protein TTHA1785
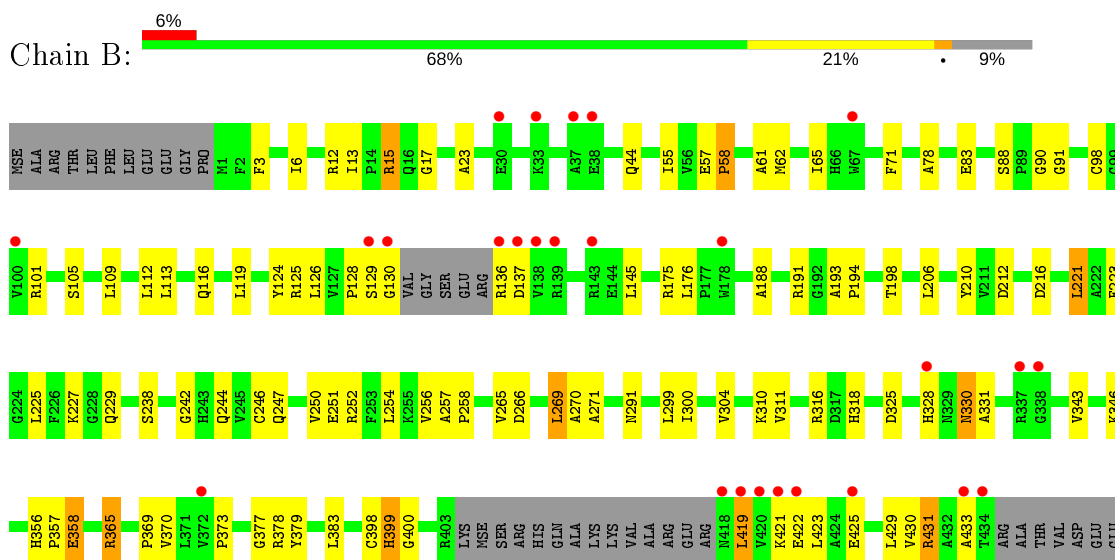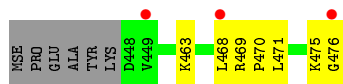
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.69Å 66.69Å 116.99Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	38.63 – 2.10 38.63 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.63-2.10) 99.1 (38.63-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.238 0.200 , 0.238	Depositor DCC
R_{free} test set	2856 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7188	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.41	0/3510	0.66	1/4728 (0.0%)
1	B	0.42	0/3529	0.67	1/4754 (0.0%)
All	All	0.42	0/7039	0.66	2/9482 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	CYS	N-CA-C	-6.39	93.73	111.00
1	B	98	CYS	N-CA-C	-5.70	95.62	111.00

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	3440	0	3444	99	0
1	B	3459	0	3458	81	0
2	A	148	0	0	8	0
2	B	141	0	0	3	0
All	All	7188	0	6902	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (179) 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:376:MSE:HE1	1:A:475:LYS:HG2	1.23	1.10
1:A:176:LEU:H	1:A:291:ASN:HD21	1.00	0.95
1:A:205:PHE:HB3	1:A:376:MSE:HE3	1.50	0.92
1:B:176:LEU:H	1:B:291:ASN:HD21	0.98	0.91
1:A:286:MSE:HE1	1:A:331:ALA:HB3	1.54	0.89
1:A:128:PRO:HB2	1:A:198:THR:HG22	1.58	0.86
1:A:376:MSE:CE	1:A:475:LYS:HG2	2.06	0.86
1:B:176:LEU:N	1:B:291:ASN:HD21	1.75	0.84
1:B:419:LEU:HA	1:B:422:GLU:HG2	1.60	0.81
1:A:31:ILE:HG23	1:A:403:ARG:HH12	1.44	0.80
1:B:176:LEU:H	1:B:291:ASN:ND2	1.80	0.78
1:A:376:MSE:HE1	1:A:475:LYS:CG	2.09	0.77
1:A:390:MSE:HE3	2:A:509:HOH:O	1.87	0.74
1:A:92:VAL:HG21	1:A:286:MSE:HE2	1.71	0.73
1:A:376:MSE:HE2	1:A:473:VAL:CG1	2.18	0.73
1:A:31:ILE:HG23	1:A:403:ARG:NH1	2.03	0.73
1:B:365:ARG:HD2	2:B:581:HOH:O	1.89	0.73
1:A:205:PHE:CB	1:A:376:MSE:HE3	2.18	0.72
1:A:6:ILE:HD11	1:A:12:ARG:HD2	1.72	0.72
1:B:475:LYS:HD2	1:B:476:GLY:O	1.92	0.70
1:A:176:LEU:N	1:A:291:ASN:HD21	1.84	0.69
1:B:136:ARG:HG3	1:B:137:ASP:H	1.57	0.68
1:B:469:ARG:HG3	1:B:470:PRO:HD2	1.76	0.67
1:A:247:GLN:O	1:A:251:GLU:HG2	1.95	0.67
1:B:145:LEU:HD13	1:B:193:ALA:HB1	1.77	0.65
1:A:328:HIS:ND1	1:A:399:HIS:HB2	2.11	0.64
1:B:328:HIS:CE1	1:B:399:HIS:HB2	2.33	0.64
1:A:418:ASN:HD22	1:A:419:LEU:N	1.96	0.64
1:A:141:SER:OG	1:A:144:GLU:HG3	1.98	0.63
1:B:128:PRO:HB2	1:B:198:THR:HG22	1.80	0.63
1:B:257:ALA:HB3	1:B:258:PRO:HD3	1.79	0.63
1:B:105:SER:HB2	1:B:318:HIS:O	1.99	0.62
1:B:62:MSE:HG2	1:B:398:CYS:HA	1.83	0.61
1:A:125:ARG:NH1	1:A:310:LYS:HE3	2.15	0.60
1:A:420:VAL:HG13	1:A:430:VAL:HG21	1.83	0.60
1:B:6:ILE:HD13	1:B:12:ARG:HB2	1.84	0.60
1:B:55:ILE:HD12	1:B:78:ALA:O	2.02	0.60
1:A:15:ARG:HH21	1:A:15:ARG:HB3	1.67	0.60
1:A:257:ALA:N	1:A:258:PRO:CD	2.65	0.59
1:A:418:ASN:HD22	1:A:419:LEU:H	1.49	0.59
1:A:200:GLY:O	1:A:476:GLY:HA3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HE	1:B:136:ARG:HA	1.69	0.57
1:A:328:HIS:CE1	1:A:399:HIS:HB2	2.39	0.57
1:B:266:ASP:O	1:B:269:LEU:HB2	2.03	0.57
1:A:116:GLN:HG2	1:A:429:LEU:CD1	2.35	0.57
1:A:176:LEU:H	1:A:291:ASN:ND2	1.85	0.56
1:B:310:LYS:HD3	1:B:310:LYS:O	2.05	0.56
1:A:28:SER:H	1:A:31:ILE:HB	1.70	0.56
1:B:370:VAL:HB	1:B:383:LEU:HB2	1.88	0.56
1:B:377:GLY:C	1:B:470:PRO:HG3	2.26	0.56
1:B:119:LEU:HA	1:B:311:VAL:HG11	1.87	0.56
1:A:11:TYR:CZ	1:A:32:LEU:HD11	2.41	0.56
1:A:116:GLN:HG2	1:A:429:LEU:HD12	1.88	0.56
1:A:61:ALA:HB1	1:A:65:ILE:HD12	1.88	0.56
1:A:362:GLU:OE1	1:B:316:ARG:HB3	2.07	0.55
1:A:105:SER:HB2	1:A:318:HIS:O	2.07	0.55
1:A:432:ALA:HB2	1:A:475:LYS:HD3	1.89	0.55
1:A:115:ARG:HA	1:A:118:GLU:OE1	2.07	0.54
1:B:225:LEU:HA	1:B:229:GLN:OE1	2.07	0.54
1:B:310:LYS:HD3	1:B:310:LYS:C	2.28	0.54
1:B:90:GLY:O	1:B:346:LYS:HE2	2.07	0.54
1:A:375:ASP:HB2	1:A:378:ARG:HG3	1.90	0.54
1:B:112:LEU:HD23	1:B:471:LEU:CD1	2.38	0.53
1:B:373:PRO:HD2	1:B:399:HIS:O	2.07	0.53
1:B:238:SER:OG	1:B:242:GLY:HA3	2.08	0.53
1:A:15:ARG:NH2	1:A:15:ARG:HB3	2.22	0.53
1:A:310:LYS:O	1:A:310:LYS:HD3	2.08	0.53
1:A:267:LYS:HE2	1:A:268:GLN:HG2	1.91	0.52
1:A:257:ALA:N	1:A:258:PRO:HD3	2.25	0.52
1:A:387:GLU:HG2	2:A:524:HOH:O	2.10	0.51
1:B:265:VAL:HG13	2:B:485:HOH:O	2.10	0.51
1:A:430:VAL:O	1:A:431:ARG:HD2	2.10	0.51
1:A:90:GLY:O	1:A:346:LYS:HE2	2.11	0.51
1:B:116:GLN:HG2	1:B:429:LEU:HD12	1.93	0.51
1:B:125:ARG:HH22	1:B:310:LYS:HE3	1.76	0.50
1:A:178:TRP:CE3	1:A:178:TRP:HA	2.46	0.50
1:B:252:ARG:O	1:B:256:VAL:HG23	2.11	0.50
1:A:192:GLY:HA3	1:A:241:LEU:HB2	1.94	0.50
1:B:101:ARG:HB2	1:B:325:ASP:OD1	2.12	0.50
1:A:378:ARG:HH21	1:A:378:ARG:HG3	1.78	0.49
1:B:124:TYR:HB2	1:B:431:ARG:CG	2.42	0.49
1:A:178:TRP:HE3	1:A:178:TRP:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:HD22	1:A:418:ASN:N	2.09	0.49
1:B:246:CYS:O	1:B:250:VAL:HG23	2.13	0.49
1:B:357:PRO:HG2	1:B:358:GLU:OE1	2.13	0.49
1:B:112:LEU:HD11	1:B:119:LEU:CD2	2.43	0.49
1:B:71:PHE:CG	1:B:91:GLY:HA2	2.48	0.49
1:A:370:VAL:HB	1:A:383:LEU:HB2	1.95	0.48
1:A:238:SER:OG	1:A:242:GLY:HA3	2.12	0.48
1:B:88:SER:HB2	1:B:271:ALA:HB2	1.95	0.48
1:A:61:ALA:CB	1:A:65:ILE:HD12	2.42	0.48
1:A:331:ALA:HA	1:A:343:VAL:O	2.14	0.48
1:B:129:SER:HB2	1:B:476:GLY:HA2	1.95	0.48
1:A:142:LYS:O	1:A:146:LYS:HB2	2.14	0.48
1:B:379:TYR:HE2	1:B:469:ARG:HB2	1.79	0.48
1:B:112:LEU:HD11	1:B:119:LEU:HD22	1.96	0.47
1:B:247:GLN:O	1:B:251:GLU:HG2	2.15	0.47
1:A:145:LEU:HD11	1:A:189:PHE:CZ	2.50	0.47
1:A:309:GLU:HA	1:A:313:PHE:O	2.14	0.47
1:B:130:GLY:N	1:B:476:GLY:HA2	2.29	0.47
1:B:378:ARG:HG3	1:B:378:ARG:HH21	1.80	0.47
1:B:421:LYS:O	1:B:425:GLU:HG3	2.15	0.47
1:A:28:SER:HB2	1:A:31:ILE:HG13	1.96	0.47
1:A:5:LYS:HE2	2:A:501:HOH:O	2.15	0.47
1:B:191:ARG:CZ	1:B:244:GLN:HG2	2.45	0.47
1:A:256:VAL:HG22	1:A:259:ARG:HD2	1.97	0.47
1:B:300:ILE:O	1:B:304:VAL:HG23	2.15	0.47
1:B:430:VAL:O	1:B:431:ARG:HD3	2.15	0.47
1:A:376:MSE:HE2	1:A:473:VAL:HG11	1.95	0.46
1:B:356:HIS:HE1	1:B:358:GLU:CD	2.18	0.46
1:B:419:LEU:CD2	1:B:423:LEU:HG	2.45	0.46
1:A:125:ARG:HH12	1:A:310:LYS:HE3	1.80	0.46
1:A:398:CYS:HA	2:A:498:HOH:O	2.15	0.46
1:B:193:ALA:N	1:B:194:PRO:HD2	2.30	0.46
1:B:57:GLU:HA	1:B:58:PRO:HA	1.71	0.46
1:B:15:ARG:HH11	1:B:17:GLY:N	2.14	0.46
1:A:29:LYS:HA	1:A:29:LYS:HD3	1.74	0.45
1:B:216:ASP:OD1	1:B:463:LYS:HD3	2.16	0.45
1:B:210:TYR:HA	1:B:229:GLN:O	2.17	0.45
1:A:52:LEU:HD11	1:A:269:LEU:HG	1.98	0.45
1:B:251:GLU:HA	1:B:254:LEU:HD12	1.98	0.45
1:A:286:MSE:CE	1:A:331:ALA:HB3	2.36	0.45
1:B:113:LEU:HD12	1:B:113:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PRO:HD2	1:A:399:HIS:O	2.17	0.44
1:B:365:ARG:HA	1:B:365:ARG:HE	1.82	0.44
1:A:126:LEU:HD12	1:A:307:ALA:HA	1.98	0.44
1:A:209:GLN:HB3	1:A:469:ARG:O	2.16	0.44
1:B:175:ARG:HA	1:B:291:ASN:ND2	2.32	0.44
1:A:330:ASN:HD22	1:A:330:ASN:HA	1.58	0.44
1:B:61:ALA:HB1	1:B:65:ILE:HD12	1.99	0.44
1:A:299:LEU:HD22	1:A:303:PHE:CZ	2.53	0.44
1:B:399:HIS:CD2	1:B:400:GLY:H	2.34	0.44
1:B:328:HIS:ND1	1:B:399:HIS:HB2	2.32	0.44
1:A:180:ASN:HB3	1:A:284:GLN:HB3	2.00	0.43
1:B:223:PHE:CZ	1:B:369:PRO:HG3	2.53	0.43
1:A:165:GLU:HG2	2:A:536:HOH:O	2.18	0.43
1:A:206:LEU:HD23	1:A:206:LEU:C	2.39	0.43
1:B:3:PHE:HB3	1:B:13:ILE:HG12	2.01	0.43
1:A:52:LEU:HA	1:A:53:PRO:HD3	1.86	0.43
1:A:44:GLN:HE21	1:A:48:ASN:ND2	2.16	0.43
1:B:269:LEU:O	1:B:270:ALA:C	2.56	0.43
1:A:418:ASN:N	1:A:418:ASN:ND2	2.66	0.43
1:B:377:GLY:O	1:B:470:PRO:HG3	2.18	0.43
1:A:6:ILE:CD1	1:A:12:ARG:HD2	2.44	0.43
1:A:189:PHE:CD1	1:A:189:PHE:C	2.92	0.43
1:A:98:CYS:HA	1:A:237:GLY:HA3	1.99	0.43
1:B:356:HIS:CE1	1:B:358:GLU:HB2	2.53	0.43
1:A:356:HIS:CE1	1:A:358:GLU:HB2	2.53	0.42
1:A:256:VAL:CG2	1:A:259:ARG:HD2	2.50	0.42
1:A:44:GLN:HE21	1:A:48:ASN:HD21	1.67	0.42
1:A:145:LEU:HG	1:A:189:PHE:CZ	2.54	0.42
1:A:418:ASN:ND2	1:A:419:LEU:N	2.66	0.42
1:A:451:LEU:HG	2:A:563:HOH:O	2.19	0.42
1:A:376:MSE:SE	1:A:475:LYS:HE3	2.70	0.42
1:B:365:ARG:HA	1:B:365:ARG:NE	2.35	0.42
1:A:88:SER:HB2	1:A:271:ALA:HB2	2.01	0.42
1:A:118:GLU:HG2	2:A:559:HOH:O	2.19	0.42
1:A:31:ILE:CG2	1:A:403:ARG:HH12	2.23	0.42
1:B:124:TYR:OH	1:B:433:ALA:HA	2.20	0.42
1:B:331:ALA:HA	1:B:343:VAL:O	2.20	0.42
1:A:57:GLU:HA	1:A:58:PRO:HA	1.79	0.42
1:B:212:ASP:O	1:B:227:LYS:HE3	2.20	0.42
1:B:399:HIS:CD2	1:B:400:GLY:N	2.88	0.42
1:A:378:ARG:NH2	1:A:378:ARG:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HB2	1:B:244:GLN:HB3	2.01	0.41
1:B:13:ILE:HB	1:B:23:ALA:HB3	2.02	0.41
1:B:71:PHE:HB3	2:B:540:HOH:O	2.20	0.41
1:A:210:TYR:HA	1:A:229:GLN:O	2.21	0.41
1:A:256:VAL:C	1:A:258:PRO:CD	2.89	0.41
1:B:112:LEU:HD23	1:B:471:LEU:HD13	2.02	0.41
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.95	0.41
1:A:172:SER:OG	1:A:332:LYS:NZ	2.36	0.41
1:B:379:TYR:CE2	1:B:469:ARG:HB2	2.56	0.41
1:A:354:PRO:HD2	1:A:387:GLU:HG3	2.03	0.41
1:B:330:ASN:HA	1:B:330:ASN:HD22	1.64	0.41
1:A:162:GLY:HA2	2:A:492:HOH:O	2.20	0.41
1:A:354:PRO:HA	1:A:364:ARG:O	2.21	0.40
1:A:115:ARG:NH2	1:A:312:GLY:HA3	2.37	0.40
1:A:398:CYS:HB3	1:A:456:VAL:HG21	2.04	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	433/487 (89%)	415 (96%)	16 (4%)	2 (0%)	29	26
1	B	436/487 (90%)	415 (95%)	21 (5%)	0	100	100
All	All	869/974 (89%)	830 (96%)	37 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
1	A	128	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	349/377 (93%)	333 (95%)	16 (5%)	27	26
1	B	351/377 (93%)	334 (95%)	17 (5%)	25	24
All	All	700/754 (93%)	667 (95%)	33 (5%)	26	25

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	35	LEU
1	A	58	PRO
1	A	83	GLU
1	A	109	LEU
1	A	113	LEU
1	A	117	LYS
1	A	145	LEU
1	A	206	LEU
1	A	209	GLN
1	A	267	LYS
1	A	299	LEU
1	A	330	ASN
1	A	358	GLU
1	A	418	ASN
1	A	468	LEU
1	B	15	ARG
1	B	44	GLN
1	B	58	PRO
1	B	83	GLU
1	B	109	LEU
1	B	126	LEU
1	B	206	LEU
1	B	221	LEU
1	B	269	LEU
1	B	299	LEU
1	B	330	ASN

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Mol	Chain	Res	Type
1	B	358	GLU
1	B	365	ARG
1	B	399	HIS
1	B	419	LEU
1	B	431	ARG
1	B	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	66	HIS
1	A	173	GLN
1	A	204	HIS
1	A	235	HIS
1	A	268	GLN
1	A	291	ASN
1	A	330	ASN
1	A	418	ASN
1	B	48	ASN
1	B	66	HIS
1	B	291	ASN
1	B	330	ASN
1	B	399	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)

There are no ligands in this entry.

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	434/487 (89%)	0.34	35 (8%)	12	15	20, 34, 66, 116	0
1	B	437/487 (89%)	0.28	29 (6%)	18	23	22, 35, 62, 103	0
All	All	871/974 (89%)	0.31	64 (7%)	15	19	20, 35, 64, 116	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	GLY	8.1
1	A	420	VAL	7.6
1	A	419	LEU	7.1
1	B	476	GLY	6.5
1	A	425	GLU	6.1
1	B	418	ASN	5.7
1	B	421	LYS	5.6
1	B	419	LEU	5.4
1	B	434	THR	5.2
1	A	449	VAL	5.0
1	A	426	ARG	4.8
1	A	422	GLU	4.8
1	A	418	ASN	4.5
1	B	420	VAL	4.5
1	B	138	VAL	4.3
1	A	427	GLY	4.0
1	B	136	ARG	3.9
1	A	67	TRP	3.9
1	A	33	LYS	3.7
1	B	38	GLU	3.6
1	A	256	VAL	3.5
1	B	37	ALA	3.5
1	A	40	TYR	3.4
1	B	129	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	421	LYS	3.2
1	A	36	GLU	3.2
1	A	136	ARG	3.2
1	A	37	ALA	3.0
1	A	424	ALA	3.0
1	A	365	ARG	3.0
1	A	433	ALA	2.9
1	A	129	SER	2.9
1	B	338	GLY	2.9
1	B	433	ALA	2.8
1	A	38	GLU	2.8
1	A	145	LEU	2.8
1	B	67	TRP	2.8
1	B	143	ARG	2.7
1	B	33	LYS	2.7
1	A	255	LYS	2.7
1	A	139	ARG	2.6
1	B	425	GLU	2.6
1	A	39	ASN	2.6
1	B	449	VAL	2.6
1	A	2	PHE	2.6
1	A	423	LEU	2.5
1	A	137	ASP	2.5
1	A	98	CYS	2.5
1	B	137	ASP	2.4
1	B	139	ARG	2.4
1	B	468	LEU	2.3
1	A	30	GLU	2.3
1	B	422	GLU	2.3
1	B	30	GLU	2.3
1	A	178	TRP	2.3
1	B	178	TRP	2.3
1	A	403	ARG	2.3
1	B	337	ARG	2.2
1	A	29	LYS	2.2
1	B	100	VAL	2.1
1	A	100	VAL	2.0
1	B	328	HIS	2.0
1	A	258	PRO	2.0
1	B	372	VAL	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.