



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:33 AM UTC

PDB ID : 2EPG / pdb_00002epg
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)

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

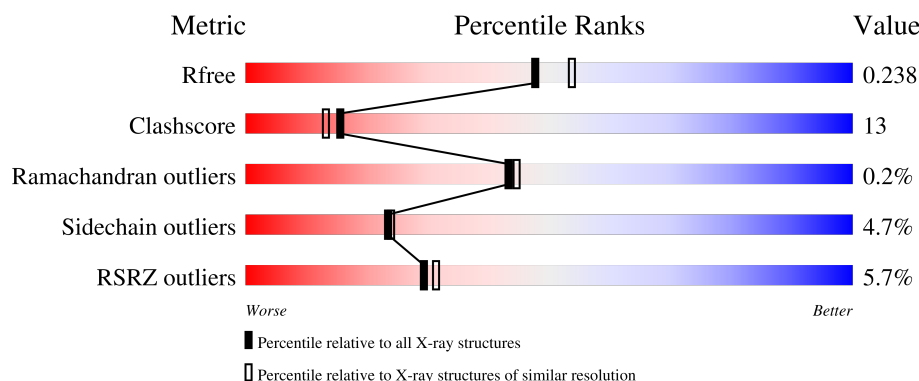
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of 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 $\leq 5\%$. 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% 66% 21% • 9%
1	B	487	4% 64% 25% • 9%

2 Entry composition

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.

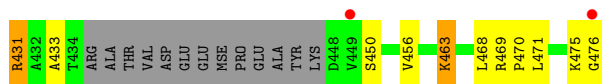
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	Se	0	0	0
			3440	2197	617	616	3	7			
1	B	444	Total	C	N	O	S	Se	0	0	0
			3459	2207	620	622	3	7			

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



4 Data and refinement statistics

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 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.63-2.10) 99.1 (38.63-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.49	0/3510	1.00	16/4728 (0.3%)
1	B	0.50	0/3529	0.99	14/4754 (0.3%)
All	All	0.49	0/7039	0.99	30/9482 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	CYS	N-CA-C	-10.98	93.73	110.10
1	B	98	CYS	N-CA-C	-9.56	95.62	109.96
1	B	350	ARG	N-CA-C	-8.03	98.60	110.48
1	A	392	VAL	N-CA-C	7.74	122.73	113.22
1	A	350	ARG	N-CA-C	-7.72	98.01	110.20
1	B	323	LEU	N-CA-C	-6.92	102.96	111.40
1	A	59	ALA	N-CA-C	-6.69	99.63	110.20
1	A	29	LYS	N-CA-C	-6.59	104.17	111.82
1	A	176	LEU	N-CA-C	-6.35	101.65	109.65
1	A	323	LEU	N-CA-C	-6.28	103.73	111.40
1	A	374	GLY	N-CA-C	-6.10	103.87	112.60
1	B	177	PRO	N-CA-C	6.04	121.81	113.65
1	B	167	VAL	N-CA-C	6.01	117.48	110.62
1	B	59	ALA	N-CA-C	-5.94	100.82	110.20
1	B	328	HIS	N-CA-C	-5.91	106.69	114.31
1	B	60	LEU	N-CA-C	5.72	118.87	109.72
1	B	364	ARG	N-CA-C	5.57	118.11	111.71
1	B	100	VAL	N-CA-C	5.43	116.49	108.45
1	B	178	TRP	N-CA-C	5.38	118.96	112.93
1	A	177	PRO	N-CA-C	5.36	120.81	113.84
1	A	60	LEU	N-CA-C	5.34	117.81	109.52
1	B	387	GLU	N-CA-C	-5.34	105.54	111.36
1	A	375	ASP	N-CA-C	-5.30	103.69	110.53
1	A	52	LEU	CA-C-N	5.19	125.10	119.76
1	A	52	LEU	C-N-CA	5.19	125.10	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	VAL	CA-C-N	5.12	126.24	119.84
1	A	127	VAL	C-N-CA	5.12	126.24	119.84
1	A	237	GLY	N-CA-C	5.09	118.86	110.77
1	B	52	LEU	CA-C-N	5.04	124.95	119.76
1	B	52	LEU	C-N-CA	5.04	124.95	119.76

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	3440	0	3444	101	0
1	B	3459	0	3458	85	0
2	A	148	0	0	8	0
2	B	141	0	0	3	0
All	All	7188	0	6902	185	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 (185) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:GLY:C	1:B:470:PRO:HG3	2.26	0.61
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:B:310:LYS:HD3	1:B:310:LYS:C	2.28	0.59
1:A:200:GLY:O	1:A:476:GLY:HA3	2.03	0.58
1:B:136:ARG:HA	1:B:136:ARG:HE	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:119:LEU:HA	1:B:311:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HB3	1:A:15:ARG:NH2	2.22	0.53
1:A:310:LYS:HD3	1:A:310:LYS:O	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:B:356:HIS:HE1	1:B:358:GLU:CD	2.18	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:HA	1:A:178:TRP:CE3	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:HG3	1:A:378:ARG:HH21	1.78	0.49
1:B:124:TYR:HB2	1:B:431:ARG:CG	2.42	0.49
1:A:178:TRP:HA	1:A:178:TRP:HE3	1.77	0.49
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:71:PHE:CG	1:B:91:GLY:HA2	2.48	0.49
1:B:112:LEU:HD11	1:B:119:LEU:CD2	2.43	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:206:LEU:C	1:A:206:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:269:LEU:O	1:B:270:ALA:C	2.56	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:A:189:PHE:C	1:A:189:PHE:CD1	2.92	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:HH21	1:B:378:ARG:HG3	1.80	0.47
1:B:421:LYS:O	1:B:425:GLU:HG3	2.15	0.47
1:A:5:LYS:HE2	2:A:501:HOH:O	2.15	0.47
1:A:28:SER:HB2	1:A:31:ILE:HG13	1.96	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: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:A:256:VAL:C	1:A:258:PRO:CD	2.89	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
1:B:115:ARG:HH22	1:B:312:GLY:C	2.25	0.45
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:256:VAL:C	1:A:258:PRO:HD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:GLU:H	1:A:118:GLU:CD	2.26	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: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: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: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:44:GLN:HE21	1:A:48:ASN:HD21	1.67	0.42
1:A:256:VAL:CG2	1:A:259:ARG:HD2	2.50	0.42
1:B:375:ASP:O	1:B:376:MSE:C	2.62	0.42
1:A:145:LEU:HG	1:A:189:PHE:CZ	2.54	0.42
1:A:376:MSE:SE	1:A:475:LYS:HE3	2.70	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: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:31:ILE:CG2	1:A:403:ARG:HH12	2.23	0.42
1:A:118:GLU:HG2	2:A:559:HOH:O	2.19	0.42
1:B:401:ALA:O	1:B:450:SER:OG	2.34	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:HG3	1:A:378:ARG:NH2	2.35	0.41
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:B:112:LEU:HD23	1:B:471:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:GLY:C	1:B:194:PRO:HD2	2.46	0.41
1:B:330:ASN:HD22	1:B:330:ASN:HA	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%)	24	22
1	B	436/487 (90%)	415 (95%)	21 (5%)	0	100	100
All	All	869/974 (89%)	830 (96%)	37 (4%)	2 (0%)	43	44

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%)	335 (96%)	14 (4%)	28	29
1	B	351/377 (93%)	332 (95%)	19 (5%)	20	18
All	All	700/754 (93%)	667 (95%)	33 (5%)	23	24

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	109	LEU
1	A	113	LEU
1	A	145	LEU
1	A	206	LEU
1	A	209	GLN
1	A	286	MSE
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	113	LEU
1	B	126	LEU
1	B	206	LEU
1	B	221	LEU
1	B	244	GLN
1	B	269	LEU
1	B	299	LEU
1	B	330	ASN
1	B	365	ARG
1	B	419	LEU
1	B	431	ARG
1	B	456	VAL
1	B	463	LYS
1	B	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	66	HIS
1	A	106	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	66	HIS
1	B	203	ASN
1	B	243	HIS
1	B	247	GLN
1	B	268	GLN
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 oligosaccharides 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

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, 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%)	0.23	32 (7%) 20 22	20, 34, 66, 116	0
1	B	437/487 (89%)	0.13	18 (4%) 41 43	22, 35, 62, 103	0
All	All	871/974 (89%)	0.18	50 (5%) 29 31	20, 35, 64, 116	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	VAL	5.8
1	A	419	LEU	5.7
1	B	138	VAL	4.5
1	A	449	VAL	4.4
1	B	476	GLY	4.3
1	B	129	SER	4.2
1	B	130	GLY	4.0
1	B	178	TRP	3.9
1	B	420	VAL	3.9
1	A	178	TRP	3.8
1	A	433	ALA	3.6
1	A	145	LEU	3.6
1	A	427	GLY	3.5
1	B	449	VAL	3.5
1	B	136	ARG	3.4
1	A	423	LEU	3.4
1	A	67	TRP	3.2
1	A	424	ALA	3.1
1	B	67	TRP	3.0
1	A	403	ARG	2.9
1	A	401	ALA	2.9
1	A	138	VAL	2.8
1	B	379	TYR	2.7
1	A	127	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	400	GLY	2.7
1	A	402	GLY	2.7
1	A	6	ILE	2.6
1	A	257	ALA	2.6
1	A	426	ARG	2.6
1	B	38	GLU	2.6
1	B	37	ALA	2.6
1	B	419	LEU	2.6
1	A	136	ARG	2.5
1	A	129	SER	2.5
1	B	259	ARG	2.5
1	A	256	VAL	2.4
1	A	28	SER	2.4
1	A	377	GLY	2.3
1	A	30	GLU	2.2
1	B	194	PRO	2.2
1	A	38	GLU	2.2
1	A	379	TYR	2.2
1	B	338	GLY	2.1
1	A	375	ASP	2.1
1	A	192	GLY	2.1
1	A	425	GLU	2.1
1	B	137	ASP	2.1
1	A	201	SER	2.1
1	A	124	TYR	2.0
1	B	94	PHE	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 oligosaccharides 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.