Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 05:16 am BST

PDB ID	:	3PE5
Title	:	Three-dimensional Structure of protein A7VV38_9CLOT from Clostridium leptum DSM 753, Northeast Structural Genomics Consortium Target QlR103
Authors	:	Kuzin, A.; Su, M.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccosanti, C.; Wang, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-10-25
Resolution	:	2.38 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

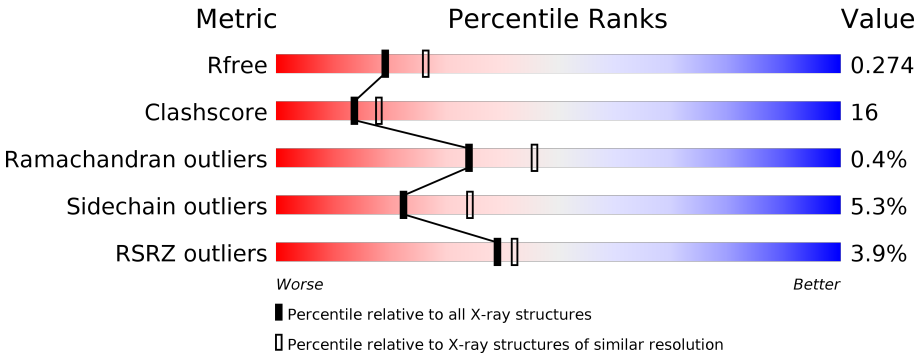
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	403	3% 51% 16% • 31%
1	B	403	2% 48% 19% • 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4402 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	Se	0	0	0
			2169	1370	357	430	12			
1	B	278	Total	C	N	O	Se	0	0	0
			2169	1370	357	430	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	LEU	-	EXPRESSION TAG	UNP A7VV38
A	397	GLU	-	EXPRESSION TAG	UNP A7VV38
A	398	HIS	-	EXPRESSION TAG	UNP A7VV38
A	399	HIS	-	EXPRESSION TAG	UNP A7VV38
A	400	HIS	-	EXPRESSION TAG	UNP A7VV38
A	401	HIS	-	EXPRESSION TAG	UNP A7VV38
A	402	HIS	-	EXPRESSION TAG	UNP A7VV38
A	403	HIS	-	EXPRESSION TAG	UNP A7VV38
B	396	LEU	-	EXPRESSION TAG	UNP A7VV38
B	397	GLU	-	EXPRESSION TAG	UNP A7VV38
B	398	HIS	-	EXPRESSION TAG	UNP A7VV38
B	399	HIS	-	EXPRESSION TAG	UNP A7VV38
B	400	HIS	-	EXPRESSION TAG	UNP A7VV38
B	401	HIS	-	EXPRESSION TAG	UNP A7VV38
B	402	HIS	-	EXPRESSION TAG	UNP A7VV38
B	403	HIS	-	EXPRESSION TAG	UNP A7VV38

- Molecule 2 is water.

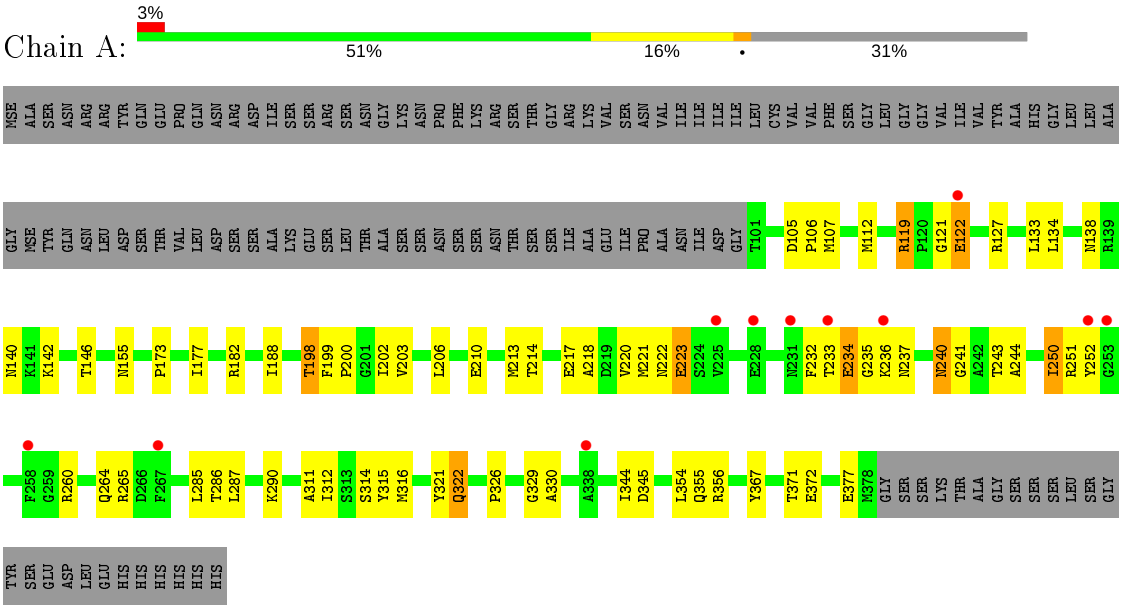
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	28	Total	O	0	0
			28	28		

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 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.

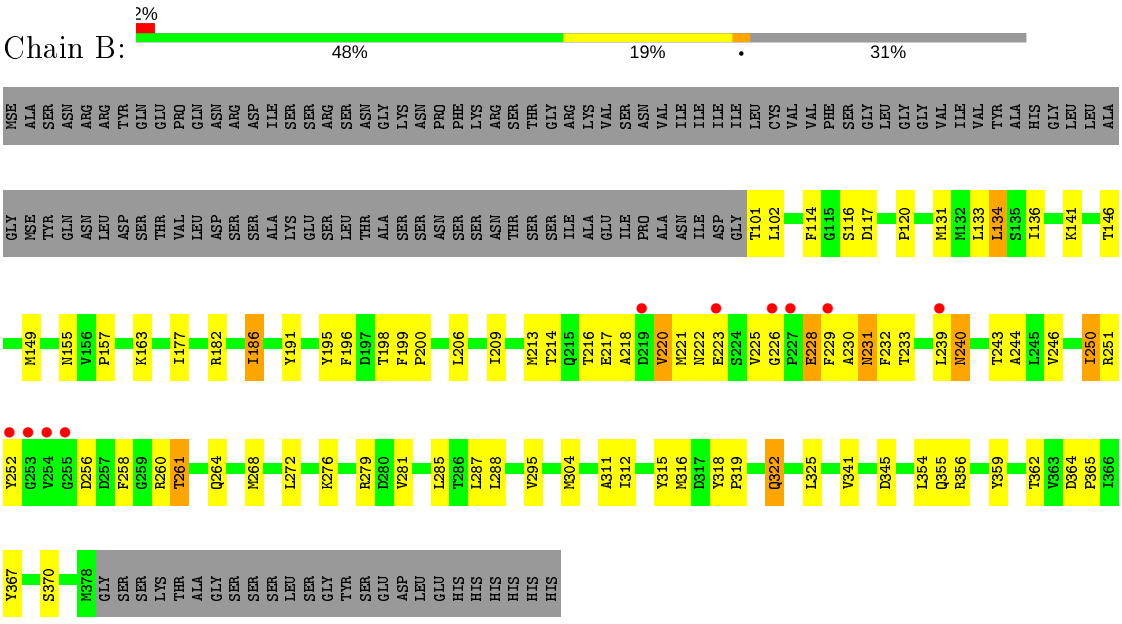
- Molecule 1: Uncharacterized protein

Chain A:



- Molecule 1: Uncharacterized protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.78Å 49.62Å 105.28Å 90.00° 106.35° 90.00°	Depositor
Resolution (Å)	35.40 – 2.38 44.54 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.8 (35.40-2.38) 95.8 (44.54-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.211 , 0.279 0.207 , 0.274	Depositor DCC
R_{free} test set	1369 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.715	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4402	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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, 0.333 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	0.43	0/2199	0.57	0/2964
1	B	0.42	0/2199	0.57	0/2964
All	All	0.42	0/4398	0.57	0/5928

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLU	Peptide
1	A	329	GLY	Peptide

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	2169	0	2107	62	0
1	B	2169	0	2107	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	0	1	0
2	B	28	0	0	0	0
All	All	4402	0	4214	135	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 16.

All (135) 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:233:THR:HG22	1:A:234:GLU:H	1.20	1.01
1:A:233:THR:HG22	1:A:234:GLU:N	1.86	0.90
1:A:233:THR:H	1:A:237:ASN:HD21	1.16	0.90
1:B:258:PHE:O	1:B:261:THR:HG22	1.71	0.90
1:B:356:ARG:HH11	1:B:356:ARG:HG3	1.39	0.86
1:A:240:ASN:ND2	1:A:243:THR:H	1.74	0.86
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.46	0.80
1:A:127:ARG:HH11	1:A:127:ARG:HG3	1.49	0.78
1:B:101:THR:HG23	1:B:102:LEU:H	1.47	0.77
1:B:220:VAL:HG11	1:B:252:TYR:CE1	2.21	0.75
1:B:240:ASN:HD21	1:B:243:THR:H	1.36	0.73
1:B:288:LEU:HD11	1:B:304:MSE:HE2	1.71	0.72
1:A:221:MSE:SE	1:A:250:ILE:HD12	2.40	0.72
1:B:228:GLU:CD	1:B:228:GLU:H	1.94	0.71
1:B:240:ASN:ND2	1:B:243:THR:H	1.90	0.70
1:B:276:LYS:HE2	1:B:318:TYR:O	1.92	0.70
1:A:232:PHE:HA	1:A:237:ASN:ND2	2.07	0.69
1:B:209:ILE:HG22	1:B:239:LEU:HB2	1.72	0.69
1:B:240:ASN:HD21	1:B:243:THR:HG23	1.56	0.69
1:B:239:LEU:HD13	1:B:244:ALA:HA	1.75	0.67
1:B:240:ASN:ND2	1:B:243:THR:HG23	2.09	0.67
1:B:225:VAL:HG23	1:B:226:GLY:H	1.59	0.67
1:A:233:THR:N	1:A:237:ASN:HD21	1.93	0.65
1:B:225:VAL:HG23	1:B:226:GLY:N	2.12	0.65
1:A:210:GLU:OE2	1:A:236:LYS:HD3	1.96	0.65
1:B:225:VAL:HG12	1:B:246:VAL:HG21	1.77	0.65
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.11	0.64
1:B:311:ALA:HA	1:B:315:TYR:HB2	1.79	0.64
1:B:252:TYR:O	1:B:256:ASP:HB3	1.98	0.64
1:B:231:ASN:N	1:B:231:ASN:ND2	2.45	0.64
1:B:221:MSE:O	1:B:225:VAL:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:HH22	1:A:322:GLN:NE2	1.97	0.63
1:A:200:PRO:HA	1:A:241:GLY:CA	2.28	0.63
1:B:222:ASN:OD1	1:B:232:PHE:HB2	1.99	0.63
1:A:311:ALA:HB1	1:A:316:MSE:HE2	1.80	0.63
1:A:155:ASN:O	1:A:182:ARG:HD3	1.98	0.62
1:B:217:GLU:HG2	1:B:252:TYR:OH	1.99	0.62
1:A:312:ILE:HD13	1:A:316:MSE:HE1	1.82	0.62
1:B:220:VAL:HG11	1:B:252:TYR:HE1	1.63	0.62
1:A:240:ASN:HD22	1:A:243:THR:H	1.45	0.61
1:B:186:ILE:H	1:B:186:ILE:HD13	1.64	0.61
1:A:311:ALA:HA	1:A:315:TYR:HB2	1.83	0.61
1:A:223:GLU:O	1:A:223:GLU:HG2	2.02	0.60
1:B:116:SER:O	1:B:195:TYR:HA	2.02	0.59
1:B:117:ASP:HB2	1:B:196:PHE:CD2	2.38	0.59
1:B:216:THR:O	1:B:220:VAL:HG12	2.03	0.58
1:B:195:TYR:O	1:B:198:THR:HG22	2.03	0.58
1:B:260:ARG:O	1:B:264:GLN:HG3	2.03	0.58
1:B:177:ILE:HD11	1:B:191:TYR:HB3	1.84	0.58
1:B:231:ASN:N	1:B:231:ASN:HD22	2.00	0.58
1:B:155:ASN:HD22	1:B:182:ARG:HH11	1.51	0.57
1:B:149:MSE:HE1	1:B:258:PHE:HE1	1.70	0.57
1:A:202:ILE:HD13	1:A:290:LYS:HB2	1.86	0.57
1:A:203:VAL:HB	1:A:241:GLY:HA2	1.88	0.56
1:B:146:THR:HG21	1:B:354:LEU:CD1	2.35	0.56
1:A:240:ASN:HD22	1:A:240:ASN:C	2.09	0.56
1:B:213:MSE:HA	1:B:217:GLU:OE1	2.06	0.55
1:B:136:ILE:N	1:B:136:ILE:HD12	2.22	0.55
1:A:206:LEU:HD21	1:A:287:LEU:HD11	1.88	0.54
1:A:222:ASN:ND2	1:A:232:PHE:HB2	2.22	0.54
1:A:177:ILE:HD12	1:A:188:ILE:HG21	1.90	0.54
1:B:225:VAL:CG1	1:B:246:VAL:HG11	2.37	0.54
1:B:218:ALA:HB2	1:B:233:THR:O	2.07	0.54
1:B:356:ARG:HG3	1:B:356:ARG:NH1	2.13	0.53
1:B:149:MSE:HG3	1:B:325:LEU:O	2.08	0.53
1:B:356:ARG:CZ	1:B:370:SER:HB2	2.38	0.53
1:B:155:ASN:ND2	1:B:182:ARG:HH11	2.06	0.53
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.19	0.53
1:A:330:ALA:HB1	2:A:438:HOH:O	2.08	0.53
1:A:218:ALA:HB2	1:A:233:THR:O	2.09	0.52
1:A:355:GLN:NE2	1:A:367:TYR:OH	2.42	0.52
1:A:286:THR:O	1:A:290:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MSE:HE1	1:B:258:PHE:CE1	2.44	0.52
1:A:233:THR:CG2	1:A:234:GLU:H	1.97	0.51
1:A:173:PRO:O	1:A:177:ILE:HG12	2.11	0.51
1:A:260:ARG:O	1:A:264:GLN:HG3	2.11	0.51
1:A:146:THR:HG21	1:A:354:LEU:CD1	2.40	0.50
1:B:279:ARG:HH12	1:B:316:MSE:CB	2.25	0.50
1:A:234:GLU:HG3	1:A:235:GLY:N	2.26	0.49
1:B:355:GLN:NE2	1:B:367:TYR:OH	2.46	0.49
1:B:157:PRO:HA	1:B:182:ARG:NH1	2.28	0.49
1:B:163:LYS:HG2	1:B:341:VAL:HG12	1.94	0.48
1:A:286:THR:HG22	1:A:290:LYS:HD3	1.96	0.48
1:B:149:MSE:CE	1:B:258:PHE:HE1	2.26	0.48
1:B:230:ALA:H	1:B:231:ASN:ND2	2.12	0.48
1:B:134:LEU:HD13	1:B:136:ILE:HD11	1.96	0.48
1:A:119:ARG:H	1:A:119:ARG:HG2	1.48	0.47
1:B:252:TYR:O	1:B:256:ASP:CB	2.63	0.47
1:B:268:MSE:O	1:B:272:LEU:HG	2.15	0.47
1:B:359:TYR:HB3	1:B:362:THR:HB	1.96	0.47
1:A:240:ASN:HD21	1:A:243:THR:H	1.56	0.46
1:A:220:VAL:HG11	1:A:252:TYR:HD2	1.80	0.46
1:A:210:GLU:CD	1:A:236:LYS:HB3	2.36	0.46
1:A:203:VAL:HB	1:A:241:GLY:CA	2.46	0.45
1:A:121:GLY:O	1:A:122:GLU:HB2	2.17	0.45
1:A:252:TYR:HD1	1:A:252:TYR:O	2.00	0.45
1:B:364:ASP:N	1:B:365:PRO:CD	2.80	0.45
1:B:281:VAL:O	1:B:285:LEU:HD23	2.18	0.44
1:A:321:TYR:CE2	1:A:377:GLU:HB2	2.52	0.44
1:B:141:LYS:O	1:B:319:PRO:HD2	2.17	0.44
1:A:322:GLN:HB2	1:A:322:GLN:HE21	1.61	0.44
1:A:326:PRO:HB3	1:A:344:ILE:HG12	2.00	0.43
1:B:114:PHE:CD1	1:B:131:MSE:HG2	2.53	0.43
1:A:285:LEU:HD13	1:B:285:LEU:HD12	1.99	0.43
1:B:356:ARG:CG	1:B:356:ARG:NH1	2.76	0.43
1:B:217:GLU:O	1:B:220:VAL:HG13	2.17	0.43
1:A:140:ASN:O	1:A:142:LYS:HG3	2.19	0.43
1:B:206:LEU:HD21	1:B:287:LEU:HD11	2.00	0.43
1:B:250:ILE:HD13	1:B:251:ARG:H	1.84	0.43
1:B:225:VAL:CG2	1:B:226:GLY:N	2.80	0.43
1:A:199:PHE:HB2	1:A:200:PRO:HD3	2.00	0.42
1:B:240:ASN:C	1:B:240:ASN:ND2	2.70	0.42
1:A:372:GLU:HA	1:A:372:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:CE	1:B:318:TYR:O	2.66	0.42
1:A:200:PRO:HA	1:A:241:GLY:HA3	1.98	0.42
1:B:228:GLU:N	1:B:228:GLU:CD	2.67	0.42
1:B:228:GLU:OE1	1:B:229:PHE:CD2	2.73	0.42
1:A:218:ALA:O	1:A:222:ASN:HB2	2.19	0.41
1:B:214:THR:OG1	1:B:217:GLU:HG3	2.20	0.41
1:A:198:THR:O	1:A:202:ILE:HG12	2.20	0.41
1:A:251:ARG:HB2	1:A:260:ARG:NH1	2.36	0.41
1:A:203:VAL:HG21	1:A:244:ALA:CB	2.50	0.41
1:A:232:PHE:HA	1:A:237:ASN:HD21	1.81	0.41
1:A:213:MSE:HB3	1:A:217:GLU:HB2	2.02	0.41
1:A:107:MSE:O	1:A:138:ASN:HB2	2.21	0.41
1:B:199:PHE:N	1:B:200:PRO:CD	2.83	0.41
1:A:105:ASP:OD1	1:A:106:PRO:HD2	2.21	0.40
1:A:200:PRO:HA	1:A:241:GLY:HA2	2.01	0.40
1:B:146:THR:HG21	1:B:354:LEU:HD13	2.03	0.40
1:B:322:GLN:HB2	1:B:322:GLN:HE21	1.63	0.40
1:B:312:ILE:N	1:B:316:MSE:HE3	2.37	0.40
1:A:112:MSE:HE2	1:A:112:MSE:HB2	1.92	0.40
1:A:221:MSE:HB3	1:A:232:PHE:CD2	2.57	0.40
1:B:311:ALA:HB1	1:B:316:MSE:HE2	2.04	0.40
1:B:191:TYR:C	1:B:191:TYR:CD1	2.94	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	276/403 (68%)	262 (95%)	13 (5%)	1 (0%)	34	46
1	B	276/403 (68%)	262 (95%)	13 (5%)	1 (0%)	34	46
All	All	552/806 (68%)	524 (95%)	26 (5%)	2 (0%)	34	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	THR
1	B	120	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	234/326 (72%)	222 (95%)	12 (5%)	24	36
1	B	234/326 (72%)	221 (94%)	13 (6%)	21	31
All	All	468/652 (72%)	443 (95%)	25 (5%)	22	34

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ARG
1	A	133	LEU
1	A	134	LEU
1	A	198	THR
1	A	223	GLU
1	A	234	GLU
1	A	240	ASN
1	A	250	ILE
1	A	314	SER
1	A	322	GLN
1	A	345	ASP
1	A	371	THR
1	B	133	LEU
1	B	134	LEU
1	B	186	ILE
1	B	220	VAL
1	B	223	GLU
1	B	228	GLU
1	B	231	ASN
1	B	240	ASN
1	B	250	ILE

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Mol	Chain	Res	Type
1	B	261	THR
1	B	295	VAL
1	B	322	GLN
1	B	345	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	155	ASN
1	A	166	HIS
1	A	215	GLN
1	A	237	ASN
1	A	240	ASN
1	A	264	GLN
1	A	322	GLN
1	A	355	GLN
1	B	138	ASN
1	B	155	ASN
1	B	215	GLN
1	B	231	ASN
1	B	240	ASN
1	B	264	GLN
1	B	322	GLN
1	B	355	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	266/403 (66%)	0.40	11 (4%)	37	40	24, 47, 88, 146	0
1	B	266/403 (66%)	0.38	10 (3%)	40	43	27, 48, 93, 132	0
All	All	532/806 (66%)	0.39	21 (3%)	39	42	24, 48, 91, 146	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	TYR	8.6
1	B	227	PRO	5.6
1	A	253	GLY	4.9
1	A	225	VAL	3.9
1	B	252	TYR	3.8
1	B	229	PHE	3.6
1	B	223	GLU	2.9
1	B	253	GLY	2.7
1	B	255	GLY	2.6
1	A	122	GLU	2.4
1	A	236	LYS	2.4
1	B	254	VAL	2.4
1	A	338	ALA	2.3
1	A	233	THR	2.3
1	B	219	ASP	2.2
1	A	231	ASN	2.2
1	A	258	PHE	2.1
1	B	226	GLY	2.1
1	B	239	LEU	2.0
1	A	228	GLU	2.0
1	A	267	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 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.