Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 06:56 am BST

PDB ID	:	5FSH
Title	:	Crystal structure of Thermus thermophilus Csm6
Authors	:	Niewoehner, O.; Jinek, M.
Deposited on	:	2016-01-06
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
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 2.30 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		10.2%
RSRZ outliers		8.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution
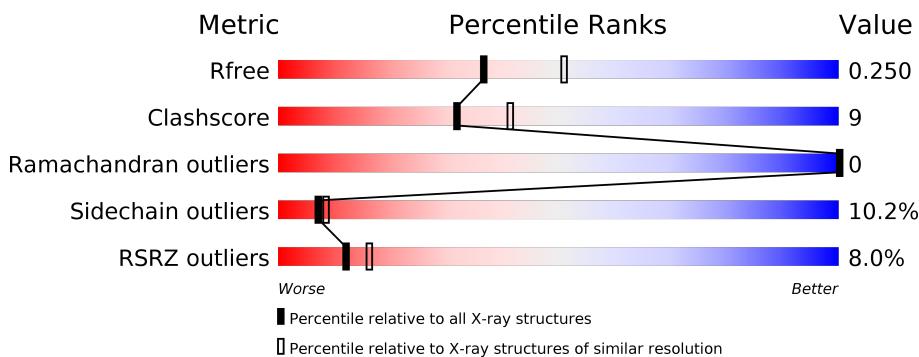
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	467	9% 74% 21% • •
1	B	467	7% 74% 18% • •
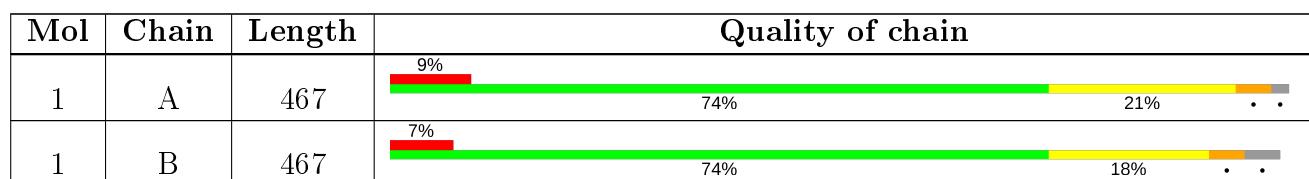
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7060 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 CSM6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total 3520	C 2267	N 621	O 627	S 5	0	0	0
1	B	448	Total 3462	C 2233	N 613	O 611	S 5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q53W17
A	-1	ASN	-	expression tag	UNP Q53W17
A	0	ALA	-	expression tag	UNP Q53W17
B	-2	SER	-	expression tag	UNP Q53W17
B	-1	ASN	-	expression tag	UNP Q53W17
B	0	ALA	-	expression tag	UNP Q53W17

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ni 1	0	0
2	A	5	Total 5	Ni 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total 39	O 39	0	0
3	B	33	Total 33	O 33	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CSM6

Chain A:

- Molecule 1: CSM6

Chain B:
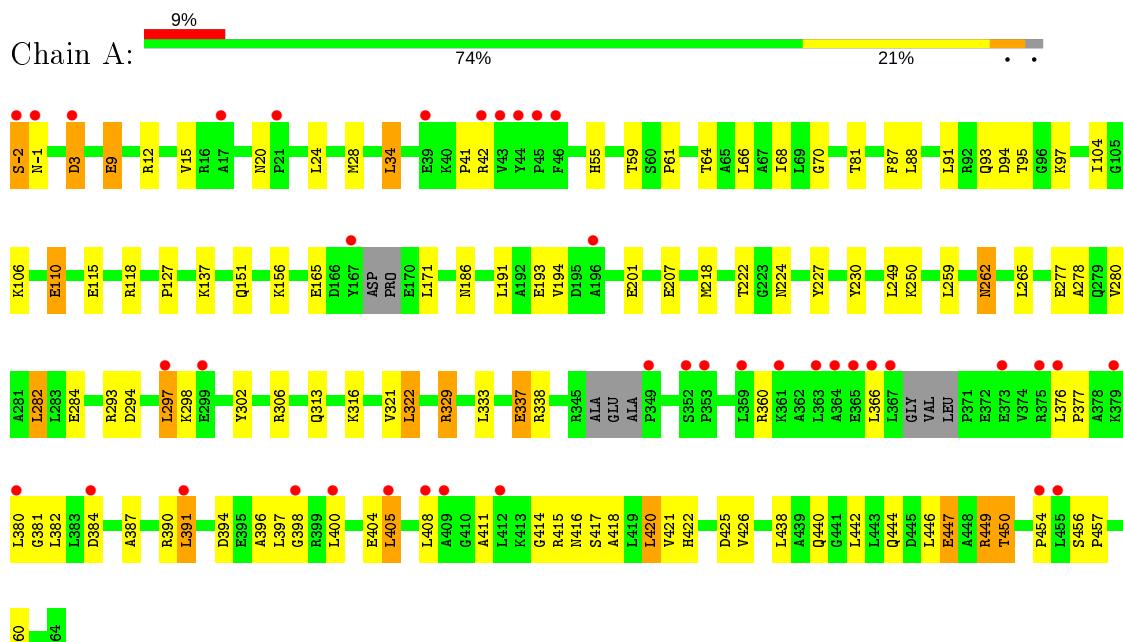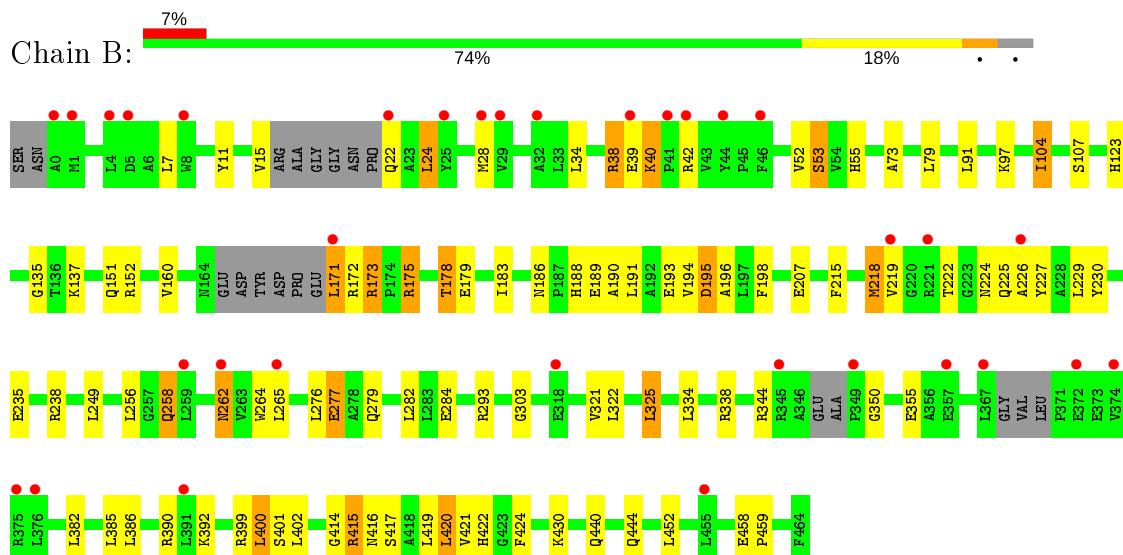
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.31Å 207.07Å 58.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.30 48.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.70-2.30) 98.3 (48.70-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.244 0.224 , 0.250	Depositor DCC
R_{free} test set	2595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7060	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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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)

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

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	0.33	1/3592 (0.0%)	0.52	2/4870 (0.0%)
1	B	0.32	0/3531	0.50	1/4781 (0.0%)
All	All	0.33	1/7123 (0.0%)	0.51	3/9651 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	ASP	CB-CG	5.80	1.64	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	ASP	CB-CG-OD2	11.64	128.78	118.30
1	A	3	ASP	CB-CG-OD1	-7.14	111.88	118.30
1	B	195	ASP	CB-CG-OD1	5.21	122.99	118.30

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	3520	0	3566	69	1
1	B	3462	0	3544	63	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	1	0	0	0	0
3	A	39	0	0	4	0
3	B	33	0	0	1	0
All	All	7060	0	7110	126	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 9.

All (126) 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:B:79:LEU:HB3	1:B:104:ILE:HD11	1.41	1.02
1:A:201:GLU:OE2	3:A:2027:HOH:O	1.88	0.92
1:A:387:ALA:O	1:A:391:LEU:HB2	1.85	0.76
1:A:-1:ASN:OD1	3:A:2001:HOH:O	2.06	0.73
1:A:110:GLU:HG3	1:B:190:ALA:HB1	1.70	0.72
1:A:12:ARG:HD2	1:A:171:LEU:HD12	1.75	0.68
1:A:278:ALA:HB2	1:A:454:PRO:HD2	1.77	0.66
1:A:298:LYS:NZ	1:A:337:GLU:OE1	2.24	0.65
1:A:24:LEU:O	1:A:28:MET:HB2	1.95	0.65
1:B:249:LEU:HD11	1:B:284:GLU:HG3	1.78	0.64
1:B:262:ASN:OD1	1:B:262:ASN:N	2.30	0.64
1:A:262:ASN:HA	1:A:265:LEU:HG	1.79	0.63
1:B:321:VAL:HG12	1:B:420:LEU:HD22	1.81	0.62
1:B:195:ASP:HA	1:B:198:PHE:HD2	1.64	0.62
1:B:382:LEU:HG	1:B:415:ARG:HG3	1.80	0.62
1:A:306:ARG:HH12	1:A:457:PRO:HA	1.65	0.62
1:B:179:GLU:N	1:B:179:GLU:OE1	2.32	0.60
1:B:186:ASN:ND2	1:B:189:GLU:OE2	2.35	0.59
1:A:338:ARG:NH1	1:A:394:ASP:OD1	2.35	0.59
1:A:81:THR:HG21	1:A:106:LYS:HE2	1.83	0.58
1:A:390:ARG:NH2	1:A:400:LEU:O	2.37	0.58
1:B:38:ARG:HB3	1:B:38:ARG:HH11	1.69	0.58
1:B:222:THR:HG22	1:B:224:ASN:HB2	1.85	0.57
1:A:137:LYS:NZ	1:B:135:GLY:O	2.34	0.57
1:A:218:MET:O	1:A:222:THR:HG22	2.04	0.57
1:B:458:GLU:HG3	1:B:459:PRO:HD2	1.87	0.57
1:B:191:LEU:O	1:B:194:VAL:HG22	2.05	0.57
1:B:225:GLN:HB2	1:B:264:TRP:HZ2	1.69	0.57
1:A:191:LEU:O	1:A:194:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLN:HB2	1:B:264:TRP:CZ2	2.40	0.56
1:B:22:GLN:HG2	1:B:173:ARG:HH21	1.70	0.56
1:B:24:LEU:O	1:B:28:MET:HB2	2.04	0.56
1:B:282:LEU:HD11	1:B:303:GLY:HA3	1.88	0.56
1:B:34:LEU:O	1:B:38:ARG:HG3	2.06	0.56
1:A:394:ASP:HB3	1:A:397:LEU:HB2	1.88	0.55
1:A:446:LEU:O	1:A:450:THR:OG1	2.25	0.55
1:A:408:LEU:HD13	1:A:438:LEU:HD22	1.89	0.55
1:A:-2:SER:OG	3:A:2002:HOH:O	2.18	0.54
1:A:420:LEU:HG	1:B:325:LEU:HD21	1.89	0.54
1:A:337:GLU:OE2	1:A:449:ARG:NH2	2.34	0.53
1:B:440:GLN:O	1:B:444:GLN:HG2	2.09	0.53
1:A:34:LEU:HD11	1:A:94:ASP:HB3	1.88	0.53
1:A:329:ARG:HD2	1:B:419:LEU:O	2.08	0.52
1:B:53:SER:HB2	1:B:73:ALA:HB3	1.90	0.52
1:A:115:GLU:OE1	1:A:118:ARG:NH1	2.43	0.52
1:B:7:LEU:HD21	1:B:28:MET:O	2.09	0.52
1:A:416:ASN:O	1:A:422:HIS:HB2	2.09	0.52
1:B:218:MET:HE2	3:B:2024:HOH:O	2.09	0.52
1:B:416:ASN:O	1:B:422:HIS:HB2	2.09	0.52
1:B:188:HIS:NE2	1:B:195:ASP:OD1	2.42	0.52
1:A:151:GLN:OE1	1:A:186:ASN:ND2	2.40	0.52
1:B:215:PHE:O	1:B:219:VAL:HG23	2.08	0.52
1:A:95:THR:HG22	1:A:97:LYS:H	1.75	0.51
1:A:421:VAL:HG13	1:A:422:HIS:H	1.75	0.51
1:B:344:ARG:NH2	1:B:350:GLY:O	2.43	0.51
1:A:394:ASP:O	1:A:398:GLY:N	2.33	0.50
1:A:127:PRO:HA	1:A:156:LYS:HB3	1.94	0.50
1:A:417:SER:OG	1:A:425:ASP:OD2	2.25	0.50
1:A:64:THR:O	1:A:68:ILE:HG12	2.11	0.50
1:B:193:GLU:O	1:B:196:ALA:HB3	2.12	0.50
1:B:282:LEU:HD13	1:B:452:LEU:HD13	1.93	0.50
1:A:293:ARG:NH1	1:B:424:PHE:HB2	2.26	0.50
1:B:344:ARG:HH12	1:B:392:LYS:NZ	2.09	0.49
1:B:256:LEU:HD21	1:B:277:GLU:HG3	1.94	0.49
1:A:41:PRO:HB3	1:A:70:GLY:HA2	1.95	0.49
1:B:279:GLN:O	1:B:282:LEU:HB3	2.12	0.49
1:A:294:ASP:O	1:A:297:LEU:HD12	2.12	0.49
1:A:321:VAL:HG12	1:A:420:LEU:HD22	1.95	0.48
1:B:24:LEU:HB2	1:B:28:MET:HE3	1.94	0.48
1:A:322:LEU:HD21	1:B:322:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:O	1:A:95:THR:HB	2.14	0.48
1:B:196:ALA:HB2	1:B:218:MET:SD	2.54	0.48
1:A:366:LEU:HD11	1:A:405:LEU:HD12	1.95	0.47
1:A:9:GLU:HA	1:A:12:ARG:HG3	1.96	0.47
1:B:11:TYR:O	1:B:15:VAL:HG23	2.14	0.47
1:B:282:LEU:HD11	1:B:303:GLY:CA	2.44	0.47
1:B:344:ARG:HH12	1:B:392:LYS:HZ3	1.61	0.47
1:A:222:THR:HG23	1:A:224:ASN:H	1.78	0.47
1:B:53:SER:HB3	1:B:55:HIS:HE1	1.80	0.47
1:B:440:GLN:OE1	1:B:444:GLN:NE2	2.48	0.47
1:B:39:GLU:HG2	1:B:40:LYS:HD2	1.96	0.47
1:A:280:VAL:O	1:A:284:GLU:HG3	2.15	0.46
1:A:381:GLY:N	1:A:384:ASP:HB3	2.30	0.46
1:A:338:ARG:HD2	1:A:442:LEU:HD22	1.98	0.46
1:B:390:ARG:NH2	1:B:400:LEU:O	2.47	0.46
1:B:227:TYR:HA	1:B:230:TYR:HD2	1.81	0.46
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.75	0.46
1:A:61:PRO:HG3	1:A:87:PHE:CD2	2.52	0.45
1:B:344:ARG:HH22	1:B:355:GLU:CD	2.20	0.45
1:A:15:VAL:HG11	1:A:171:LEU:HD21	1.98	0.45
1:A:417:SER:O	1:A:417:SER:OG	2.35	0.44
1:B:229:LEU:HD11	1:B:258:GLN:HG2	1.99	0.44
1:A:404:GLU:O	1:A:408:LEU:HG	2.16	0.44
1:B:249:LEU:CD1	1:B:284:GLU:HG3	2.47	0.44
1:A:193:GLU:HB2	3:A:2025:HOH:O	2.18	0.44
1:A:302:TYR:CE1	1:A:447:GLU:HB2	2.53	0.44
1:A:227:TYR:HA	1:A:230:TYR:HD2	1.83	0.44
1:A:55:HIS:CD2	1:A:68:ILE:HD13	2.53	0.44
1:A:306:ARG:HH12	1:A:457:PRO:CA	2.30	0.43
1:B:334:LEU:O	1:B:338:ARG:HG2	2.17	0.43
1:B:22:GLN:HG2	1:B:173:ARG:NH2	2.33	0.43
1:A:313:GLN:HA	1:A:316:LYS:HE3	1.99	0.43
1:B:160:VAL:HG12	1:B:183:ILE:HG12	2.00	0.42
1:A:81:THR:HA	1:A:104:ILE:O	2.19	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.89	0.42
1:B:175:ARG:O	1:B:178:THR:OG1	2.36	0.42
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.79	0.42
1:A:408:LEU:O	1:A:411:ALA:N	2.52	0.42
1:A:376:LEU:HA	1:A:377:PRO:HD3	1.84	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD22	1.90	0.42
1:A:59:THR:O	1:A:61:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LYS:HA	1:B:137:LYS:HD3	1.91	0.42
1:A:95:THR:HG22	1:A:97:LYS:N	2.35	0.41
1:B:420:LEU:HA	1:B:420:LEU:HD12	1.85	0.41
1:A:360:ARG:HE	1:A:376:LEU:HD22	1.84	0.41
1:A:338:ARG:NH1	1:A:396:ALA:HB3	2.36	0.41
1:A:414:GLY:HA2	1:A:417:SER:HB3	2.03	0.41
1:A:418:ALA:HA	1:A:425:ASP:HB2	2.02	0.41
1:A:250:LYS:HE3	1:A:250:LYS:HB2	1.69	0.41
1:B:226:ALA:O	1:B:229:LEU:HB2	2.21	0.41
1:B:52:VAL:HG21	1:B:123:HIS:CG	2.55	0.41
1:A:382:LEU:HD23	1:A:382:LEU:HA	1.84	0.41
1:A:249:LEU:CD1	1:A:284:GLU:HG2	2.51	0.40
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.85	0.40
1:B:195:ASP:HA	1:B:198:PHE:CD2	2.50	0.40
1:B:414:GLY:HA2	1:B:417:SER:HB3	2.03	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:A:-1:ASN:ND2	1:B:195:ASP:OD2[1_556]	2.08	0.12

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	451/467 (97%)	436 (97%)	15 (3%)	0	100	100
1	B	438/467 (94%)	424 (97%)	14 (3%)	0	100	100
All	All	889/934 (95%)	860 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	340/358 (95%)	307 (90%)	33 (10%)	8	9
1	B	337/358 (94%)	301 (89%)	36 (11%)	6	7
All	All	677/716 (95%)	608 (90%)	69 (10%)	7	8

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	3	ASP
1	A	9	GLU
1	A	20	ASN
1	A	34	LEU
1	A	42	ARG
1	A	66	LEU
1	A	93	GLN
1	A	110	GLU
1	A	165	GLU
1	A	207	GLU
1	A	259	LEU
1	A	262	ASN
1	A	277	GLU
1	A	282	LEU
1	A	297	LEU
1	A	322	LEU
1	A	329	ARG
1	A	333	LEU
1	A	337	GLU
1	A	380	LEU
1	A	391	LEU
1	A	405	LEU
1	A	415	ARG
1	A	420	LEU
1	A	426	VAL
1	A	440	GLN

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Mol	Chain	Res	Type
1	A	444	GLN
1	A	447	GLU
1	A	449	ARG
1	A	450	THR
1	A	456	SER
1	A	460	VAL
1	B	24	LEU
1	B	38	ARG
1	B	40	LYS
1	B	42	ARG
1	B	53	SER
1	B	97	LYS
1	B	104	ILE
1	B	107	SER
1	B	151	GLN
1	B	152	ARG
1	B	171	LEU
1	B	172	ARG
1	B	173	ARG
1	B	175	ARG
1	B	178	THR
1	B	207	GLU
1	B	218	MET
1	B	235	GLU
1	B	238	ARG
1	B	258	GLN
1	B	262	ASN
1	B	265	LEU
1	B	276	LEU
1	B	277	GLU
1	B	293	ARG
1	B	325	LEU
1	B	385	LEU
1	B	386	LEU
1	B	399	ARG
1	B	400	LEU
1	B	401	SER
1	B	402	LEU
1	B	415	ARG
1	B	420	LEU
1	B	421	VAL
1	B	430	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	B	55	HIS
1	B	151	GLN
1	B	444	GLN

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 6 ligands modelled in this entry, 6 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(Å²)	Q<0.9
1	A	459/467 (98%)	0.54	40 (8%)	10	14	39, 69, 128, 154	0
1	B	448/467 (95%)	0.44	33 (7%)	14	19	40, 73, 132, 159	0
All	All	907/934 (97%)	0.49	73 (8%)	12	16	39, 71, 130, 159	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	MET	6.8
1	B	29	VAL	5.9
1	A	167	TYR	5.7
1	B	4	LEU	5.4
1	A	367	LEU	5.1
1	A	454	PRO	5.1
1	A	44	TYR	4.9
1	B	25	TYR	4.8
1	A	-2	SER	4.6
1	A	366	LEU	4.6
1	B	262	ASN	4.6
1	A	379	LYS	4.4
1	B	219	VAL	4.2
1	B	8	TRP	4.2
1	A	365	GLU	4.1
1	A	364	ALA	4.0
1	B	0	ALA	3.9
1	B	374	VAL	3.7
1	B	372	GLU	3.7
1	B	46	PHE	3.5
1	A	376	LEU	3.4
1	A	391	LEU	3.4
1	A	455	LEU	3.2
1	A	384	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	3.1
1	A	45	PRO	3.1
1	A	400	LEU	3.0
1	A	39	GLU	3.0
1	B	44	TYR	3.0
1	A	412	LEU	3.0
1	B	39	GLU	3.0
1	A	21	PRO	3.0
1	A	297	LEU	2.9
1	B	42	ARG	2.9
1	B	367	LEU	2.9
1	A	17	ALA	2.8
1	A	42	ARG	2.8
1	A	405	LEU	2.8
1	B	345	ARG	2.7
1	A	46	PHE	2.7
1	A	359	LEU	2.7
1	A	398	GLY	2.7
1	A	353	PRO	2.6
1	B	5	ASP	2.6
1	B	375	ARG	2.6
1	A	352	SER	2.6
1	A	363	LEU	2.6
1	B	41	PRO	2.6
1	B	259	LEU	2.5
1	B	455	LEU	2.5
1	A	361	LYS	2.5
1	B	349	PRO	2.5
1	A	299	GLU	2.4
1	B	318	GLU	2.4
1	B	391	LEU	2.4
1	A	380	LEU	2.3
1	A	409	ALA	2.3
1	A	349	PRO	2.3
1	B	221	ARG	2.3
1	B	357	GLU	2.3
1	B	265	LEU	2.3
1	B	1	MET	2.2
1	B	22	GLN	2.2
1	A	373	GLU	2.2
1	B	376	LEU	2.2
1	A	3	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	226	ALA	2.2
1	A	-1	ASN	2.1
1	B	171	LEU	2.1
1	A	408	LEU	2.1
1	A	375	ARG	2.1
1	A	196	ALA	2.0
1	B	32	ALA	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. 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	B-factors(Å^2)	Q<0.9
2	NI	A	1467	1/1	-0.21	0.33	92,92,92,92	1
2	NI	B	1465	1/1	0.32	0.14	112,112,112,112	0
2	NI	A	1465	1/1	0.68	0.16	68,68,68,68	0
2	NI	A	1466	1/1	0.76	0.12	72,72,72,72	1
2	NI	A	1469	1/1	0.78	0.22	111,111,111,111	0
2	NI	A	1468	1/1	0.82	0.10	91,91,91,91	1

6.5 Other polymers (i)

There are no such residues in this entry.