Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:06 pm BST

PDB ID	:	3ZHE
Title	:	Structure of the C. elegans SMG5-SMG7 complex
Authors	:	Jonas, S.; Weichenrieder, O.; Izaurralde, E.
Deposited on	:	2012-12-21
Resolution	:	3.00 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 following versions of software and data (see references ①) were used in the production of this report:

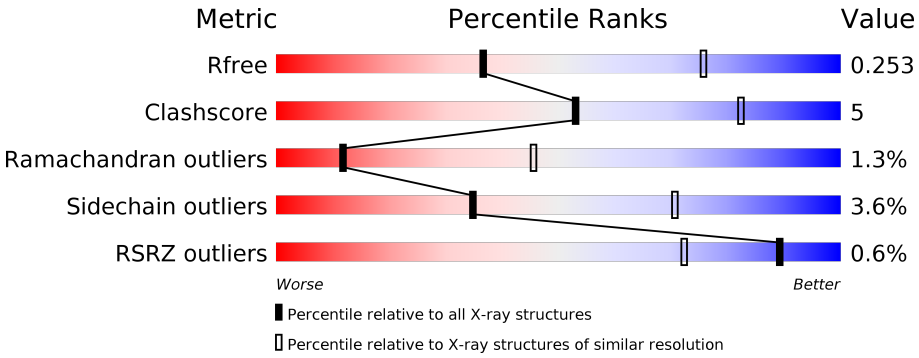
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	420	% 77% 17% • 5%
1	C	420	79% 12% • 8%
2	B	395	83% 16% ••
2	D	395	% 83% 13% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12141 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 NONSENSE-MEDIATED MRNA DECAY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3110	1997	517	572	24			
1	C	388	Total	C	N	O	S	0	0	0
			3019	1943	500	553	23			

- Molecule 2 is a protein called PROTEIN SMG-7.

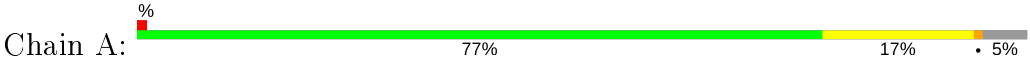
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	0	0
			3037	1941	503	573	20			
2	D	387	Total	C	N	O	S	0	0	0
			2975	1905	492	560	18			

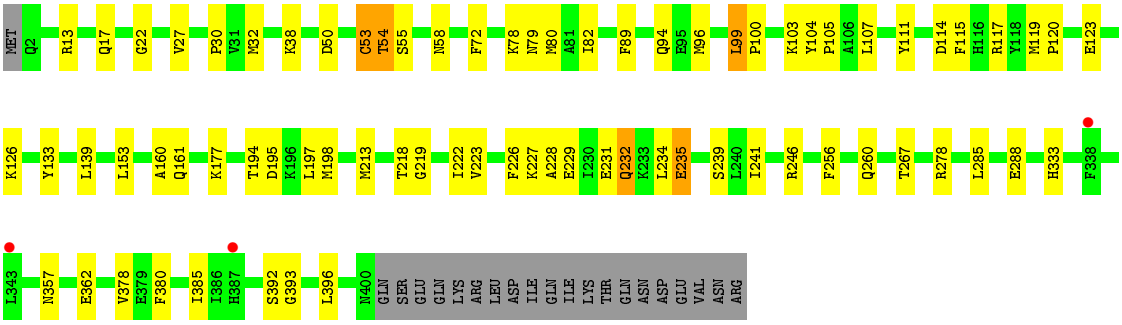
3 Residue-property plots (i)

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: NONSENSE-MEDIATED MRNA DECAY PROTEIN

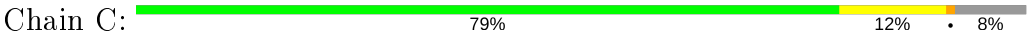
Chain A:

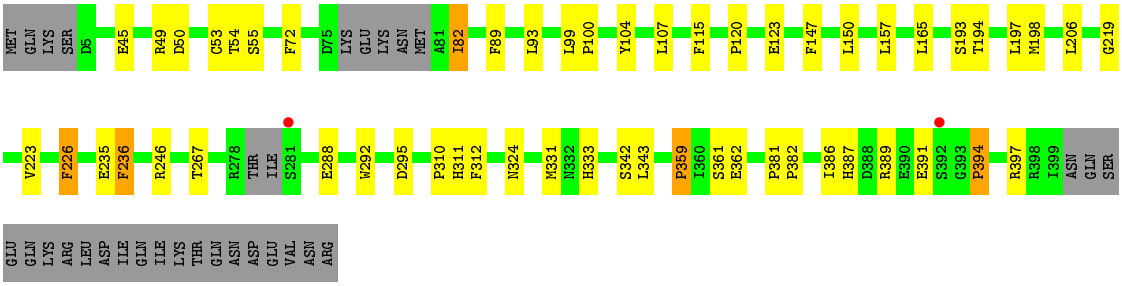




- Molecule 1: NONSENSE-MEDIATED MRNA DECAY PROTEIN

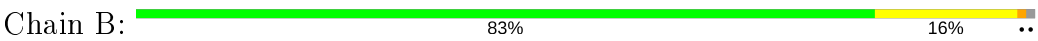
Chain C:

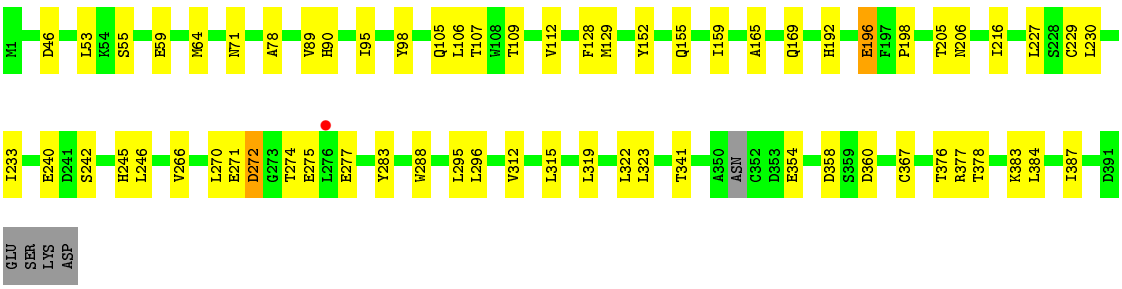




- Molecule 2: PROTEIN SMG-7

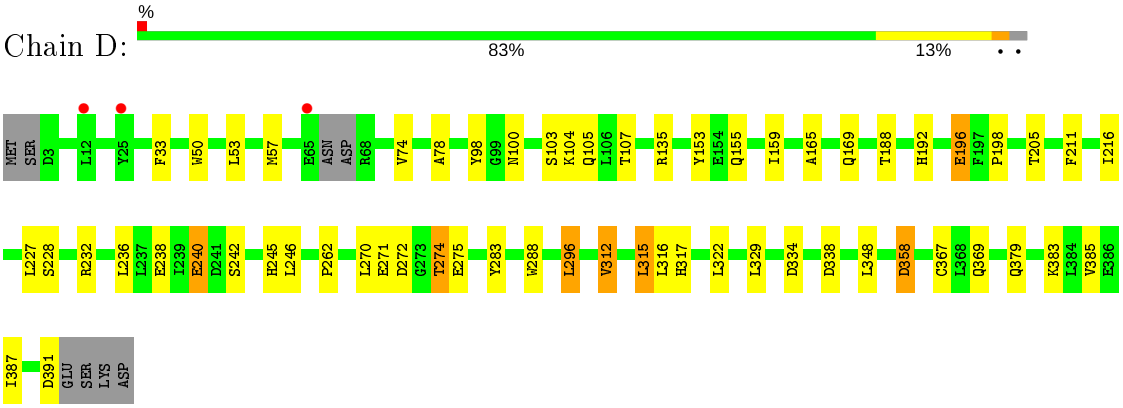
Chain B:





• Molecule 2: PROTEIN SMG-7

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.16Å 82.00Å 154.51Å 90.00° 116.88° 90.00°	Depositor
Resolution (Å)	49.34 – 3.00 49.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.34-3.00) 99.9 (49.34-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.222 , 0.249 0.227 , 0.253	Depositor DCC
R_{free} test set	2828 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	94.3	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12141	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	0.23	0/3180	0.41	0/4320
1	C	0.23	0/3088	0.43	0/4192
2	B	0.22	0/3104	0.39	0/4226
2	D	0.22	0/3042	0.40	0/4151
All	All	0.23	0/12414	0.41	0/16889

There are no bond length outliers.

There are no bond angle outliers.

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	3110	0	2973	43	0
1	C	3019	0	2870	25	0
2	B	3037	0	2883	32	0
2	D	2975	0	2777	33	0
All	All	12141	0	11503	128	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 5.

All (128) 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:72:PHE:HE2	1:A:82:ILE:HG22	1.54	0.71
1:A:120:PRO:HG2	1:A:123:GLU:HG3	1.72	0.71
2:B:192:HIS:CG	2:B:367:CYS:HB2	2.30	0.66
1:C:53:CYS:O	1:C:55:SER:N	2.29	0.66
1:A:17:GLN:NE2	2:D:338:ASP:OD1	2.30	0.65
1:A:96:MET:HA	1:A:99:LEU:HD23	1.80	0.64
1:A:53:CYS:O	1:A:55:SER:N	2.30	0.64
2:D:103:SER:OG	2:D:105:GLN:OE1	2.16	0.64
1:A:197:LEU:HD11	1:A:229:GLU:HG3	1.81	0.62
1:C:246:ARG:NH1	1:C:295:ASP:OD2	2.33	0.62
1:C:99:LEU:HD12	1:C:100:PRO:HD2	1.83	0.60
2:B:53:LEU:HD21	2:B:78:ALA:HB1	1.83	0.60
1:A:94:GLN:HE21	2:B:105:GLN:HB3	1.67	0.60
1:A:223:VAL:HG22	1:A:267:THR:HG23	1.84	0.58
1:C:223:VAL:HG22	1:C:267:THR:HG23	1.84	0.58
1:A:246:ARG:NE	1:A:288:GLU:OE2	2.31	0.57
1:A:50:ASP:OD1	1:A:50:ASP:N	2.33	0.56
1:C:386:ILE:HD12	1:C:394:PRO:HD2	1.87	0.56
2:B:323:LEU:HG	2:B:387:ILE:HG13	1.88	0.56
1:A:105:PRO:HB2	1:A:139:LEU:HD13	1.87	0.56
1:C:310:PRO:O	1:C:312:PHE:N	2.33	0.56
2:B:246:LEU:HD11	2:B:283:TYR:HD1	1.71	0.55
2:B:55:SER:O	2:B:59:GLU:HG2	2.07	0.55
2:D:57:MET:HA	2:D:74:VAL:HG21	1.89	0.55
2:B:376:THR:HG22	2:B:378:THR:H	1.72	0.55
1:A:72:PHE:CE1	1:A:78:LYS:HG2	2.43	0.53
1:A:256:PHE:HD2	1:A:260:GLN:HG2	1.73	0.53
1:C:246:ARG:NE	1:C:288:GLU:OE2	2.41	0.53
1:C:104:TYR:HB3	1:C:107:LEU:HD12	1.91	0.53
1:C:331:MET:HG3	1:C:397:ARG:HG3	1.91	0.53
2:D:53:LEU:HD21	2:D:78:ALA:HB1	1.92	0.52
1:C:359:PRO:O	1:C:361:SER:N	2.39	0.52
2:D:246:LEU:HD11	2:D:283:TYR:HD1	1.74	0.52
2:D:192:HIS:CG	2:D:367:CYS:HB2	2.44	0.52
2:B:165:ALA:O	2:B:169:GLN:HG2	2.11	0.51
2:D:329:LEU:HD12	2:D:387:ILE:HD13	1.93	0.51
1:A:78:LYS:HZ2	1:A:80:MET:H	1.59	0.51
2:B:155:GLN:O	2:B:159:ILE:HG12	2.11	0.51
1:A:117:ARG:HG3	1:A:153:LEU:HD21	1.93	0.50
1:A:72:PHE:CE2	1:A:82:ILE:HG22	2.42	0.50
1:A:392:SER:OG	1:A:393:GLY:N	2.40	0.50
2:B:274:THR:OG1	2:B:277:GLU:OE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:HD11	2:B:152:TYR:HE1	1.76	0.49
2:D:165:ALA:O	2:D:169:GLN:HG2	2.13	0.48
1:A:198:MET:HG3	1:A:241:ILE:HG23	1.95	0.48
1:A:161:GLN:NE2	1:A:357:ASN:O	2.47	0.48
2:B:354:GLU:HG2	2:B:377:ARG:HB3	1.95	0.48
1:C:197:LEU:HD13	1:C:226:PHE:HA	1.96	0.48
1:A:13:ARG:NH2	2:D:334:ASP:OD1	2.48	0.47
2:D:98:TYR:HB3	2:D:159:ILE:HD12	1.97	0.47
1:C:342:SER:HB2	1:C:391:GLU:H	1.80	0.47
1:A:378:VAL:HG12	1:A:380:PHE:H	1.80	0.46
2:D:288:TRP:CZ2	2:D:322:LEU:HA	2.51	0.46
1:A:89:PHE:HB3	1:A:115:PHE:CE2	2.50	0.46
1:A:114:ASP:OD1	1:A:117:ARG:NH1	2.47	0.46
2:B:90:HIS:CE1	2:B:107:THR:HA	2.50	0.46
1:A:58:ASN:OD1	1:A:111:TYR:OH	2.34	0.46
2:B:288:TRP:CZ2	2:B:322:LEU:HA	2.51	0.46
2:D:358:ASP:N	2:D:358:ASP:OD1	2.47	0.46
2:B:98:TYR:HB3	2:B:159:ILE:HD12	1.97	0.46
2:D:155:GLN:O	2:D:159:ILE:HG12	2.17	0.45
2:B:246:LEU:HD11	2:B:283:TYR:CD1	2.51	0.45
1:A:228:ALA:O	1:A:232:GLN:HB2	2.17	0.45
2:B:89:VAL:HG21	2:B:128:PHE:CZ	2.51	0.45
1:C:324:ASN:OD1	1:C:397:ARG:NH2	2.50	0.45
2:B:319:LEU:HD21	2:B:384:LEU:HD11	1.98	0.45
1:A:104:TYR:HB3	1:A:107:LEU:HD12	1.99	0.45
1:A:119:MET:O	1:A:126:LYS:NZ	2.41	0.45
2:D:379:GLN:O	2:D:383:LYS:HG2	2.17	0.44
1:A:160:ALA:HB2	1:A:198:MET:HE1	1.99	0.44
1:C:194:THR:HG21	1:C:236:PHE:CZ	2.53	0.44
1:A:78:LYS:HA	1:A:78:LYS:HD2	1.85	0.44
1:A:385:ILE:H	1:A:385:ILE:HG13	1.52	0.44
2:D:246:LEU:HD11	2:D:283:TYR:CD1	2.52	0.44
1:A:78:LYS:HZ2	1:A:79:ASN:H	1.66	0.43
2:B:196:GLU:O	2:B:198:PRO:HD3	2.18	0.43
2:D:227:LEU:HA	2:D:227:LEU:HD23	1.82	0.43
1:C:194:THR:HG21	1:C:236:PHE:HZ	1.84	0.43
1:C:198:MET:HB2	1:C:198:MET:HE2	1.89	0.43
1:A:53:CYS:HB3	1:A:54:THR:H	1.56	0.43
2:B:270:LEU:O	2:B:272:ASP:N	2.51	0.43
2:D:196:GLU:O	2:D:198:PRO:HD3	2.18	0.43
2:D:236:LEU:HD21	2:D:270:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:NH1	1:A:133:TYR:OH	2.51	0.43
1:C:150:LEU:HA	1:C:150:LEU:HD23	1.89	0.43
2:D:274:THR:HG22	2:D:275:GLU:H	1.83	0.43
2:D:57:MET:HG2	2:D:74:VAL:HG22	2.00	0.43
1:A:99:LEU:HD12	1:A:100:PRO:O	2.19	0.43
2:B:295:LEU:HD11	2:B:315:LEU:HG	2.00	0.43
1:C:72:PHE:HE2	1:C:82:ILE:HG22	1.83	0.43
1:C:381:PRO:HA	1:C:382:PRO:HD3	1.86	0.42
2:D:315:LEU:HA	2:D:315:LEU:HD12	1.86	0.42
1:A:38:LYS:NZ	2:D:391:ASP:OD1	2.39	0.42
2:B:315:LEU:HA	2:B:315:LEU:HD12	1.93	0.42
1:C:120:PRO:HB2	1:C:123:GLU:HG3	2.00	0.42
1:C:219:GLY:O	1:C:223:VAL:HG23	2.19	0.42
1:A:219:GLY:O	1:A:223:VAL:HG23	2.20	0.42
1:C:147:PHE:HB3	1:C:165:LEU:O	2.20	0.42
1:A:218:THR:O	1:A:222:ILE:HG13	2.20	0.42
1:A:22:GLY:HA2	1:A:32:MET:SD	2.59	0.42
2:B:274:THR:HG22	2:B:275:GLU:H	1.85	0.42
2:D:211:PHE:HB3	2:D:228:SER:HA	2.02	0.42
2:B:109:THR:O	2:B:112:VAL:HG22	2.20	0.42
2:B:46:ASP:N	2:B:46:ASP:OD1	2.53	0.41
2:D:216:ILE:HG22	2:D:245:HIS:CE1	2.55	0.41
2:B:216:ILE:HG22	2:B:245:HIS:CE1	2.55	0.41
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.89	0.41
2:B:90:HIS:CD2	2:B:95:ILE:HB	2.56	0.41
2:B:383:LYS:O	2:B:387:ILE:HG12	2.21	0.41
2:D:312:VAL:O	2:D:316:LEU:HG	2.20	0.41
2:B:229:CYS:O	2:B:233:ILE:HG13	2.21	0.41
2:D:317:HIS:CE1	2:D:358:ASP:HB3	2.56	0.41
1:C:89:PHE:HB3	1:C:115:PHE:CE2	2.56	0.41
2:D:192:HIS:ND1	2:D:367:CYS:HB2	2.36	0.41
2:D:50:TRP:CE2	2:D:135:ARG:HD2	2.56	0.41
1:A:227:LYS:O	1:A:231:GLU:HG2	2.21	0.40
2:B:358:ASP:C	2:B:360:ASP:H	2.23	0.40
1:C:246:ARG:HG3	1:C:292:TRP:HE3	1.87	0.40
2:D:232:ARG:NH1	2:D:238:GLU:O	2.50	0.40
1:A:103:LYS:HB2	1:A:104:TYR:CE2	2.56	0.40
1:A:234:LEU:O	1:A:235:GLU:HB2	2.21	0.40
2:D:296:LEU:HA	2:D:296:LEU:HD12	1.82	0.40
1:A:194:THR:OG1	1:A:195:ASP:N	2.55	0.40
2:B:230:LEU:HD11	2:B:266:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:TYR:CZ	2:D:169:GLN:HB3	2.56	0.40
2:D:188:THR:HG21	2:D:262:PRO:HA	2.03	0.40
1:A:30:PRO:HB2	2:D:385:VAL:HG21	2.03	0.40
1:C:93:LEU:HA	1:C:93:LEU:HD23	1.93	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	397/420 (94%)	373 (94%)	20 (5%)	4 (1%)	15 53
1	C	382/420 (91%)	354 (93%)	23 (6%)	5 (1%)	12 45
2	B	386/395 (98%)	367 (95%)	14 (4%)	5 (1%)	12 45
2	D	383/395 (97%)	366 (96%)	11 (3%)	6 (2%)	9 40
All	All	1548/1630 (95%)	1460 (94%)	68 (4%)	20 (1%)	12 45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	271	GLU
1	C	359	PRO
1	C	394	PRO
2	D	271	GLU
1	A	177	LYS
1	A	235	GLU
2	B	240	GLU
1	C	54	THR
2	D	240	GLU
2	D	369	GLN
2	B	196	GLU

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Mol	Chain	Res	Type
2	B	242	SER
2	D	196	GLU
2	D	242	SER
2	D	272	ASP
1	A	54	THR
1	A	362	GLU
1	C	311	HIS
1	C	362	GLU
2	B	272	ASP

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	326/384 (85%)	315 (97%)	11 (3%)	37	72
1	C	314/384 (82%)	300 (96%)	14 (4%)	27	64
2	B	317/356 (89%)	309 (98%)	8 (2%)	47	79
2	D	302/356 (85%)	290 (96%)	12 (4%)	31	68
All	All	1259/1480 (85%)	1214 (96%)	45 (4%)	35	70

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	53	CYS
1	A	99	LEU
1	A	213	MET
1	A	226	PHE
1	A	232	GLN
1	A	239	SER
1	A	278	ARG
1	A	285	LEU
1	A	333	HIS
1	A	396	LEU
2	B	64	MET

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Mol	Chain	Res	Type
2	B	71	ASN
2	B	129	MET
2	B	205	THR
2	B	206	ASN
2	B	296	LEU
2	B	312	VAL
2	B	341	THR
1	C	45	GLU
1	C	49	ARG
1	C	50	ASP
1	C	82	ILE
1	C	157	LEU
1	C	193	SER
1	C	206	LEU
1	C	226	PHE
1	C	235	GLU
1	C	236	PHE
1	C	333	HIS
1	C	343	LEU
1	C	387	HIS
1	C	389	ARG
2	D	33	PHE
2	D	100	ASN
2	D	104	LYS
2	D	107	THR
2	D	205	THR
2	D	240	GLU
2	D	274	THR
2	D	296	LEU
2	D	312	VAL
2	D	315	LEU
2	D	348	LEU
2	D	358	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	94	GLN
1	A	224	ASN
1	A	327	ASN
2	B	90	HIS

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Mol	Chain	Res	Type
2	B	97	ASN
2	B	169	GLN
1	C	142	ASN
1	C	335	ASN
2	D	169	GLN
2	D	245	HIS
2	D	335	GLN
2	D	379	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	399/420 (95%)	-0.23	3 (0%)	86	65	67, 99, 167, 199	0
1	C	388/420 (92%)	-0.19	2 (0%)	91	75	66, 103, 157, 191	0
2	B	390/395 (98%)	-0.17	1 (0%)	94	84	66, 100, 141, 171	0
2	D	387/395 (97%)	-0.17	3 (0%)	86	65	69, 102, 148, 194	0
All	All	1564/1630 (95%)	-0.19	9 (0%)	89	72	66, 101, 157, 199	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	3.0
2	D	25	TYR	2.9
2	B	276	LEU	2.8
1	C	281	SER	2.7
1	C	392	SER	2.6
2	D	65	GLU	2.4
2	D	12	LEU	2.4
1	A	338	PHE	2.2
1	A	387	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.