Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:44 AM EDT

PDB ID	:	5C6G
Title	:	Structural Insights into the Scc2-Scc4 Cohesin Loader
Authors	:	Singleton, M.R.; Chao, W.C.H.
Deposited on	:	2015-06-23
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

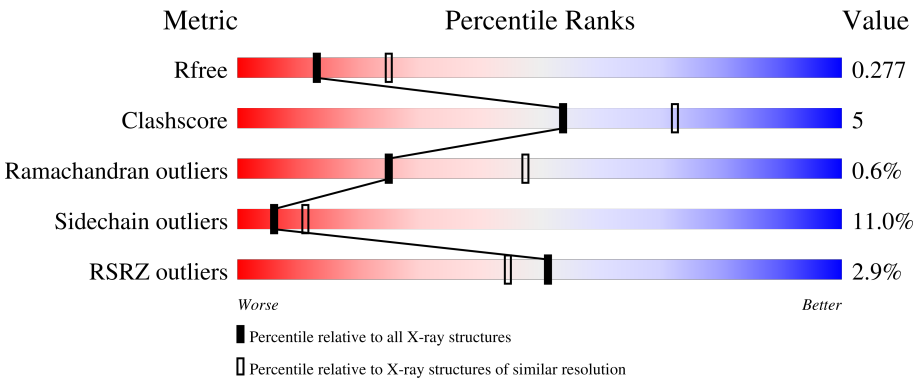
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	620	79% 17% • •
1	C	620	5% 77% 15% • 5%
2	B	218	% 40% 12% 5% 42%
2	D	218	4% 42% 13% 44%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11563 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 AGR133Cp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	605	4854	3097	833	901	23	0	0	0
1	C	588	4725	3016	811	875	23	0	0	0

- Molecule 2 is a protein called Sister chromatid cohesion protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	126	1006	629	180	195	2	0	0	0
2	D	121	968	606	174	186	2	0	0	0

- Molecule 3 is water.

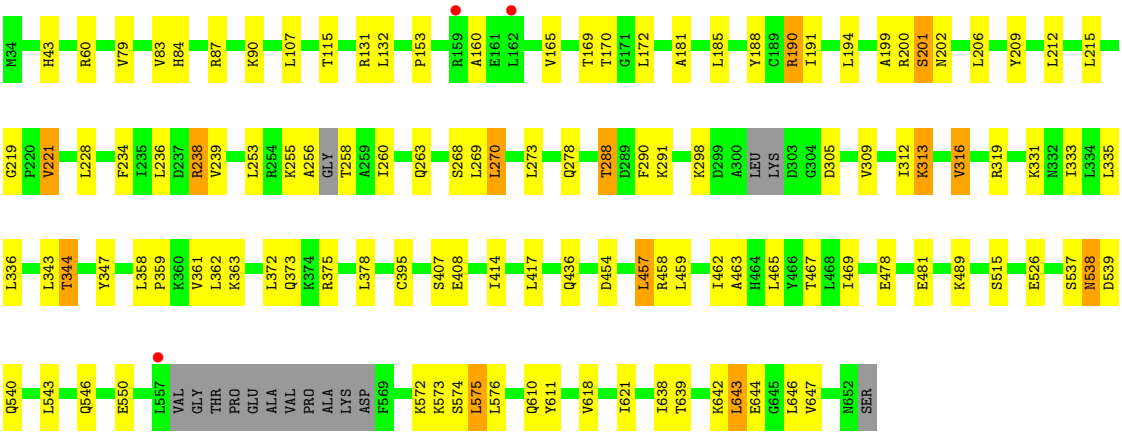
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
3	B	3	3	3	0	0
3	C	4	4	4	0	0
3	D	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

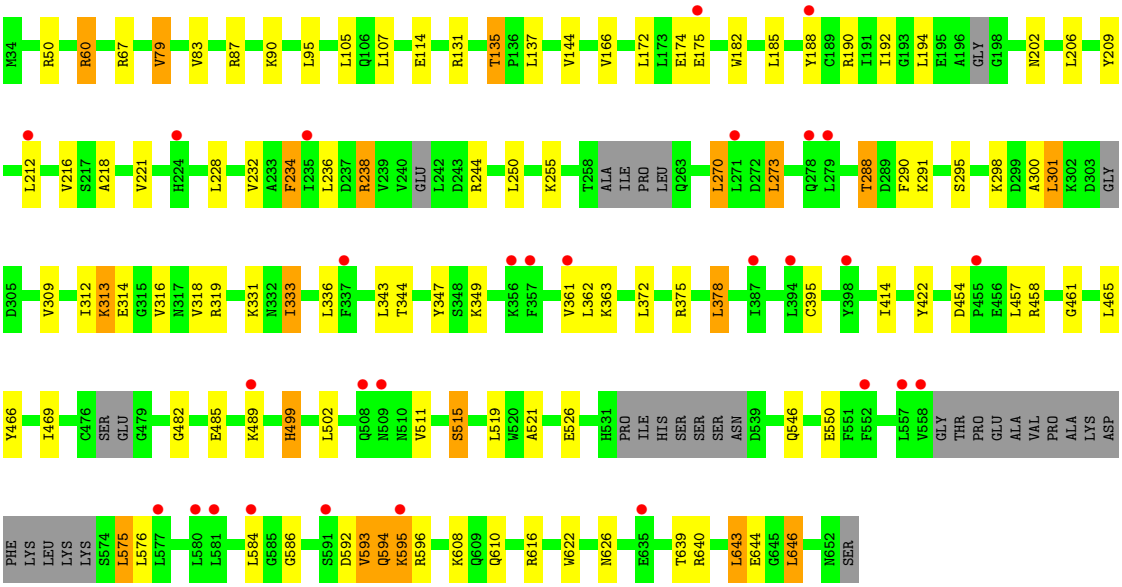
• Molecule 1: AGR133Cp

Chain A: 79% 17% • •



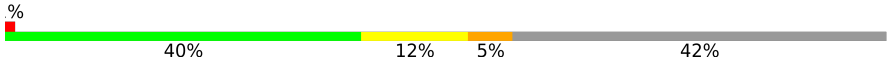
• Molecule 1: AGR133Cp

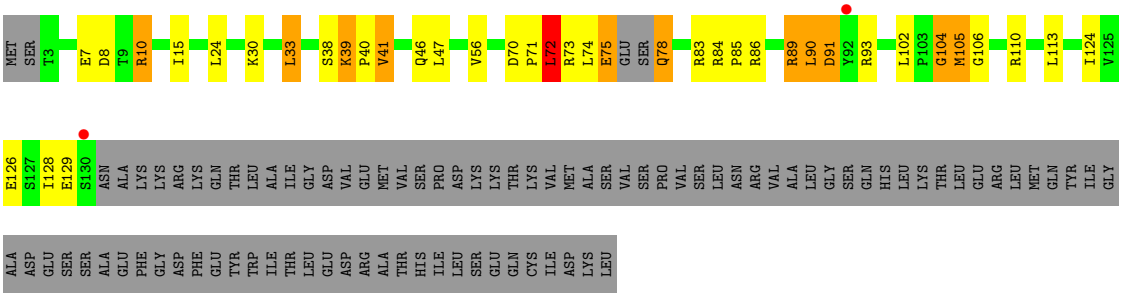
Chain C: 5% 77% 15% • 5%



• Molecule 2: Sister chromatid cohesion protein 2

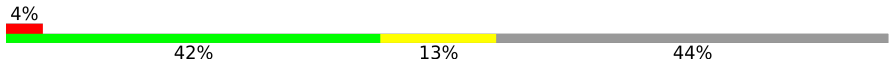
Chain B:

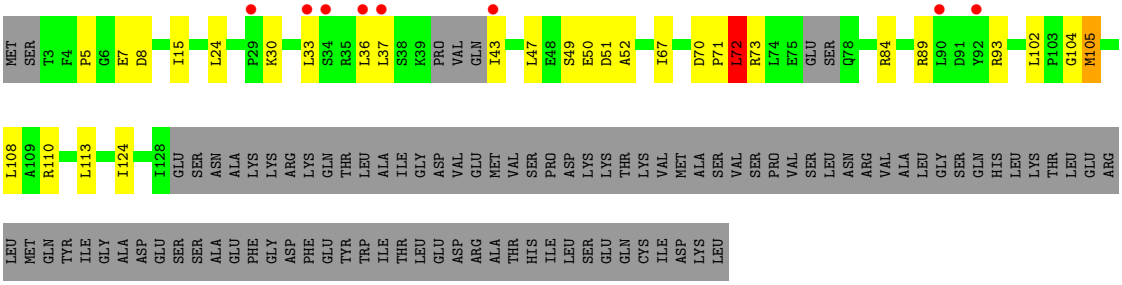




• Molecule 2: Sister chromatid cohesion protein 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.24Å 88.81Å 116.00Å 90.00° 118.49° 90.00°	Depositor
Resolution (Å)	98.65 – 2.60 98.65 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.7 (98.65-2.60) 96.8 (98.65-2.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.274 0.231 , 0.277	Depositor DCC
R_{free} test set	3198 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-l,k,h 0.008 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 (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	0.53	0/4939	0.65	0/6684
1	C	0.35	0/4802	0.53	1/6493 (0.0%)
2	B	0.48	0/1026	0.76	1/1391 (0.1%)
2	D	0.34	0/986	0.64	1/1334 (0.1%)
All	All	0.44	0/11753	0.61	3/15902 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	LEU	CA-CB-CG	5.39	127.71	115.30
2	D	36	LEU	CA-CB-CG	5.31	127.52	115.30
2	B	104	GLY	N-CA-C	-5.05	100.48	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	72	LEU	Peptide

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	4854	0	4922	46	0
1	C	4725	0	4792	46	0
2	B	1006	0	999	25	0
2	D	968	0	963	14	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	2	0
3	D	1	0	0	0	0
All	All	11563	0	11676	122	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 (122) 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:181:ALA:HB1	1:A:312:ILE:HD12	1.66	0.77
1:C:309:VAL:HG12	1:C:319:ARG:HG2	1.76	0.68
1:A:309:VAL:HG12	1:A:319:ARG:HG2	1.77	0.66
1:C:135:THR:HG23	1:C:137:LEU:H	1.61	0.66
1:A:221:VAL:HG13	1:A:260:ILE:HD13	1.79	0.65
2:D:104:GLY:HA2	2:D:105:MET:HB3	1.78	0.64
1:C:422:TYR:HE1	1:C:457:LEU:HD11	1.64	0.62
1:C:616:ARG:HD3	1:C:646:LEU:HD11	1.82	0.61
1:A:170:THR:OG1	1:A:190:ARG:NH1	2.34	0.61
1:A:465:LEU:O	1:A:469:ILE:HG12	2.01	0.60
1:C:234:PHE:HE1	1:C:238:ARG:HH11	1.49	0.60
2:B:30:LYS:O	2:B:33:LEU:HB2	2.00	0.60
1:C:67:ARG:HH11	2:D:93:ARG:HH12	1.49	0.59
2:B:84:ARG:NH1	2:B:124:ILE:O	2.37	0.58
1:A:191:ILE:HD13	1:A:209:TYR:CZ	2.39	0.57
1:A:199:ALA:C	1:A:201:SER:H	2.07	0.56
1:C:465:LEU:O	1:C:469:ILE:HG12	2.06	0.56
1:A:361:VAL:HG23	1:A:395:CYS:SG	2.45	0.56
2:B:84:ARG:HB2	2:B:124:ILE:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:SER:O	2:B:38:SER:OG	2.20	0.56
2:B:75:GLU:O	2:B:78:GLN:N	2.38	0.56
2:D:70:ASP:OD1	2:D:73:ARG:N	2.40	0.55
2:D:105:MET:O	2:D:110:ARG:NH1	2.40	0.55
1:C:232:VAL:HG21	1:C:250:LEU:HD13	1.90	0.53
1:C:575:LEU:HD23	1:C:610:GLN:HG2	1.90	0.53
2:B:38:SER:O	2:B:40:PRO:HD3	2.07	0.53
2:B:70:ASP:OD1	2:B:73:ARG:N	2.42	0.53
1:C:270:LEU:HD13	1:C:290:PHE:HZ	1.73	0.53
1:C:288:THR:HA	1:C:291:LYS:HD2	1.91	0.53
1:A:618:VAL:HG21	2:B:15:ILE:HD12	1.91	0.52
2:B:89:ARG:NH2	2:B:91:ASP:HB2	2.25	0.52
1:A:537:SER:N	1:A:538:ASN:HA	2.25	0.51
2:B:89:ARG:O	2:B:89:ARG:HG3	2.10	0.51
1:C:270:LEU:HD13	1:C:290:PHE:CZ	2.47	0.50
1:C:640:ARG:HG3	2:D:5:PRO:HG3	1.93	0.50
1:A:572:LYS:O	1:A:573:LYS:HB2	2.12	0.49
1:C:174:GLU:HA	1:C:175:GLU:HA	1.61	0.49
2:D:84:ARG:NH1	2:D:124:ILE:O	2.46	0.49
1:A:43:HIS:HB3	2:B:56:VAL:HG12	1.95	0.49
2:B:39:LYS:HD3	2:B:39:LYS:H	1.78	0.48
2:B:86:ARG:HH11	2:B:126:GLU:HB3	1.78	0.48
1:A:153:PRO:HG3	1:A:165:VAL:HG21	1.94	0.48
2:D:7:GLU:O	2:D:8:ASP:HB2	2.14	0.48
1:A:263:GLN:NE2	1:A:305:ASP:O	2.47	0.47
1:A:373:GLN:HG3	1:A:375:ARG:HH22	1.78	0.47
1:C:466:TYR:HE2	1:C:519:LEU:HB3	1.78	0.47
1:A:256:ALA:O	1:A:258:THR:N	2.47	0.47
1:A:288:THR:HA	1:A:291:LYS:HD2	1.96	0.47
1:C:295:SER:HA	1:C:298:LYS:HG3	1.97	0.47
1:A:335:LEU:HB3	1:A:361:VAL:CG1	2.45	0.47
1:A:160:ALA:HB1	2:D:8:ASP:HB3	1.97	0.46
1:A:373:GLN:HG3	1:A:375:ARG:NH2	2.30	0.46
1:C:461:GLY:O	1:C:465:LEU:HB2	2.15	0.46
2:D:67:ILE:HD12	2:D:108:LEU:HD11	1.97	0.46
2:B:106:GLY:O	2:B:110:ARG:HG3	2.16	0.46
2:D:84:ARG:HB2	2:D:124:ILE:HG22	1.98	0.46
1:C:511:VAL:O	1:C:515:SER:OG	2.30	0.46
1:A:313:LYS:HD2	1:A:316:VAL:HG13	1.98	0.46
1:C:188:TYR:O	1:C:192:ILE:HG12	2.16	0.46
2:B:71:PRO:O	2:B:72:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:LEU:HD12	2:B:73:ARG:HG2	1.98	0.45
1:C:79:VAL:O	1:C:83:VAL:HG23	2.17	0.45
1:A:188:TYR:O	1:A:191:ILE:HG13	2.16	0.45
1:A:458:ARG:O	1:A:462:ILE:HG13	2.15	0.45
1:A:269:LEU:HG	1:A:290:PHE:CE2	2.51	0.45
1:C:592:ASP:OD1	1:C:594:GLN:N	2.49	0.45
1:A:185:LEU:HD11	1:A:312:ILE:HD13	1.98	0.45
2:B:10:ARG:H	2:B:10:ARG:HG3	1.51	0.45
2:B:39:LYS:HZ1	2:B:41:VAL:HG22	1.81	0.45
1:A:347:TYR:CZ	1:A:575:LEU:HD13	2.51	0.45
1:C:216:VAL:C	1:C:218:ALA:H	2.20	0.44
1:A:239:VAL:HG12	1:A:278:GLN:NE2	2.33	0.44
2:B:104:GLY:HA2	2:B:105:MET:HB3	1.99	0.44
1:C:521:ALA:HB3	1:C:584:LEU:HD21	1.97	0.44
1:A:269:LEU:HG	1:A:290:PHE:CZ	2.52	0.44
2:B:90:LEU:HD12	2:B:90:LEU:HA	1.84	0.44
1:A:373:GLN:HE21	1:A:375:ARG:HH22	1.66	0.44
1:C:361:VAL:HG23	1:C:395:CYS:SG	2.58	0.44
1:C:454:ASP:HB3	1:C:457:LEU:HB2	1.99	0.44
1:A:234:PHE:CE1	1:A:238:ARG:HD3	2.53	0.44
1:A:643:LEU:O	1:A:647:VAL:HG13	2.18	0.44
2:B:91:ASP:OD1	2:B:93:ARG:HG2	2.17	0.44
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.89	0.43
1:C:626:ASN:ND2	3:C:701:HOH:O	2.50	0.43
1:A:115:THR:O	2:B:83:ARG:NE	2.47	0.43
1:C:319:ARG:O	2:D:43:ILE:HA	2.18	0.43
1:C:575:LEU:HD12	1:C:575:LEU:HA	1.77	0.43
1:C:166:VAL:HG13	1:C:190:ARG:HG3	2.00	0.43
1:C:50:ARG:HD3	1:C:50:ARG:HA	1.72	0.42
1:C:185:LEU:HD21	1:C:318:VAL:HG21	2.00	0.42
1:C:333:ILE:HD13	2:D:37:LEU:HD21	2.00	0.42
1:C:596:ARG:O	3:C:701:HOH:O	2.21	0.42
1:C:499:HIS:HA	1:C:502:LEU:HD12	2.01	0.42
1:A:537:SER:H	1:A:538:ASN:HA	1.83	0.42
1:A:639:THR:HG22	1:A:643:LEU:HD22	2.00	0.42
2:B:7:GLU:O	2:B:8:ASP:CG	2.57	0.42
1:C:593:VAL:HG13	1:C:596:ARG:NH2	2.35	0.42
1:A:344:THR:HG21	1:A:574:SER:OG	2.18	0.42
1:A:199:ALA:C	1:A:201:SER:N	2.73	0.42
1:A:454:ASP:HB3	1:A:457:LEU:HB2	2.00	0.42
1:A:638:ILE:HG13	1:A:642:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HD21	1:C:144:VAL:HG22	2.01	0.41
1:A:408:GLU:HB2	1:A:611:TYR:CZ	2.55	0.41
1:C:60:ARG:NH2	1:C:114:GLU:OE1	2.35	0.41
1:A:358:LEU:N	1:A:359:PRO:HD2	2.35	0.41
1:C:312:ILE:HG13	1:C:313:LYS:N	2.36	0.41
2:B:84:ARG:HA	2:B:85:PRO:HD3	1.92	0.41
1:A:270:LEU:HD13	1:A:290:PHE:HZ	1.85	0.41
1:C:592:ASP:HB3	1:C:595:LYS:HG2	2.02	0.41
1:A:575:LEU:HD23	1:A:610:GLN:HG2	2.03	0.41
1:C:586:GLY:HA3	1:C:622:TRP:HH2	1.86	0.41
2:D:71:PRO:O	2:D:72:LEU:HD23	2.21	0.41
1:C:349:LYS:HD2	1:C:349:LYS:HA	1.93	0.40
1:A:270:LEU:HD13	1:A:290:PHE:CZ	2.56	0.40
1:A:463:ALA:O	1:A:467:THR:HG23	2.21	0.40
1:C:347:TYR:CE2	1:C:575:LEU:HD22	2.56	0.40
1:C:639:THR:O	1:C:643:LEU:HB2	2.22	0.40
1:A:84:HIS:NE2	2:B:74:LEU:HD13	2.36	0.40
1:C:482:GLY:O	1:C:485:GLU:HG2	2.21	0.40
1:A:79:VAL:O	1:A:83:VAL:HG23	2.22	0.40
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.80	0.40
2:D:30:LYS:O	2:D:33:LEU:HB2	2.21	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	597/620 (96%)	576 (96%)	20 (3%)	1 (0%)	47 71
1	C	572/620 (92%)	552 (96%)	19 (3%)	1 (0%)	47 71
2	B	122/218 (56%)	111 (91%)	8 (7%)	3 (2%)	5 9
2	D	115/218 (53%)	103 (90%)	8 (7%)	4 (4%)	3 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1406/1676 (84%)	1342 (95%)	55 (4%)	9 (1%)	25 47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLY
2	B	72	LEU
2	D	72	LEU
2	D	51	ASP
2	B	105	MET
1	C	300	ALA
2	D	52	ALA
2	D	105	MET
2	B	41	VAL

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	541/552 (98%)	480 (89%)	61 (11%)	6 10
1	C	526/552 (95%)	470 (89%)	56 (11%)	6 12
2	B	113/194 (58%)	97 (86%)	16 (14%)	3 5
2	D	108/194 (56%)	99 (92%)	9 (8%)	11 22
All	All	1288/1492 (86%)	1146 (89%)	142 (11%)	6 11

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	87	ARG
1	A	90	LYS
1	A	107	LEU
1	A	131	ARG
1	A	132	LEU

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Mol	Chain	Res	Type
1	A	169	THR
1	A	172	LEU
1	A	190	ARG
1	A	194	LEU
1	A	200	ARG
1	A	201	SER
1	A	202	ASN
1	A	206	LEU
1	A	212	LEU
1	A	215	LEU
1	A	221	VAL
1	A	228	LEU
1	A	236	LEU
1	A	238	ARG
1	A	253	LEU
1	A	255	LYS
1	A	268	SER
1	A	270	LEU
1	A	273	LEU
1	A	288	THR
1	A	298	LYS
1	A	313	LYS
1	A	316	VAL
1	A	331	LYS
1	A	333	ILE
1	A	336	LEU
1	A	343	LEU
1	A	344	THR
1	A	362	LEU
1	A	363	LYS
1	A	372	LEU
1	A	378	LEU
1	A	407	SER
1	A	414	ILE
1	A	417	LEU
1	A	436	GLN
1	A	457	LEU
1	A	459	LEU
1	A	478	GLU
1	A	481	GLU
1	A	489	LYS
1	A	515	SER

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Mol	Chain	Res	Type
1	A	526	GLU
1	A	538	ASN
1	A	539	ASP
1	A	540	GLN
1	A	543	LEU
1	A	546	GLN
1	A	550	GLU
1	A	575	LEU
1	A	576	LEU
1	A	621	ILE
1	A	643	LEU
1	A	644	GLU
1	A	646	LEU
2	B	10	ARG
2	B	24	LEU
2	B	33	LEU
2	B	39	LYS
2	B	46	GLN
2	B	47	LEU
2	B	72	LEU
2	B	75	GLU
2	B	78	GLN
2	B	89	ARG
2	B	90	LEU
2	B	91	ASP
2	B	102	LEU
2	B	113	LEU
2	B	128	ILE
2	B	129	GLU
1	C	60	ARG
1	C	79	VAL
1	C	87	ARG
1	C	90	LYS
1	C	95	LEU
1	C	107	LEU
1	C	131	ARG
1	C	135	THR
1	C	172	LEU
1	C	182	TRP
1	C	194	LEU
1	C	202	ASN
1	C	206	LEU

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Mol	Chain	Res	Type
1	C	209	TYR
1	C	212	LEU
1	C	221	VAL
1	C	228	LEU
1	C	234	PHE
1	C	236	LEU
1	C	238	ARG
1	C	244	ARG
1	C	255	LYS
1	C	270	LEU
1	C	273	LEU
1	C	288	THR
1	C	301	LEU
1	C	313	LYS
1	C	314	GLU
1	C	316	VAL
1	C	331	LYS
1	C	333	ILE
1	C	336	LEU
1	C	343	LEU
1	C	344	THR
1	C	362	LEU
1	C	363	LYS
1	C	372	LEU
1	C	375	ARG
1	C	378	LEU
1	C	414	ILE
1	C	458	ARG
1	C	489	LYS
1	C	499	HIS
1	C	515	SER
1	C	526	GLU
1	C	546	GLN
1	C	550	GLU
1	C	575	LEU
1	C	576	LEU
1	C	593	VAL
1	C	594	GLN
1	C	595	LYS
1	C	608	LYS
1	C	643	LEU
1	C	644	GLU

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Mol	Chain	Res	Type
1	C	646	LEU
2	D	15	ILE
2	D	24	LEU
2	D	47	LEU
2	D	49	SER
2	D	50	GLU
2	D	72	LEU
2	D	89	ARG
2	D	102	LEU
2	D	113	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	106	GLN
1	A	202	ASN
1	A	366	GLN
1	A	373	GLN
1	A	380	HIS
1	A	441	HIS
1	A	541	GLN
1	A	623	HIS
2	B	42	GLN
1	C	53	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 monosaccharides 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	605/620 (97%)	-0.16	3 (0%)	91	89	46, 65, 102, 136	0
1	C	588/620 (94%)	0.31	29 (4%)	29	23	61, 116, 150, 179	0
2	B	126/218 (57%)	-0.09	2 (1%)	72	68	49, 70, 112, 137	0
2	D	121/218 (55%)	0.18	8 (6%)	18	13	70, 106, 143, 162	0
All	All	1440/1676 (85%)	0.06	42 (2%)	51	45	46, 88, 141, 179	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	558	VAL	5.1
1	A	557	LEU	4.9
1	C	557	LEU	4.5
1	C	595	LYS	4.1
1	C	580	LEU	3.9
1	C	356	LYS	3.7
1	C	357	PHE	3.6
2	D	92	TYR	3.6
1	C	577	LEU	3.3
1	A	159	ARG	3.2
1	C	455	PRO	3.2
2	D	90	LEU	3.2
2	D	34	SER	3.2
1	C	552	PHE	3.2
2	D	29	PRO	3.1
1	C	212	LEU	2.9
1	C	337	PHE	2.8
1	C	188	TYR	2.7
2	D	36	LEU	2.7
1	C	581	LEU	2.6
1	C	271	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	387	ILE	2.5
2	D	33	LEU	2.5
1	C	584	LEU	2.4
2	D	43	ILE	2.4
1	C	224	HIS	2.3
1	C	278	GLN	2.3
1	C	398	TYR	2.3
1	C	489	LYS	2.3
1	C	508	GLN	2.3
1	C	509	ASN	2.3
2	D	37	LEU	2.3
1	A	162	LEU	2.2
1	C	175	GLU	2.2
1	C	635	GLU	2.2
1	C	361	VAL	2.2
1	C	279	LEU	2.1
1	C	591	SER	2.1
2	B	92	TYR	2.1
2	B	130	SER	2.1
1	C	235	ILE	2.1
1	C	394	LEU	2.1

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 monosaccharides 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.