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wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 06:41 pm BST

PDB ID	:	4LCT
Title	:	Crystal Structure and Versatile Functional Roles of the COP9 Signalosome Subunit 1
Authors	:	Lee, J.-H.; Yi, L.; Li, J.; Schweitzer, K.; Borgmann, M.; Naumann, M.; Wu, H.
Deposited on	:	2013-06-23
Resolution	:	2.70 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 (i)) were used in the production of this report:

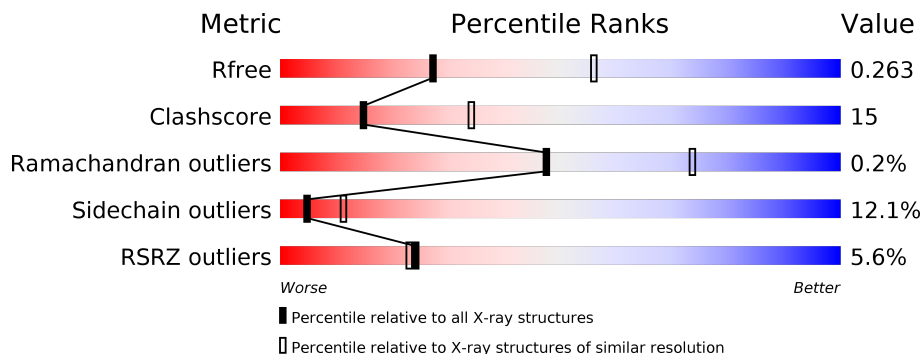|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.70 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		0.263
Clashscore		15
Ramachandran outliers		0.2%
Sidechain outliers		12.1%
RSRZ outliers		5.6%

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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.

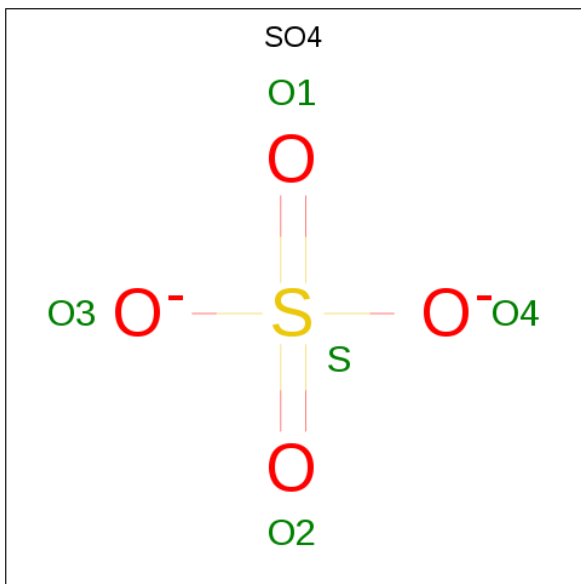| Mol	Chain	Length	Quality of chain
1	A	348	71% 18% •• 9%
1	B	348	3% 72% 24% ••
1	C	348	9% 57% 27% 7% 8%
1	D	348	9% 61% 32% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10840 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2568	1631	444	476	17			
1	B	348	Total	C	N	O	S	0	0	0
			2796	1775	479	524	18			
1	C	321	Total	C	N	O	S	0	0	0
			2592	1648	447	480	17			
1	D	348	Total	C	N	O	S	0	0	0
			2796	1775	479	524	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	23	Total 23	O 23	0	0
3	C	10	Total 10	O 10	0	0
3	D	16	Total 16	O 16	0	0

3 Residue-property plots ⓘ

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.
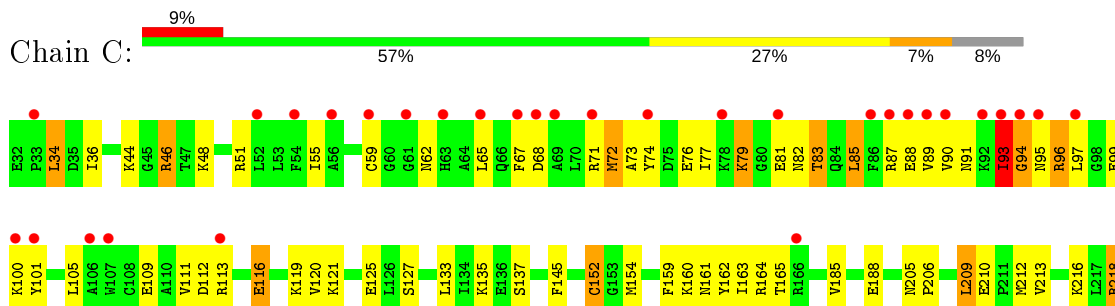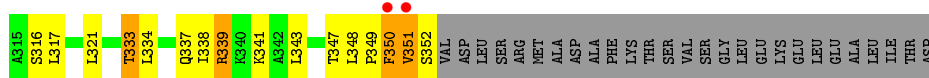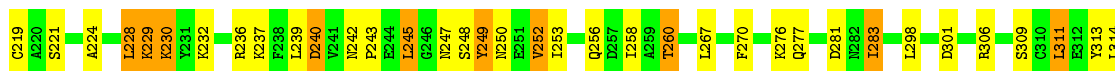
- Molecule 1: COP9 signalosome complex subunit 1
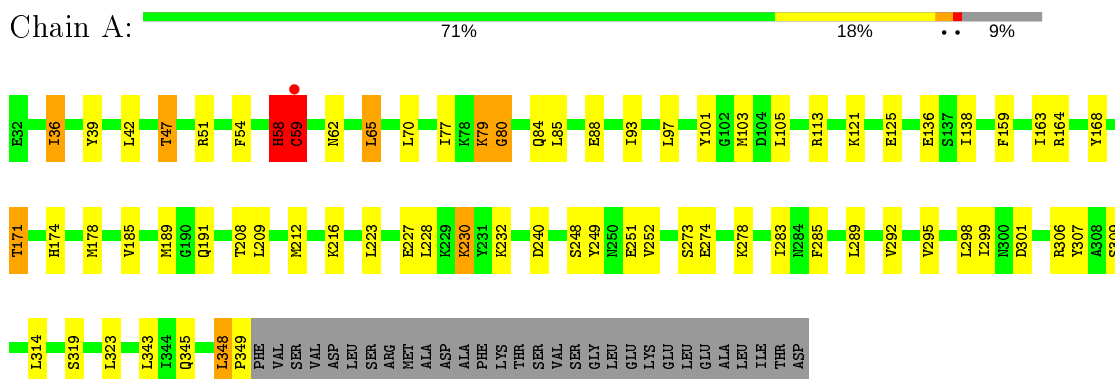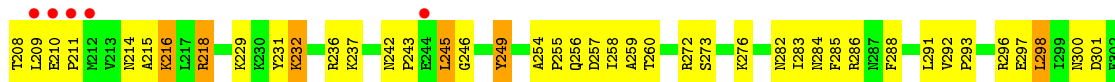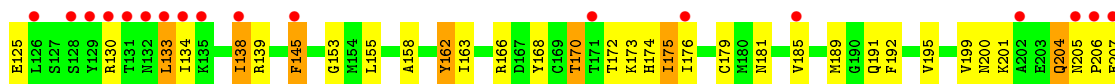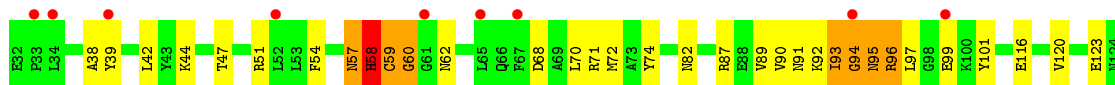

- Molecule 1: COP9 signalosome complex subunit 1

- Molecule 1: COP9 signalosome complex subunit 1

• Molecule 1: COP9 signalosome complex subunit 1

Chain D:
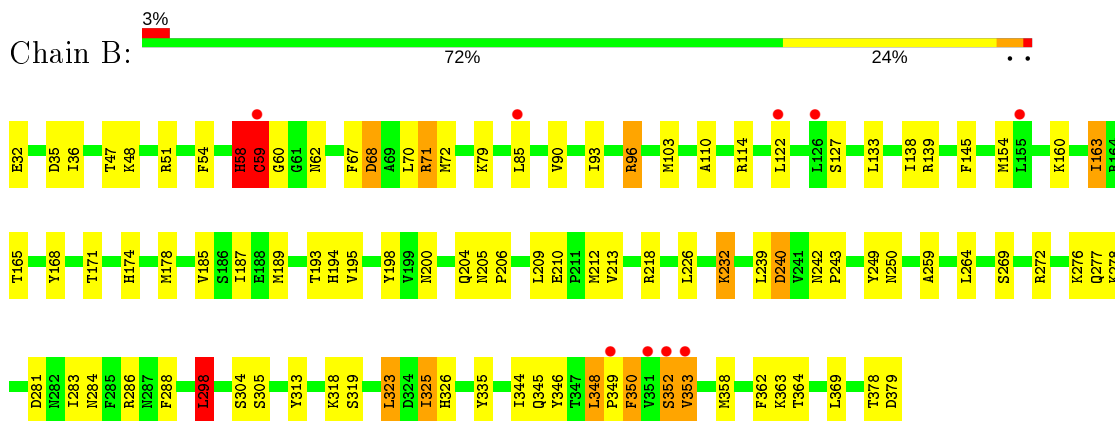
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	202.21Å 87.09Å 133.60Å 90.00° 105.47° 90.00°	Depositor
Resolution (Å)	48.70 – 2.70 48.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.70-2.70) 99.7 (48.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.224 , 0.272 0.214 , 0.263	Depositor DCC
R_{free} test set	3078 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.0	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	0.94	EDS
Total number of atoms	10840	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: SO4

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	0.52	0/2616	0.69	4/3526 (0.1%)
1	B	0.49	1/2846 (0.0%)	0.66	2/3836 (0.1%)
1	C	0.47	0/2641	0.62	0/3560
1	D	0.44	0/2846	0.61	2/3836 (0.1%)
All	All	0.48	1/10949 (0.0%)	0.64	8/14758 (0.1%)

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
1	B	0	3
1	C	0	3
1	D	0	6
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	CYS	CB-SG	5.59	1.91	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	CYS	N-CA-C	-7.33	91.20	111.00
1	A	79	LYS	N-CA-C	6.61	128.86	111.00
1	D	59	CYS	N-CA-C	-6.45	93.59	111.00
1	B	298	LEU	CA-CB-CG	6.39	129.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	LYS	C-N-CA	6.33	135.60	122.30
1	A	59	CYS	N-CA-C	-5.39	96.44	111.00
1	A	80	GLY	N-CA-C	-5.19	100.11	113.10
1	D	60	GLY	N-CA-C	-5.16	100.20	113.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	HIS	Peptide
1	A	79	LYS	Peptide
1	B	352	SER	Peptide
1	B	58	HIS	Peptide
1	B	79	LYS	Peptide
1	C	351	VAL	Peptide
1	C	59	CYS	Peptide
1	C	94	GLY	Peptide
1	D	206	PRO	Peptide
1	D	208	THR	Peptide
1	D	57	ASN	Peptide
1	D	58	HIS	Peptide
1	D	94	GLY	Peptide
1	D	95	ASN	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	2568	0	2563	49	0
1	B	2796	0	2793	96	0
1	C	2592	0	2586	96	0
1	D	2796	0	2793	92	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	0	1	0
3	C	10	0	0	1	0
3	D	16	0	0	1	0
All	All	10840	0	10735	327	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 15.

All (327) 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:D:93:ILE:HG12	1:D:94:GLY:H	1.06	1.17
1:D:200:ASN:O	1:D:204:GLN:HB2	1.40	1.14
1:B:350:PHE:HB2	1:B:353:VAL:HA	1.31	1.08
1:B:344:ILE:O	1:B:348:LEU:HD12	1.63	0.97
1:D:93:ILE:CG1	1:D:94:GLY:N	2.30	0.94
1:B:348:LEU:C	1:B:348:LEU:HD13	1.87	0.94
1:C:62:ASN:HB2	1:C:65:LEU:HB2	1.48	0.94
1:D:93:ILE:HG12	1:D:94:GLY:N	1.76	0.94
1:A:348:LEU:HD12	1:A:349:PRO:HD2	1.48	0.93
1:D:130:ARG:O	1:D:133:LEU:HD12	1.71	0.91
1:B:348:LEU:O	1:B:348:LEU:HD13	1.69	0.91
1:C:73:ALA:O	1:C:77:ILE:HB	1.71	0.90
1:B:54:PHE:CE1	1:B:58:HIS:HE1	1.91	0.88
1:C:46:ARG:HD3	1:C:188:GLU:HG2	1.56	0.88
1:C:267:LEU:HD23	1:C:338:ILE:HD13	1.56	0.87
1:A:103:MET:HE2	1:A:105:LEU:HD23	1.56	0.87
1:D:59:CYS:SG	1:D:60:GLY:N	2.48	0.86
1:B:348:LEU:HD21	1:B:350:PHE:CD1	2.12	0.84
1:B:54:PHE:CE1	1:B:58:HIS:CE1	2.66	0.84
1:A:171:THR:HG22	1:A:174:HIS:H	1.42	0.83
1:B:348:LEU:HD22	1:B:349:PRO:N	1.94	0.83
1:C:93:ILE:HG23	1:C:94:GLY:H	1.43	0.83
1:D:93:ILE:CG1	1:D:94:GLY:H	1.86	0.82
1:B:59:CYS:HB2	1:B:323:LEU:HD11	1.62	0.81
1:C:216:LYS:HE2	1:C:248:SER:OG	1.81	0.81
1:A:230:LYS:HE3	1:A:232:LYS:HB3	1.62	0.81
1:B:348:LEU:HD21	1:B:350:PHE:CG	2.15	0.81
1:C:97:LEU:HB3	1:C:101:TYR:HD2	1.46	0.80
1:D:57:ASN:HD21	1:D:92:LYS:HD2	1.46	0.80
1:C:350:PHE:CD1	1:C:351:VAL:HA	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:VAL:HG22	1:C:352:SER:C	2.04	0.78
1:C:77:ILE:HD11	1:C:85:LEU:HB3	1.66	0.77
1:C:351:VAL:HG13	1:C:352:SER:N	1.99	0.77
1:A:97:LEU:HB2	1:A:101:TYR:HB2	1.68	0.76
1:C:67:PHE:CE1	1:C:97:LEU:HD22	2.21	0.76
1:A:59:CYS:HB2	1:A:323:LEU:HD21	1.67	0.75
1:A:54:PHE:CE1	1:A:58:HIS:CE1	2.75	0.75
1:A:185:VAL:HG12	1:A:189:MET:CE	2.17	0.74
1:C:159:PHE:HB2	1:C:185:VAL:HG11	1.69	0.74
1:C:89:VAL:O	1:C:93:ILE:HG22	1.86	0.73
1:C:34:LEU:O	1:C:34:LEU:HD23	1.88	0.73
1:A:54:PHE:CD1	1:A:58:HIS:HE1	2.06	0.73
1:C:67:PHE:HE1	1:C:97:LEU:HD22	1.54	0.72
1:A:36:ILE:H	1:A:36:ILE:HD13	1.54	0.71
1:D:255:PRO:HA	1:D:258:ILE:HD12	1.73	0.70
1:B:51:ARG:CZ	1:B:325:ILE:HD11	2.21	0.69
1:D:70:LEU:HD22	1:D:93:ILE:CG2	2.22	0.69
1:B:350:PHE:CB	1:B:353:VAL:HA	2.19	0.69
1:B:163:ILE:HD11	1:B:198:TYR:CE2	2.27	0.69
1:B:54:PHE:CD1	1:B:58:HIS:HE1	2.11	0.68
1:C:77:ILE:HD11	1:C:85:LEU:C	2.13	0.68
1:C:253:ILE:CD1	1:C:258:ILE:HG13	2.24	0.67
1:B:36:ILE:HD11	1:B:68:ASP:HB3	1.77	0.66
1:B:193:THR:HG23	1:B:194:HIS:CD2	2.31	0.66
1:D:170:THR:H	1:D:174:HIS:HD2	1.43	0.66
1:C:301:ASP:OD1	1:C:306:ARG:HD2	1.96	0.66
1:B:193:THR:HG23	1:B:194:HIS:HD2	1.61	0.65
1:C:95:ASN:O	1:C:96:ARG:HD3	1.97	0.65
1:A:185:VAL:HG12	1:A:189:MET:HE2	1.77	0.65
1:D:87:ARG:O	1:D:91:ASN:HB2	1.95	0.65
1:D:276:LYS:HG3	1:D:303:TYR:OH	1.97	0.65
1:C:350:PHE:CG	1:C:351:VAL:HA	2.33	0.64
1:C:97:LEU:HD23	1:C:101:TYR:CE2	2.32	0.64
1:D:70:LEU:HD22	1:D:93:ILE:HG21	1.79	0.64
1:C:252:VAL:HG12	1:C:253:ILE:HG22	1.77	0.64
1:B:243:PRO:HG3	1:B:284:ASN:HB3	1.79	0.63
1:D:283:ILE:O	1:D:286:ARG:HB2	1.97	0.63
1:C:351:VAL:HG13	1:C:352:SER:H	1.64	0.63
1:A:54:PHE:CD1	1:A:58:HIS:CE1	2.87	0.63
1:B:139:ARG:HG3	1:B:165:THR:HB	1.81	0.63
1:D:243:PRO:HG3	1:D:284:ASN:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:HD13	1:B:286:ARG:NH1	2.14	0.63
1:B:348:LEU:HD21	1:B:350:PHE:CE1	2.34	0.62
1:D:166:ARG:HH12	1:D:201:LYS:HE2	1.63	0.62
1:B:218:ARG:NH2	1:B:240:ASP:HB3	2.14	0.62
1:B:36:ILE:HD12	1:B:72:MET:HE3	1.81	0.62
1:B:193:THR:HG23	1:B:194:HIS:N	2.14	0.62
1:C:256:GLN:O	1:C:260:THR:HG22	2.01	0.61
1:B:160:LYS:O	1:B:163:ILE:HG22	2.00	0.61
1:C:270:PHE:O	1:C:341:LYS:HE2	2.01	0.61
1:B:54:PHE:CZ	1:B:58:HIS:CE1	2.89	0.61
1:C:152:CYS:SG	1:C:154:MET:HG2	2.40	0.61
1:C:247:ASN:HB2	1:C:250:ASN:HB3	1.83	0.60
1:B:350:PHE:HD1	1:B:353:VAL:HG12	1.66	0.60
1:A:298:LEU:HD11	1:A:314:LEU:HD23	1.83	0.60
1:C:298:LEU:HD11	1:C:314:LEU:HG	1.83	0.60
1:C:348:LEU:HD12	1:C:349:PRO:HD2	1.82	0.60
1:C:74:TYR:O	1:C:77:ILE:HG22	2.00	0.60
1:C:253:ILE:HD11	1:C:258:ILE:HG13	1.83	0.59
1:C:113:ARG:O	1:C:116:GLU:HG3	2.02	0.59
1:A:274:GLU:HG3	1:A:278:LYS:HD2	1.83	0.59
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.68	0.58
1:B:348:LEU:HD21	1:B:350:PHE:CD2	2.38	0.58
1:B:93:ILE:O	1:B:96:ARG:HG3	2.01	0.58
1:A:343:LEU:HD23	1:B:362:PHE:CE1	2.39	0.58
1:C:73:ALA:O	1:C:77:ILE:CB	2.49	0.58
1:D:354:ASP:OD2	1:D:357:ARG:HG3	2.03	0.58
1:D:89:VAL:O	1:D:93:ILE:HG23	2.04	0.57
1:C:232:LYS:HE3	1:C:236:ARG:NH2	2.18	0.57
1:A:185:VAL:HG12	1:A:189:MET:HE3	1.85	0.57
1:B:138:ILE:HG21	1:B:168:TYR:CE1	2.40	0.57
1:D:216:LYS:HG3	1:D:249:TYR:CG	2.40	0.57
1:C:36:ILE:HG12	1:C:72:MET:HE2	1.88	0.56
1:C:97:LEU:HD23	1:C:101:TYR:HE2	1.68	0.56
1:D:298:LEU:HD12	1:D:313:TYR:HB3	1.88	0.56
1:B:259:ALA:HB2	1:B:288:PHE:HB3	1.87	0.56
1:C:121:LYS:O	1:C:125:GLU:HG3	2.06	0.56
1:B:59:CYS:SG	1:B:323:LEU:HD13	2.45	0.56
1:B:283:ILE:HD13	1:B:286:ARG:HH12	1.70	0.55
1:C:212:MET:O	1:C:216:LYS:HG3	2.05	0.55
1:B:71:ARG:HG2	1:B:71:ARG:NH1	2.20	0.55
1:B:171:THR:HG22	1:B:174:HIS:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:HG23	3:B:519:HOH:O	2.07	0.55
1:C:313:TYR:O	1:C:317:LEU:HG	2.06	0.55
1:D:254:ALA:O	1:D:257:ASP:HB2	2.06	0.55
1:D:96:ARG:C	1:D:97:LEU:HD23	2.27	0.55
1:C:210:GLU:HG2	1:C:213:VAL:HG23	1.88	0.55
1:B:350:PHE:CD1	1:B:353:VAL:HG12	2.41	0.55
1:C:83:THR:HG21	1:C:112:ASP:OD1	2.06	0.55
1:C:162:TYR:O	1:C:165:THR:HB	2.07	0.55
1:D:54:PHE:CZ	1:D:58:HIS:NE2	2.74	0.55
1:D:181:ASN:O	1:D:185:VAL:HG23	2.06	0.55
1:D:93:ILE:HG13	1:D:94:GLY:N	2.22	0.54
1:A:348:LEU:CD1	1:A:349:PRO:HD2	2.29	0.54
1:B:51:ARG:HG2	1:B:325:ILE:HG12	1.88	0.54
1:C:90:VAL:HG12	1:C:91:ASN:N	2.21	0.54
1:A:301:ASP:OD2	1:A:309:SER:OG	2.20	0.54
1:C:36:ILE:HG12	1:C:72:MET:CE	2.36	0.54
1:D:341:LYS:O	1:D:345:GLN:HG3	2.07	0.54
1:B:185:VAL:O	1:B:189:MET:HG3	2.07	0.54
1:B:193:THR:HG23	1:B:194:HIS:H	1.73	0.54
1:C:224:ALA:O	1:C:228:LEU:HD22	2.08	0.54
1:D:256:GLN:O	1:D:260:THR:HG23	2.07	0.54
1:A:295:VAL:O	1:A:299:ILE:HG13	2.08	0.54
1:D:243:PRO:HA	1:D:288:PHE:CE2	2.43	0.54
1:B:200:ASN:O	1:B:204:GLN:HG3	2.08	0.54
1:B:350:PHE:CD1	1:B:353:VAL:O	2.60	0.54
1:C:82:ASN:ND2	1:C:85:LEU:HD23	2.24	0.53
1:D:116:GLU:O	1:D:120:VAL:HG23	2.07	0.53
1:C:77:ILE:HD11	1:C:85:LEU:O	2.08	0.53
1:D:97:LEU:HD23	1:D:97:LEU:N	2.24	0.53
1:C:242:ASN:OD1	1:C:243:PRO:HD2	2.08	0.53
1:C:93:ILE:O	1:C:96:ARG:NH1	2.42	0.53
1:A:227:GLU:HA	1:A:227:GLU:OE1	2.09	0.53
1:C:245:LEU:HD11	1:C:249:TYR:HB2	1.91	0.53
1:C:95:ASN:C	1:C:96:ARG:HD3	2.29	0.53
1:D:232:LYS:HG3	1:D:236:ARG:HE	1.74	0.53
1:D:207:GLU:O	1:D:209:LEU:HD13	2.09	0.52
1:D:304:SER:O	1:D:305:SER:HB2	2.08	0.52
1:B:36:ILE:HG13	1:B:72:MET:HE1	1.91	0.52
1:C:161:ASN:HA	1:C:164:ARG:HB2	1.91	0.52
1:C:76:GLU:O	1:C:79:LYS:HB2	2.10	0.52
1:D:54:PHE:CG	1:D:325:ILE:HG13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HE2	1:A:125:GLU:OE2	2.10	0.52
1:B:298:LEU:C	1:B:298:LEU:HD23	2.30	0.52
1:D:211:PRO:O	1:D:214:ASN:HB2	2.09	0.52
1:B:171:THR:HG22	1:B:174:HIS:CG	2.45	0.51
1:D:138:ILE:HD11	1:D:168:TYR:CD1	2.45	0.51
1:A:136:GLU:OE1	1:A:136:GLU:HA	2.10	0.51
1:A:159:PHE:HB2	1:A:189:MET:HE2	1.93	0.51
1:D:185:VAL:O	1:D:189:MET:HG3	2.10	0.51
1:D:82:ASN:ND2	1:D:153:GLY:HA3	2.26	0.51
1:B:218:ARG:CZ	1:B:240:ASP:HB3	2.41	0.51
1:C:46:ARG:NH1	1:C:188:GLU:HG3	2.26	0.51
1:D:260:THR:HG22	1:D:292:VAL:HG11	1.92	0.51
1:C:333:THR:O	1:C:337:GLN:HG3	2.11	0.51
1:B:318:LYS:HG3	1:B:335:TYR:CE1	2.47	0.50
1:D:288:PHE:O	1:D:291:LEU:HB2	2.11	0.50
1:D:200:ASN:O	1:D:204:GLN:CB	2.34	0.50
1:B:47:THR:OG1	1:B:51:ARG:NH2	2.44	0.50
1:C:252:VAL:HG12	1:C:253:ILE:N	2.27	0.50
1:C:74:TYR:CD2	1:C:101:TYR:HD1	2.29	0.50
1:D:158:ALA:O	1:D:162:TYR:HB2	2.12	0.50
1:A:97:LEU:HB2	1:A:101:TYR:CB	2.40	0.50
1:A:58:HIS:ND1	1:A:58:HIS:N	2.58	0.50
1:C:160:LYS:HE3	1:C:164:ARG:NH1	2.27	0.49
1:B:350:PHE:HD1	1:B:353:VAL:CB	2.25	0.49
1:B:36:ILE:HD12	1:B:72:MET:CE	2.42	0.49
1:B:193:THR:CG2	1:B:194:HIS:N	2.76	0.49
1:C:87:ARG:O	1:C:91:ASN:HB2	2.12	0.49
1:A:171:THR:CG2	1:A:174:HIS:H	2.20	0.49
1:D:158:ALA:O	1:D:162:TYR:CD1	2.66	0.48
1:B:276:LYS:HE2	1:B:281:ASP:OD2	2.13	0.48
1:D:246:GLY:O	1:D:255:PRO:HG3	2.13	0.48
1:D:60:GLY:C	1:D:62:ASN:H	2.16	0.48
1:B:277:GLN:HG2	1:B:278:LYS:HG3	1.95	0.48
1:D:191:GLN:O	1:D:195:VAL:HG23	2.13	0.48
1:D:255:PRO:HB2	1:D:291:LEU:HD12	1.95	0.48
1:D:218:ARG:NH1	1:D:237:LYS:NZ	2.61	0.48
1:D:59:CYS:C	1:D:60:GLY:O	2.52	0.48
1:A:230:LYS:HD2	1:A:230:LYS:C	2.33	0.48
1:B:348:LEU:C	1:B:348:LEU:HD22	2.32	0.48
1:C:62:ASN:CB	1:C:65:LEU:HB2	2.32	0.48
1:B:358:MET:HB3	1:B:369:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ARG:HH11	1:C:188:GLU:CG	2.27	0.47
1:D:340:LYS:HD3	1:D:370:GLU:HB3	1.95	0.47
1:D:175:ILE:HG12	1:D:175:ILE:H	1.46	0.47
1:D:301:ASP:OD2	1:D:309:SER:HB3	2.14	0.47
1:D:232:LYS:CG	1:D:236:ARG:HE	2.28	0.47
1:D:47:THR:HG23	1:D:51:ARG:HE	1.80	0.47
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.70	0.47
1:D:282:ASN:ND2	1:D:285:PHE:HB2	2.30	0.47
1:A:285:PHE:CE2	1:A:289:LEU:HG	2.50	0.47
1:A:47:THR:OG1	1:A:51:ARG:NH2	2.48	0.47
1:C:83:THR:HG22	1:C:111:VAL:HG11	1.97	0.47
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.28	0.47
1:C:339:ARG:HH21	1:D:362:PHE:HB3	1.80	0.47
1:D:313:TYR:O	1:D:317:LEU:HG	2.15	0.47
1:B:350:PHE:HD1	1:B:353:VAL:CG1	2.27	0.46
1:C:253:ILE:HD13	1:C:258:ILE:HG13	1.96	0.46
1:C:343:LEU:O	1:C:347:THR:HG23	2.15	0.46
1:D:54:PHE:CD1	1:D:325:ILE:HG13	2.50	0.46
1:A:84:GLN:OE1	1:A:84:GLN:HA	2.16	0.46
1:B:239:LEU:HD13	1:B:278:LYS:O	2.16	0.46
1:D:68:ASP:O	1:D:72:MET:HG3	2.14	0.46
1:D:218:ARG:NH1	3:D:502:HOH:O	2.49	0.46
1:D:58:HIS:N	1:D:58:HIS:CD2	2.83	0.46
1:B:90:VAL:HG11	1:B:103:MET:HB2	1.97	0.46
1:B:193:THR:CG2	1:B:194:HIS:H	2.27	0.46
1:B:242:ASN:OD1	1:B:243:PRO:HD2	2.16	0.46
1:B:325:ILE:HD12	1:B:326:HIS:CD2	2.50	0.46
1:D:97:LEU:HB2	1:D:101:TYR:HB2	1.98	0.45
1:C:51:ARG:O	1:C:55:ILE:HG13	2.17	0.45
1:C:62:ASN:HB3	1:C:65:LEU:H	1.81	0.45
1:D:139:ARG:NH1	1:D:174:HIS:NE2	2.63	0.45
1:B:210:GLU:HB2	1:B:213:VAL:HG23	1.99	0.45
1:C:218:ARG:HE	1:C:240:ASP:HB3	1.81	0.45
1:D:89:VAL:HG13	1:D:90:VAL:N	2.32	0.45
1:A:77:ILE:O	1:A:80:GLY:HA3	2.16	0.45
1:B:232:LYS:HG3	1:B:269:SER:HB3	1.99	0.45
1:B:171:THR:HG22	1:B:174:HIS:CE1	2.52	0.45
1:C:228:LEU:O	1:C:229:LYS:HB2	2.15	0.45
1:D:195:VAL:O	1:D:199:VAL:HG23	2.16	0.45
1:D:87:ARG:O	1:D:91:ASN:CB	2.61	0.45
1:C:283:ILE:HG12	3:C:505:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ILE:CD1	1:C:85:LEU:HB3	2.43	0.45
1:A:178:MET:HG2	1:A:178:MET:O	2.14	0.45
1:D:255:PRO:HB2	1:D:291:LEU:CD1	2.48	0.44
1:B:348:LEU:HD22	1:B:350:PHE:N	2.32	0.44
1:C:67:PHE:CZ	1:C:97:LEU:HD22	2.51	0.44
1:B:349:PRO:O	1:B:350:PHE:CD2	2.71	0.44
1:A:343:LEU:HD23	1:B:362:PHE:CZ	2.53	0.44
1:D:229:LYS:HG2	1:D:231:TYR:OH	2.17	0.44
1:D:353:VAL:O	1:D:354:ASP:HB3	2.18	0.44
1:A:138:ILE:HG21	1:A:168:TYR:CE1	2.53	0.44
1:D:176:ILE:O	1:D:179:CYS:HB2	2.17	0.44
1:D:293:PRO:HB3	1:D:296:ARG:HH12	1.82	0.44
1:B:323:LEU:HA	1:B:323:LEU:HD12	1.71	0.44
1:B:60:GLY:C	1:B:62:ASN:H	2.21	0.44
1:C:276:LYS:O	1:C:281:ASP:HB2	2.17	0.44
1:D:378:THR:O	1:D:379:ASP:HB2	2.18	0.43
1:C:94:GLY:O	1:C:96:ARG:NH2	2.51	0.43
1:A:58:HIS:HD1	1:A:58:HIS:H	1.66	0.43
1:B:378:THR:O	1:B:379:ASP:HB2	2.18	0.43
1:C:209:LEU:HD12	1:C:209:LEU:HA	1.75	0.43
1:A:348:LEU:HD13	1:A:348:LEU:HA	1.87	0.43
1:C:317:LEU:O	1:C:321:LEU:HG	2.18	0.43
1:D:324:ASP:HB3	1:D:327:LEU:HB3	2.00	0.43
1:B:205:ASN:HA	1:B:206:PRO:HD3	1.76	0.43
1:B:59:CYS:SG	1:B:323:LEU:CD1	3.06	0.43
1:C:232:LYS:O	1:C:236:ARG:HG3	2.19	0.43
1:A:212:MET:O	1:A:216:LYS:HG3	2.19	0.43
1:A:77:ILE:HG12	1:A:85:LEU:HD13	2.01	0.43
1:B:349:PRO:O	1:B:350:PHE:HD2	2.02	0.43
1:D:145:PHE:HD2	1:D:145:PHE:HA	1.77	0.43
1:D:38:ALA:O	1:D:42:LEU:HG	2.19	0.43
1:B:346:TYR:CZ	1:C:205:ASN:HA	2.54	0.42
1:C:216:LYS:O	1:C:219:CYS:HB2	2.19	0.42
1:A:301:ASP:HA	1:A:306:ARG:HH11	1.84	0.42
1:C:230:LYS:HG2	1:C:230:LYS:H	1.54	0.42
1:D:39:TYR:O	1:D:42:LEU:HB2	2.19	0.42
1:C:232:LYS:HE2	1:C:232:LYS:HB3	1.76	0.42
1:D:304:SER:O	1:D:305:SER:CB	2.66	0.42
1:D:70:LEU:HD22	1:D:93:ILE:HG22	2.00	0.42
1:A:70:LEU:HD13	1:A:93:ILE:HG12	2.01	0.42
1:B:70:LEU:HD23	1:B:70:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:CG	1:A:65:LEU:HB2	2.39	0.42
1:B:36:ILE:CD1	1:B:72:MET:HE1	2.50	0.42
1:C:334:LEU:O	1:C:338:ILE:HG13	2.19	0.42
1:D:216:LYS:HG3	1:D:249:TYR:CD1	2.54	0.42
1:B:139:ARG:HB2	1:B:168:TYR:HB2	2.02	0.42
1:B:59:CYS:HB2	1:B:323:LEU:CD1	2.43	0.42
1:B:348:LEU:HD22	1:B:349:PRO:CA	2.49	0.42
1:B:36:ILE:CD1	1:B:72:MET:CE	2.97	0.42
1:C:228:LEU:HD12	1:C:228:LEU:HA	1.84	0.42
1:B:154:MET:HE3	1:B:154:MET:HB2	1.96	0.41
1:B:348:LEU:HD21	1:B:350:PHE:CZ	2.56	0.41
1:C:112:ASP:O	1:C:116:GLU:HG2	2.20	0.41
1:C:46:ARG:HD3	1:C:188:GLU:CG	2.37	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.88	0.41
1:A:58:HIS:HD1	1:A:58:HIS:N	2.18	0.41
1:B:348:LEU:CD2	1:B:350:PHE:CE2	3.04	0.41
1:C:74:TYR:HA	1:C:77:ILE:HG22	2.01	0.41
1:D:192:PHE:HA	1:D:195:VAL:HG23	2.02	0.41
1:D:215:ALA:HB1	1:D:245:LEU:HD13	2.01	0.41
1:D:242:ASN:HA	1:D:243:PRO:HD3	1.77	0.41
1:A:251:GLU:HG2	1:A:252:VAL:HG23	2.02	0.41
1:C:298:LEU:HD12	1:C:313:TYR:HB3	2.02	0.41
1:D:218:ARG:HD3	1:D:218:ARG:HA	1.50	0.41
1:A:232:LYS:HB3	1:A:232:LYS:HE2	1.77	0.41
1:B:171:THR:CG2	1:B:174:HIS:CD2	3.03	0.41
1:C:94:GLY:O	1:C:95:ASN:C	2.58	0.41
1:D:300:ASN:O	1:D:304:SER:HB2	2.20	0.41
1:A:307:TYR:OH	1:A:345:GLN:HB3	2.21	0.41
1:B:348:LEU:HD22	1:B:349:PRO:C	2.41	0.41
1:B:346:TYR:CE1	1:C:205:ASN:HA	2.56	0.41
1:C:44:LYS:HD3	1:C:250:ASN:OD1	2.20	0.41
1:A:39:TYR:O	1:A:42:LEU:HB2	2.21	0.41
1:B:304:SER:O	1:B:305:SER:HB2	2.20	0.41
1:B:348:LEU:HA	1:B:349:PRO:HD2	1.83	0.40
1:D:209:LEU:HD22	1:D:209:LEU:N	2.36	0.40
1:D:292:VAL:HA	1:D:293:PRO:HD3	1.86	0.40
1:D:74:TYR:HE1	1:D:90:VAL:HG22	1.85	0.40
1:B:187:ILE:HG13	1:B:195:VAL:HG21	2.03	0.40
1:C:205:ASN:OD1	1:C:206:PRO:HD2	2.21	0.40
1:C:221:SER:HB3	1:C:237:LYS:HD2	2.03	0.40
1:D:155:LEU:HA	1:D:155:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:O	1:B:114:ARG:HG2	2.22	0.40
1:B:348:LEU:CD2	1:B:350:PHE:CZ	3.05	0.40
1:B:67:PHE:HA	1:B:70:LEU:HB2	2.02	0.40
1:C:159:PHE:HB2	1:C:185:VAL:CG1	2.46	0.40
1:B:133:LEU:HD23	1:B:133:LEU:HA	1.90	0.40
1:D:218:ARG:HH11	1:D:237:LYS:CD	2.35	0.40
1:D:47:THR:O	1:D:51:ARG:HG3	2.21	0.40
1:A:348:LEU:HD22	1:C:135:LYS:HB2	2.03	0.40
1:C:311:LEU:HD12	1:C:311:LEU:HA	1.93	0.40
1:D:259:ALA:HB2	1:D:288:PHE:HB3	2.03	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	316/348 (91%)	306 (97%)	10 (3%)	0	100	100
1	B	346/348 (99%)	332 (96%)	14 (4%)	0	100	100
1	C	319/348 (92%)	290 (91%)	28 (9%)	1 (0%)	41	66
1	D	346/348 (99%)	327 (94%)	18 (5%)	1 (0%)	41	66
All	All	1327/1392 (95%)	1255 (95%)	70 (5%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	ILE
1	D	95	ASN

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	276/302 (91%)	253 (92%)	23 (8%)	11	25
1	B	302/302 (100%)	267 (88%)	35 (12%)	5	12
1	C	279/302 (92%)	234 (84%)	45 (16%)	2	6
1	D	302/302 (100%)	265 (88%)	37 (12%)	4	11
All	All	1159/1208 (96%)	1019 (88%)	140 (12%)	5	11

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	47	THR
1	A	58	HIS
1	A	59	CYS
1	A	65	LEU
1	A	88	GLU
1	A	113	ARG
1	A	163	ILE
1	A	164	ARG
1	A	171	THR
1	A	191	GLN
1	A	208	THR
1	A	209	LEU
1	A	228	LEU
1	A	230	LYS
1	A	240	ASP
1	A	248	SER
1	A	249	TYR
1	A	273	SER
1	A	283	ILE
1	A	292	VAL
1	A	319	SER
1	A	348	LEU
1	B	32	GLU

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Mol	Chain	Res	Type
1	B	35	ASP
1	B	48	LYS
1	B	58	HIS
1	B	59	CYS
1	B	68	ASP
1	B	71	ARG
1	B	85	LEU
1	B	96	ARG
1	B	122	LEU
1	B	127	SER
1	B	145	PHE
1	B	163	ILE
1	B	178	MET
1	B	209	LEU
1	B	212	MET
1	B	226	LEU
1	B	232	LYS
1	B	240	ASP
1	B	249	TYR
1	B	250	ASN
1	B	264	LEU
1	B	272	ARG
1	B	298	LEU
1	B	313	TYR
1	B	319	SER
1	B	323	LEU
1	B	325	ILE
1	B	345	GLN
1	B	348	LEU
1	B	350	PHE
1	B	352	SER
1	B	353	VAL
1	B	363	LYS
1	B	364	THR
1	C	34	LEU
1	C	46	ARG
1	C	48	LYS
1	C	68	ASP
1	C	71	ARG
1	C	72	MET
1	C	79	LYS
1	C	81	GLU

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Mol	Chain	Res	Type
1	C	83	THR
1	C	85	LEU
1	C	88	GLU
1	C	93	ILE
1	C	96	ARG
1	C	99	GLU
1	C	100	LYS
1	C	105	LEU
1	C	109	GLU
1	C	116	GLU
1	C	119	LYS
1	C	120	VAL
1	C	127	SER
1	C	133	LEU
1	C	137	SER
1	C	145	PHE
1	C	152	CYS
1	C	163	ILE
1	C	209	LEU
1	C	218	ARG
1	C	228	LEU
1	C	229	LYS
1	C	230	LYS
1	C	239	LEU
1	C	240	ASP
1	C	245	LEU
1	C	249	TYR
1	C	252	VAL
1	C	260	THR
1	C	277	GLN
1	C	283	ILE
1	C	309	SER
1	C	311	LEU
1	C	316	SER
1	C	333	THR
1	C	339	ARG
1	C	350	PHE
1	D	44	LYS
1	D	58	HIS
1	D	71	ARG
1	D	93	ILE
1	D	96	ARG

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Mol	Chain	Res	Type
1	D	99	GLU
1	D	123	GLU
1	D	125	GLU
1	D	133	LEU
1	D	134	ILE
1	D	138	ILE
1	D	145	PHE
1	D	162	TYR
1	D	163	ILE
1	D	170	THR
1	D	172	THR
1	D	173	LYS
1	D	175	ILE
1	D	204	GLN
1	D	205	ASN
1	D	210	GLU
1	D	216	LYS
1	D	218	ARG
1	D	232	LYS
1	D	245	LEU
1	D	249	TYR
1	D	272	ARG
1	D	273	SER
1	D	297	GLU
1	D	298	LEU
1	D	304	SER
1	D	306	ARG
1	D	316	SER
1	D	319	SER
1	D	323	LEU
1	D	363	LYS
1	D	371	LYS

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

Mol	Chain	Res	Type
1	A	58	HIS
1	A	191	GLN
1	B	58	HIS
1	B	194	HIS
1	C	57	ASN
1	C	84	GLN

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Mol	Chain	Res	Type
1	C	345	GLN
1	D	57	ASN
1	D	143	ASN
1	D	174	HIS
1	D	181	ASN

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	C	401	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	D	401	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	A	401	-	4,4,4	0.18	0	6,6,6	0.16	0
2	SO4	B	401	-	4,4,4	0.16	0	6,6,6	0.08	0

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	318/348 (91%)	0.29	1 (0%)	94	95	32, 47, 65, 88	0
1	B	348/348 (100%)	0.44	9 (2%)	56	57	38, 58, 94, 102	0
1	C	321/348 (92%)	0.64	33 (10%)	6	5	44, 67, 119, 136	0
1	D	348/348 (100%)	0.71	32 (9%)	9	7	42, 73, 108, 132	0
All	All	1335/1392 (95%)	0.52	75 (5%)	24	23	32, 61, 107, 136	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	SER	7.9
1	B	351	VAL	7.8
1	C	67	PHE	7.2
1	D	94	GLY	7.0
1	D	209	LEU	6.6
1	C	94	GLY	6.2
1	C	78	LYS	5.8
1	D	134	ILE	5.7
1	D	131	THR	5.6
1	D	133	LEU	4.9
1	D	207	GLU	4.4
1	D	130	ARG	4.2
1	B	59	CYS	4.2
1	C	69	ALA	4.1
1	B	126	LEU	4.0
1	A	59	CYS	4.0
1	B	349	PRO	3.9
1	C	97	LEU	3.9
1	C	33	PRO	3.9
1	C	87	ARG	3.8
1	D	65	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	56	ALA	3.7
1	D	34	LEU	3.6
1	C	74	TYR	3.6
1	C	95	ASN	3.5
1	C	351	VAL	3.4
1	C	89	VAL	3.4
1	C	101	TYR	3.4
1	D	129	TYR	3.3
1	D	210	GLU	3.3
1	D	206	PRO	3.2
1	D	132	ASN	3.2
1	B	122	LEU	3.1
1	D	176	ILE	3.0
1	C	106	ALA	2.9
1	D	211	PRO	2.9
1	D	126	LEU	2.8
1	D	138	ILE	2.7
1	C	90	VAL	2.7
1	B	85	LEU	2.6
1	D	145	PHE	2.6
1	C	350	PHE	2.6
1	C	71	ARG	2.6
1	D	202	ALA	2.5
1	D	205	ASN	2.5
1	C	54	PHE	2.4
1	C	93	ILE	2.4
1	D	135	LYS	2.4
1	C	63	HIS	2.4
1	C	65	LEU	2.4
1	C	107	TRP	2.4
1	D	128	SER	2.4
1	C	113	ARG	2.4
1	C	86	PHE	2.4
1	D	99	GLU	2.4
1	D	52	LEU	2.3
1	D	33	PRO	2.3
1	C	52	LEU	2.3
1	D	171	THR	2.3
1	C	59	CYS	2.3
1	C	81	GLU	2.3
1	D	61	GLY	2.2
1	C	68	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	67	PHE	2.2
1	D	185	VAL	2.2
1	D	39	TYR	2.2
1	B	353	VAL	2.2
1	D	212	MET	2.2
1	D	244	GLU	2.2
1	C	61	GLY	2.1
1	C	166	ARG	2.1
1	C	92	LYS	2.1
1	B	155	LEU	2.1
1	C	88	GLU	2.1
1	C	100	LYS	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 ⓘ

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	SO4	D	401	5/5	0.79	0.19	81,100,116,126	0
2	SO4	C	401	5/5	0.93	0.11	77,88,104,105	0
2	SO4	B	401	5/5	0.93	0.15	83,86,94,105	0
2	SO4	A	401	5/5	0.95	0.15	75,77,89,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.