



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:42 PM UTC

PDB ID : 4F7O / pdb_00004f7o
Title : Crystal structure of CSN5
Authors : Echalier, A.; Birol, M.; Hoh, F.; Dumas, C.
Deposited on : 2012-05-16
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

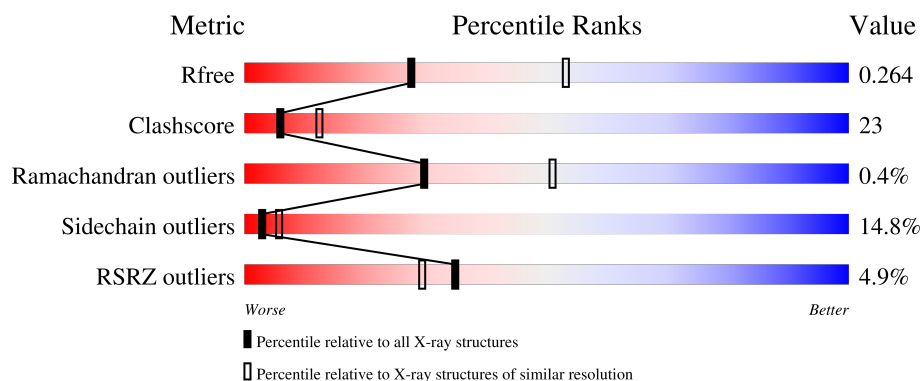
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	257	
1	B	257	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3807 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.

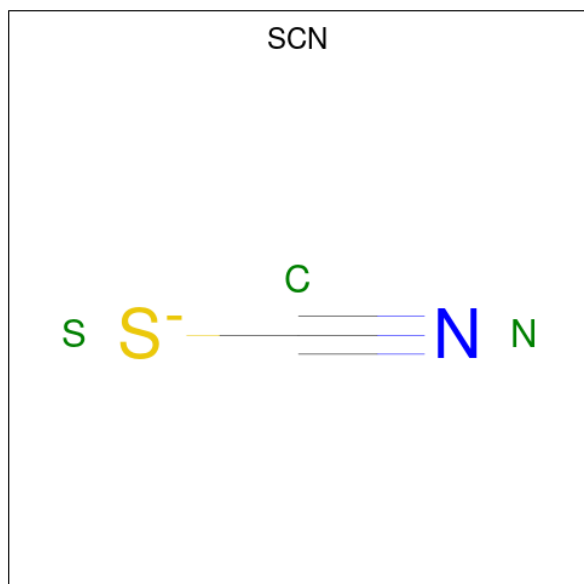
- Molecule 1 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	Se	0	1	0
			1872	1200	311	348	2	11			
1	B	235	Total	C	N	O	S	Se	0	1	0
			1872	1200	311	348	2	11			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N S 3 1 1 1	0	0
3	A	1	Total C N S 3 1 1 1	0	0
3	B	1	Total C N S 3 1 1 1	0	0

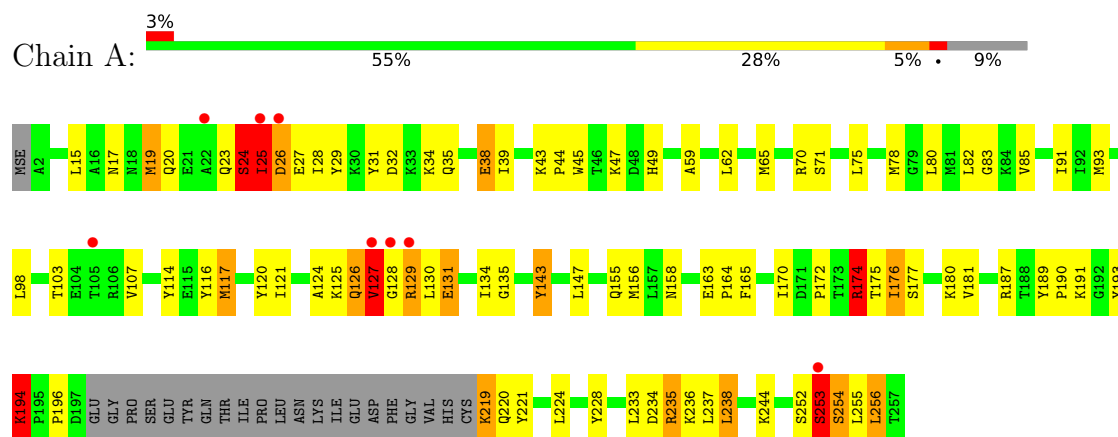
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	22	Total O 22 22	0	0

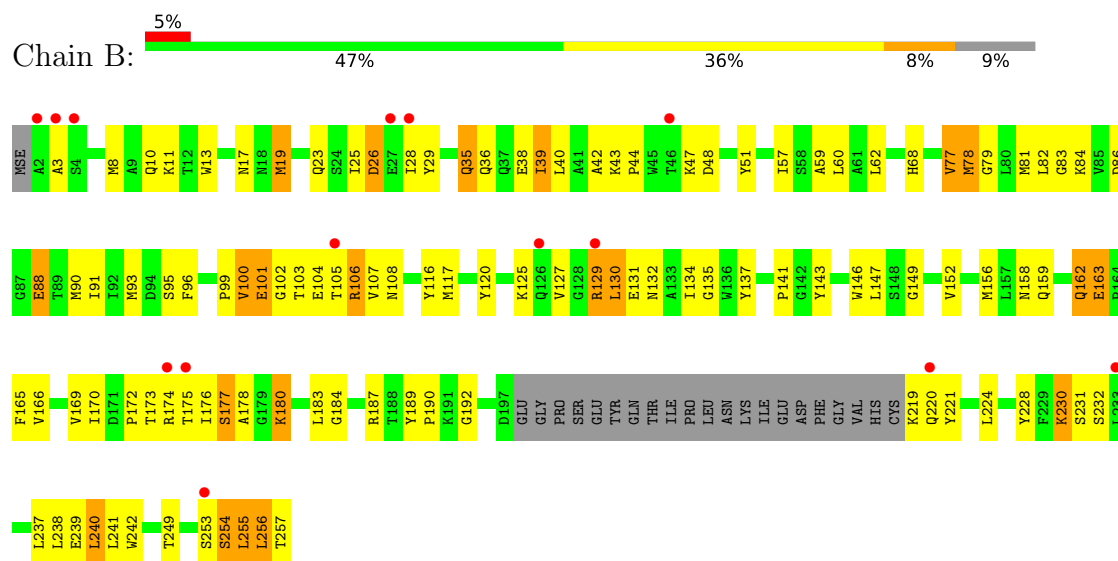
3 Residue-property plots [i](#)

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: COP9 signalosome complex subunit 5



- Molecule 1: COP9 signalosome complex subunit 5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.73Å 46.51Å 71.26Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	29.00 – 2.60 29.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.00-2.60) 92.2 (29.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.216 , 0.274 0.211 , 0.264	Depositor DCC
R_{free} test set	897 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtrriage
Anisotropy	0.297	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3807	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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

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	0.44	0/1906	0.94	6/2560 (0.2%)
1	B	0.41	0/1906	0.93	5/2560 (0.2%)
All	All	0.43	0/3812	0.93	11/5120 (0.2%)

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	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	N-CA-C	6.80	118.35	111.07
1	A	194	LYS	CA-C-N	6.60	127.18	120.38
1	A	194	LYS	C-N-CA	6.60	127.18	120.38
1	B	101	GLU	N-CA-C	-6.36	103.64	111.40
1	A	174	ARG	CB-CA-C	-6.02	109.65	116.63
1	A	24	SER	CA-C-N	5.90	132.58	121.97
1	A	24	SER	C-N-CA	5.90	132.58	121.97
1	B	163	GLU	CA-C-N	-5.54	112.92	119.84
1	B	163	GLU	C-N-CA	-5.54	112.92	119.84
1	B	189	TYR	CA-C-N	5.23	124.89	119.56
1	B	189	TYR	C-N-CA	5.23	124.89	119.56

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	VAL	Peptide
1	A	131	GLU	Peptide
1	A	24	SER	Peptide
1	A	253	SER	Peptide
1	B	162	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1872	0	1847	88	1
1	B	1872	0	1847	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	0	0
3	B	3	0	0	0	0
4	A	30	0	0	1	0
4	B	22	0	0	0	1
All	All	3807	0	3694	171	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 23.

All (171) 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:24:SER:O	1:A:25:ILE:HG12	1.63	0.98
1:A:129:ARG:HB2	1:B:130:LEU:HA	1.46	0.98
1:A:125:LYS:HA	1:A:130:LEU:HA	1.53	0.89
1:A:177:SER:HB3	1:A:256:LEU:HD22	1.60	0.84
1:A:25:ILE:HG23	1:A:29:TYR:HD2	1.45	0.82
1:B:152:VAL:HG12	1:B:156:MSE:HE2	1.61	0.81
1:A:174:ARG:HD2	1:A:175:THR:N	1.95	0.81
1:A:219:LYS:HE3	1:A:220:GLN:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:MSE:HE2	1:A:189:TYR:O	1.82	0.78
1:A:25:ILE:HG23	1:A:29:TYR:CD2	2.16	0.78
1:A:23:GLN:H	1:A:26:ASP:HB2	1.48	0.77
1:A:82:LEU:HD11	1:A:129:ARG:HH22	1.49	0.76
1:A:127:VAL:O	1:A:130:LEU:HD12	1.85	0.75
1:A:129:ARG:HD3	1:B:130:LEU:HD12	1.68	0.75
1:B:187:ARG:HG3	1:B:224:LEU:HD11	1.67	0.75
1:B:163:GLU:O	1:B:165:PHE:N	2.23	0.72
1:B:19:MSE:SE	1:B:59:ALA:HB2	2.40	0.71
1:A:125:LYS:C	1:A:127:VAL:H	1.97	0.71
1:B:68:HIS:CE1	1:B:77:VAL:HG13	2.26	0.70
1:B:81:MSE:HE1	1:B:166:VAL:HG13	1.75	0.69
1:B:36:GLN:O	1:B:40:LEU:HB2	1.93	0.68
1:A:35:GLN:HA	1:A:38:GLU:HG3	1.75	0.67
1:A:23:GLN:H	1:A:26:ASP:CB	2.08	0.66
1:A:24:SER:O	1:A:25:ILE:CG1	2.42	0.65
1:A:49:HIS:CD2	1:A:190:PRO:HG2	2.33	0.64
1:B:253:SER:HB2	1:B:256:LEU:HB2	1.78	0.63
1:A:82:LEU:HD11	1:A:129:ARG:NH2	2.14	0.63
1:A:194:LYS:O	1:A:196:PRO:HD3	2.00	0.62
1:B:44:PRO:O	1:B:47:LYS:HB3	1.99	0.61
1:A:23:GLN:HB2	1:A:26:ASP:HB2	1.81	0.61
1:A:34:LYS:O	1:A:38:GLU:HG2	2.01	0.61
1:A:23:GLN:HA	1:A:23:GLN:OE1	2.01	0.60
1:A:80:LEU:HD21	1:A:117:MSE:HG3	1.83	0.59
1:B:78:MSE:HB2	1:B:100:VAL:HG13	1.84	0.59
1:B:62:LEU:HD22	1:B:228:TYR:CD1	2.38	0.59
1:B:79:GLY:HA3	1:B:137:TYR:CE2	2.37	0.59
1:B:125:LYS:HA	1:B:129:ARG:O	2.03	0.59
1:B:3:ALA:HA	1:B:8:MSE:HB2	1.85	0.57
1:B:8:MSE:HE2	1:B:11:LYS:HD3	1.85	0.57
1:A:62:LEU:HA	1:A:65:MSE:HE3	1.87	0.57
1:A:49:HIS:HD2	1:A:190:PRO:CD	2.19	0.56
1:B:135:GLY:HA2	1:B:165:PHE:CD1	2.40	0.56
1:A:129:ARG:H	1:B:132:ASN:HD22	1.52	0.56
1:A:24:SER:C	1:A:25:ILE:HG12	2.31	0.56
1:A:103:THR:O	1:A:107:VAL:HG12	2.06	0.55
1:A:253:SER:O	1:A:254:SER:HB3	2.05	0.55
1:B:255:LEU:HD13	1:B:256:LEU:HD13	1.88	0.55
1:B:39:ILE:HA	1:B:42:ALA:HB3	1.89	0.54
1:B:152:VAL:HG11	1:B:220:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD13	1:A:116:TYR:CE2	2.43	0.54
1:A:174:ARG:HD2	1:A:174:ARG:C	2.33	0.54
1:A:31:TYR:HB3	1:A:35:GLN:HG3	1.90	0.54
1:B:190:PRO:C	1:B:192:GLY:H	2.14	0.54
1:B:25:ILE:HG13	1:B:29:TYR:HD2	1.73	0.54
1:A:62:LEU:HD22	1:A:228:TYR:CD1	2.44	0.53
1:A:23:GLN:HG2	1:A:26:ASP:OD2	2.09	0.53
1:B:220:GLN:N	1:B:220:GLN:OE1	2.42	0.52
1:A:83:GLY:HA3	1:A:91:ILE:O	2.08	0.52
1:A:129:ARG:NH1	1:B:129:ARG:HG2	2.24	0.52
1:A:43:LYS:O	1:A:45:TRP:O	2.27	0.52
1:B:149:GLY:HA2	1:B:152:VAL:HB	1.92	0.52
1:B:174:ARG:NH1	1:B:176:ILE:HG22	2.24	0.51
1:A:125:LYS:CA	1:A:130:LEU:HA	2.33	0.51
1:A:125:LYS:C	1:A:127:VAL:N	2.65	0.51
1:B:39:ILE:O	1:B:44:PRO:HD3	2.10	0.51
1:B:104:GLU:CD	1:B:108:ASN:HD21	2.18	0.51
1:A:23:GLN:N	1:A:26:ASP:HB2	2.20	0.51
1:B:79:GLY:HA3	1:B:137:TYR:CZ	2.46	0.51
1:A:39:ILE:HG23	1:A:44:PRO:HG2	1.91	0.51
1:B:43:LYS:N	1:B:44:PRO:HD3	2.25	0.51
1:A:126:GLN:HG2	1:A:127:VAL:HG22	1.92	0.51
1:A:234:ASP:HB3	1:A:238:LEU:HD23	1.92	0.51
1:A:23:GLN:HG2	1:A:26:ASP:CG	2.36	0.51
1:B:135:GLY:HA2	1:B:165:PHE:CE1	2.45	0.51
1:A:25:ILE:O	1:A:28:ILE:HG12	2.12	0.50
1:A:26:ASP:O	1:A:27:GLU:HB3	2.11	0.50
1:B:130:LEU:C	1:B:132:ASN:H	2.19	0.50
1:B:254:SER:O	1:B:257:THR:HG22	2.12	0.50
1:B:90:MSE:HE2	1:B:134:ILE:HG13	1.94	0.50
1:B:152:VAL:O	1:B:156:MSE:HG3	2.11	0.49
1:A:143:TYR:N	1:A:143:TYR:CD2	2.80	0.49
1:B:99:PRO:HD2	1:B:116:TYR:OH	2.12	0.49
1:B:60:LEU:HD23	1:B:241:LEU:HD22	1.93	0.49
1:B:146:TRP:O	1:B:169:VAL:HG21	2.13	0.49
1:B:253:SER:HB3	1:B:256:LEU:HD22	1.94	0.49
1:B:35:GLN:O	1:B:38:GLU:HB3	2.12	0.49
1:B:84:LYS:HE3	1:B:93[B]:MSE:SE	2.63	0.49
1:B:25:ILE:HA	1:B:29:TYR:CE2	2.47	0.49
1:A:147:LEU:HB2	1:A:221:TYR:CE2	2.47	0.49
1:B:68:HIS:CE1	1:B:77:VAL:CG1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HG13	1:B:29:TYR:CD2	2.48	0.48
1:B:17:ASN:OD1	1:B:180:LYS:HA	2.13	0.48
1:B:130:LEU:O	1:B:131:GLU:HB2	2.14	0.48
1:B:35:GLN:O	1:B:39:ILE:HG12	2.13	0.48
1:A:187:ARG:HG3	1:A:224:LEU:HD11	1.95	0.48
1:B:13:TRP:CA	1:B:178:ALA:HB1	2.44	0.47
1:B:230:LYS:HG2	1:B:231:SER:H	1.79	0.47
1:A:121:ILE:CG2	1:A:125:LYS:HE2	2.44	0.47
1:A:45:TRP:C	1:A:47:LYS:H	2.23	0.47
1:B:174:ARG:HG3	1:B:176:ILE:HG23	1.97	0.47
1:B:47:LYS:HG2	1:B:48:ASP:N	2.29	0.47
1:B:141:PRO:HA	1:B:172:PRO:HD2	1.95	0.47
1:B:183:LEU:HD23	1:B:184:GLY:N	2.30	0.46
1:A:114:TYR:CD2	1:A:114:TYR:C	2.90	0.46
1:B:83:GLY:HA3	1:B:91:ILE:O	2.15	0.46
1:B:240:LEU:HD22	1:B:240:LEU:HA	1.85	0.46
1:B:39:ILE:HG12	1:B:39:ILE:H	1.46	0.46
1:A:129:ARG:HB3	1:B:82:LEU:HD13	1.97	0.46
1:A:49:HIS:NE2	1:A:190:PRO:HG2	2.30	0.45
1:B:100:VAL:HG12	1:B:102:GLY:CA	2.46	0.45
1:A:237:LEU:HD11	1:B:120:TYR:HA	1.97	0.45
1:A:253:SER:HA	1:A:255:LEU:H	1.81	0.45
1:A:23:GLN:CB	1:A:26:ASP:HB2	2.47	0.45
1:B:10:GLN:HB2	1:B:242:TRP:CD1	2.51	0.45
1:B:28:ILE:HG13	1:B:29:TYR:N	2.31	0.45
1:B:173:THR:HG22	1:B:174:ARG:N	2.32	0.45
1:A:219:LYS:HA	1:A:219:LYS:HD2	1.73	0.45
1:B:19:MSE:SE	1:B:59:ALA:CB	3.12	0.45
1:A:129:ARG:HB2	1:B:130:LEU:CA	2.32	0.45
1:B:23:GLN:HG2	1:B:232:SER:HB3	1.99	0.45
1:A:93[A]:MSE:HE3	4:A:418:HOH:O	2.17	0.44
1:A:128:GLY:HA2	1:B:132:ASN:ND2	2.33	0.44
1:A:244:LYS:HE3	1:B:100:VAL:O	2.18	0.44
1:B:187:ARG:O	1:B:221:TYR:HB2	2.17	0.44
1:A:23:GLN:O	1:A:24:SER:HB3	2.18	0.44
1:A:24:SER:C	1:A:25:ILE:CG1	2.91	0.44
1:B:117:MSE:HE1	1:B:158:ASN:HD21	1.83	0.44
1:A:17:ASN:OD1	1:A:181:VAL:HG22	2.18	0.43
1:B:95:SER:O	1:B:96:PHE:HB3	2.17	0.43
1:B:117:MSE:CE	1:B:158:ASN:HD21	2.30	0.43
1:A:129:ARG:NH1	1:B:129:ARG:CG	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:HIS:CD2	1:A:190:PRO:CG	3.01	0.43
1:A:135:GLY:HA2	1:A:165:PHE:CD1	2.53	0.43
1:B:253:SER:CB	1:B:256:LEU:HB2	2.47	0.43
1:B:13:TRP:N	1:B:178:ALA:HB1	2.33	0.43
1:A:121:ILE:HG22	1:A:125:LYS:HE2	2.01	0.43
1:B:36:GLN:NE2	1:B:86:ASP:OD1	2.50	0.43
1:A:124:ALA:HB3	1:A:131:GLU:OE2	2.19	0.43
1:A:19:MSE:SE	1:A:59:ALA:HB2	2.69	0.42
1:A:114:TYR:HD1	1:A:158:ASN:OD1	2.02	0.42
1:B:130:LEU:HB3	1:B:131:GLU:H	1.44	0.42
1:A:129:ARG:NH1	1:A:130:LEU:O	2.53	0.42
1:B:176:ILE:O	1:B:176:ILE:HG13	2.20	0.42
1:A:70:ARG:HG2	1:A:172:PRO:HB2	2.00	0.42
1:A:163:GLU:HG3	1:A:164:PRO:HA	2.01	0.42
1:A:163:GLU:OE2	1:A:164:PRO:HA	2.20	0.42
1:B:147:LEU:HD12	1:B:221:TYR:CG	2.55	0.42
1:B:159:GLN:HE22	1:B:187:ARG:HB3	1.84	0.42
1:B:159:GLN:O	1:B:163:GLU:HB2	2.19	0.42
1:A:85:VAL:HG23	1:A:134:ILE:HD11	2.02	0.42
1:A:175:THR:HG21	1:A:180:LYS:O	2.20	0.42
1:B:241:LEU:O	1:B:242:TRP:C	2.62	0.42
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.80	0.41
1:B:125:LYS:HE3	1:B:131:GLU:HA	2.02	0.41
1:A:256:LEU:HD23	1:A:256:LEU:N	2.35	0.41
1:B:105:THR:HG23	1:B:106:ARG:HG2	2.02	0.41
1:B:51:TYR:O	1:B:88:GLU:HB3	2.19	0.41
1:A:78:MSE:SE	1:A:117:MSE:HE1	2.71	0.41
1:B:190:PRO:C	1:B:192:GLY:N	2.79	0.41
1:A:125:LYS:O	1:A:126:GLN:CB	2.69	0.41
1:B:23:GLN:O	1:B:26:ASP:HB3	2.20	0.41
1:A:120:TYR:CD2	1:A:120:TYR:C	3.00	0.40
1:A:43:LYS:N	1:A:44:PRO:HD3	2.35	0.40
1:B:177:SER:HB2	1:B:178:ALA:H	1.63	0.40
1:B:237:LEU:HA	1:B:237:LEU:HD23	1.91	0.40
1:B:238:LEU:O	1:B:239:GLU:C	2.63	0.40
1:A:130:LEU:O	1:A:131:GLU:CB	2.69	0.40
1:A:135:GLY:HA2	1:A:165:PHE:CE1	2.56	0.40
1:A:155:GLN:OE1	1:A:155:GLN:HA	2.20	0.40
1:B:134:ILE:O	1:B:165:PHE:HA	2.21	0.40
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:OG	4:B:401:HOH:O[2_657]	2.11	0.09

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	232/257 (90%)	207 (89%)	23 (10%)	2 (1%)	14	30
1	B	232/257 (90%)	210 (90%)	22 (10%)	0	100	100
All	All	464/514 (90%)	417 (90%)	45 (10%)	2 (0%)	30	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	176	ILE

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	197/205 (96%)	168 (85%)	29 (15%)	3	6
1	B	197/205 (96%)	168 (85%)	29 (15%)	3	6
All	All	394/410 (96%)	336 (85%)	58 (15%)	3	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	19	MSE
1	A	20	GLN
1	A	25	ILE
1	A	26	ASP
1	A	32	ASP
1	A	38	GLU
1	A	71	SER
1	A	75	LEU
1	A	117	MSE
1	A	126	GLN
1	A	127	VAL
1	A	129	ARG
1	A	143	TYR
1	A	170	ILE
1	A	174	ARG
1	A	176	ILE
1	A	191	LYS
1	A	193	TYR
1	A	194	LYS
1	A	219	LYS
1	A	233	LEU
1	A	235	ARG
1	A	236	LYS
1	A	238	LEU
1	A	252	SER
1	A	253	SER
1	A	254	SER
1	A	256	LEU
1	B	19	MSE
1	B	26	ASP
1	B	35	GLN
1	B	39	ILE
1	B	57	ILE
1	B	77	VAL
1	B	78	MSE
1	B	88	GLU
1	B	100	VAL
1	B	101	GLU
1	B	103	THR
1	B	106	ARG
1	B	107	VAL

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Mol	Chain	Res	Type
1	B	127	VAL
1	B	129	ARG
1	B	130	LEU
1	B	143	TYR
1	B	162	GLN
1	B	170	ILE
1	B	175	THR
1	B	177	SER
1	B	180	LYS
1	B	219	LYS
1	B	230	LYS
1	B	240	LEU
1	B	249	THR
1	B	254	SER
1	B	255	LEU
1	B	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	248	ASN
1	B	108	ASN
1	B	123	ASN
1	B	132	ASN
1	B	159	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	SCN	A	302	-	1,2,2	0.97	0	0,1,1	-	-
3	SCN	B	302	-	1,2,2	0.96	0	0,1,1	-	-
3	SCN	A	303	-	1,2,2	0.98	0	0,1,1	-	-

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

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, 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	225/257 (87%)	0.02	8 (3%)	46	40	18, 52, 104, 165	0
1	B	225/257 (87%)	0.28	14 (6%)	26	21	23, 58, 115, 163	0
All	All	450/514 (87%)	0.15	22 (4%)	35	29	18, 54, 112, 165	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	SER	3.3
1	B	3	ALA	3.3
1	A	128	GLY	3.2
1	B	2	ALA	3.2
1	A	25	ILE	3.0
1	A	253	SER	2.9
1	A	22	ALA	2.9
1	A	129	ARG	2.8
1	B	174	ARG	2.6
1	A	105	THR	2.5
1	B	175	THR	2.5
1	A	127	VAL	2.5
1	B	233	LEU	2.4
1	B	105	THR	2.3
1	A	26	ASP	2.2
1	B	27	GLU	2.2
1	B	28	ILE	2.1
1	B	220	GLN	2.1
1	B	4	SER	2.0
1	B	46	THR	2.0
1	B	126	GLN	2.0
1	B	129	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SCN	B	302	3/3	0.72	0.17	73,73,75,93	0
3	SCN	A	303	3/3	0.86	0.13	52,52,54,113	0
3	SCN	A	302	3/3	0.90	0.10	54,54,55,65	0
2	ZN	B	301	1/1	0.99	0.03	34,34,34,34	0
2	ZN	A	301	1/1	0.99	0.01	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.