Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2024 – 07:22 pm BST

PDB ID	:	9EOR
Title	:	SARS-CoV2 major protease in complex with a covalent inhibitor SLL12.
Authors	:	Moche, M.; Lennerstrand, J.; Nyman, T.; Strandback, E.; Akaberi, D.
Deposited on	:	2024-03-15
Resolution	:	2.25 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:

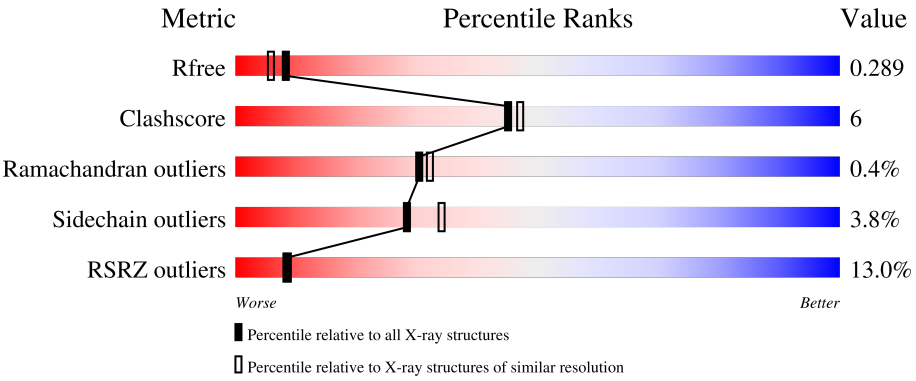
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	306	13% 85% 13% ·
1	B	306	8% 85% 15%
1	C	306	23% 84% 15% ·
1	D	306	17% 82% 17% ·
1	E	306	9% 83% 16% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	306	8% 82% 16%
2	G	4	75% 25%
2	H	4	25% 75%
2	I	4	75% 25%
2	J	4	75% 25%
2	K	4	50% 50%
2	L	4	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14761 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 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	1	0
			2368	1498	403	445	22			
1	B	306	Total	C	N	O	S	0	0	0
			2355	1490	399	444	22			
1	C	305	Total	C	N	O	S	0	0	0
			2351	1488	400	441	22			
1	D	306	Total	C	N	O	S	0	0	0
			2361	1493	402	444	22			
1	E	305	Total	C	N	O	S	0	0	0
			2351	1488	400	441	22			
1	F	305	Total	C	N	O	S	0	0	0
			2345	1485	397	441	22			

- Molecule 2 is a protein called Inhibitor SLL12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			46	34	8	4			
2	H	4	Total	C	N	O	0	0	0
			46	34	8	4			
2	I	4	Total	C	N	O	0	0	0
			46	34	8	4			
2	J	4	Total	C	N	O	0	0	0
			46	34	8	4			
2	K	4	Total	C	N	O	0	0	0
			46	34	8	4			
2	L	4	Total	C	N	O	0	0	0
			46	34	8	4			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0
3	F	1	Total K 1 1	0	0

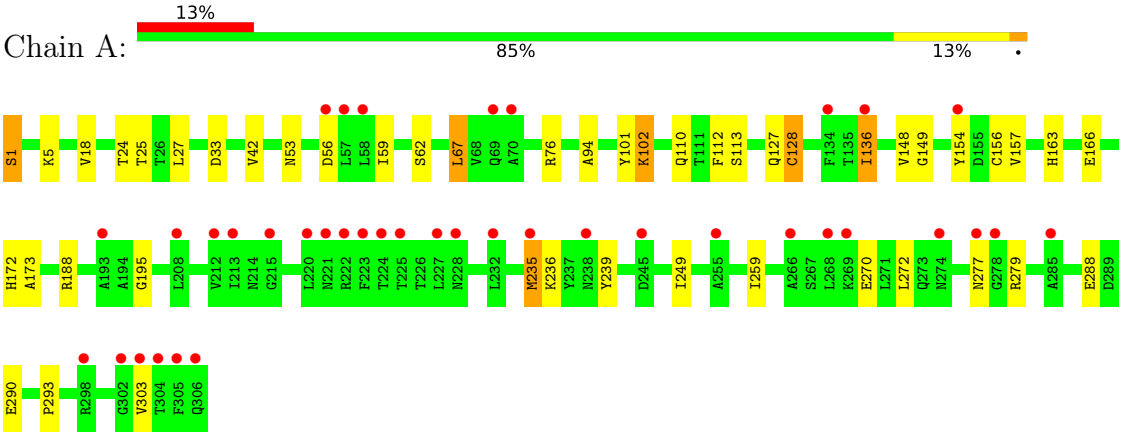
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	59	Total O 59 59	0	0
4	C	42	Total O 42 42	0	0
4	D	46	Total O 46 46	0	0
4	E	63	Total O 63 63	0	0
4	F	63	Total O 63 63	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0
4	I	2	Total O 2 2	0	0
4	J	3	Total O 3 3	0	0
4	K	2	Total O 2 2	0	0
4	L	1	Total O 1 1	0	0

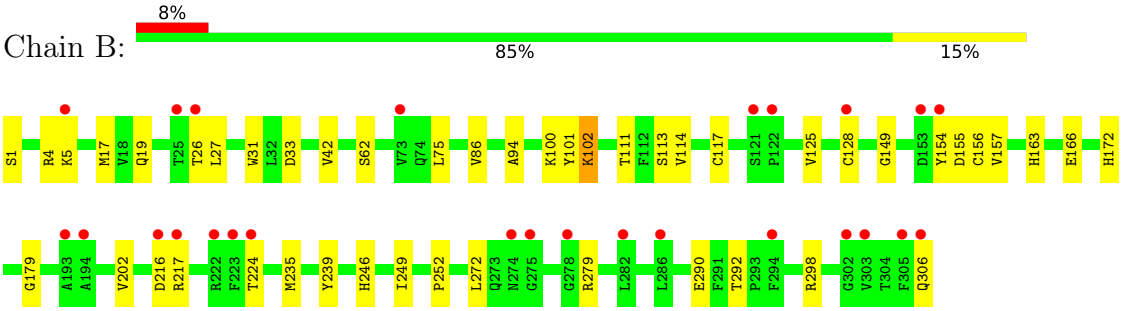
3 Residue-property plots (i)

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.

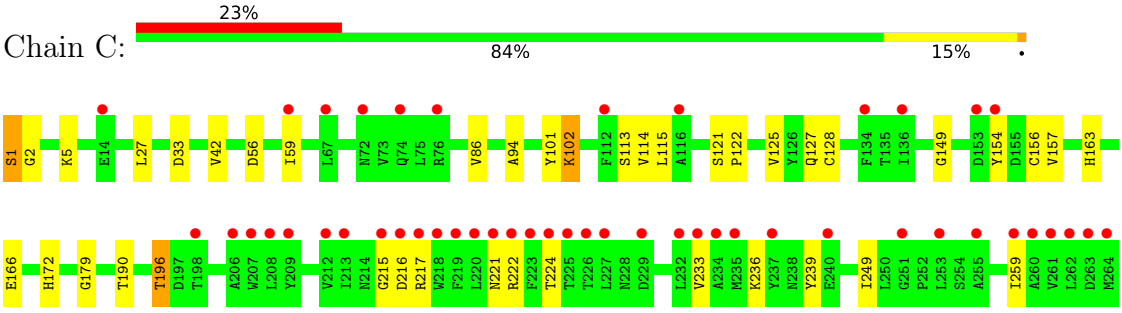
• Molecule 1: 3C-like proteinase nsp5

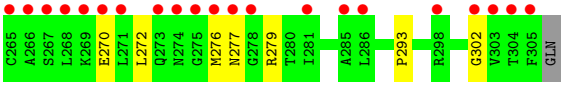


• Molecule 1: 3C-like proteinase nsp5

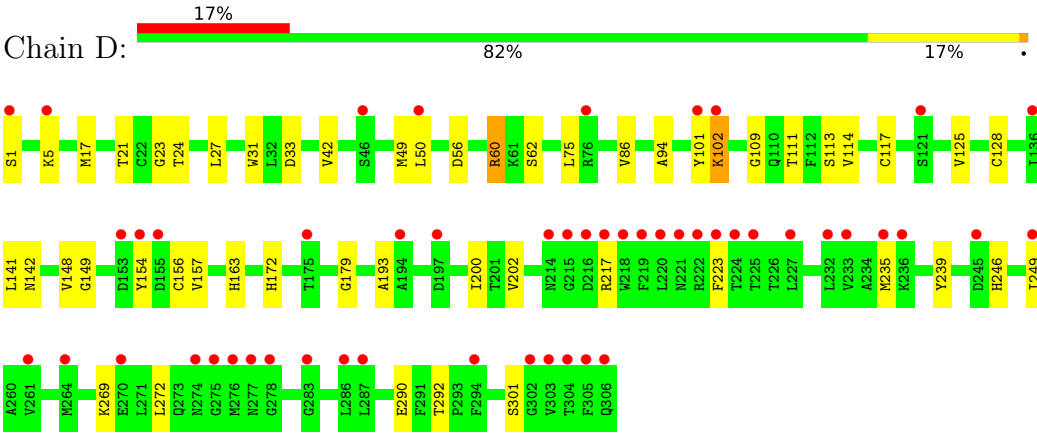


• Molecule 1: 3C-like proteinase nsp5

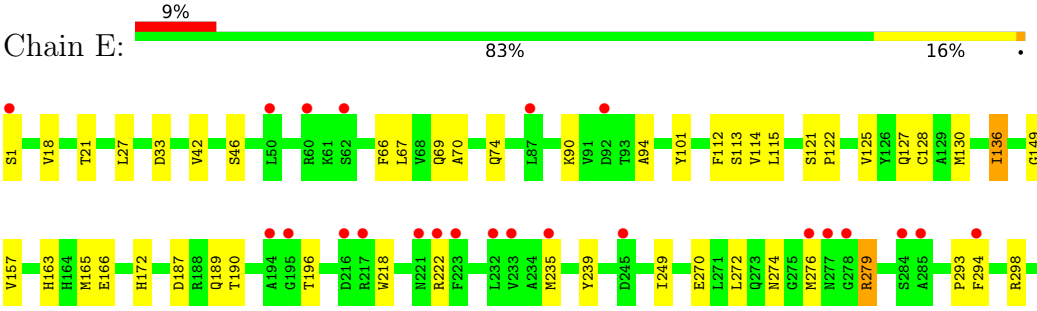




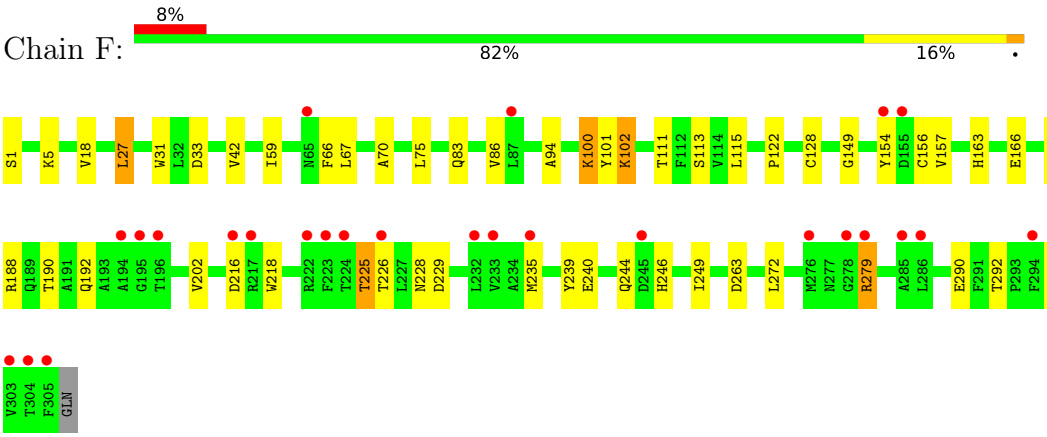
• Molecule 1: 3C-like proteinase nsp5



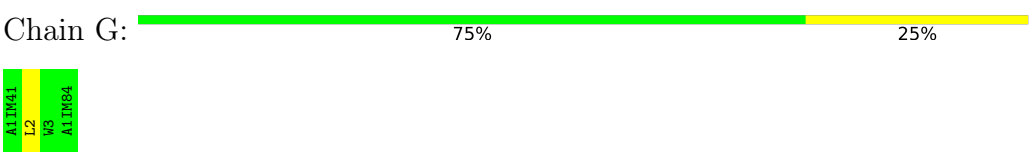
• Molecule 1: 3C-like proteinase nsp5



• Molecule 1: 3C-like proteinase nsp5



• Molecule 2: Inhibitor SLL12



• Molecule 2: Inhibitor SLL12

Chain H:

• Molecule 2: Inhibitor SLL12

Chain I:

• Molecule 2: Inhibitor SLL12

Chain J:

• Molecule 2: Inhibitor SLL12

Chain K:

• Molecule 2: Inhibitor SLL12

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.83Å 85.56Å 93.67Å 78.96° 87.18° 83.17°	Depositor
Resolution (Å)	43.91 – 2.25 43.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	58.8 (43.91-2.25) 58.8 (43.91-2.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.241 , 0.289 0.243 , 0.289	Depositor DCC
R_{free} test set	4942 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14761	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.15% 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

Bond lengths and bond angles in the following residue types are not validated in this section: A1IM8, A1IM4, K, DNE, HT7

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	0.39	0/2420	0.68	0/3288
1	B	0.41	0/2407	0.69	0/3271
1	C	0.40	0/2403	0.67	0/3266
1	D	0.40	0/2413	0.70	1/3278 (0.0%)
1	E	0.39	0/2403	0.69	1/3266 (0.0%)
1	F	0.40	0/2397	0.68	0/3259
All	All	0.40	0/14443	0.69	2/19628 (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
1	A	0	2
1	B	0	2
1	C	0	1
1	E	0	1
2	G	0	1
2	H	0	1
2	J	0	1
2	K	0	1
2	L	0	1
All	All	0	11

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	298	ARG	NE-CZ-NH1	-5.71	117.44	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	217	ARG	CB-CG-CD	5.28	125.31	111.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ARG	Sidechain
1	A	279	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	279	ARG	Sidechain
1	C	217	ARG	Sidechain
1	E	222	ARG	Sidechain
2	G	2	DNE	Peptide
2	H	2	DNE	Peptide
2	J	2	DNE	Peptide
2	K	2	DNE	Peptide
2	L	2	DNE	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	2368	0	2314	28	0
1	B	2355	0	2295	26	0
1	C	2351	0	2298	31	0
1	D	2361	0	2305	35	0
1	E	2351	0	2298	32	0
1	F	2345	0	2287	32	0
2	G	46	0	21	0	0
2	H	46	0	21	1	0
2	I	46	0	21	1	0
2	J	46	0	21	4	0
2	K	46	0	21	2	0
2	L	46	0	21	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	1	0
4	A	64	0	0	8	0
4	B	59	0	0	1	0
4	C	42	0	0	6	0
4	D	46	0	0	2	0
4	E	63	0	0	2	0
4	F	63	0	0	3	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
4	I	2	0	0	0	0
4	J	3	0	0	1	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
All	All	14761	0	13923	163	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 6.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:NZ	1:B:156:CYS:SG	2.08	1.26
1:C:224:THR:HB	4:C:510:HOH:O	1.62	1.00
1:B:100:LYS:NZ	4:B:501:HOH:O	2.06	0.84
1:A:110:GLN:HG3	4:A:506:HOH:O	1.74	0.84
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.64	0.79
1:C:166:GLU:OE2	1:D:1:SER:HA	1.82	0.79
1:D:223:PHE:O	4:D:501:HOH:O	2.00	0.78
2:H:1:A1IM4:N3	4:H:101:HOH:O	2.18	0.76
1:C:42:VAL:O	4:C:501:HOH:O	2.03	0.76
1:F:263:ASP:OD1	3:F:401:K:K	1.98	0.74
1:E:115:LEU:HD11	1:E:122:PRO:HB3	1.71	0.71
1:C:221:ASN:OD1	4:C:502:HOH:O	2.09	0.70
1:A:235:MET:HG2	1:A:236:LYS:N	2.07	0.69
1:B:33:ASP:OD2	1:C:222:ARG:NH1	2.26	0.67
1:A:288:GLU:HB2	4:A:527:HOH:O	1.94	0.66
2:J:1:A1IM4:N3	4:J:101:HOH:O	2.29	0.66
1:A:1:SER:HB2	1:B:166:GLU:OE2	1.96	0.65
1:B:101:TYR:O	1:C:222:ARG:HB2	1.97	0.65
1:F:225:THR:HG23	1:F:226:THR:O	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE2	1:B:1:SER:HA	1.98	0.64
1:D:24:THR:HB	1:E:21:THR:HG21	1.80	0.63
1:C:279:ARG:HG3	1:C:279:ARG:HH11	1.64	0.63
1:A:24:THR:HG21	1:D:50:LEU:HD22	1.81	0.62
1:F:67:LEU:HD12	1:F:67:LEU:N	2.14	0.62
1:A:25:THR:HG21	4:A:517:HOH:O	1.99	0.61
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.82	0.61
1:C:5:LYS:HG3	1:C:127:GLN:HB3	1.83	0.60
1:D:24:THR:HG22	1:E:21:THR:OG1	2.01	0.60
1:F:86:VAL:HG13	1:F:179:GLY:HA2	1.84	0.60
1:C:233:VAL:HA	1:C:236:LYS:HD2	1.84	0.59
1:A:127:GLN:O	1:B:4:ARG:NH2	2.36	0.59
1:F:218:TRP:CE2	1:F:279:ARG:HD2	2.37	0.59
1:A:1:SER:CB	1:B:166:GLU:OE2	2.51	0.59
1:C:56:ASP:HA	1:C:59:ILE:HG12	1.83	0.59
1:A:56:ASP:HA	1:A:59:ILE:HG12	1.85	0.59
1:E:166:GLU:OE2	1:F:1:SER:HA	2.04	0.58
1:F:5:LYS:HE2	1:F:290:GLU:HB2	1.86	0.58
1:E:218:TRP:CE2	1:E:279:ARG:HD2	2.39	0.58
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.86	0.57
1:D:21:THR:HG23	1:E:67:LEU:HD13	1.86	0.57
1:D:56:ASP:O	1:D:60:ARG:HD2	2.05	0.56
1:E:66:PHE:C	1:E:67:LEU:HD23	2.26	0.56
1:F:100:LYS:HA	4:F:524:HOH:O	2.06	0.56
1:B:19:GLN:HE21	1:B:26:THR:HG21	1.71	0.54
1:D:5:LYS:HE2	1:D:290:GLU:HB2	1.89	0.54
1:D:102:LYS:HD3	1:D:156:CYS:SG	2.49	0.53
1:C:196:THR:HB	4:C:524:HOH:O	2.09	0.53
1:C:2:GLY:HA3	1:D:138:GLY:O	2.10	0.52
1:E:249:ILE:HG22	1:E:293:PRO:HG2	1.92	0.51
1:E:279:ARG:HH11	1:E:279:ARG:HG3	1.75	0.51
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.92	0.51
1:A:18:VAL:HA	4:A:533:HOH:O	2.10	0.51
1:A:53:ASN:HB2	4:A:512:HOH:O	2.11	0.51
1:F:27:LEU:HD21	1:F:42:VAL:HB	1.92	0.51
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.93	0.50
1:D:27:LEU:HD21	1:D:42:VAL:HB	1.94	0.50
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.93	0.49
1:B:31:TRP:CE2	1:B:75:LEU:HD21	2.47	0.49
1:F:226:THR:HG23	1:F:229:ASP:H	1.77	0.49
1:C:27:LEU:HD21	1:C:42:VAL:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:TRP:CE2	1:D:75:LEU:HD21	2.47	0.49
1:F:244:GLN:NE2	4:F:505:HOH:O	2.43	0.49
1:F:31:TRP:CE2	1:F:75:LEU:HD21	2.47	0.49
1:C:279:ARG:HG3	1:C:279:ARG:NH1	2.26	0.49
1:D:246:HIS:HA	1:D:249:ILE:HG12	1.95	0.49
1:E:67:LEU:HD23	1:E:67:LEU:N	2.27	0.49
1:E:33:ASP:O	1:E:94:ALA:HA	2.13	0.48
1:A:33:ASP:O	1:A:94:ALA:HA	2.14	0.48
1:B:33:ASP:O	1:B:94:ALA:HA	2.14	0.48
1:C:33:ASP:O	1:C:94:ALA:HA	2.14	0.48
1:E:101:TYR:HA	1:E:157:VAL:O	2.14	0.48
1:F:33:ASP:O	1:F:94:ALA:HA	2.13	0.48
1:F:295:ASP:OD1	1:F:298:ARG:NH1	2.45	0.48
1:C:239:TYR:CZ	1:C:272:LEU:HD21	2.49	0.48
1:E:18:VAL:HG12	1:E:70:ALA:CB	2.44	0.47
1:D:33:ASP:O	1:D:94:ALA:HA	2.13	0.47
1:C:101:TYR:HA	1:C:157:VAL:O	2.15	0.47
1:D:101:TYR:HA	1:D:157:VAL:O	2.15	0.47
1:B:246:HIS:HA	1:B:249:ILE:HG12	1.95	0.47
1:F:188:ARG:NH2	1:F:190:THR:HG21	2.29	0.47
1:D:23:GLY:HA2	1:E:69:GLN:OE1	2.15	0.47
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.50	0.47
1:C:190:THR:O	2:I:3:HT7:HT2	2.15	0.46
1:E:113:SER:O	1:E:149:GLY:HA2	2.15	0.46
1:A:101:TYR:HA	1:A:157:VAL:O	2.15	0.46
1:A:127:GLN:HG2	4:A:514:HOH:O	2.15	0.46
1:B:101:TYR:HA	1:B:157:VAL:O	2.16	0.46
1:B:111:THR:HG23	1:B:292:THR:HG23	1.97	0.46
1:F:101:TYR:HA	1:F:157:VAL:O	2.15	0.46
1:C:302:GLY:CA	1:D:141:LEU:HD12	2.45	0.46
1:F:18:VAL:HG12	1:F:70:ALA:CB	2.45	0.46
1:D:23:GLY:H	1:E:74:GLN:HE21	1.62	0.46
1:D:113:SER:O	1:D:149:GLY:HA2	2.16	0.46
1:F:113:SER:O	1:F:149:GLY:HA2	2.16	0.46
1:C:1:SER:N	1:D:140:PHE:O	2.48	0.45
1:E:112:PHE:HZ	1:E:136:ILE:HG12	1.81	0.45
1:A:102:LYS:HD3	1:A:156:CYS:SG	2.56	0.45
1:B:155:ASP:HB3	1:B:306:GLN:OXT	2.17	0.45
1:B:113:SER:O	1:B:149:GLY:HA2	2.16	0.45
1:C:102:LYS:HD3	1:C:156:CYS:SG	2.57	0.45
1:D:148:VAL:HG22	4:D:503:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:GLN:HG3	2:K:2:DNE:HB3	1.99	0.45
1:E:190:THR:O	2:K:3:HT7:HT2	2.17	0.44
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.52	0.44
1:A:113:SER:O	1:A:149:GLY:HA2	2.17	0.44
1:A:67:LEU:HD11	1:D:193:ALA:HA	1.99	0.44
1:C:113:SER:O	1:C:149:GLY:HA2	2.17	0.44
1:B:5:LYS:HE3	1:B:290:GLU:HB2	2.00	0.44
1:F:190:THR:O	2:L:3:HT7:HT2	2.17	0.44
1:A:249:ILE:HG22	1:A:293:PRO:HG2	1.99	0.43
1:A:5:LYS:HE2	1:A:290:GLU:HB2	2.00	0.43
1:A:128:CYS:SG	1:A:136:ILE:CD1	3.06	0.43
1:C:127:GLN:HG2	4:C:521:HOH:O	2.18	0.43
1:D:111:THR:HG23	1:D:292:THR:HG23	2.00	0.43
1:D:239:TYR:CZ	1:D:272:LEU:HD21	2.53	0.43
1:B:202:VAL:HG21	1:B:249:ILE:HD11	2.01	0.43
1:D:163:HIS:CE1	1:D:172:HIS:HB3	2.53	0.43
1:F:163:HIS:CE1	1:F:172:HIS:HB3	2.53	0.43
1:F:246:HIS:HA	1:F:249:ILE:HG12	2.00	0.43
1:E:130:MET:HA	1:E:136:ILE:CD1	2.47	0.43
1:F:67:LEU:N	1:F:67:LEU:CD1	2.81	0.43
1:D:202:VAL:HG21	1:D:249:ILE:HD11	2.01	0.43
1:D:23:GLY:N	1:E:74:GLN:NE2	2.66	0.43
1:E:163:HIS:CE1	1:E:172:HIS:HB3	2.54	0.43
1:F:239:TYR:CZ	1:F:272:LEU:HD21	2.53	0.43
1:F:192:GLN:HE21	2:L:3:HT7:HT2	1.84	0.43
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.53	0.42
1:F:115:LEU:HD11	1:F:122:PRO:HB3	2.01	0.42
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.54	0.42
1:D:109:GLY:HA2	1:D:200:ILE:HD13	2.02	0.42
1:D:142:ASN:ND2	2:J:4:A1IM8:O	2.42	0.42
1:B:101:TYR:O	1:C:222:ARG:CB	2.67	0.42
1:B:17:MET:HG3	1:B:117:CYS:SG	2.60	0.42
1:D:49:MET:HE1	2:J:2:DNE:HE3	2.00	0.42
1:D:86:VAL:HG23	1:D:179:GLY:HA2	2.00	0.42
1:C:163:HIS:CE1	1:C:172:HIS:HB3	2.55	0.42
1:D:17:MET:HG3	1:D:117:CYS:SG	2.59	0.42
1:C:121:SER:HA	1:C:122:PRO:HD3	1.93	0.42
1:D:114:VAL:O	1:D:125:VAL:HA	2.20	0.42
1:E:239:TYR:CZ	1:E:272:LEU:HD21	2.55	0.42
1:E:279:ARG:HG3	1:E:279:ARG:NH1	2.35	0.42
1:A:112:PHE:N	1:A:112:PHE:CD1	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:MET:CE	2:J:2:DNE:HE3	2.50	0.41
1:E:1:SER:HB2	1:F:166:GLU:OE2	2.20	0.41
1:E:114:VAL:O	1:E:125:VAL:HA	2.21	0.41
1:C:114:VAL:O	1:C:125:VAL:HA	2.21	0.41
1:E:113:SER:OG	1:E:127:GLN:NE2	2.53	0.41
1:A:148:VAL:HG22	4:A:510:HOH:O	2.20	0.41
1:D:24:THR:C	1:E:67:LEU:HD12	2.40	0.41
1:E:294:PHE:HB2	4:E:550:HOH:O	2.20	0.41
1:F:102:LYS:HD3	1:F:156:CYS:SG	2.61	0.41
1:F:202:VAL:HG21	1:F:249:ILE:HD11	2.02	0.41
1:A:173:ALA:HA	4:A:511:HOH:O	2.20	0.41
1:B:114:VAL:O	1:B:125:VAL:HA	2.21	0.41
1:F:66:PHE:C	1:F:67:LEU:HD12	2.41	0.41
1:A:1:SER:HB2	1:B:166:GLU:CD	2.41	0.40
1:C:249:ILE:HG22	1:C:293:PRO:HG2	2.02	0.40
1:E:165:MET:CE	1:E:187:ASP:HA	2.51	0.40
1:F:83:GLN:O	1:F:86:VAL:HG22	2.22	0.40
1:C:215:GLY:CA	4:C:504:HOH:O	2.69	0.40
1:E:155:ASP:O	4:E:502:HOH:O	2.22	0.40
1:F:5:LYS:HB2	4:F:555:HOH:O	2.22	0.40
1:F:111:THR:HG23	1:F:292:THR:HG23	2.02	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	305/306 (100%)	297 (97%)	6 (2%)	2 (1%)	19	18
1	B	304/306 (99%)	295 (97%)	8 (3%)	1 (0%)	37	41
1	C	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	37	41
1	D	304/306 (99%)	294 (97%)	9 (3%)	1 (0%)	37	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	37	41
1	F	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	37	41
All	All	1822/1836 (99%)	1768 (97%)	47 (3%)	7 (0%)	30	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	B	154	TYR
1	C	154	TYR
1	D	154	TYR
1	E	154	TYR
1	F	154	TYR
1	A	195	GLY

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	263/263 (100%)	251 (95%)	12 (5%)	23	25
1	B	261/263 (99%)	253 (97%)	8 (3%)	35	43
1	C	261/263 (99%)	252 (97%)	9 (3%)	32	40
1	D	262/263 (100%)	254 (97%)	8 (3%)	35	43
1	E	261/263 (99%)	250 (96%)	11 (4%)	25	29
1	F	260/263 (99%)	248 (95%)	12 (5%)	23	25
All	All	1568/1578 (99%)	1508 (96%)	60 (4%)	28	34

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	62	SER
1	A	67	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	ARG
1	A	102	LYS
1	A	128	CYS
1	A	136	ILE
1	A	235	MET
1	A	259	ILE
1	A	270	GLU
1	A	277	ASN
1	A	303	VAL
1	B	62	SER
1	B	102	LYS
1	B	128	CYS
1	B	216	ASP
1	B	224	THR
1	B	235	MET
1	B	252	PRO
1	B	298	ARG
1	C	1	SER
1	C	102	LYS
1	C	128	CYS
1	C	196	THR
1	C	216	ASP
1	C	259	ILE
1	C	270	GLU
1	C	276	MET
1	C	277	ASN
1	D	60	ARG
1	D	62	SER
1	D	102	LYS
1	D	128	CYS
1	D	235	MET
1	D	252	PRO
1	D	269	LYS
1	D	301	SER
1	E	46	SER
1	E	90	LYS
1	E	121	SER
1	E	128	CYS
1	E	136	ILE
1	E	196	THR
1	E	235	MET
1	E	270	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	274	ASN
1	E	276	MET
1	E	279	ARG
1	F	27	LEU
1	F	59	ILE
1	F	100	LYS
1	F	102	LYS
1	F	128	CYS
1	F	216	ASP
1	F	225	THR
1	F	228	ASN
1	F	235	MET
1	F	240	GLU
1	F	279	ARG
1	F	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	B	19	GLN
1	B	189	GLN
1	B	306	GLN
1	C	51	ASN
1	C	127	GLN
1	D	69	GLN
1	D	119	ASN
1	D	189	GLN
1	D	214	ASN
1	E	64	HIS
1	E	74	GLN
1	E	119	ASN
1	E	127	GLN
1	F	244	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

18 non-standard protein/DNA/RNA residues 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	HT7	J	3	2	15,16,17	0.93	1 (6%)	14,21,23	1.19	1 (7%)
2	HT7	I	3	2	15,16,17	0.78	0	14,21,23	1.07	1 (7%)
2	DNE	K	2	2	6,7,8	0.45	0	2,7,9	0.29	0
2	HT7	K	3	2	15,16,17	0.78	0	14,21,23	1.17	2 (14%)
2	HT7	L	3	2	15,16,17	0.78	0	14,21,23	1.05	0
2	A1IM8	G	4	2	13,13,13	0.28	0	16,16,16	0.45	0
2	A1IM8	I	4	2	13,13,13	0.26	0	16,16,16	0.63	0
2	A1IM8	L	4	2	13,13,13	0.30	0	16,16,16	0.60	0
2	DNE	I	2	2	6,7,8	0.58	0	2,7,9	0.11	0
2	DNE	J	2	2	6,7,8	0.45	0	2,7,9	0.21	0
2	DNE	L	2	2	6,7,8	0.50	0	2,7,9	0.08	0
2	DNE	G	2	2	6,7,8	0.52	0	2,7,9	0.36	0
2	HT7	G	3	2	15,16,17	0.74	0	14,21,23	1.12	0
2	A1IM8	J	4	2	13,13,13	0.26	0	16,16,16	0.61	0
2	A1IM8	H	4	2	13,13,13	0.31	0	16,16,16	0.54	0
2	DNE	H	2	2	6,7,8	0.48	0	2,7,9	0.13	0
2	HT7	H	3	2	15,16,17	0.75	0	14,21,23	1.16	2 (14%)
2	A1IM8	K	4	2	13,13,13	0.26	0	16,16,16	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HT7	J	3	2	-	0/6/7/8	0/2/2/2
2	HT7	I	3	2	-	1/6/7/8	0/2/2/2
2	DNE	K	2	2	-	4/5/6/8	-
2	HT7	K	3	2	-	0/6/7/8	0/2/2/2
2	HT7	L	3	2	-	0/6/7/8	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IM8	G	4	2	-	9/10/10/10	0/1/1/1
2	A1IM8	I	4	2	-	6/10/10/10	0/1/1/1
2	A1IM8	L	4	2	-	6/10/10/10	0/1/1/1
2	DNE	I	2	2	-	4/5/6/8	-
2	DNE	J	2	2	-	2/5/6/8	-
2	DNE	L	2	2	-	5/5/6/8	-
2	DNE	G	2	2	-	4/5/6/8	-
2	HT7	G	3	2	-	0/6/7/8	0/2/2/2
2	A1IM8	J	4	2	-	4/10/10/10	0/1/1/1
2	A1IM8	H	4	2	-	4/10/10/10	0/1/1/1
2	DNE	H	2	2	-	4/5/6/8	-
2	HT7	H	3	2	-	0/6/7/8	0/2/2/2
2	A1IM8	K	4	2	-	5/10/10/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	HT7	CA-CB	2.27	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	HT7	CT2-CH2-CZ2	-2.53	116.44	120.08
2	H	3	HT7	CA-CB-CG	2.41	114.30	110.81
2	J	3	HT7	CT2-CH2-CZ2	-2.39	116.64	120.08
2	H	3	HT7	CT2-CH2-CZ2	-2.34	116.71	120.08
2	I	3	HT7	CT2-CH2-CZ2	-2.29	116.79	120.08
2	K	3	HT7	CH3-CZ3-CE2	-2.15	117.91	120.89

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	DNE	O-C-CA-CB
2	H	2	DNE	N-CA-CB-CG
2	I	2	DNE	O-C-CA-CB
2	K	2	DNE	N-CA-CB-CG
2	K	2	DNE	C-CA-CB-CG
2	L	2	DNE	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	2	DNE	N-CA-CB-CG
2	L	2	DNE	C-CA-CB-CG
2	I	3	HT7	C-CA-CB-N
2	G	4	A1IM8	N5-C-CA-N
2	G	4	A1IM8	N5-C-CA-CB2
2	G	4	A1IM8	CA-C-N5-C13
2	G	4	A1IM8	O-C-N5-C13
2	H	4	A1IM8	CA-C-N5-C13
2	H	4	A1IM8	O-C-N5-C13
2	I	4	A1IM8	CA-C-N5-C13
2	I	4	A1IM8	O-C-N5-C13
2	J	4	A1IM8	CA-C-N5-C13
2	J	4	A1IM8	O-C-N5-C13
2	K	4	A1IM8	CA-C-N5-C13
2	K	4	A1IM8	O-C-N5-C13
2	L	4	A1IM8	N5-C-CA-N
2	L	4	A1IM8	CA-C-N5-C13
2	L	4	A1IM8	O-C-N5-C13
2	L	2	DNE	CA-CB-CG-CD
2	G	2	DNE	CA-CB-CG-CD
2	K	2	DNE	CA-CB-CG-CD
2	J	2	DNE	CA-CB-CG-CD
2	H	2	DNE	CA-CB-CG-CD
2	I	4	A1IM8	O-C-CA-N
2	K	4	A1IM8	O-C-CA-N
2	L	4	A1IM8	O-C-CA-N
2	G	4	A1IM8	N-CA-CB2-CG2
2	I	4	A1IM8	N5-C-CA-N
2	K	4	A1IM8	N5-C-CA-N
2	G	4	A1IM8	CA-CB2-CG2-CD2
2	G	4	A1IM8	CA-CB2-CG2-C4
2	I	4	A1IM8	CA-CB2-CG2-C4
2	I	4	A1IM8	CA-CB2-CG2-CD2
2	L	2	DNE	CE-CD-CG-CB
2	H	4	A1IM8	CA-CB2-CG2-CD2
2	I	2	DNE	CA-CB-CG-CD
2	G	2	DNE	N-CA-CB-CG
2	I	2	DNE	N-CA-CB-CG
2	J	2	DNE	N-CA-CB-CG
2	H	4	A1IM8	CA-CB2-CG2-C4
2	G	4	A1IM8	O-C-CA-N
2	J	4	A1IM8	CA-CB2-CG2-CD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	4	A1IM8	CA-CB2-CG2-C4
2	L	4	A1IM8	CA-CB2-CG2-C4
2	K	2	DNE	CE-CD-CG-CB
2	L	4	A1IM8	CA-CB2-CG2-CD2
2	G	4	A1IM8	C-CA-CB2-CG2
2	G	2	DNE	C-CA-CB-CG
2	H	2	DNE	C-CA-CB-CG
2	I	2	DNE	C-CA-CB-CG
2	G	2	DNE	CE-CD-CG-CB
2	K	4	A1IM8	CA-CB2-CG2-C4

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	HT7	1	0
2	K	2	DNE	1	0
2	K	3	HT7	1	0
2	L	3	HT7	2	0
2	J	2	DNE	2	0
2	J	4	A1IM8	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	306/306 (100%)	1.04	39 (12%) 9 9	8, 33, 58, 100	1 (0%)
1	B	306/306 (100%)	0.77	26 (8%) 18 18	14, 29, 52, 75	0
1	C	305/306 (99%)	1.18	69 (22%) 3 3	18, 34, 66, 85	0
1	D	306/306 (100%)	1.09	52 (16%) 5 5	16, 34, 67, 89	0
1	E	305/306 (99%)	0.70	27 (8%) 17 16	14, 29, 60, 82	0
1	F	305/306 (99%)	0.74	26 (8%) 18 18	14, 29, 62, 91	0
2	G	0/4	-	-	-	-
2	H	0/4	-	-	-	-
2	I	0/4	-	-	-	-
2	J	0/4	-	-	-	-
2	K	0/4	-	-	-	-
2	L	0/4	-	-	-	-
All	All	1833/1860 (98%)	0.92	239 (13%) 9 8	8, 31, 63, 100	1 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	5.9
1	D	216	ASP	5.8
1	F	305	PHE	5.6
1	C	266	ALA	5.3
1	D	223	PHE	5.2
1	A	304	THR	4.9
1	D	235	MET	4.8
1	C	275	GLY	4.7
1	D	154	TYR	4.6
1	E	154	TYR	4.6
1	D	155	ASP	4.5
1	C	303	VAL	4.5
1	F	223	PHE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	305	PHE	4.4
1	B	223	PHE	4.2
1	D	215	GLY	4.2
1	A	303	VAL	4.1
1	A	223	PHE	4.1
1	D	305	PHE	4.1
1	C	223	PHE	4.1
1	C	286	LEU	4.1
1	C	220	LEU	4.0
1	C	59	ILE	4.0
1	C	219	PHE	3.9
1	A	232	LEU	3.9
1	C	262	LEU	3.9
1	D	224	THR	3.9
1	C	278	GLY	3.8
1	D	218	TRP	3.8
1	C	269	LYS	3.8
1	F	303	VAL	3.8
1	C	268	LEU	3.8
1	D	233	VAL	3.7
1	B	193	ALA	3.7
1	D	220	LEU	3.7
1	A	222	ARG	3.6
1	C	72	ASN	3.6
1	C	264	MET	3.6
1	D	294	PHE	3.6
1	E	294	PHE	3.6
1	C	305	PHE	3.6
1	C	261	VAL	3.6
1	D	276	MET	3.6
1	A	220	LEU	3.6
1	C	260	ALA	3.5
1	E	50	LEU	3.4
1	F	87	LEU	3.4
1	E	303	VAL	3.4
1	F	217	ARG	3.4
1	A	213	ILE	3.3
1	C	281	ILE	3.3
1	F	154	TYR	3.3
1	D	306	GLN	3.3
1	C	276	MET	3.3
1	E	235	MET	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	222	ARG	3.3
1	A	227	LEU	3.3
1	C	209	TYR	3.3
1	E	195	GLY	3.3
1	F	235	MET	3.3
1	C	224	THR	3.2
1	C	215	GLY	3.2
1	C	232	LEU	3.2
1	F	278	GLY	3.2
1	E	216	ASP	3.2
1	F	285	ALA	3.2
1	B	26	THR	3.2
1	C	227	LEU	3.2
1	C	221	ASN	3.1
1	F	222	ARG	3.1
1	C	218	TRP	3.1
1	A	298	ARG	3.1
1	B	305	PHE	3.1
1	D	225	THR	3.1
1	A	235	MET	3.1
1	B	153	ASP	3.1
1	F	276	MET	3.1
1	B	222	ARG	3.1
1	B	154	TYR	3.0
1	C	116	ALA	3.0
1	E	284	SER	3.0
1	C	212	VAL	3.0
1	F	155	ASP	3.0
1	B	224	THR	2.9
1	C	302	GLY	2.9
1	C	277	ASN	2.9
1	D	153	ASP	2.9
1	E	60	ARG	2.9
1	D	214	ASN	2.9
1	A	154	TYR	2.9
1	A	228	ASN	2.9
1	C	233	VAL	2.8
1	D	303	VAL	2.8
1	C	259	ILE	2.8
1	C	235	MET	2.8
1	A	274	ASN	2.8
1	C	216	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	245	ASP	2.8
1	C	234	ALA	2.8
1	B	25	THR	2.8
1	D	283	GLY	2.8
1	C	213	ILE	2.7
1	D	102	LYS	2.7
1	C	265	CYS	2.7
1	A	221	ASN	2.7
1	A	277	ASN	2.7
1	D	274	ASN	2.7
1	A	56	ASP	2.7
1	A	212	VAL	2.7
1	B	217	ARG	2.7
1	C	255	ALA	2.7
1	D	302	GLY	2.7
1	F	196	THR	2.7
1	C	74	GLN	2.7
1	C	298	ARG	2.6
1	F	294	PHE	2.6
1	C	274	ASN	2.6
1	D	222	ARG	2.6
1	A	215	GLY	2.6
1	F	195	GLY	2.6
1	B	122	PRO	2.6
1	D	76	ARG	2.6
1	E	285	ALA	2.6
1	A	136	ILE	2.6
1	B	5	LYS	2.6
1	E	245	ASP	2.6
1	C	76	ARG	2.6
1	B	294	PHE	2.5
1	C	206	ALA	2.5
1	D	227	LEU	2.5
1	D	232	LEU	2.5
1	E	1	SER	2.5
1	B	216	ASP	2.5
1	D	304	THR	2.5
1	D	259	ILE	2.5
1	D	264	MET	2.5
1	A	268	LEU	2.5
1	C	225	THR	2.5
1	C	285	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	233	VAL	2.5
1	F	286	LEU	2.5
1	A	245	ASP	2.4
1	D	270	GLU	2.4
1	E	276	MET	2.4
1	A	69	GLN	2.4
1	D	277	ASN	2.4
1	C	154	TYR	2.4
1	D	46	SER	2.4
1	D	275	GLY	2.4
1	A	208	LEU	2.4
1	E	194	ALA	2.4
1	E	232	LEU	2.4
1	D	5	LYS	2.4
1	A	302	GLY	2.4
1	C	217	ARG	2.4
1	B	306	GLN	2.4
1	A	285	ALA	2.4
1	F	224	THR	2.4
1	E	217	ARG	2.4
1	A	238	ASN	2.4
1	C	208	LEU	2.4
1	C	226	THR	2.3
1	D	219	PHE	2.3
1	F	226	THR	2.3
1	C	14	GLU	2.3
1	A	269	LYS	2.3
1	A	306	GLN	2.3
1	A	70	ALA	2.3
1	B	274	ASN	2.3
1	D	221	ASN	2.3
1	D	136	ILE	2.3
1	C	237	TYR	2.3
1	A	224	THR	2.3
1	B	73	VAL	2.3
1	C	229	ASP	2.3
1	B	278	GLY	2.3
1	B	303	VAL	2.3
1	C	273	GLN	2.3
1	D	278	GLY	2.3
1	D	286	LEU	2.2
1	A	225	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	304	THR	2.2
1	C	267	SER	2.2
1	B	194	ALA	2.2
1	E	233	VAL	2.2
1	C	134	PHE	2.2
1	C	263	ASP	2.2
1	C	270	GLU	2.2
1	A	58	LEU	2.2
1	B	282	LEU	2.2
1	D	194	ALA	2.2
1	B	302	GLY	2.2
1	C	240	GLU	2.2
1	C	251	GLY	2.2
1	D	217	ARG	2.2
1	E	277	ASN	2.2
1	C	304	THR	2.2
1	D	197	ASP	2.2
1	D	245	ASP	2.2
1	F	279	ARG	2.1
1	C	67	LEU	2.1
1	C	253	LEU	2.1
1	E	92	ASP	2.1
1	D	1	SER	2.1
1	C	136	ILE	2.1
1	A	255	ALA	2.1
1	A	134	PHE	2.1
1	C	112	PHE	2.1
1	B	121	SER	2.1
1	E	62	SER	2.1
1	B	128	CYS	2.1
1	D	50	LEU	2.1
1	E	87	LEU	2.1
1	A	266	ALA	2.1
1	E	223	PHE	2.1
1	E	155	ASP	2.1
1	D	121	SER	2.1
1	E	278	GLY	2.1
1	A	193	ALA	2.1
1	D	175	THR	2.1
1	F	194	ALA	2.1
1	B	275	GLY	2.0
1	C	153	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	2.0
1	F	65	ASN	2.0
1	C	198	THR	2.0
1	C	207	TRP	2.0
1	E	222	ARG	2.0
1	D	261	VAL	2.0
1	D	101	TYR	2.0
1	A	278	GLY	2.0
1	F	216	ASP	2.0
1	D	236	LYS	2.0
1	D	249	ILE	2.0
1	B	286	LEU	2.0
1	C	271	LEU	2.0
1	D	287	LEU	2.0
1	E	221	ASN	2.0
1	F	232	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	A1IM8	J	4	13/13	0.82	0.12	21,27,31,33	0
2	A1IM8	H	4	13/13	0.83	0.12	22,29,38,50	0
2	DNE	K	2	8/9	0.86	0.11	22,23,30,32	0
2	A1IM8	I	4	13/13	0.88	0.13	27,32,44,45	0
2	HT7	J	3	15/16	0.88	0.12	15,27,32,32	0
2	A1IM8	K	4	13/13	0.88	0.13	30,39,46,46	0
2	A1IM8	L	4	13/13	0.88	0.10	28,30,36,39	0
2	HT7	I	3	15/16	0.89	0.10	19,22,33,34	0
2	DNE	I	2	8/9	0.89	0.12	22,25,27,27	0
2	HT7	L	3	15/16	0.89	0.10	22,23,27,27	0
2	DNE	L	2	8/9	0.89	0.11	29,32,41,47	0
2	HT7	G	3	15/16	0.90	0.10	16,18,24,27	0
2	HT7	H	3	15/16	0.90	0.10	20,26,32,32	0
2	A1IM8	G	4	13/13	0.90	0.10	25,26,33,36	0
2	DNE	H	2	8/9	0.90	0.12	16,21,23,25	0
2	HT7	K	3	15/16	0.91	0.11	17,19,23,25	0
2	DNE	J	2	8/9	0.91	0.10	18,19,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DNE	G	2	8/9	0.92	0.09	19,20,23,25	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
3	K	F	401	1/1	0.86	0.13	83,83,83,83	0
3	K	A	401	1/1	0.87	0.08	52,52,52,52	0
3	K	A	402	1/1	0.88	0.14	51,51,51,51	0
3	K	E	401	1/1	0.92	0.12	51,51,51,51	0
3	K	B	401	1/1	0.92	0.13	59,59,59,59	0
3	K	B	402	1/1	0.94	0.06	56,56,56,56	0
3	K	D	401	1/1	0.95	0.08	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.