



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:05 PM UTC

PDB ID : 9EOR / pdb_00009eor
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 ⓘ 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

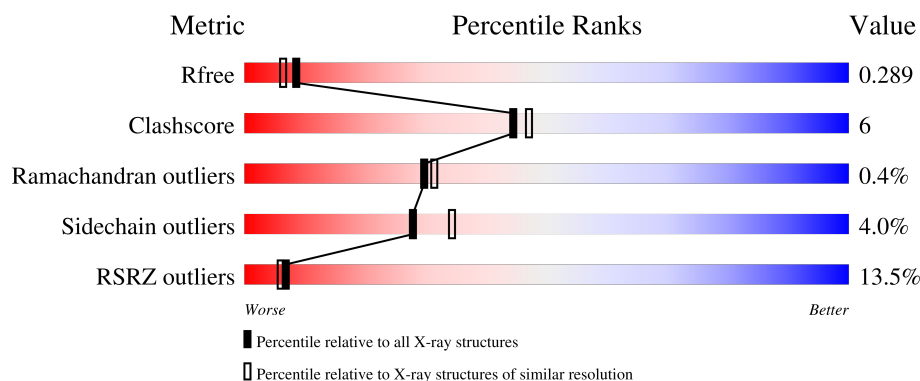
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	

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Mol	Chain	Length	Quality of chain
1	F	306	 8% 81% 17%
2	G	4	 75% 25%
2	H	4	 25% 75%
2	I	4	 75% 25%
2	J	4	 75% 25%
2	K	4	 50% 25% 25%
2	L	4	 50% 50%

2 Entry composition

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 (CCD ID: 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

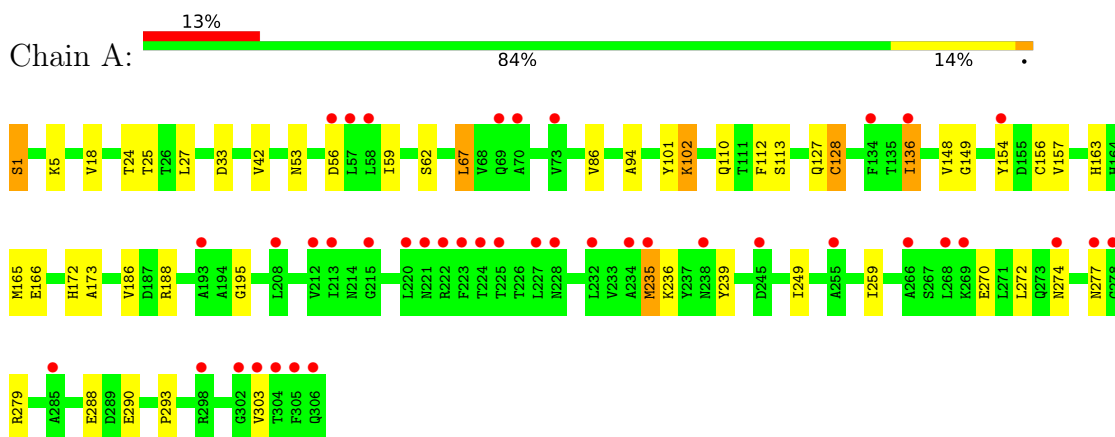
- Molecule 4 is water.

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

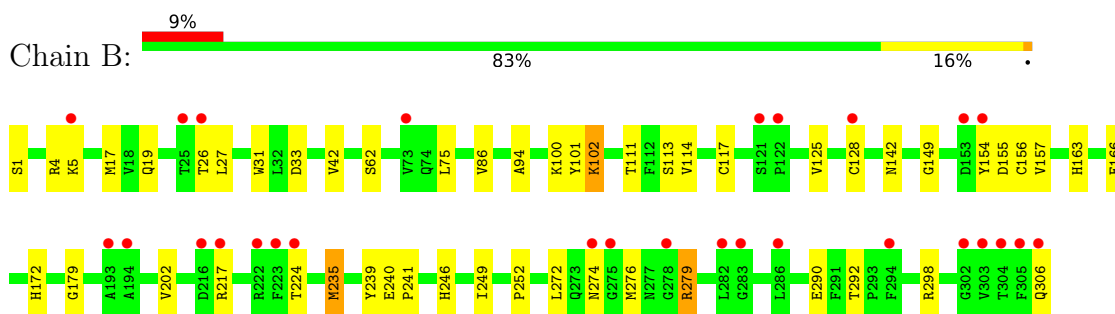
3 Residue-property plots [i](#)

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.

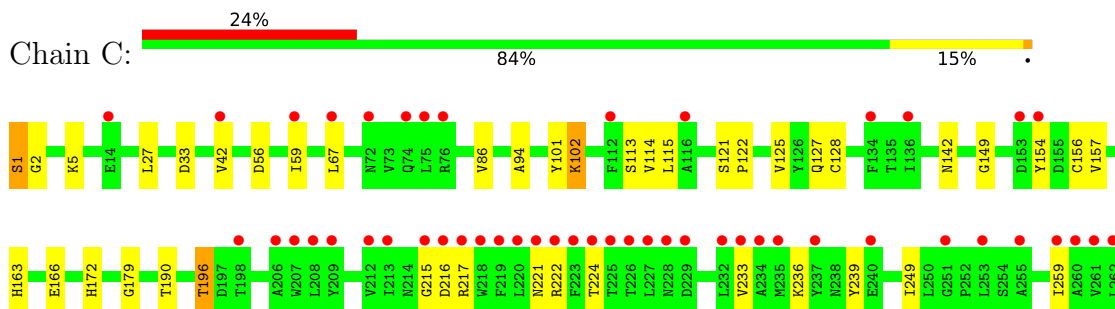
- Molecule 1: 3C-like proteinase nsp5

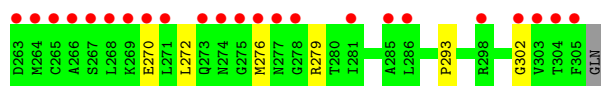


- Molecule 1: 3C-like proteinase nsp5

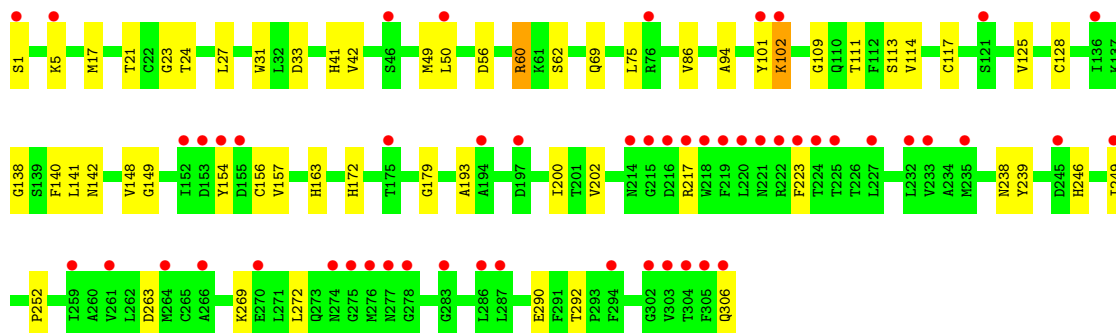
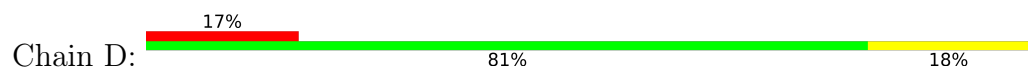


- Molecule 1: 3C-like proteinase nsp5

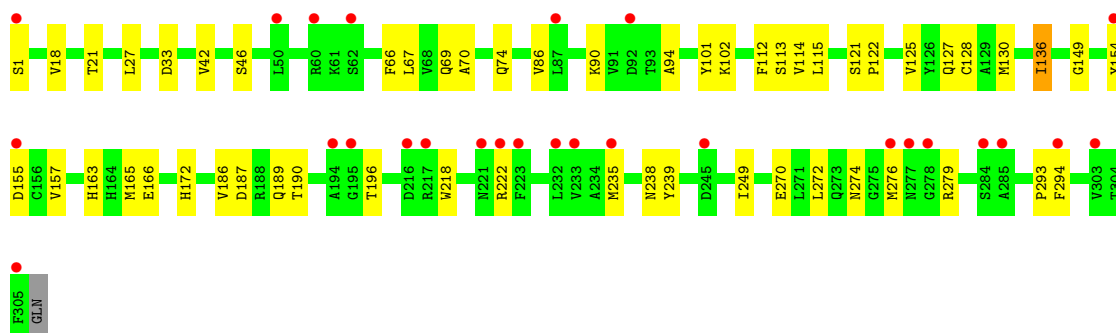
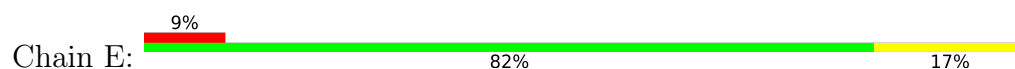




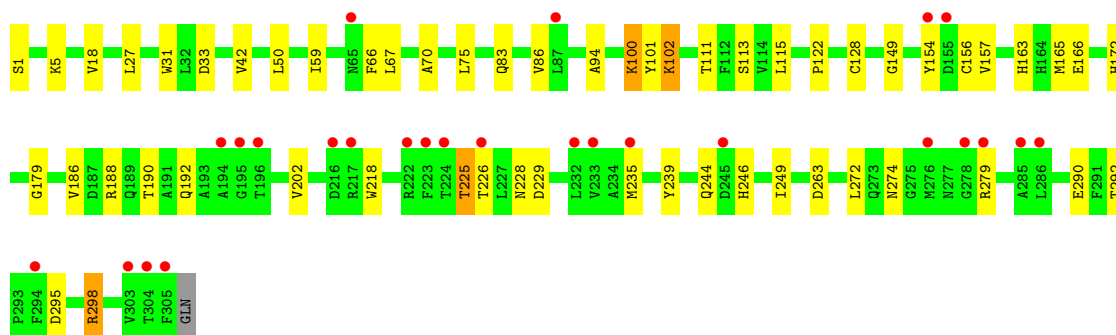
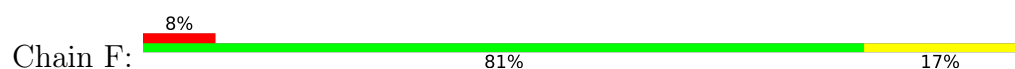
• Molecule 1: 3C-like proteinase nsp5



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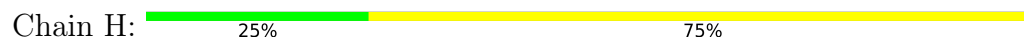


• Molecule 2: Inhibitor SLL12





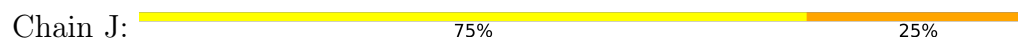
- Molecule 2: Inhibitor SLL12



- Molecule 2: Inhibitor SLL12



- Molecule 2: Inhibitor SLL12



- Molecule 2: Inhibitor SLL12



- Molecule 2: Inhibitor SLL12



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2918 reflections (2.92%)	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)	0.31 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.*

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: HT7, DNE, K, A1IM4, A1IM8

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	0.57	0/2420	0.94	0/3288
1	B	0.57	0/2407	0.94	1/3271 (0.0%)
1	C	0.56	0/2403	0.94	1/3266 (0.0%)
1	D	0.57	0/2413	0.95	2/3278 (0.1%)
1	E	0.55	0/2403	0.94	0/3266
1	F	0.56	0/2397	0.95	0/3259
All	All	0.56	0/14443	0.94	4/19628 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ASP	CA-CB-CG	7.50	120.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	217	ARG	CB-CG-CD	6.09	125.31	111.30
1	C	142	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	142	ASN	CB-CA-C	5.15	118.12	109.89

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

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	29	0
1	B	2355	0	2295	28	0
1	C	2351	0	2298	32	0
1	D	2361	0	2305	36	0
1	E	2351	0	2298	34	0
1	F	2345	0	2287	33	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	3	0
2	K	46	0	21	2	0
2	L	46	0	21	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	D	1	0	0	0	0
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	170	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 (170) 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:D:49:MET:HE2	2:J:2:DNE:HE3	1.55	0.89
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:E:165:MET:HE1	1:E:186:VAL:O	1.86	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:66:PHE:C	1:E:67:LEU:HD23	2.26	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:F:165:MET:HE1	1:F:186:VAL:O	2.03	0.57
1:A:165:MET:HE1	1:A:186:VAL:O	2.04	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: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:B:235:MET:HE1	1:B:241:PRO:HD3	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:24:THR:C	1:E:67:LEU:HD12	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:SER:O	1:F:149:GLY:HA2	2.16	0.46
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:F:66:PHE:C	1:F:67:LEU:HD12	2.41	0.45
1:A:1:SER:HB2	1:B:166:GLU:CD	2.41	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
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:D:41:HIS:HB2	1:D:49:MET:HE1	2.00	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:276:MET:HE2	1:B:279:ARG:O	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:C:121:SER:OG	1:D:306:GLN:CD	2.61	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:C:1:SER:N	1:D:140:PHE:O	2.48	0.42
1:E:165:MET:HE1	1:E:187:ASP:HA	2.01	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	18	17
1	B	304/306 (99%)	295 (97%)	8 (3%)	1 (0%)	36	40
1	C	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	36	40
1	D	304/306 (99%)	294 (97%)	9 (3%)	1 (0%)	36	40
1	E	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	36	40
1	F	303/306 (99%)	294 (97%)	8 (3%)	1 (0%)	36	40
All	All	1822/1836 (99%)	1768 (97%)	47 (3%)	7 (0%)	30	31

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 ⓘ

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%)	250 (95%)	13 (5%)	22	24
1	B	261/263 (99%)	252 (97%)	9 (3%)	32	40
1	C	261/263 (99%)	252 (97%)	9 (3%)	32	40
1	D	262/263 (100%)	254 (97%)	8 (3%)	35	44
1	E	261/263 (99%)	248 (95%)	13 (5%)	22	24
1	F	260/263 (99%)	250 (96%)	10 (4%)	29	36
All	All	1568/1578 (99%)	1506 (96%)	62 (4%)	28	34

All (62) 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
1	A	86	VAL
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	274	ASN
1	A	277	ASN
1	A	303	VAL
1	B	62	SER
1	B	102	LYS
1	B	128	CYS
1	B	224	THR
1	B	235	MET
1	B	240	GLU
1	B	252	PRO
1	B	274	ASN
1	B	298	ARG
1	C	1	SER
1	C	67	LEU
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	D	60	ARG
1	D	62	SER
1	D	69	GLN
1	D	102	LYS
1	D	128	CYS
1	D	238	ASN
1	D	252	PRO
1	D	269	LYS
1	E	46	SER
1	E	86	VAL
1	E	90	LYS

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Mol	Chain	Res	Type
1	E	102	LYS
1	E	121	SER
1	E	128	CYS
1	E	136	ILE
1	E	196	THR
1	E	235	MET
1	E	238	ASN
1	E	270	GLU
1	E	274	ASN
1	E	276	MET
1	F	50	LEU
1	F	59	ILE
1	F	100	LYS
1	F	102	LYS
1	F	128	CYS
1	F	225	THR
1	F	228	ASN
1	F	235	MET
1	F	274	ASN
1	F	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	127	GLN
1	A	142	ASN
1	B	19	GLN
1	B	189	GLN
1	B	238	ASN
1	B	244	GLN
1	B	306	GLN
1	C	127	GLN
1	D	69	GLN
1	D	189	GLN
1	E	74	GLN
1	E	119	ASN
1	E	127	GLN
1	F	142	ASN
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 ⓘ

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	DNE	G	2	2	6,7,8	0.54	0	2,7,9	0.34	0
2	DNE	I	2	2	6,7,8	0.61	0	2,7,9	0.11	0
2	HT7	G	3	2	16,16,17	0.54	0	18,21,23	0.80	0
2	HT7	L	3	2	16,16,17	0.53	0	18,21,23	0.74	0
2	A1IM8	I	4	2	13,13,13	0.26	0	16,16,16	0.66	0
2	A1IM8	K	4	2	13,13,13	0.26	0	16,16,16	0.66	0
2	HT7	J	3	2	16,16,17	0.80	1 (6%)	18,21,23	0.80	0
2	HT7	H	3	2	16,16,17	0.58	0	18,21,23	0.80	1 (5%)
2	A1IM8	J	4	2	13,13,13	0.26	0	16,16,16	0.64	0
2	A1IM8	L	4	2	13,13,13	0.29	0	16,16,16	0.63	0
2	DNE	J	2	2	6,7,8	0.48	0	2,7,9	0.20	0
2	HT7	I	3	2	16,16,17	0.55	0	18,21,23	0.69	0
2	HT7	K	3	2	16,16,17	0.58	0	18,21,23	0.73	0
2	A1IM8	G	4	2	13,13,13	0.28	0	16,16,16	0.48	0
2	DNE	L	2	2	6,7,8	0.52	0	2,7,9	0.10	0
2	DNE	H	2	2	6,7,8	0.50	0	2,7,9	0.12	0
2	DNE	K	2	2	6,7,8	0.46	0	2,7,9	0.32	0
2	A1IM8	H	4	2	13,13,13	0.31	0	16,16,16	0.57	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	DNE	G	2	2	-	4/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DNE	I	2	2	-	4/5/6/8	-
2	HT7	G	3	2	-	0/7/7/8	0/2/2/2
2	HT7	L	3	2	-	0/7/7/8	0/2/2/2
2	A1IM8	I	4	2	-	6/10/10/10	0/1/1/1
2	A1IM8	K	4	2	-	5/10/10/10	0/1/1/1
2	HT7	J	3	2	-	0/7/7/8	0/2/2/2
2	HT7	H	3	2	-	0/7/7/8	0/2/2/2
2	A1IM8	J	4	2	-	4/10/10/10	0/1/1/1
2	A1IM8	L	4	2	-	6/10/10/10	0/1/1/1
2	DNE	J	2	2	-	2/5/6/8	-
2	HT7	I	3	2	-	1/7/7/8	0/2/2/2
2	HT7	K	3	2	-	0/7/7/8	0/2/2/2
2	A1IM8	G	4	2	-	9/10/10/10	0/1/1/1
2	DNE	L	2	2	-	5/5/6/8	-
2	DNE	H	2	2	-	4/5/6/8	-
2	DNE	K	2	2	-	4/5/6/8	-
2	A1IM8	H	4	2	-	4/10/10/10	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	2.30	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	HT7	CA-CB-CG	2.46	114.30	110.82

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
2	L	2	DNE	N-CA-CB-CG

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

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

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	HT7	2	0
2	J	4	A1IM8	1	0
2	J	2	DNE	1	0
2	I	3	HT7	1	0
2	K	3	HT7	1	0
2	K	2	DNE	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, 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	306/306 (100%)	1.11	41 (13%) 7 6	8, 33, 58, 100	1 (0%)
1	B	306/306 (100%)	0.84	28 (9%) 14 13	14, 29, 52, 75	0
1	C	305/306 (99%)	1.25	72 (23%) 2 1	18, 34, 66, 85	0
1	D	306/306 (100%)	1.15	53 (17%) 4 3	16, 34, 67, 89	0
1	E	305/306 (99%)	0.77	27 (8%) 15 14	14, 29, 60, 82	0
1	F	305/306 (99%)	0.81	26 (8%) 16 15	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%)	0.99	247 (13%) 7 6	8, 31, 63, 100	1 (0%)

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	6.0
1	D	216	ASP	5.7
1	F	305	PHE	5.6
1	C	266	ALA	5.4
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	E	154	TYR	4.7
1	D	154	TYR	4.7
1	C	303	VAL	4.5
1	E	305	PHE	4.5
1	F	223	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	155	ASP	4.4
1	B	223	PHE	4.2
1	A	223	PHE	4.2
1	D	305	PHE	4.2
1	D	215	GLY	4.2
1	C	223	PHE	4.1
1	C	286	LEU	4.1
1	A	303	VAL	4.1
1	C	220	LEU	4.1
1	C	219	PHE	4.1
1	C	59	ILE	4.0
1	A	232	LEU	4.0
1	C	262	LEU	3.9
1	C	278	GLY	3.9
1	D	218	TRP	3.9
1	D	224	THR	3.9
1	F	303	VAL	3.9
1	C	268	LEU	3.9
1	D	233	VAL	3.8
1	B	193	ALA	3.8
1	E	294	PHE	3.8
1	D	220	LEU	3.7
1	C	269	LYS	3.7
1	C	264	MET	3.7
1	C	305	PHE	3.7
1	D	294	PHE	3.7
1	C	261	VAL	3.7
1	A	220	LEU	3.6
1	C	260	ALA	3.6
1	C	72	ASN	3.6
1	A	222	ARG	3.6
1	D	276	MET	3.5
1	F	87	LEU	3.5
1	E	50	LEU	3.5
1	F	154	TYR	3.4
1	C	281	ILE	3.4
1	E	303	VAL	3.4
1	E	195	GLY	3.4
1	A	213	ILE	3.4
1	C	209	TYR	3.4
1	A	227	LEU	3.3
1	F	217	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	276	MET	3.3
1	E	235	MET	3.3
1	C	215	GLY	3.3
1	F	235	MET	3.3
1	C	224	THR	3.3
1	D	306	GLN	3.3
1	C	222	ARG	3.3
1	C	218	TRP	3.3
1	F	285	ALA	3.2
1	C	232	LEU	3.2
1	F	278	GLY	3.2
1	C	227	LEU	3.2
1	B	26	THR	3.2
1	B	305	PHE	3.2
1	C	221	ASN	3.2
1	E	216	ASP	3.2
1	D	225	THR	3.2
1	B	154	TYR	3.1
1	A	298	ARG	3.1
1	F	276	MET	3.1
1	C	116	ALA	3.1
1	C	212	VAL	3.1
1	F	222	ARG	3.1
1	A	235	MET	3.1
1	B	153	ASP	3.1
1	C	302	GLY	3.1
1	A	154	TYR	3.0
1	C	259	ILE	3.0
1	B	222	ARG	3.0
1	B	224	THR	3.0
1	F	155	ASP	3.0
1	D	303	VAL	2.9
1	D	214	ASN	2.9
1	E	284	SER	2.9
1	C	234	ALA	2.9
1	C	233	VAL	2.9
1	A	228	ASN	2.9
1	C	277	ASN	2.9
1	D	153	ASP	2.9
1	B	25	THR	2.9
1	C	235	MET	2.9
1	E	60	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	212	VAL	2.8
1	F	245	ASP	2.8
1	D	283	GLY	2.8
1	A	274	ASN	2.8
1	C	216	ASP	2.8
1	D	274	ASN	2.8
1	C	265	CYS	2.8
1	C	255	ALA	2.8
1	A	221	ASN	2.7
1	A	277	ASN	2.7
1	C	213	ILE	2.7
1	F	196	THR	2.7
1	D	302	GLY	2.7
1	F	294	PHE	2.7
1	A	56	ASP	2.7
1	F	195	GLY	2.7
1	D	102	LYS	2.7
1	B	217	ARG	2.7
1	C	74	GLN	2.7
1	A	136	ILE	2.7
1	E	285	ALA	2.6
1	C	274	ASN	2.6
1	A	215	GLY	2.6
1	C	298	ARG	2.6
1	C	206	ALA	2.6
1	B	294	PHE	2.6
1	B	122	PRO	2.6
1	D	232	LEU	2.6
1	E	1	SER	2.6
1	D	227	LEU	2.6
1	D	222	ARG	2.6
1	C	285	ALA	2.6
1	D	304	THR	2.6
1	F	233	VAL	2.6
1	C	154	TYR	2.6
1	D	259	ILE	2.6
1	E	245	ASP	2.5
1	C	225	THR	2.5
1	B	5	LYS	2.5
1	C	76	ARG	2.5
1	D	76	ARG	2.5
1	F	286	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	264	MET	2.5
1	A	285	ALA	2.5
1	B	216	ASP	2.5
1	A	268	LEU	2.5
1	E	276	MET	2.5
1	A	245	ASP	2.5
1	E	194	ALA	2.5
1	A	302	GLY	2.5
1	A	208	LEU	2.5
1	E	232	LEU	2.5
1	D	277	ASN	2.5
1	A	69	GLN	2.5
1	D	275	GLY	2.5
1	F	226	THR	2.4
1	B	73	VAL	2.4
1	C	208	LEU	2.4
1	A	70	ALA	2.4
1	D	270	GLU	2.4
1	D	46	SER	2.4
1	A	238	ASN	2.4
1	C	226	THR	2.4
1	F	224	THR	2.4
1	D	136	ILE	2.4
1	D	219	PHE	2.4
1	B	306	GLN	2.4
1	C	217	ARG	2.4
1	B	274	ASN	2.4
1	E	217	ARG	2.4
1	C	237	TYR	2.3
1	D	5	LYS	2.3
1	A	224	THR	2.3
1	B	303	VAL	2.3
1	A	306	GLN	2.3
1	D	286	LEU	2.3
1	C	14	GLU	2.3
1	D	221	ASN	2.3
1	A	269	LYS	2.3
1	B	278	GLY	2.3
1	C	134	PHE	2.3
1	E	233	VAL	2.3
1	A	58	LEU	2.3
1	C	229	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	278	GLY	2.3
1	B	194	ALA	2.3
1	A	225	THR	2.3
1	F	304	THR	2.3
1	C	273	GLN	2.3
1	D	194	ALA	2.3
1	C	267	SER	2.3
1	B	282	LEU	2.2
1	C	263	ASP	2.2
1	B	302	GLY	2.2
1	C	251	GLY	2.2
1	C	136	ILE	2.2
1	C	67	LEU	2.2
1	C	253	LEU	2.2
1	A	255	ALA	2.2
1	A	134	PHE	2.2
1	E	277	ASN	2.2
1	B	128	CYS	2.2
1	C	270	GLU	2.2
1	A	266	ALA	2.2
1	F	194	ALA	2.2
1	D	1	SER	2.2
1	D	217	ARG	2.2
1	E	87	LEU	2.2
1	C	112	PHE	2.2
1	D	197	ASP	2.2
1	C	240	GLU	2.2
1	B	275	GLY	2.2
1	B	121	SER	2.2
1	C	304	THR	2.2
1	D	50	LEU	2.1
1	D	245	ASP	2.1
1	E	223	PHE	2.1
1	E	278	GLY	2.1
1	A	193	ALA	2.1
1	C	198	THR	2.1
1	D	121	SER	2.1
1	D	175	THR	2.1
1	E	62	SER	2.1
1	F	279	ARG	2.1
1	F	232	LEU	2.1
1	E	92	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	207	TRP	2.1
1	D	266	ALA	2.1
1	A	57	LEU	2.1
1	B	286	LEU	2.1
1	C	271	LEU	2.1
1	D	101	TYR	2.1
1	D	261	VAL	2.1
1	A	278	GLY	2.1
1	D	152	ILE	2.1
1	D	249	ILE	2.1
1	E	221	ASN	2.1
1	F	216	ASP	2.1
1	B	304	THR	2.0
1	D	287	LEU	2.0
1	E	155	ASP	2.0
1	F	65	ASN	2.0
1	A	73	VAL	2.0
1	C	42	VAL	2.0
1	B	283	GLY	2.0
1	A	234	ALA	2.0
1	C	75	LEU	2.0
1	C	153	ASP	2.0
1	C	228	ASN	2.0
1	E	222	ARG	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, 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	A1IM8	H	4	13/13	0.82	0.12	22,29,38,50	0
2	A1IM8	J	4	13/13	0.82	0.12	21,27,31,33	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	DNE	L	2	8/9	0.89	0.11	29,32,41,47	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HT7	L	3	15/16	0.89	0.10	22,23,27,27	0
2	A1IM8	L	4	13/13	0.89	0.10	28,30,36,39	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
2	DNE	G	2	8/9	0.92	0.09	19,20,23,25	0

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	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	0.13	51,51,51,51	0
3	K	B	401	1/1	0.92	0.12	59,59,59,59	0
3	K	E	401	1/1	0.93	0.12	51,51,51,51	0
3	K	B	402	1/1	0.94	0.06	56,56,56,56	0
3	K	D	401	1/1	0.95	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.