



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:56 AM UTC

PDB ID : 9EO6 / pdb_00009eo6
Title : SARS-CoV2 major protease in complex with a covalent inhibitor SLL11.
Authors : Moche, M.; Lennerstrand, J.; Nyman, T.; Strandback, E.; Akaberi, D.
Deposited on : 2024-03-14
Resolution : 2.11 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

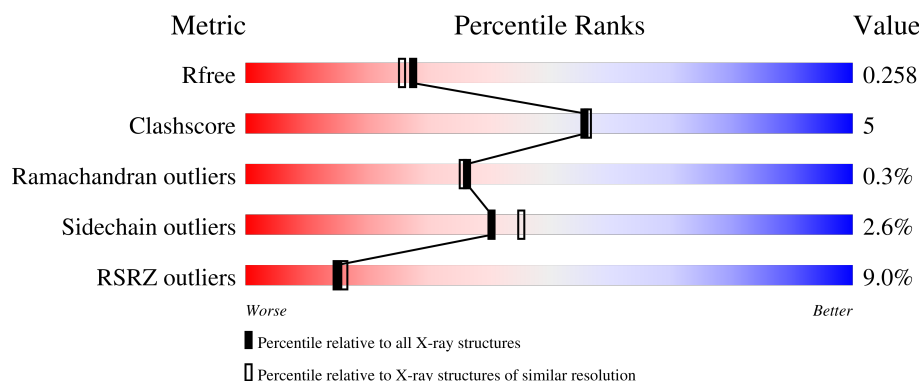
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	6% 91% 8%
1	B	306	4% 89% 11%
1	C	306	18% 85% 14%
1	D	306	15% 87% 13%
1	E	306	5% 88% 11%

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Mol	Chain	Length	Quality of chain
1	F	306	6% 86% 12%
2	G	4	75% 25%
2	H	4	50% 25% 25%
2	I	4	75% 25%
2	J	4	50% 25% 25%
2	K	4	75% 25%
2	L	4	25% 25% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14978 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	2	0
			2379	1504	407	446	22			
1	B	306	Total	C	N	O	S	0	2	0
			2377	1502	407	446	22			
1	C	305	Total	C	N	O	S	0	1	0
			2357	1491	401	443	22			
1	D	306	Total	C	N	O	S	0	0	0
			2355	1490	399	444	22			
1	E	305	Total	C	N	O	S	0	2	0
			2365	1495	405	444	21			
1	F	305	Total	C	N	O	S	0	2	0
			2355	1490	402	442	21			

- Molecule 2 is a protein called Inhibitor SLL11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			47	35	8	4			
2	H	4	Total	C	N	O	0	0	0
			47	35	8	4			
2	I	4	Total	C	N	O	0	0	0
			47	35	8	4			
2	J	4	Total	C	N	O	0	0	0
			47	35	8	4			
2	K	4	Total	C	N	O	0	0	0
			47	35	8	4			
2	L	4	Total	C	N	O	0	0	0
			47	35	8	4			

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	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

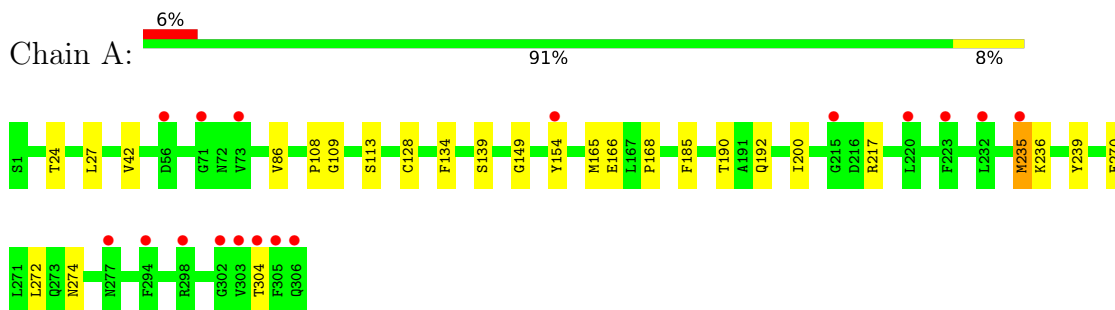
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	97	Total O 97 97	0	0
4	C	81	Total O 81 81	0	0
4	D	61	Total O 61 61	0	0
4	E	85	Total O 85 85	0	0
4	F	88	Total O 88 88	0	0
4	G	2	Total O 2 2	0	0
4	H	4	Total O 4 4	0	0
4	I	1	Total O 1 1	0	0
4	J	3	Total O 3 3	0	0
4	K	2	Total O 2 2	0	0
4	L	3	Total O 3 3	0	0

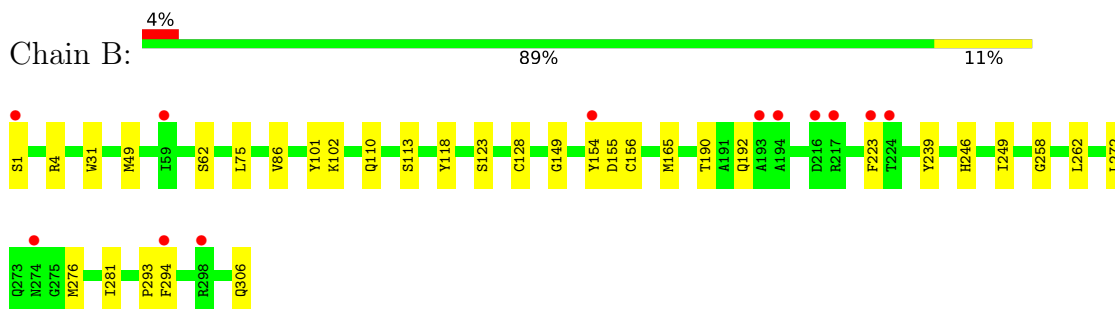
3 Residue-property plots [i](#)

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.

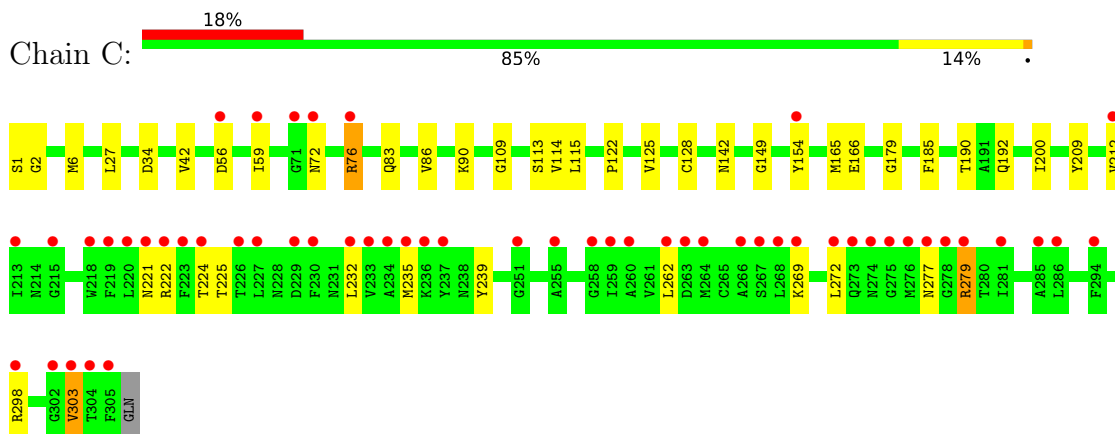
- Molecule 1: 3C-like proteinase nsp5



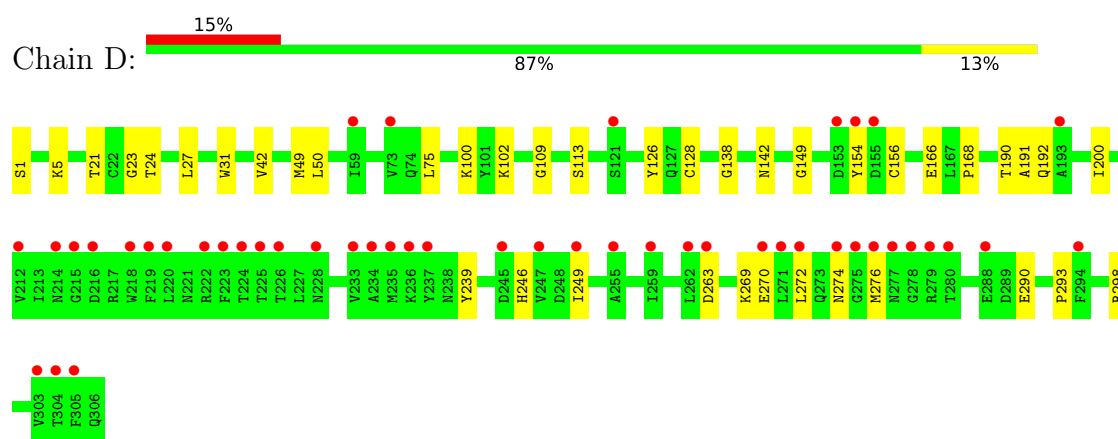
- Molecule 1: 3C-like proteinase nsp5



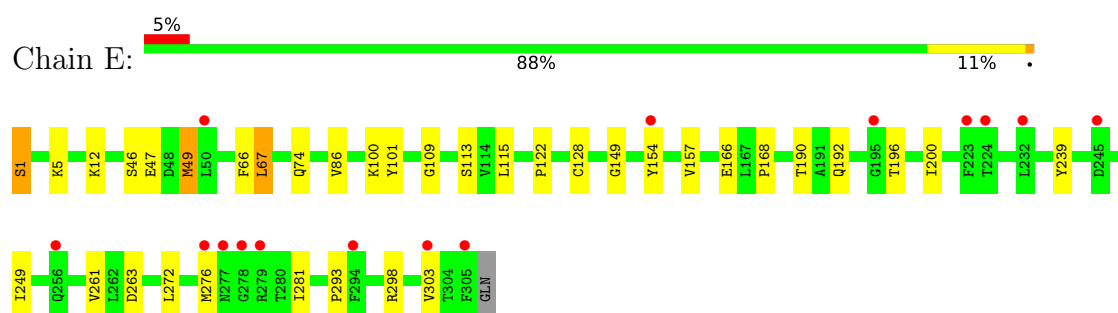
- Molecule 1: 3C-like proteinase nsp5



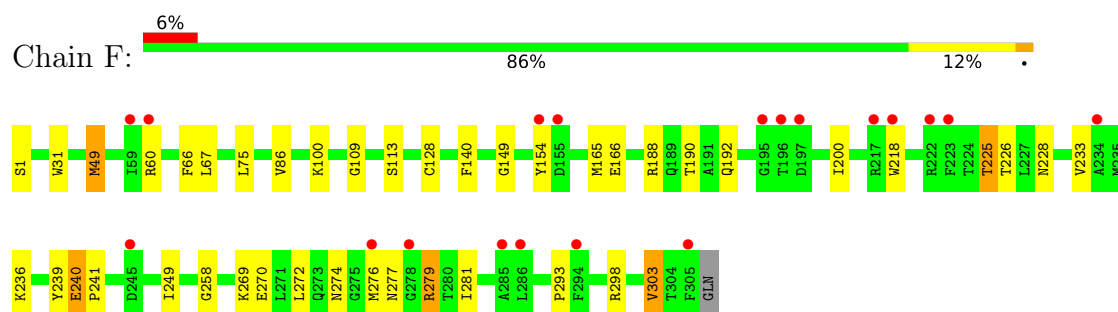
- Molecule 1: 3C-like proteinase nsp5



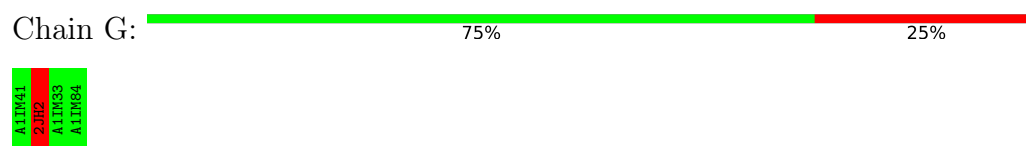
- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



- Molecule 2: Inhibitor SLL11



- Molecule 2: Inhibitor SLL11



- Molecule 2: Inhibitor SLL11

Chain I:  75% 25%

A1IM41
2JH2
A1IM33
A1IM84

- Molecule 2: Inhibitor SLL11

Chain J:  50% 25% 25%

A1IM41
2JH2
A1IM33
A1IM84

- Molecule 2: Inhibitor SLL11

Chain K:  75% 25%

A1IM41
2JH2
A1IM33
A1IM84

- Molecule 2: Inhibitor SLL11

Chain L:  25% 25% 50%

A1IM41
2JH2
A1IM33
A1IM84

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.81Å 85.74Å 93.91Å 79.25° 87.44° 83.86°	Depositor
Resolution (Å)	46.16 – 2.11 46.16 – 2.11	Depositor EDS
% Data completeness (in resolution range)	63.1 (46.16-2.11) 63.1 (46.16-2.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.208 , 0.257 0.212 , 0.258	Depositor DCC
R_{free} test set	6026 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14978	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.40% 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: K, 2JH, A1IM8, A1IM4, A1IM3

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	0.56	0/2431	0.90	0/3302
1	B	0.57	0/2429	0.90	0/3299
1	C	0.56	0/2409	0.91	0/3274
1	D	0.57	0/2407	0.91	0/3271
1	E	0.54	0/2417	0.88	0/3285
1	F	0.55	0/2407	0.90	0/3274
All	All	0.56	0/14500	0.90	0/19705

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	F	0	1
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	60	ARG	Sidechain
2	G	2	2JH	Peptide
2	H	2	2JH	Peptide
2	I	2	2JH	Peptide
2	J	2	2JH	Peptide
2	K	2	2JH	Peptide
2	L	2	2JH	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	2379	0	2326	18	0
1	B	2377	0	2319	24	0
1	C	2357	0	2302	32	0
1	D	2355	0	2294	29	0
1	E	2365	0	2307	25	0
1	F	2355	0	2293	28	0
2	G	47	0	9	1	0
2	H	47	0	9	1	0
2	I	47	0	9	0	0
2	J	47	0	9	1	0
2	K	47	0	9	0	0
2	L	47	0	9	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	76	0	0	2	0
4	B	97	0	0	5	0
4	C	81	0	0	3	0
4	D	61	0	0	1	0
4	E	85	0	0	2	0
4	F	88	0	0	2	0
4	G	2	0	0	0	0
4	H	4	0	0	0	0
4	I	1	0	0	0	0
4	J	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	2	0	0	0	0
4	L	3	0	0	0	0
All	All	14978	0	13895	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HD2	1:D:156:CYS:SG	2.06	0.94
1:B:102:LYS:NZ	1:B:156:CYS:SG	2.44	0.90
1:B:192:GLN:O	4:B:502:HOH:O	2.01	0.78
1:B:223:PHE:O	4:B:501:HOH:O	1.99	0.78
1:F:233:VAL:HG21	1:F:269:LYS:HD2	1.65	0.77
1:C:142:ASN:OD1	4:C:501:HOH:O	2.04	0.76
1:B:49:MET:HE3	1:B:49:MET:HA	1.72	0.72
1:C:221:ASN:OD1	4:C:502:HOH:O	2.08	0.71
1:B:155:ASP:HB3	1:B:306:GLN:OXT	1.92	0.70
1:D:102:LYS:NZ	1:D:156:CYS:SG	2.59	0.69
1:D:49:MET:HE3	1:D:49:MET:HA	1.73	0.69
1:E:1:SER:HB3	1:F:166:GLU:OE2	1.93	0.69
1:C:166:GLU:OE2	1:D:1:SER:HA	1.94	0.67
1:C:232:LEU:HA	1:C:235:MET:HE2	1.79	0.65
1:F:225:THR:HG23	1:F:226:THR:O	1.96	0.65
1:A:235:MET:HG2	1:A:236:LYS:N	2.11	0.64
1:B:294:PHE:HD2	4:B:587:HOH:O	1.80	0.64
1:F:188:ARG:HG3	4:F:554:HOH:O	1.98	0.63
1:A:166:GLU:OE2	1:B:1:SER:HA	1.98	0.63
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.81	0.63
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.82	0.62
1:E:166:GLU:OE2	1:F:1:SER:HA	2.01	0.61
1:D:102:LYS:CD	1:D:156:CYS:SG	2.88	0.60
1:C:269:LYS:HD2	4:C:579:HOH:O	2.01	0.59
1:E:115:LEU:HD11	1:E:122:PRO:HB3	1.84	0.59
1:E:1:SER:N	1:F:140:PHE:O	2.35	0.59
1:D:21:THR:HG23	1:E:67:LEU:HD13	1.86	0.57
1:D:23:GLY:H	1:E:74:GLN:NE2	2.03	0.57
1:B:258:GLY:HA3	1:E:168:PRO:HG3	1.86	0.56
1:A:24:THR:HG21	1:D:50:LEU:HD22	1.88	0.55
1:B:101:TYR:O	1:C:222:ARG:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:HB3	4:B:582:HOH:O	2.06	0.54
1:F:298[A]:ARG:HG3	1:F:303:VAL:HG22	1.88	0.54
1:D:142:ASN:ND2	2:L:4:A1IM8:O	2.38	0.54
1:D:24:THR:C	1:E:67:LEU:HD12	2.33	0.53
1:F:279:ARG:HH21	1:F:279:ARG:HG3	1.72	0.53
1:D:23:GLY:N	1:E:74:GLN:NE2	2.56	0.53
1:C:298:ARG:HA	1:C:303:VAL:HG13	1.91	0.52
1:E:12:LYS:HE3	4:E:508:HOH:O	2.09	0.52
1:A:270:GLU:HG2	1:A:274:ASN:ND2	2.24	0.52
1:F:66:PHE:C	1:F:67:LEU:HD12	2.35	0.52
1:C:2:GLY:HA3	1:D:138:GLY:O	2.10	0.51
1:A:304:THR:HG21	1:B:118:TYR:HB2	1.93	0.50
1:B:165:MET:HB3	2:H:2:2JH:H11	1.94	0.50
1:C:6:MET:HE2	1:D:126:TYR:CD2	2.47	0.50
1:C:298:ARG:HG3	1:C:303:VAL:HG22	1.94	0.50
1:D:113:SER:O	1:D:149:GLY:HA2	2.12	0.50
1:A:190:THR:O	1:A:192:GLN:HG3	2.12	0.50
1:B:113:SER:O	1:B:149:GLY:HA2	2.12	0.49
1:F:190:THR:O	1:F:192:GLN:HG3	2.13	0.49
1:B:246:HIS:HA	1:B:249:ILE:HG12	1.95	0.49
1:E:190:THR:O	1:E:192:GLN:HG3	2.12	0.49
1:F:109:GLY:HA2	1:F:200:ILE:HD13	1.95	0.49
1:C:113:SER:O	1:C:149:GLY:HA2	2.13	0.48
1:C:224:THR:HG22	1:C:225:THR:N	2.28	0.48
1:C:190:THR:O	1:C:192:GLN:HG3	2.13	0.48
1:F:67:LEU:HD12	1:F:67:LEU:N	2.27	0.48
1:F:113:SER:O	1:F:149:GLY:HA2	2.12	0.48
1:B:276:MET:HE3	1:B:281:ILE:HG13	1.95	0.48
1:A:165:MET:HB3	2:G:2:2JH:H11	1.96	0.48
1:E:113:SER:O	1:E:149:GLY:HA2	2.13	0.48
1:B:190:THR:O	1:B:192:GLN:HG3	2.14	0.47
1:D:168:PRO:HD2	4:D:501:HOH:O	2.12	0.47
1:A:168:PRO:HG3	1:F:258:GLY:HA3	1.96	0.47
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.96	0.47
1:C:224:THR:HG22	1:C:225:THR:H	1.80	0.47
1:D:249:ILE:HD12	1:D:293:PRO:HG2	1.97	0.47
1:E:276:MET:HE3	1:E:281:ILE:HG13	1.97	0.47
1:F:49:MET:HA	1:F:49:MET:HE2	1.97	0.47
1:C:1:SER:HB2	1:D:166:GLU:OE2	2.15	0.46
1:A:113:SER:O	1:A:149:GLY:HA2	2.15	0.46
1:D:190:THR:O	1:D:192:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLN:O	1:C:86:VAL:HG22	2.15	0.46
1:D:23:GLY:H	1:E:74:GLN:HE21	1.63	0.46
1:D:100:LYS:HE2	1:D:102:LYS:HZ1	1.80	0.46
1:D:246:HIS:HA	1:D:249:ILE:HG12	1.97	0.46
1:E:261:VAL:HG23	4:E:524:HOH:O	2.16	0.46
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.51	0.45
1:C:239:TYR:CZ	1:C:272:LEU:HD21	2.51	0.45
1:F:188:ARG:CG	4:F:554:HOH:O	2.60	0.45
1:E:109:GLY:HA2	1:E:200:ILE:HD13	1.99	0.45
1:F:233:VAL:CG2	1:F:269:LYS:HD2	2.39	0.45
1:E:1:SER:HB3	1:F:166:GLU:CD	2.41	0.45
1:A:108:PRO:HG3	1:A:134:PHE:CE1	2.53	0.44
1:D:239:TYR:CZ	1:D:272:LEU:HD21	2.53	0.44
1:F:218:TRP:CE2	1:F:279:ARG:HD2	2.53	0.44
1:C:279:ARG:HG3	1:C:279:ARG:HH11	1.83	0.44
1:B:262:LEU:HG	4:B:558:HOH:O	2.17	0.44
1:F:67:LEU:N	1:F:67:LEU:CD1	2.81	0.44
1:F:249:ILE:HG22	1:F:293:PRO:HG2	1.99	0.43
1:C:56:ASP:HA	1:C:59:ILE:HG12	1.99	0.43
1:C:279:ARG:HG3	1:C:279:ARG:NH1	2.33	0.43
1:E:66:PHE:C	1:E:67:LEU:HD23	2.43	0.43
1:C:76:ARG:HA	1:C:76:ARG:HD3	1.82	0.43
1:D:109:GLY:HA2	1:D:200:ILE:HD13	2.00	0.43
1:E:49:MET:HA	1:E:49:MET:HE2	2.01	0.43
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.54	0.43
1:C:225:THR:O	1:C:262:LEU:HD13	2.17	0.43
1:E:49:MET:HA	1:E:49:MET:CE	2.49	0.43
1:F:165:MET:SD	2:J:2:2JH:H10	2.59	0.43
1:C:34:ASP:OD2	1:C:90:LYS:HD2	2.18	0.43
1:D:5:LYS:HE2	1:D:290:GLU:HB2	2.00	0.42
1:A:304:THR:HG22	1:B:123:SER:HB2	2.01	0.42
1:E:249:ILE:HG22	1:E:293:PRO:HG2	2.01	0.42
1:F:276:MET:HE2	1:F:281:ILE:HD12	2.02	0.42
1:B:249:ILE:HD12	1:B:293:PRO:HG2	2.02	0.42
1:F:239:TYR:CZ	1:F:272:LEU:HD21	2.55	0.41
1:F:240:GLU:HG3	1:F:241:PRO:HD2	2.02	0.41
1:C:6:MET:HE2	1:D:126:TYR:CE2	2.55	0.41
1:C:232:LEU:HA	1:C:235:MET:CE	2.48	0.41
1:D:27:LEU:HD21	1:D:42:VAL:HB	2.03	0.41
1:E:67:LEU:HD23	1:E:67:LEU:N	2.35	0.41
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:TRP:CE2	1:D:75:LEU:HD21	2.55	0.41
1:A:27:LEU:HD21	1:A:42:VAL:HB	2.02	0.41
1:B:258:GLY:HA3	1:E:168:PRO:CG	2.51	0.41
1:C:27:LEU:HD21	1:C:42:VAL:HB	2.02	0.41
1:F:270:GLU:HG3	1:F:274:ASN:ND2	2.36	0.41
1:A:304:THR:CG2	1:B:118:TYR:HB2	2.50	0.41
1:B:31:TRP:CE2	1:B:75:LEU:HD21	2.55	0.41
1:C:114:VAL:O	1:C:125:VAL:HA	2.21	0.41
1:E:239:TYR:CZ	1:E:272:LEU:HD21	2.56	0.41
1:F:279:ARG:HG3	1:F:279:ARG:NH2	2.36	0.41
4:A:516:HOH:O	1:D:191:ALA:HB3	2.21	0.40
1:C:165:MET:CE	1:C:185:PHE:HB3	2.51	0.40
1:F:31:TRP:CE2	1:F:75:LEU:HD21	2.56	0.40
1:A:217:ARG:NH1	4:A:510:HOH:O	2.54	0.40
1:C:209:TYR:O	1:C:212:VAL:HG22	2.20	0.40
1:E:101:TYR:HA	1:E:157:VAL:O	2.22	0.40
1:A:139:SER:HB2	1:B:4:ARG:HG2	2.04	0.40
1:A:165:MET:CE	1:A:185:PHE:HB3	2.51	0.40
1:D:270:GLU:HG2	1:D:274:ASN:HD21	1.87	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	306/306 (100%)	298 (97%)	7 (2%)	1 (0%)	36	36
1	B	306/306 (100%)	298 (97%)	7 (2%)	1 (0%)	36	36
1	C	304/306 (99%)	296 (97%)	7 (2%)	1 (0%)	36	36
1	D	304/306 (99%)	296 (97%)	7 (2%)	1 (0%)	36	36
1	E	305/306 (100%)	297 (97%)	7 (2%)	1 (0%)	36	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	305/306 (100%)	297 (97%)	7 (2%)	1 (0%)	36	36
All	All	1830/1836 (100%)	1782 (97%)	42 (2%)	6 (0%)	36	36

All (6) Ramachandran outliers are listed below:

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

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	264/263 (100%)	261 (99%)	3 (1%)	65	74
1	B	263/263 (100%)	260 (99%)	3 (1%)	65	74
1	C	262/263 (100%)	256 (98%)	6 (2%)	44	50
1	D	261/263 (99%)	256 (98%)	5 (2%)	50	57
1	E	262/263 (100%)	248 (95%)	14 (5%)	20	18
1	F	260/263 (99%)	249 (96%)	11 (4%)	26	27
All	All	1572/1578 (100%)	1530 (97%)	42 (3%)	40	44

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	128	CYS
1	A	235	MET
1	B	62	SER
1	B	86	VAL

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Mol	Chain	Res	Type
1	B	128	CYS
1	C	72	ASN
1	C	76	ARG
1	C	128	CYS
1	C	277	ASN
1	C	279	ARG
1	C	303	VAL
1	D	128	CYS
1	D	263	ASP
1	D	269	LYS
1	D	276	MET
1	D	298	ARG
1	E	1	SER
1	E	5	LYS
1	E	46	SER
1	E	47	GLU
1	E	49	MET
1	E	67	LEU
1	E	86	VAL
1	E	100	LYS
1	E	128	CYS
1	E	196	THR
1	E	263	ASP
1	E	298[A]	ARG
1	E	298[B]	ARG
1	E	303	VAL
1	F	49	MET
1	F	86	VAL
1	F	100	LYS
1	F	128	CYS
1	F	225	THR
1	F	228	ASN
1	F	236	LYS
1	F	240	GLU
1	F	277	ASN
1	F	279	ARG
1	F	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	274	ASN
1	B	64	HIS
1	B	119	ASN
1	B	189	GLN
1	B	244	GLN
1	C	119	ASN
1	C	127	GLN
1	D	69	GLN
1	D	180	ASN
1	D	189	GLN
1	D	244	GLN
1	D	274	ASN
1	D	306	GLN
1	E	74	GLN
1	E	107	GLN
1	E	119	ASN
1	E	127	GLN
1	E	142	ASN
1	F	69	GLN
1	F	74	GLN
1	F	110	GLN
1	F	180	ASN
1	F	244	GLN
1	F	274	ASN
1	F	277	ASN

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	2JH	J	2	2	7,9,10	0.44	0	7,11,13	1.40	2 (28%)
2	A1IM3	K	3	2	16,16,17	0.58	0	18,21,23	0.76	0
2	A1IM8	K	4	2	13,13,13	0.24	0	16,16,16	0.56	0
2	A1IM3	L	3	2	16,16,17	0.56	0	18,21,23	1.12	3 (16%)
2	2JH	L	2	2	7,9,10	0.45	0	7,11,13	1.60	2 (28%)
2	A1IM3	J	3	2	16,16,17	0.39	0	18,21,23	0.71	0
2	2JH	H	2	2	7,9,10	0.63	0	7,11,13	1.77	1 (14%)
2	A1IM3	H	3	2	16,16,17	0.51	0	18,21,23	0.94	2 (11%)
2	A1IM8	J	4	2	13,13,13	0.30	0	16,16,16	0.85	1 (6%)
2	A1IM3	I	3	2	16,16,17	0.42	0	18,21,23	0.82	0
2	A1IM8	L	4	2	13,13,13	0.25	0	16,16,16	1.00	1 (6%)
2	2JH	G	2	2	7,9,10	0.53	0	7,11,13	1.94	2 (28%)
2	A1IM3	G	3	2	16,16,17	0.47	0	18,21,23	0.74	0
2	A1IM8	G	4	2	13,13,13	0.29	0	16,16,16	0.54	0
2	A1IM8	H	4	2	13,13,13	0.33	0	16,16,16	0.70	0
2	2JH	K	2	2	7,9,10	0.44	0	7,11,13	1.33	2 (28%)
2	2JH	I	2	2	7,9,10	0.42	0	7,11,13	1.78	2 (28%)
2	A1IM8	I	4	2	13,13,13	0.29	0	16,16,16	0.76	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	2JH	J	2	2	-	0/5/12/14	0/1/1/1
2	A1IM3	K	3	2	-	4/7/7/8	0/2/2/2
2	A1IM8	K	4	2	-	8/10/10/10	0/1/1/1
2	A1IM3	L	3	2	-	4/7/7/8	0/2/2/2
2	2JH	L	2	2	-	1/5/12/14	0/1/1/1
2	A1IM3	J	3	2	-	3/7/7/8	0/2/2/2
2	2JH	H	2	2	-	1/5/12/14	0/1/1/1
2	A1IM3	H	3	2	-	3/7/7/8	0/2/2/2
2	A1IM8	J	4	2	-	8/10/10/10	0/1/1/1
2	A1IM3	I	3	2	-	4/7/7/8	0/2/2/2
2	A1IM8	L	4	2	-	6/10/10/10	0/1/1/1
2	2JH	G	2	2	-	1/5/12/14	0/1/1/1
2	A1IM3	G	3	2	-	4/7/7/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IM8	G	4	2	-	9/10/10/10	0/1/1/1
2	A1IM8	H	4	2	-	2/10/10/10	0/1/1/1
2	2JH	K	2	2	-	2/5/12/14	0/1/1/1
2	2JH	I	2	2	-	1/5/12/14	0/1/1/1
2	A1IM8	I	4	2	-	7/10/10/10	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	2JH	CG-CB-CA	-4.27	108.78	114.52
2	G	2	2JH	CB-CA-C	3.89	116.97	110.99
2	L	2	2JH	CG-CB-CA	-3.67	109.58	114.52
2	I	2	2JH	CG-CB-CA	-3.64	109.63	114.52
2	G	2	2JH	CG-CB-CA	-3.26	110.13	114.52
2	L	3	A1IM3	CA-CB-CG	-2.96	106.64	110.82
2	I	2	2JH	CB-CA-C	2.77	115.26	110.99
2	L	4	A1IM8	CA-C-N5	2.64	119.67	116.18
2	J	2	2JH	CG-CB-CA	-2.63	110.98	114.52
2	H	3	A1IM3	O-C-CA	-2.35	118.55	125.38
2	L	3	A1IM3	O-C-CA	-2.31	118.65	125.38
2	J	4	A1IM8	CA-C-N5	2.20	119.08	116.18
2	J	2	2JH	CB-CA-C	2.19	114.37	110.99
2	K	2	2JH	CG-CB-CA	-2.16	111.62	114.52
2	L	3	A1IM3	CB-CA-C	2.04	115.46	112.17
2	K	2	2JH	CB-CA-C	2.01	114.08	110.99
2	L	2	2JH	CB-CA-C	2.01	114.08	110.99
2	H	3	A1IM3	CA-CB-CG	-2.01	107.99	110.82

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	2JH	CA-CB-CG-CD2
2	G	3	A1IM3	N-CB-CG-CD
2	H	3	A1IM3	CA-CB-CG-CD
2	H	3	A1IM3	O-C-CA-CB
2	I	3	A1IM3	C-CA-CB-N
2	J	3	A1IM3	CA-CB-CG-CD
2	K	3	A1IM3	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
2	K	3	A1IM3	O-C-CA-CB
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	I	4	A1IM8	O-C-CA-N
2	I	4	A1IM8	N5-C-CA-N
2	I	4	A1IM8	O-C-CA-CB2
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	CA-C-N5-C13
2	L	4	A1IM8	O-C-N5-C13
2	H	3	A1IM3	N-CB-CG-CD
2	I	3	A1IM3	N-CB-CG-CD
2	K	3	A1IM3	N-CB-CG-CD
2	L	3	A1IM3	N-CB-CG-CD
2	G	4	A1IM8	O-C-CA-N
2	J	4	A1IM8	N-CA-CB2-CG2
2	K	4	A1IM8	N-CA-CB2-CG2
2	G	4	A1IM8	N5-C-CA-CB2
2	I	4	A1IM8	N5-C-CA-CB2
2	H	4	A1IM8	CA-CB2-CG2-C4
2	H	4	A1IM8	CA-CB2-CG2-CD2
2	L	4	A1IM8	CA-CB2-CG2-C4
2	L	4	A1IM8	CA-CB2-CG2-CD2
2	K	4	A1IM8	CA-CB2-CG2-CD2
2	K	4	A1IM8	CA-CB2-CG2-C4
2	I	4	A1IM8	CA-CB2-CG2-C4
2	J	4	A1IM8	C-CA-CB2-CG2
2	G	4	A1IM8	CA-CB2-CG2-C4
2	G	4	A1IM8	CA-CB2-CG2-CD2
2	J	3	A1IM3	N-CB-CG-CD
2	G	3	A1IM3	CA-CB-CG-CD
2	I	3	A1IM3	CA-CB-CG-CD
2	L	3	A1IM3	CA-CB-CG-CD
2	J	4	A1IM8	CA-CB2-CG2-CD2
2	I	4	A1IM8	CA-CB2-CG2-CD2
2	J	4	A1IM8	CA-CB2-CG2-C4
2	G	3	A1IM3	O-C-CA-CB
2	J	3	A1IM3	O-C-CA-CB
2	L	3	A1IM3	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	K	2	2JH	C-CA-CB-CG
2	G	4	A1IM8	O-C-CA-CB2
2	G	4	A1IM8	N-CA-CB2-CG2
2	I	4	A1IM8	N-CA-CB2-CG2
2	G	2	2JH	CA-CB-CG-CD2
2	I	2	2JH	CA-CB-CG-CD2
2	L	2	2JH	CA-CB-CG-CD2
2	G	3	A1IM3	C-CA-CB-N
2	L	3	A1IM3	C-CA-CB-N
2	I	3	A1IM3	O-C-CA-CB
2	J	4	A1IM8	O-C-CA-N
2	K	4	A1IM8	O-C-CA-N
2	L	4	A1IM8	O-C-CA-N
2	K	2	2JH	N-CA-CB-CG
2	K	4	A1IM8	C-CA-CB2-CG2
2	J	4	A1IM8	N5-C-CA-N
2	K	4	A1IM8	N5-C-CA-N
2	L	4	A1IM8	N5-C-CA-N
2	K	3	A1IM3	C-CA-CB-N

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	2JH	1	0
2	H	2	2JH	1	0
2	L	4	A1IM8	1	0
2	G	2	2JH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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%)	0.50	17 (5%)	30 33	8, 31, 53, 83	2 (0%)
1	B	306/306 (100%)	0.37	12 (3%)	43 46	15, 28, 50, 78	2 (0%)
1	C	305/306 (99%)	0.83	55 (18%)	3 4	15, 33, 63, 88	1 (0%)
1	D	306/306 (100%)	0.83	47 (15%)	5 5	17, 33, 70, 87	0
1	E	305/306 (99%)	0.35	15 (4%)	35 37	16, 28, 55, 79	2 (0%)
1	F	305/306 (99%)	0.41	19 (6%)	26 29	10, 28, 55, 90	2 (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%)	0.55	165 (9%)	15 16	8, 30, 59, 90	9 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	5.9
1	F	223	PHE	5.4
1	C	260	ALA	5.0
1	B	223	PHE	4.9
1	D	218	TRP	4.8
1	D	294	PHE	4.7
1	E	294	PHE	4.7
1	D	216	ASP	4.7
1	F	305	PHE	4.6
1	C	303	VAL	4.5
1	C	305	PHE	4.4
1	D	215	GLY	4.3
1	C	266	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	233	VAL	4.2
1	C	278	GLY	4.1
1	B	294	PHE	4.1
1	B	224	THR	4.1
1	F	155	ASP	4.0
1	D	219	PHE	3.9
1	C	262	LEU	3.9
1	F	294	PHE	3.8
1	C	220	LEU	3.8
1	D	223	PHE	3.7
1	C	234	ALA	3.7
1	F	222	ARG	3.7
1	C	223	PHE	3.7
1	D	224	THR	3.6
1	D	220	LEU	3.6
1	F	154	TYR	3.6
1	C	219	PHE	3.6
1	C	259	ILE	3.6
1	E	303	VAL	3.5
1	D	214	ASN	3.5
1	D	154	TYR	3.4
1	C	218	TRP	3.4
1	C	221	ASN	3.3
1	C	275	GLY	3.3
1	D	222	ARG	3.3
1	C	255	ALA	3.3
1	D	278	GLY	3.3
1	D	259	ILE	3.2
1	E	154	TYR	3.2
1	D	305	PHE	3.1
1	E	223	PHE	3.1
1	C	235	MET	3.1
1	C	232	LEU	3.1
1	C	273	GLN	3.1
1	F	217	ARG	3.1
1	A	294	PHE	3.0
1	E	305	PHE	3.0
1	C	304	THR	3.0
1	E	278	GLY	2.9
1	B	193	ALA	2.9
1	E	232	LEU	2.9
1	C	285	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	274	ASN	2.8
1	D	228	ASN	2.8
1	C	237	TYR	2.8
1	A	298[A]	ARG	2.7
1	D	155	ASP	2.7
1	A	304	THR	2.7
1	C	59	ILE	2.7
1	F	196	THR	2.7
1	A	306	GLN	2.7
1	C	212	VAL	2.7
1	C	276	MET	2.7
1	F	285	ALA	2.7
1	C	267	SER	2.7
1	D	279	ARG	2.7
1	C	272	LEU	2.6
1	C	233	VAL	2.6
1	B	298[A]	ARG	2.6
1	D	226	THR	2.6
1	A	220	LEU	2.6
1	E	245	ASP	2.6
1	A	154	TYR	2.6
1	B	216	ASP	2.6
1	D	153	ASP	2.6
1	C	56	ASP	2.6
1	D	272	LEU	2.6
1	A	223	PHE	2.5
1	D	212	VAL	2.5
1	A	302	GLY	2.5
1	D	237	TYR	2.5
1	D	235	MET	2.5
1	F	278	GLY	2.5
1	D	193	ALA	2.5
1	A	232	LEU	2.5
1	F	286	LEU	2.5
1	A	303	VAL	2.5
1	D	59	ILE	2.5
1	D	247	VAL	2.5
1	C	236	LYS	2.5
1	C	277	ASN	2.5
1	E	195	GLY	2.5
1	C	268	LEU	2.5
1	A	235	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	286	LEU	2.4
1	D	275	GLY	2.4
1	A	277	ASN	2.4
1	B	274	ASN	2.4
1	E	277	ASN	2.4
1	D	249	ILE	2.4
1	E	256	GLN	2.4
1	C	154	TYR	2.4
1	C	224	THR	2.4
1	D	280	THR	2.4
1	D	262	LEU	2.4
1	A	215	GLY	2.4
1	C	302	GLY	2.4
1	F	197	ASP	2.4
1	A	73	VAL	2.4
1	C	281	ILE	2.4
1	D	234	ALA	2.4
1	C	263	ASP	2.4
1	F	245	ASP	2.4
1	C	269	LYS	2.4
1	D	276	MET	2.4
1	E	276	MET	2.4
1	C	213	ILE	2.3
1	C	222	ARG	2.3
1	D	277	ASN	2.3
1	B	194	ALA	2.3
1	C	229	ASP	2.3
1	D	263	ASP	2.3
1	D	303	VAL	2.3
1	D	304	THR	2.3
1	C	72	ASN	2.3
1	F	276	MET	2.3
1	B	154	TYR	2.3
1	D	255	ALA	2.2
1	B	1	SER	2.2
1	C	258	GLY	2.2
1	B	59	ILE	2.2
1	D	225	THR	2.2
1	C	264	MET	2.2
1	C	215	GLY	2.2
1	C	226	THR	2.2
1	F	59	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	73	VAL	2.1
1	B	217[A]	ARG	2.1
1	C	227	LEU	2.1
1	D	274	ASN	2.1
1	D	270	GLU	2.1
1	E	224	THR	2.1
1	C	294	PHE	2.1
1	C	279	ARG	2.1
1	F	234	ALA	2.1
1	D	236	LYS	2.1
1	F	218	TRP	2.1
1	D	121	SER	2.1
1	E	50	LEU	2.1
1	D	288	GLU	2.1
1	C	76	ARG	2.1
1	C	251	GLY	2.1
1	D	271	LEU	2.0
1	A	56	ASP	2.0
1	C	71	GLY	2.0
1	C	230	PHE	2.0
1	D	245	ASP	2.0
1	C	298	ARG	2.0
1	E	279	ARG	2.0
1	F	60	ARG	2.0
1	A	71	GLY	2.0
1	F	195	GLY	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	2JH	J	2	9/10	0.86	0.13	34,35,37,39	0
2	2JH	K	2	9/10	0.89	0.11	30,30,37,37	0
2	A1IM8	K	4	13/13	0.89	0.12	33,34,47,49	0
2	A1IM8	J	4	13/13	0.90	0.09	23,26,42,48	0
2	A1IM3	I	3	15/16	0.90	0.09	24,25,34,39	0
2	A1IM3	J	3	15/16	0.91	0.10	29,31,34,35	0
2	A1IM3	K	3	15/16	0.91	0.10	21,23,31,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1IM3	L	3	15/16	0.92	0.09	22,25,30,30	0
2	A1IM8	I	4	13/13	0.92	0.11	19,24,49,52	0
2	2JH	I	2	9/10	0.92	0.09	22,24,25,28	0
2	2JH	G	2	9/10	0.92	0.09	21,23,24,25	0
2	A1IM8	L	4	13/13	0.92	0.08	20,22,30,34	0
2	A1IM3	H	3	15/16	0.93	0.08	17,19,20,21	0
2	A1IM8	H	4	13/13	0.93	0.07	23,25,33,33	0
2	A1IM3	G	3	15/16	0.93	0.09	23,23,27,32	0
2	A1IM8	G	4	13/13	0.94	0.08	20,23,40,44	0
2	2JH	H	2	9/10	0.94	0.08	19,20,21,22	0
2	2JH	L	2	9/10	0.94	0.08	22,23,24,25	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	0.83	0.12	73,73,73,73	0
3	K	B	401	1/1	0.90	0.14	71,71,71,71	0
3	K	E	401	1/1	0.91	0.07	68,68,68,68	0
3	K	A	401	1/1	0.94	0.08	49,49,49,49	0
3	K	D	401	1/1	0.96	0.11	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.