



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:49 PM UTC

PDB ID : 8DS1 / pdb_00008ds1
Title : Structure of SARS-CoV-2 Mpro in complex with nsp12-nsp13 (C12) cut site sequence
Authors : Lee, J.; Kenward, C.; Worrall, L.J.; Vuckovic, M.; Paetzel, M.; Strynadka, N.C.J.
Deposited on : 2022-07-21
Resolution : 2.19 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

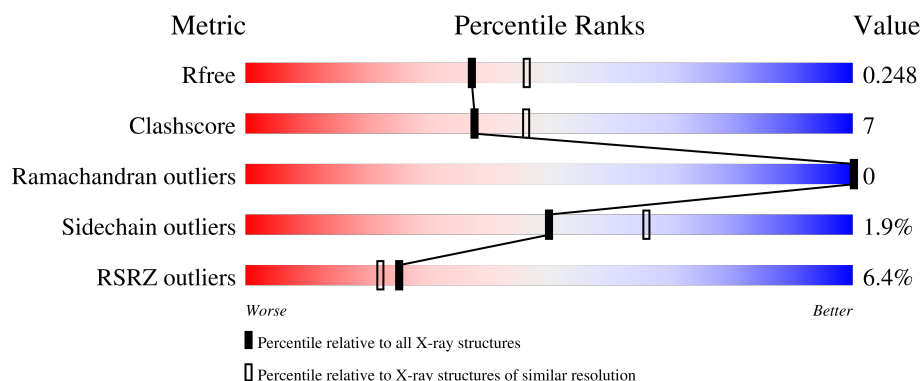
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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.





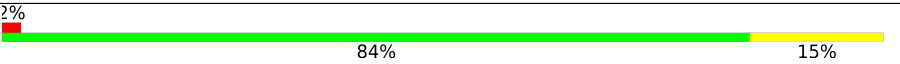
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	<div> <div>2%</div> <div>81%18%</div> <div>.</div> </div>
1	B	306	<div> <div>4%</div> <div>77%21%</div> <div>..</div> </div>
1	C	306	<div> <div>21%</div> <div>74%24%</div> <div>.</div> </div>
1	D	306	<div> <div>19%</div> <div>78%21%</div> <div>.</div> </div>
1	E	306	<div> <div>6%</div> <div>82%16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	306	
1	G	306	
1	H	306	
1	I	306	
1	J	306	
1	K	306	
1	L	306	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28279 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	302	Total	C	N	O	S	0	0	0
			2335	1479	397	437	22			
1	B	302	Total	C	N	O	S	0	1	0
			2343	1484	400	437	22			
1	C	302	Total	C	N	O	S	0	0	0
			2285	1451	385	428	21			
1	D	306	Total	C	N	O	S	0	0	0
			2288	1446	388	434	20			
1	E	302	Total	C	N	O	S	0	0	0
			2326	1473	394	437	22			
1	F	302	Total	C	N	O	S	0	0	0
			2332	1476	397	437	22			
1	G	302	Total	C	N	O	S	0	0	0
			2320	1471	395	432	22			
1	H	302	Total	C	N	O	S	0	1	0
			2343	1484	400	437	22			
1	I	306	Total	C	N	O	S	0	0	0
			2367	1500	404	441	22			
1	J	306	Total	C	N	O	S	0	0	0
			2347	1484	400	441	22			
1	K	302	Total	C	N	O	S	0	1	0
			2337	1481	396	438	22			
1	L	302	Total	C	N	O	S	0	0	0
			2330	1475	397	436	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	PRO	-	expression tag	UNP P0DTD1
A	302	HIS	-	expression tag	UNP P0DTD1
A	303	THR	-	expression tag	UNP P0DTD1
A	304	VAL	-	expression tag	UNP P0DTD1
A	305	LEU	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	306	GLN	-	expression tag	UNP P0DTD1
B	301	PRO	-	expression tag	UNP P0DTD1
B	302	HIS	-	expression tag	UNP P0DTD1
B	303	THR	-	expression tag	UNP P0DTD1
B	304	VAL	-	expression tag	UNP P0DTD1
B	305	LEU	-	expression tag	UNP P0DTD1
B	306	GLN	-	expression tag	UNP P0DTD1
C	301	PRO	-	expression tag	UNP P0DTD1
C	302	HIS	-	expression tag	UNP P0DTD1
C	303	THR	-	expression tag	UNP P0DTD1
C	304	VAL	-	expression tag	UNP P0DTD1
C	305	LEU	-	expression tag	UNP P0DTD1
C	306	GLN	-	expression tag	UNP P0DTD1
D	301	PRO	-	expression tag	UNP P0DTD1
D	302	HIS	-	expression tag	UNP P0DTD1
D	303	THR	-	expression tag	UNP P0DTD1
D	304	VAL	-	expression tag	UNP P0DTD1
D	305	LEU	-	expression tag	UNP P0DTD1
D	306	GLN	-	expression tag	UNP P0DTD1
E	301	PRO	-	expression tag	UNP P0DTD1
E	302	HIS	-	expression tag	UNP P0DTD1
E	303	THR	-	expression tag	UNP P0DTD1
E	304	VAL	-	expression tag	UNP P0DTD1
E	305	LEU	-	expression tag	UNP P0DTD1
E	306	GLN	-	expression tag	UNP P0DTD1
F	301	PRO	-	expression tag	UNP P0DTD1
F	302	HIS	-	expression tag	UNP P0DTD1
F	303	THR	-	expression tag	UNP P0DTD1
F	304	VAL	-	expression tag	UNP P0DTD1
F	305	LEU	-	expression tag	UNP P0DTD1
F	306	GLN	-	expression tag	UNP P0DTD1
G	301	PRO	-	expression tag	UNP P0DTD1
G	302	HIS	-	expression tag	UNP P0DTD1
G	303	THR	-	expression tag	UNP P0DTD1
G	304	VAL	-	expression tag	UNP P0DTD1
G	305	LEU	-	expression tag	UNP P0DTD1
G	306	GLN	-	expression tag	UNP P0DTD1
H	301	PRO	-	expression tag	UNP P0DTD1
H	302	HIS	-	expression tag	UNP P0DTD1
H	303	THR	-	expression tag	UNP P0DTD1
H	304	VAL	-	expression tag	UNP P0DTD1
H	305	LEU	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	306	GLN	-	expression tag	UNP P0DTD1
I	301	PRO	-	expression tag	UNP P0DTD1
I	302	HIS	-	expression tag	UNP P0DTD1
I	303	THR	-	expression tag	UNP P0DTD1
I	304	VAL	-	expression tag	UNP P0DTD1
I	305	LEU	-	expression tag	UNP P0DTD1
I	306	GLN	-	expression tag	UNP P0DTD1
J	301	PRO	-	expression tag	UNP P0DTD1
J	302	HIS	-	expression tag	UNP P0DTD1
J	303	THR	-	expression tag	UNP P0DTD1
J	304	VAL	-	expression tag	UNP P0DTD1
J	305	LEU	-	expression tag	UNP P0DTD1
J	306	GLN	-	expression tag	UNP P0DTD1
K	301	PRO	-	expression tag	UNP P0DTD1
K	302	HIS	-	expression tag	UNP P0DTD1
K	303	THR	-	expression tag	UNP P0DTD1
K	304	VAL	-	expression tag	UNP P0DTD1
K	305	LEU	-	expression tag	UNP P0DTD1
K	306	GLN	-	expression tag	UNP P0DTD1
L	301	PRO	-	expression tag	UNP P0DTD1
L	302	HIS	-	expression tag	UNP P0DTD1
L	303	THR	-	expression tag	UNP P0DTD1
L	304	VAL	-	expression tag	UNP P0DTD1
L	305	LEU	-	expression tag	UNP P0DTD1
L	306	GLN	-	expression tag	UNP P0DTD1

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	K	1	Total Na 1 1	0	0
2	L	1	Total Na 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	22	Total O 22 22	0	0
4	C	8	Total O 8 8	0	0
4	D	1	Total O 1 1	0	0
4	E	22	Total O 22 22	0	0
4	F	12	Total O 12 12	0	0
4	G	58	Total O 58 58	0	0

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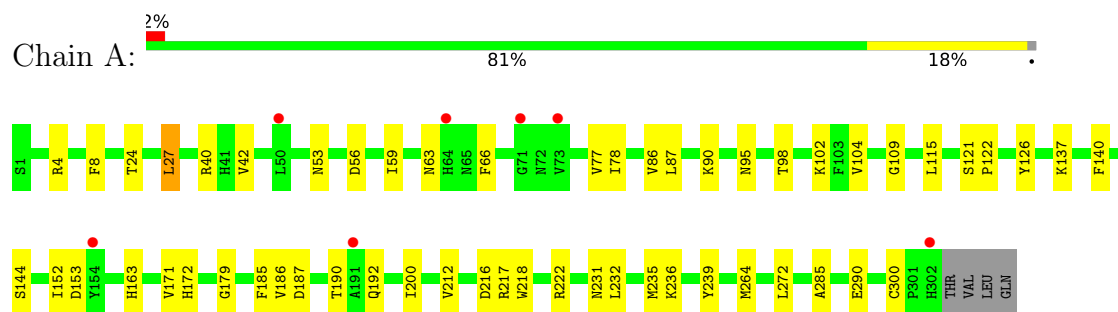
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	50	Total 50	O 50	0	0
4	I	26	Total 26	O 26	0	0
4	J	13	Total 13	O 13	0	0
4	K	22	Total 22	O 22	0	0
4	L	23	Total 23	O 23	0	0

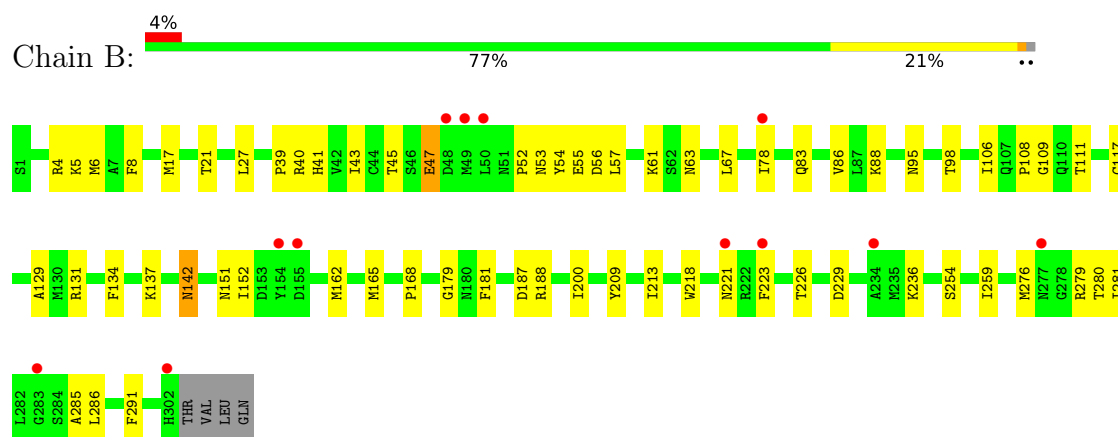
3 Residue-property plots [i](#)

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.

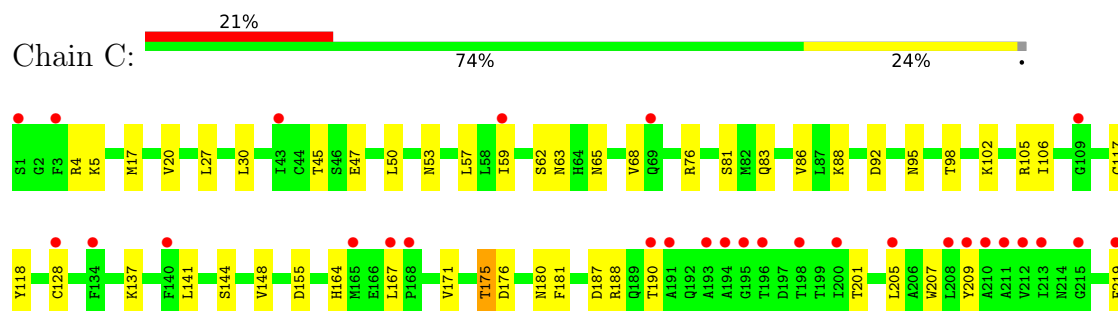
• Molecule 1: 3C-like proteinase nsp5

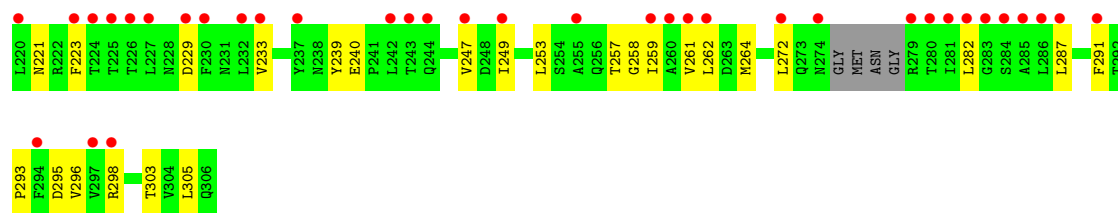


• Molecule 1: 3C-like proteinase nsp5

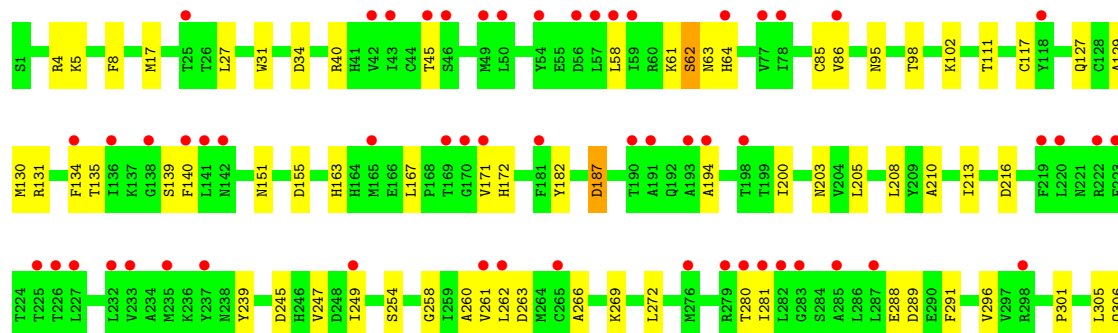
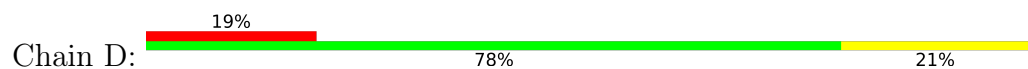


• Molecule 1: 3C-like proteinase nsp5

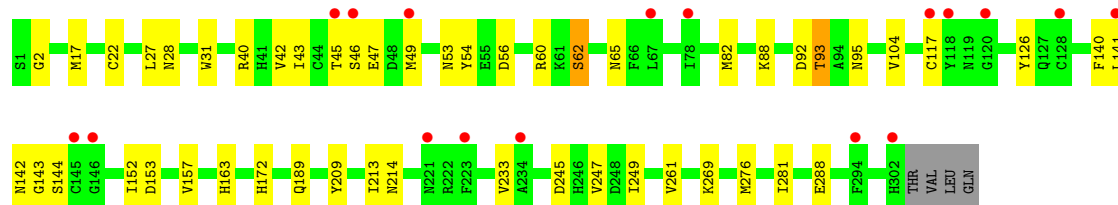
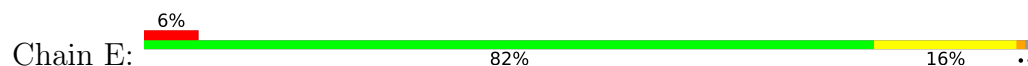




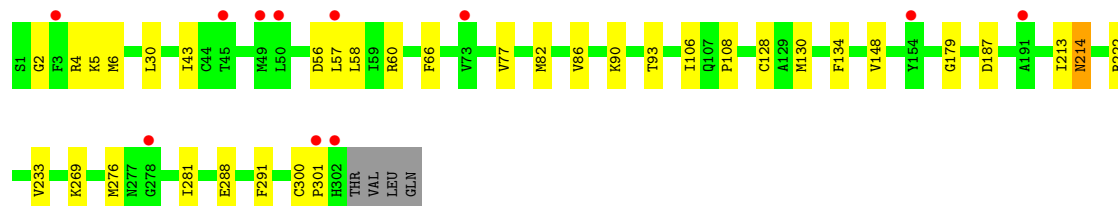
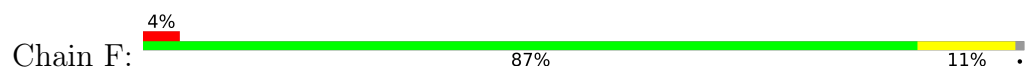
• Molecule 1: 3C-like proteinase nsp5



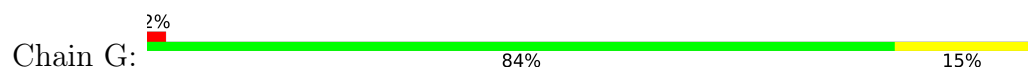
• Molecule 1: 3C-like proteinase nsp5



• Molecule 1: 3C-like proteinase nsp5

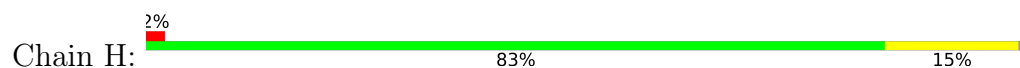


• Molecule 1: 3C-like proteinase nsp5

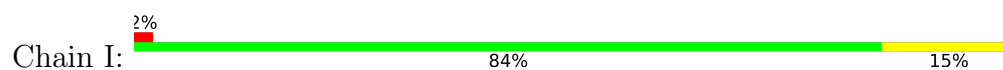




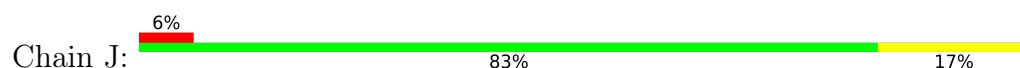
- Molecule 1: 3C-like proteinase nsp5



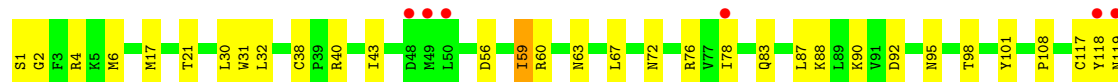
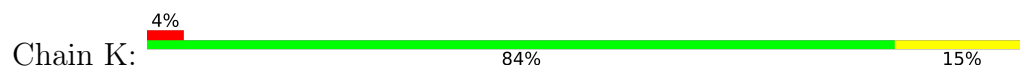
- Molecule 1: 3C-like proteinase nsp5



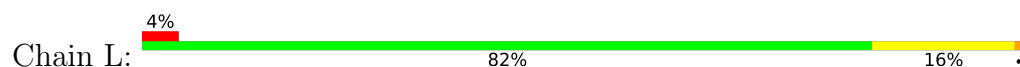
- Molecule 1: 3C-like proteinase nsp5

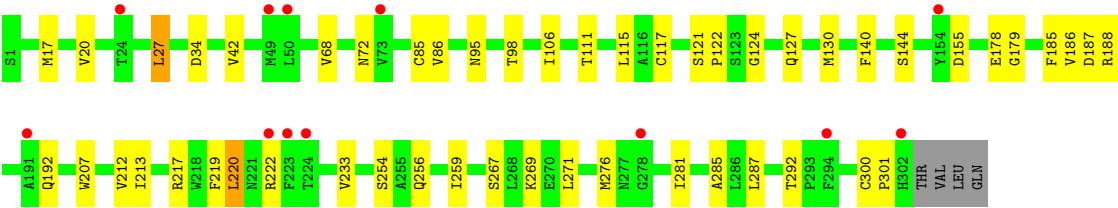


- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.00Å 105.78Å 276.34Å 90.00° 90.93° 90.00°	Depositor
Resolution (Å)	48.52 – 2.19 48.52 – 2.19	Depositor EDS
% Data completeness (in resolution range)	67.3 (48.52-2.19) 67.3 (48.52-2.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.248 0.198 , 0.248	Depositor DCC
R_{free} test set	6703 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28279	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2929e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.09	0/2388	0.26	0/3247
1	B	0.12	0/2399	0.29	0/3261
1	C	0.12	0/2337	0.29	0/3186
1	D	0.10	0/2340	0.29	0/3193
1	E	0.10	0/2379	0.28	0/3236
1	F	0.09	0/2385	0.27	0/3243
1	G	0.10	0/2373	0.28	0/3228
1	H	0.10	0/2399	0.27	0/3261
1	I	0.10	0/2421	0.27	0/3293
1	J	0.10	0/2401	0.28	0/3267
1	K	0.10	0/2393	0.27	0/3254
1	L	0.10	0/2383	0.27	0/3240
All	All	0.10	0/28598	0.28	0/38909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2335	0	2282	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2343	0	2294	43	0
1	C	2285	0	2190	51	0
1	D	2288	0	2159	42	0
1	E	2326	0	2262	34	0
1	F	2332	0	2273	23	0
1	G	2320	0	2256	28	0
1	H	2343	0	2294	31	0
1	I	2367	0	2318	38	0
1	J	2347	0	2264	39	0
1	K	2337	0	2282	28	0
1	L	2330	0	2268	32	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	7	0	10	0	0
3	F	7	0	10	2	0
3	G	7	0	10	1	0
3	I	7	0	10	2	0
3	L	7	0	10	0	0
4	A	29	0	0	3	0
4	B	22	0	0	1	0
4	C	8	0	0	0	0
4	D	1	0	0	0	0
4	E	22	0	0	0	0
4	F	12	0	0	0	0
4	G	58	0	0	2	0
4	H	50	0	0	0	0
4	I	26	0	0	0	0
4	J	13	0	0	1	0
4	K	22	0	0	0	0
4	L	23	0	0	1	0
All	All	28279	0	27192	387	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 7.

All (387) 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:J:138:GLY:O	1:J:172:HIS:HE1	1.58	0.86
1:I:4:ARG:H	1:I:299:GLN:HE22	1.22	0.85
1:C:257:THR:HG23	1:C:259:ILE:H	1.45	0.81
1:E:62:SER:H	1:E:65:ASN:HD22	1.29	0.80
1:A:186:VAL:H	1:A:192:GLN:HE22	1.29	0.79
1:B:276:MET:HE1	1:B:281:ILE:HD12	1.66	0.78
1:D:102:LYS:HD2	1:F:222:ARG:HB2	1.65	0.78
1:E:247:VAL:HG13	1:E:261:VAL:HG21	1.68	0.74
1:G:5:LYS:HD2	3:G:402:PEG:H22	1.68	0.73
1:F:276:MET:HE1	1:F:281:ILE:HG13	1.72	0.72
1:H:233:VAL:HG21	1:H:269:LYS:HD2	1.72	0.72
1:E:54:TYR:HB3	1:E:82:MET:HE1	1.70	0.72
1:F:288:GLU:HG2	1:F:291:PHE:HE1	1.55	0.71
1:L:212:VAL:HG22	1:L:217:ARG:HG2	1.72	0.71
1:A:8:PHE:HB3	1:A:152:ILE:HD12	1.73	0.70
1:D:247:VAL:HB	1:D:261:VAL:HG11	1.72	0.70
1:J:138:GLY:O	1:J:172:HIS:CE1	2.44	0.69
1:H:63:ASN:ND2	1:H:78:ILE:O	2.26	0.69
1:I:284:SER:HA	1:J:286:LEU:HD22	1.73	0.68
1:D:258:GLY:HA3	1:E:46:SER:O	1.94	0.67
1:C:4:ARG:NH2	1:D:127:GLN:O	2.27	0.67
1:G:63:ASN:ND2	1:G:78:ILE:O	2.28	0.67
1:I:53:ASN:HD22	1:I:56:ASP:HB2	1.59	0.66
1:B:276:MET:HE2	1:B:285:ALA:HA	1.77	0.66
1:C:105:ARG:NH1	1:C:176:ASP:OD2	2.28	0.66
1:J:40:ARG:HD3	1:J:85:CYS:HA	1.78	0.66
1:E:276:MET:HE1	1:E:281:ILE:HG13	1.79	0.64
1:B:165:MET:HB3	1:C:305:LEU:HD23	1.78	0.64
1:H:226:THR:HG23	1:H:229:ASP:H	1.63	0.64
1:J:305:LEU:HD23	1:K:165:MET:HB3	1.81	0.63
1:L:276:MET:HE1	1:L:281:ILE:HG13	1.81	0.63
1:F:213:ILE:HG21	1:F:300:CYS:HB3	1.80	0.62
1:C:261:VAL:HG13	1:C:262:LEU:HD22	1.80	0.62
1:C:247:VAL:HG13	1:C:261:VAL:HG11	1.82	0.61
1:G:17:MET:HG3	1:G:117:CYS:SG	2.39	0.61
1:L:20:VAL:HG22	1:L:68:VAL:HG22	1.81	0.61
1:F:2:GLY:H	1:F:214:ASN:HD21	1.48	0.61
1:L:127:GLN:NE2	4:L:502:HOH:O	2.34	0.60
1:B:54:TYR:HA	1:B:57:LEU:HD12	1.83	0.60
1:B:279:ARG:HG3	1:B:280:THR:H	1.66	0.60
1:J:153:ASP:OD2	1:L:217:ARG:NH2	2.33	0.60
1:G:78:ILE:HD11	1:G:92:ASP:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HE2	1:A:104:VAL:HG22	1.83	0.60
1:J:52:PRO:HD2	1:J:188:ARG:HG2	1.83	0.60
1:L:186:VAL:HG22	1:L:192:GLN:HE22	1.67	0.60
1:C:167:LEU:HD12	1:C:171:VAL:HG23	1.84	0.59
1:E:49:MET:HB3	1:E:189:GLN:HG3	1.84	0.59
1:A:40:ARG:HA	1:A:87:LEU:HG	1.83	0.59
1:I:4:ARG:HD2	1:J:138:GLY:HA2	1.84	0.59
1:A:285:ALA:HB2	1:B:286:LEU:HG	1.85	0.58
1:I:4:ARG:NH2	1:J:290:GLU:OE1	2.36	0.58
3:I:401:PEG:H22	1:J:5:LYS:HE3	1.84	0.58
1:B:8:PHE:HB3	1:B:152:ILE:HD12	1.85	0.58
1:E:28:ASN:ND2	1:E:143:GLY:O	2.37	0.58
1:C:137:LYS:HG3	1:C:171:VAL:HG12	1.85	0.58
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.86	0.57
1:D:187:ASP:OD1	1:D:187:ASP:N	2.25	0.57
1:D:205:LEU:HA	1:D:208:LEU:HD13	1.86	0.57
1:J:303:THR:HG21	1:K:165:MET:SD	2.43	0.57
1:B:21:THR:HB	1:B:67:LEU:HB3	1.85	0.57
1:G:2:GLY:H	1:G:214:ASN:ND2	2.03	0.57
1:E:245:ASP:O	1:E:249:ILE:HG13	2.05	0.57
1:I:76:ARG:HB3	1:I:92:ASP:OD2	2.05	0.57
1:I:266:ALA:O	1:I:269:LYS:HG2	2.04	0.57
1:K:163:HIS:HE1	1:K:172:HIS:HB3	1.69	0.56
1:B:86:VAL:HG23	1:B:179:GLY:HA2	1.87	0.56
1:J:78:ILE:HD11	1:J:92:ASP:HA	1.87	0.56
1:B:17:MET:HG3	1:B:117:CYS:SG	2.45	0.56
1:F:58:LEU:HD22	1:F:82:MET:HE2	1.87	0.56
1:I:8:PHE:HE2	1:I:151:ASN:HD22	1.53	0.56
1:J:63:ASN:ND2	1:J:78:ILE:O	2.37	0.56
1:C:207:TRP:HE1	1:C:282:LEU:HD23	1.70	0.56
1:G:288:GLU:HG2	1:G:291:PHE:HE2	1.70	0.56
1:B:53:ASN:HD21	1:B:55:GLU:HB2	1.71	0.56
1:E:53:ASN:HB3	1:E:56:ASP:HB2	1.88	0.56
1:L:111:THR:HG23	1:L:292:THR:HG23	1.88	0.56
1:J:231:ASN:HD21	1:J:242:LEU:H	1.54	0.55
1:L:256:GLN:NE2	1:L:301:PRO:O	2.39	0.55
1:A:137:LYS:HD3	1:A:171:VAL:HG12	1.88	0.55
1:B:53:ASN:HD22	1:B:56:ASP:H	1.55	0.55
1:H:165:MET:HB3	1:I:305:LEU:HD23	1.88	0.55
1:B:27:LEU:HD13	1:B:39:PRO:HD2	1.88	0.55
1:H:165:MET:SD	1:I:303:THR:HG21	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:ASP:OD2	1:I:60:ARG:NH2	2.37	0.54
1:I:163:HIS:CE1	1:I:172:HIS:HB3	2.42	0.54
1:A:185:PHE:HA	1:A:192:GLN:NE2	2.23	0.54
1:J:145:CYS:SG	4:J:412:HOH:O	2.59	0.54
1:D:130:MET:HE1	1:D:182:TYR:CG	2.42	0.54
1:D:266:ALA:HA	1:D:269:LYS:HE3	1.89	0.54
1:A:63:ASN:ND2	1:A:78:ILE:O	2.40	0.54
1:I:17:MET:HG3	1:I:117:CYS:SG	2.48	0.54
1:E:22:CYS:HB3	1:E:42:VAL:HG22	1.90	0.54
1:F:2:GLY:N	1:F:214:ASN:HD21	2.06	0.54
1:D:163:HIS:CE1	1:D:172:HIS:HB3	2.43	0.53
1:G:188:ARG:HG3	1:G:190:THR:HG23	1.90	0.53
1:H:8:PHE:HB3	1:H:152:ILE:HD12	1.90	0.53
1:A:232:LEU:O	1:A:236:LYS:HD2	2.09	0.53
1:E:47:GLU:N	1:E:47:GLU:OE1	2.42	0.53
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.89	0.53
1:H:58:LEU:HD22	1:H:82:MET:HB2	1.91	0.53
1:B:63:ASN:ND2	1:B:78:ILE:O	2.42	0.53
1:F:233:VAL:HG21	1:F:269:LYS:HD2	1.91	0.53
1:G:285:ALA:HB2	1:H:286:LEU:HG	1.90	0.53
1:G:145:CYS:SG	4:G:548:HOH:O	2.59	0.52
1:J:198:THR:OG1	1:J:240:GLU:HG3	2.10	0.52
1:H:271:LEU:HD13	1:H:287:LEU:HD21	1.91	0.52
1:F:288:GLU:HG2	1:F:291:PHE:CE1	2.41	0.52
1:F:187:ASP:OD1	1:F:187:ASP:N	2.43	0.51
1:D:288:GLU:HG2	1:D:291:PHE:HE1	1.74	0.51
1:B:209:TYR:O	1:B:213:ILE:HG13	2.10	0.51
1:F:30:LEU:HD22	1:F:148:VAL:HG11	1.92	0.51
1:D:155:ASP:OD1	1:D:155:ASP:N	2.39	0.51
1:B:41:HIS:HA	1:B:54:TYR:HE1	1.75	0.51
1:D:210:ALA:HA	1:D:213:ILE:HD12	1.93	0.51
1:D:288:GLU:HG2	1:D:291:PHE:CE1	2.46	0.51
1:F:4:ARG:HD3	3:F:402:PEG:H12	1.91	0.51
1:I:187:ASP:OD1	1:I:187:ASP:N	2.36	0.51
1:K:78:ILE:N	1:K:90:LYS:O	2.31	0.50
1:L:86:VAL:HG13	1:L:179:GLY:HA2	1.94	0.50
1:D:305:LEU:HD13	1:E:189:GLN:HG2	1.92	0.50
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.93	0.50
1:C:30:LEU:HD22	1:C:148:VAL:HG11	1.93	0.50
1:E:152:ILE:HG12	1:E:157:VAL:HG22	1.93	0.50
1:C:219:PHE:CE1	1:C:264:MET:HE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:ASN:O	1:H:146:GLY:HA3	2.12	0.50
1:I:52:PRO:HD2	1:I:188:ARG:HG2	1.93	0.50
1:J:30:LEU:HD22	1:J:148:VAL:HG11	1.93	0.50
1:H:163:HIS:HE1	1:H:172:HIS:HB3	1.77	0.50
1:G:288:GLU:HG2	1:G:291:PHE:CE2	2.46	0.49
1:A:231:ASN:O	1:A:235:MET:HG3	2.12	0.49
1:H:209:TYR:O	1:H:213:ILE:HG13	2.12	0.49
1:K:21:THR:HB	1:K:67:LEU:HB3	1.94	0.49
1:K:40:ARG:O	1:K:43:ILE:HG12	2.11	0.49
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.47	0.49
1:B:226:THR:HG23	1:B:229:ASP:H	1.77	0.49
1:C:95:ASN:HB3	1:C:98:THR:OG1	2.11	0.49
1:C:209:TYR:CD1	1:C:257:THR:HG21	2.48	0.49
1:E:56:ASP:O	1:E:60:ARG:HG3	2.12	0.49
1:C:141:LEU:HD13	1:D:301:PRO:HG3	1.94	0.49
1:E:163:HIS:CE1	1:E:172:HIS:HB3	2.48	0.49
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.94	0.49
1:C:209:TYR:CE1	1:C:257:THR:HG21	2.48	0.49
1:K:76:ARG:NH1	1:K:92:ASP:OD2	2.46	0.49
1:C:155:ASP:OD1	1:C:155:ASP:N	2.35	0.49
1:B:5:LYS:HG3	1:B:291:PHE:CZ	2.48	0.48
1:I:225:THR:HG22	1:I:226:THR:O	2.14	0.48
1:I:269:LYS:O	1:I:273:GLN:HG2	2.13	0.48
1:B:8:PHE:HE2	1:B:151:ASN:HD22	1.60	0.48
1:C:188:ARG:HH11	1:C:188:ARG:HG2	1.79	0.48
1:D:40:ARG:HD3	1:D:85:CYS:HA	1.96	0.48
1:K:163:HIS:CE1	1:K:172:HIS:HB3	2.47	0.48
1:H:86:VAL:HG13	1:H:179:GLY:HA2	1.96	0.48
1:A:186:VAL:N	1:A:192:GLN:HE22	2.02	0.48
1:B:168:PRO:HD3	1:C:303:THR:HG22	1.95	0.48
1:C:229:ASP:O	1:C:233:VAL:HG23	2.13	0.48
1:D:261:VAL:HG13	1:D:262:LEU:HD22	1.95	0.48
1:G:218:TRP:O	1:I:100:LYS:NZ	2.47	0.48
1:I:273:GLN:HG3	1:I:274:ASN:OD1	2.13	0.48
1:E:141:LEU:HD21	1:F:301:PRO:HD3	1.96	0.48
1:G:247:VAL:HG22	1:G:261:VAL:HG11	1.96	0.48
1:H:2:GLY:H	1:H:214:ASN:HD21	1.61	0.48
1:I:266:ALA:HA	1:I:269:LYS:HD2	1.95	0.48
1:K:165:MET:HE2	1:K:181:PHE:CZ	2.49	0.48
1:B:187:ASP:N	1:B:187:ASP:OD1	2.47	0.48
1:B:52:PRO:HD2	1:B:188[B]:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:SER:OG	1:B:259:ILE:O	2.30	0.47
1:I:163:HIS:HE1	1:I:172:HIS:HB3	1.77	0.47
1:D:111:THR:HG22	1:D:129:ALA:HB2	1.96	0.47
1:H:167:LEU:HA	1:I:303:THR:HG23	1.96	0.47
1:F:5:LYS:HE3	3:F:402:PEG:H32	1.95	0.47
1:I:115:LEU:HD11	1:I:122:PRO:HB3	1.96	0.47
1:K:72:ASN:OD1	1:K:72:ASN:N	2.43	0.47
1:K:117:CYS:O	1:K:144:SER:HA	2.14	0.47
1:L:185:PHE:HA	1:L:192:GLN:NE2	2.29	0.47
1:J:40:ARG:HA	1:J:87:LEU:HG	1.95	0.47
1:K:2:GLY:H	1:K:214:ASN:ND2	2.12	0.47
1:K:30:LEU:HD13	1:K:148:VAL:HG21	1.95	0.47
1:L:72:ASN:OD1	1:L:72:ASN:N	2.47	0.47
1:L:187:ASP:OD1	1:L:187:ASP:N	2.46	0.47
1:D:135:THR:HG21	1:D:194:ALA:HB2	1.96	0.47
1:D:130:MET:HE3	1:D:134:PHE:HD1	1.80	0.47
1:D:200:ILE:HB	1:D:203:ASN:HB2	1.95	0.47
1:D:239:TYR:CZ	1:D:272:LEU:HD21	2.49	0.47
1:G:86:VAL:HG13	1:G:179:GLY:HA2	1.97	0.47
1:J:21:THR:HB	1:J:67:LEU:HB2	1.95	0.47
1:B:86:VAL:HG22	1:B:162:MET:HE3	1.97	0.47
1:D:8:PHE:HE2	1:D:151:ASN:HD22	1.62	0.47
1:I:210:ALA:HB2	1:I:296:VAL:HG13	1.96	0.47
1:J:165:MET:HE3	1:J:165:MET:HB3	1.83	0.47
1:J:276:MET:HG3	1:J:279:ARG:O	2.15	0.47
1:A:212:VAL:HG21	1:A:264:MET:HE1	1.97	0.46
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.97	0.46
1:F:106:ILE:HD11	1:F:130:MET:HE3	1.98	0.46
1:J:86:VAL:HG13	1:J:179:GLY:HA2	1.97	0.46
1:L:213:ILE:HG21	1:L:300:CYS:HB3	1.98	0.46
1:F:66:PHE:HB2	1:F:77:VAL:HG21	1.98	0.46
1:J:137:LYS:NZ	1:J:197:ASP:OD2	2.49	0.46
1:D:140:PHE:HB2	1:D:172:HIS:NE2	2.30	0.46
1:D:254:SER:O	1:D:258:GLY:N	2.47	0.46
1:I:4:ARG:H	1:I:299:GLN:NE2	2.03	0.46
1:J:286:LEU:HD23	1:J:286:LEU:H	1.79	0.46
1:L:17:MET:HG3	1:L:117:CYS:SG	2.56	0.46
1:C:253:LEU:HD21	1:C:296:VAL:HB	1.98	0.46
1:I:6:MET:HG3	1:J:126:TYR:HD2	1.80	0.46
1:K:6:MET:HG2	1:L:124:GLY:HA3	1.98	0.46
1:B:40:ARG:O	1:B:43:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ARG:HG3	1:B:280:THR:N	2.31	0.46
1:E:2:GLY:H	1:E:214:ASN:ND2	2.14	0.46
1:J:102:LYS:HB3	1:L:222:ARG:HG3	1.98	0.46
1:L:34:ASP:OD1	1:L:34:ASP:N	2.41	0.46
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.15	0.46
1:C:17:MET:HG3	1:C:117:CYS:SG	2.55	0.46
1:C:83:GLN:OE1	1:C:88:LYS:HD2	2.15	0.46
1:D:131:ARG:HH12	1:D:289:ASP:CG	2.24	0.46
1:E:31:TRP:CE2	1:E:95:ASN:HB2	2.51	0.46
1:B:111:THR:HG22	1:B:129:ALA:HB2	1.98	0.45
1:H:108:PRO:HG3	1:H:134:PHE:CE1	2.51	0.45
1:L:186:VAL:HG21	1:L:188:ARG:HE	1.81	0.45
1:L:220:LEU:HD21	1:L:259:ILE:HD11	1.98	0.45
1:C:137:LYS:O	1:D:4:ARG:HD3	2.16	0.45
1:F:86:VAL:HG13	1:F:179:GLY:HA2	1.99	0.45
1:G:95:ASN:HB3	1:G:98:THR:OG1	2.16	0.45
1:A:290:GLU:CD	1:B:4:ARG:HH22	2.25	0.45
1:D:62:SER:OG	1:D:63:ASN:N	2.49	0.45
1:I:83:GLN:NE2	1:I:88:LYS:HE2	2.32	0.45
1:J:247:VAL:HG13	1:J:261:VAL:HG21	1.97	0.45
1:D:216:ASP:HB3	1:D:281:ILE:HD13	1.97	0.45
1:H:61:LYS:HA	1:H:61:LYS:HD3	1.74	0.45
1:L:106:ILE:HD12	1:L:130:MET:HB2	1.99	0.45
1:A:163:HIS:HE1	1:A:172:HIS:HB3	1.81	0.45
1:G:60:ARG:HG2	1:G:60:ARG:HH11	1.81	0.45
1:K:83:GLN:OE1	1:K:88:LYS:HE2	2.17	0.45
1:B:61:LYS:HA	1:B:61:LYS:HD3	1.72	0.45
1:C:53:ASN:O	1:C:57:LEU:HG	2.17	0.45
1:E:140:PHE:HB2	1:E:172:HIS:NE2	2.32	0.45
1:F:276:MET:HE3	1:F:276:MET:HB3	1.83	0.45
1:C:76:ARG:NH1	1:C:92:ASP:OD2	2.50	0.45
1:F:43:ILE:HD12	1:F:57:LEU:HB3	1.99	0.45
1:F:108:PRO:HG3	1:F:134:PHE:CE1	2.52	0.44
1:H:163:HIS:CE1	1:H:172:HIS:HB3	2.52	0.44
1:E:163:HIS:HE1	1:E:172:HIS:HB3	1.81	0.44
1:G:60:ARG:HG2	1:G:60:ARG:NH1	2.32	0.44
1:K:38:CYS:SG	1:K:87:LEU:HD23	2.57	0.44
1:K:95:ASN:HB3	1:K:98:THR:OG1	2.17	0.44
1:L:178:GLU:OE1	1:L:178:GLU:HA	2.18	0.44
1:K:56:ASP:O	1:K:60:ARG:HD3	2.17	0.44
1:A:4:ARG:NH1	4:B:401:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:276:MET:HE2	1:L:285:ALA:HA	1.99	0.44
1:C:118:TYR:CE1	1:C:144:SER:HB3	2.53	0.44
1:D:260:ALA:HB3	1:D:263:ASP:OD1	2.17	0.44
1:J:269:LYS:HA	1:J:272:LEU:HD12	1.99	0.44
1:C:201:THR:HG22	1:C:239:TYR:HD2	1.82	0.44
1:I:188:ARG:HH21	1:I:190:THR:HG21	1.83	0.44
1:J:40:ARG:HG3	1:J:54:TYR:CE1	2.52	0.44
1:L:115:LEU:HD11	1:L:122:PRO:HB3	2.00	0.44
1:F:56:ASP:OD2	1:F:60:ARG:NH2	2.50	0.44
1:L:85:CYS:HB2	1:L:179:GLY:O	2.17	0.44
1:D:61:LYS:HA	1:D:61:LYS:HD3	1.72	0.44
1:E:117:CYS:O	1:E:144:SER:HA	2.17	0.44
1:A:66:PHE:HB2	1:A:77:VAL:HG21	2.00	0.44
1:C:106:ILE:H	1:C:106:ILE:HG13	1.63	0.44
1:G:4:ARG:O	1:G:299:GLN:NE2	2.48	0.44
1:I:225:THR:HG21	1:I:269:LYS:NZ	2.33	0.44
1:K:63:ASN:ND2	1:K:78:ILE:O	2.51	0.44
1:E:233:VAL:HG11	1:E:269:LYS:HG3	2.00	0.43
1:I:247:VAL:HG13	1:I:261:VAL:HG11	2.00	0.43
1:A:95:ASN:HB3	1:A:98:THR:OG1	2.18	0.43
1:A:217:ARG:N	4:A:503:HOH:O	2.41	0.43
1:A:285:ALA:HB1	1:B:285:ALA:HB3	1.99	0.43
1:D:5:LYS:HD2	1:D:291:PHE:CZ	2.53	0.43
1:A:187:ASP:OD1	1:A:187:ASP:N	2.51	0.43
1:G:4:ARG:NH2	1:H:127:GLN:O	2.41	0.43
1:L:95:ASN:HB3	1:L:98:THR:OG1	2.18	0.43
1:B:109:GLY:HA2	1:B:200:ILE:HD13	2.00	0.43
1:E:40:ARG:O	1:E:43:ILE:HG12	2.18	0.43
1:E:189:GLN:HE21	1:E:189:GLN:HB3	1.58	0.43
1:H:45:THR:OG1	1:H:48:ASP:OD1	2.28	0.43
1:A:300:CYS:SG	4:A:509:HOH:O	2.61	0.43
1:C:207:TRP:HZ3	1:C:287:LEU:HD23	1.83	0.43
1:C:207:TRP:NE1	1:C:282:LEU:HD23	2.33	0.43
1:E:92:ASP:OD1	1:E:93:THR:N	2.51	0.43
1:A:90:LYS:HE2	1:A:90:LYS:HB2	1.76	0.43
1:E:209:TYR:O	1:E:213:ILE:HG13	2.18	0.43
1:F:90:LYS:HB2	1:F:90:LYS:HE2	1.60	0.43
1:H:213:ILE:HD13	1:H:256:GLN:NE2	2.33	0.43
1:B:165:MET:HE2	1:B:181:PHE:CZ	2.54	0.43
1:C:59:ILE:HD13	1:C:59:ILE:HA	1.91	0.43
1:G:35:VAL:HG11	1:G:88:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:ARG:O	1:H:43:ILE:HG12	2.18	0.43
1:K:108:PRO:HG3	1:K:134:PHE:CE1	2.53	0.43
1:B:83:GLN:HE21	1:B:88:LYS:HD2	1.83	0.43
1:C:221:ASN:ND2	1:C:223:PHE:HD2	2.17	0.43
1:D:131:ARG:NH1	1:D:289:ASP:OD2	2.52	0.43
1:K:31:TRP:CE2	1:K:95:ASN:HB2	2.54	0.43
1:B:47:GLU:HA	1:C:258:GLY:HA3	2.01	0.42
1:C:295:ASP:HA	1:C:298:ARG:NE	2.34	0.42
1:J:162:MET:O	1:J:164:HIS:HD2	2.02	0.42
1:I:53:ASN:ND2	1:I:56:ASP:HB2	2.30	0.42
1:K:17:MET:HG3	1:K:117:CYS:SG	2.59	0.42
1:A:222:ARG:HA	1:C:102:LYS:HE2	2.00	0.42
1:D:245:ASP:O	1:D:249:ILE:HG13	2.19	0.42
1:H:165:MET:HE2	1:H:181:PHE:CZ	2.54	0.42
1:I:227:LEU:HD11	1:I:242:LEU:O	2.20	0.42
1:C:118:TYR:CE1	1:C:141:LEU:HB2	2.54	0.42
1:K:32:LEU:HD13	1:K:101:TYR:CE2	2.55	0.42
1:C:65:ASN:OD1	1:C:65:ASN:N	2.53	0.42
1:D:306:GLN:HB3	1:E:142:ASN:HA	2.00	0.42
1:H:46:SER:O	1:I:258:GLY:HA3	2.19	0.42
1:A:53:ASN:OD1	1:A:56:ASP:HB3	2.20	0.42
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.54	0.42
1:B:221:ASN:HD22	1:B:223:PHE:HE1	1.66	0.42
1:C:187:ASP:C	1:C:188:ARG:HD2	2.44	0.42
1:E:141:LEU:O	1:E:144:SER:OG	2.35	0.42
1:G:131:ARG:HD3	1:G:137:LYS:HG3	2.01	0.42
1:G:152:ILE:HG12	1:G:157:VAL:HG22	2.01	0.42
1:H:76:ARG:NH2	1:H:92:ASP:OD2	2.53	0.42
1:I:105:ARG:NH1	1:I:176:ASP:OD2	2.50	0.42
1:J:58:LEU:HD21	1:J:80:HIS:HD2	1.84	0.42
1:B:142:ASN:HD22	1:B:142:ASN:HA	1.66	0.42
1:C:209:TYR:CE1	1:C:264:MET:HG3	2.54	0.42
1:H:130:MET:HE2	1:H:130:MET:HB2	1.93	0.42
1:H:217:ARG:HB3	1:H:220:LEU:HD12	2.01	0.42
1:B:218:TRP:CE2	1:B:279:ARG:HG2	2.55	0.42
1:E:17:MET:HE2	1:E:117:CYS:SG	2.60	0.42
1:E:88:LYS:HB3	1:E:88:LYS:HE3	1.76	0.42
1:L:207:TRP:CZ3	1:L:287:LEU:HA	2.55	0.42
1:D:34:ASP:OD1	1:D:34:ASP:N	2.48	0.42
1:G:76:ARG:HB3	1:G:92:ASP:OD2	2.19	0.42
1:E:45:THR:OG1	1:E:46:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:ASP:O	1:J:59:ILE:HG22	2.19	0.41
1:J:231:ASN:HD22	1:J:231:ASN:HA	1.61	0.41
1:A:140:PHE:HB3	1:A:144:SER:OG	2.20	0.41
1:J:242:LEU:HD23	1:J:246:HIS:HB2	2.01	0.41
1:J:268:LEU:O	1:J:272:LEU:HD12	2.20	0.41
1:C:45:THR:HG23	1:C:47:GLU:H	1.86	0.41
1:C:176:ASP:OD2	1:C:180:ASN:HB3	2.20	0.41
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.20	0.41
1:I:6:MET:HE3	1:I:298:ARG:NH2	2.35	0.41
1:I:245:ASP:OD1	1:I:245:ASP:N	2.52	0.41
1:J:298:ARG:HA	1:J:298:ARG:HD2	1.73	0.41
1:L:233:VAL:HG11	1:L:269:LYS:HG3	2.03	0.41
1:C:62:SER:OG	1:C:63:ASN:N	2.53	0.41
1:C:207:TRP:CZ3	1:C:287:LEU:HA	2.54	0.41
1:D:31:TRP:CE2	1:D:95:ASN:HB2	2.55	0.41
1:D:163:HIS:HE1	1:D:172:HIS:HB3	1.82	0.41
1:K:56:ASP:O	1:K:59:ILE:HG22	2.21	0.41
1:B:236:LYS:HG3	1:D:64:HIS:O	2.20	0.41
1:C:205:LEU:HD23	1:C:261:VAL:HG23	2.02	0.41
1:J:85:CYS:HB2	1:J:179:GLY:O	2.21	0.41
1:K:118:TYR:CE1	1:K:144:SER:HB3	2.56	0.41
1:B:106:ILE:H	1:B:106:ILE:HG13	1.69	0.41
1:H:114:VAL:O	1:H:125:VAL:HA	2.21	0.41
1:L:254:SER:OG	1:L:259:ILE:O	2.25	0.41
1:B:108:PRO:HG3	1:B:134:PHE:CE1	2.55	0.41
1:C:247:VAL:HG22	1:C:261:VAL:HG21	2.01	0.41
1:H:55:GLU:OE1	1:H:55:GLU:N	2.50	0.41
1:A:126:TYR:HD2	1:B:6:MET:HG3	1.84	0.41
1:B:131:ARG:HD3	1:B:137:LYS:HE3	2.02	0.41
1:J:276:MET:HG2	1:J:278:GLY:H	1.84	0.41
1:K:1:SER:N	1:L:140:PHE:O	2.45	0.41
1:L:117:CYS:O	1:L:144:SER:HA	2.21	0.41
1:L:219:PHE:HB2	1:L:271:LEU:HD11	2.03	0.41
1:A:218:TRP:N	4:A:503:HOH:O	2.51	0.41
1:C:50:LEU:HD22	1:C:50:LEU:H	1.86	0.41
1:D:167:LEU:HD12	1:D:171:VAL:HG23	2.03	0.41
1:G:31:TRP:CD2	1:G:95:ASN:HB2	2.56	0.41
1:G:140:PHE:HB3	1:G:144:SER:OG	2.21	0.41
1:J:266:ALA:O	1:J:269:LYS:HG2	2.20	0.41
1:K:4:ARG:O	1:K:299:GLN:NE2	2.44	0.41
1:C:20:VAL:HG22	1:C:68:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:HIS:CD2	1:C:175:THR:HG23	2.55	0.40
1:C:188:ARG:HB3	1:C:190:THR:HG23	2.03	0.40
1:C:249:ILE:HG22	1:C:293:PRO:HB2	2.03	0.40
1:E:140:PHE:HD2	1:E:172:HIS:CG	2.39	0.40
1:L:27:LEU:HD21	1:L:42:VAL:HB	2.04	0.40
1:G:45:THR:OG1	1:G:48:ASP:OD1	2.35	0.40
1:G:163:HIS:CE1	1:G:172:HIS:HB3	2.55	0.40
1:G:175:THR:HG22	1:G:181:PHE:HA	2.04	0.40
1:H:2:GLY:H	1:H:214:ASN:ND2	2.19	0.40
1:I:55:GLU:H	1:I:55:GLU:CD	2.28	0.40
1:K:164:HIS:CD2	1:K:175:THR:HG23	2.56	0.40
1:C:5:LYS:HG2	1:C:291:PHE:CZ	2.57	0.40
1:G:298:ARG:NH1	4:G:508:HOH:O	2.49	0.40
1:I:5:LYS:HD3	3:I:401:PEG:H42	2.02	0.40
1:D:17:MET:HG3	1:D:117:CYS:SG	2.61	0.40
1:E:126:TYR:HD1	1:F:6:MET:HG3	1.87	0.40
1:H:31:TRP:CE2	1:H:95:ASN:HB2	2.56	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	300/306 (98%)	296 (99%)	4 (1%)	0	100	100
1	B	301/306 (98%)	295 (98%)	6 (2%)	0	100	100
1	C	298/306 (97%)	293 (98%)	5 (2%)	0	100	100
1	D	304/306 (99%)	293 (96%)	11 (4%)	0	100	100
1	E	300/306 (98%)	291 (97%)	9 (3%)	0	100	100
1	F	300/306 (98%)	291 (97%)	9 (3%)	0	100	100
1	G	300/306 (98%)	296 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	301/306 (98%)	293 (97%)	8 (3%)	0	100	100
1	I	304/306 (99%)	303 (100%)	1 (0%)	0	100	100
1	J	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	K	301/306 (98%)	295 (98%)	6 (2%)	0	100	100
1	L	300/306 (98%)	294 (98%)	6 (2%)	0	100	100
All	All	3613/3672 (98%)	3539 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	259/264 (98%)	252 (97%)	7 (3%)	39	53
1	B	260/264 (98%)	257 (99%)	3 (1%)	63	78
1	C	247/264 (94%)	239 (97%)	8 (3%)	34	47
1	D	242/264 (92%)	233 (96%)	9 (4%)	30	41
1	E	257/264 (97%)	252 (98%)	5 (2%)	50	66
1	F	258/264 (98%)	255 (99%)	3 (1%)	63	78
1	G	254/264 (96%)	249 (98%)	5 (2%)	48	64
1	H	260/264 (98%)	259 (100%)	1 (0%)	84	92
1	I	263/264 (100%)	259 (98%)	4 (2%)	57	73
1	J	257/264 (97%)	253 (98%)	4 (2%)	55	71
1	K	259/264 (98%)	254 (98%)	5 (2%)	50	66
1	L	257/264 (97%)	252 (98%)	5 (2%)	50	66
All	All	3073/3168 (97%)	3014 (98%)	59 (2%)	50	66

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	27	LEU
1	A	59	ILE
1	A	121	SER
1	A	153	ASP
1	A	190	THR
1	A	216	ASP
1	B	45	THR
1	B	47	GLU
1	B	142	ASN
1	C	27	LEU
1	C	81	SER
1	C	86	VAL
1	C	128	CYS
1	C	175	THR
1	C	181	PHE
1	C	240	GLU
1	C	272	LEU
1	D	27	LEU
1	D	45	THR
1	D	58	LEU
1	D	62	SER
1	D	86	VAL
1	D	139	SER
1	D	187	ASP
1	D	280	THR
1	D	296	VAL
1	E	62	SER
1	E	93	THR
1	E	104	VAL
1	E	153	ASP
1	E	288	GLU
1	F	93	THR
1	F	128	CYS
1	F	214	ASN
1	G	59	ILE
1	G	104	VAL
1	G	106	ILE
1	G	192	GLN
1	G	216	ASP
1	H	225	THR
1	I	5	LYS
1	I	86	VAL

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Mol	Chain	Res	Type
1	I	243	THR
1	I	280	THR
1	J	121	SER
1	J	169	THR
1	J	198	THR
1	J	280	THR
1	K	59	ILE
1	K	119	ASN
1	K	137	LYS
1	K	155	ASP
1	K	238	ASN
1	L	27	LEU
1	L	121	SER
1	L	155	ASP
1	L	220	LEU
1	L	267	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	163	HIS
1	A	192	GLN
1	A	256	GLN
1	A	274	ASN
1	B	19	GLN
1	B	41	HIS
1	B	53	ASN
1	B	69	GLN
1	B	72	ASN
1	B	83	GLN
1	B	84	ASN
1	B	110	GLN
1	B	119	ASN
1	B	142	ASN
1	B	164	HIS
1	B	180	ASN
1	B	221	ASN
1	B	228	ASN
1	B	273	GLN
1	C	19	GLN
1	C	63	ASN

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Mol	Chain	Res	Type
1	C	64	HIS
1	C	142	ASN
1	C	163	HIS
1	C	164	HIS
1	C	214	ASN
1	C	273	GLN
1	D	53	ASN
1	D	69	GLN
1	D	72	ASN
1	D	74	GLN
1	D	83	GLN
1	D	84	ASN
1	D	110	GLN
1	D	151	ASN
1	D	244	GLN
1	D	256	GLN
1	D	273	GLN
1	E	19	GLN
1	E	41	HIS
1	E	53	ASN
1	E	65	ASN
1	E	69	GLN
1	E	127	GLN
1	E	189	GLN
1	E	214	ASN
1	E	256	GLN
1	F	19	GLN
1	F	63	ASN
1	F	72	ASN
1	F	74	GLN
1	F	107	GLN
1	F	214	ASN
1	F	273	GLN
1	F	274	ASN
1	G	41	HIS
1	G	53	ASN
1	G	74	GLN
1	G	107	GLN
1	G	163	HIS
1	G	214	ASN
1	G	228	ASN
1	H	41	HIS

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Mol	Chain	Res	Type
1	H	64	HIS
1	H	69	GLN
1	H	214	ASN
1	H	277	ASN
1	I	53	ASN
1	I	74	GLN
1	I	83	GLN
1	I	142	ASN
1	I	164	HIS
1	I	256	GLN
1	I	299	GLN
1	J	107	GLN
1	J	164	HIS
1	J	172	HIS
1	J	180	ASN
1	J	231	ASN
1	J	238	ASN
1	K	41	HIS
1	K	74	GLN
1	K	151	ASN
1	K	164	HIS
1	K	214	ASN
1	L	110	GLN
1	L	192	GLN
1	L	228	ASN
1	L	244	GLN
1	L	274	ASN
1	L	277	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PEG	A	402	-	6,6,6	0.11	0	5,5,5	0.10	0
3	PEG	G	402	-	6,6,6	0.13	0	5,5,5	0.06	0
3	PEG	F	402	-	6,6,6	0.10	0	5,5,5	0.11	0
3	PEG	L	402	-	6,6,6	0.12	0	5,5,5	0.09	0
3	PEG	I	401	-	6,6,6	0.11	0	5,5,5	0.10	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
3	PEG	A	402	-	-	3/4/4/4	-
3	PEG	G	402	-	-	1/4/4/4	-
3	PEG	F	402	-	-	2/4/4/4	-
3	PEG	L	402	-	-	0/4/4/4	-
3	PEG	I	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	PEG	O1-C1-C2-O2
3	F	402	PEG	O2-C3-C4-O4
3	G	402	PEG	C1-C2-O2-C3
3	A	402	PEG	C1-C2-O2-C3
3	A	402	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	402	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	402	PEG	1	0
3	F	402	PEG	2	0
3	I	401	PEG	2	0

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	302/306 (98%)	0.07	7 (2%) 61 58	26, 42, 78, 108	0
1	B	302/306 (98%)	0.34	12 (3%) 42 39	30, 49, 85, 127	1 (0%)
1	C	302/306 (98%)	1.09	65 (21%) 2 2	34, 70, 117, 152	0
1	D	306/306 (100%)	1.17	57 (18%) 3 2	39, 75, 121, 139	0
1	E	302/306 (98%)	0.43	17 (5%) 30 27	28, 50, 78, 127	0
1	F	302/306 (98%)	0.36	11 (3%) 46 43	27, 51, 90, 137	0
1	G	302/306 (98%)	-0.12	7 (2%) 61 58	19, 33, 77, 121	0
1	H	302/306 (98%)	-0.04	7 (2%) 61 58	19, 35, 64, 115	1 (0%)
1	I	306/306 (100%)	0.26	7 (2%) 61 58	25, 46, 86, 113	0
1	J	306/306 (100%)	0.41	18 (5%) 28 25	27, 53, 104, 178	0
1	K	302/306 (98%)	0.27	12 (3%) 42 39	27, 45, 74, 130	1 (0%)
1	L	302/306 (98%)	0.43	12 (3%) 42 39	29, 50, 91, 140	0
All	All	3636/3672 (99%)	0.39	232 (6%) 25 22	19, 49, 100, 178	3 (0%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	223	PHE	5.6
1	D	141	LEU	5.0
1	B	283	GLY	4.7
1	C	283	GLY	4.5
1	L	224	THR	4.4
1	K	50	LEU	4.3
1	C	285	ALA	4.2
1	D	191	ALA	4.1
1	L	302	HIS	4.0
1	J	286	LEU	4.0
1	F	302	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	73	VAL	3.9
1	D	136	ILE	3.9
1	E	146	GLY	3.9
1	C	294	PHE	3.8
1	I	223	PHE	3.8
1	D	140	PHE	3.8
1	D	223	PHE	3.8
1	B	50	LEU	3.7
1	A	302	HIS	3.7
1	C	220	LEU	3.6
1	K	302	HIS	3.6
1	A	154	TYR	3.6
1	B	223	PHE	3.4
1	D	283	GLY	3.4
1	C	165	MET	3.4
1	C	261	VAL	3.4
1	J	230	PHE	3.4
1	C	190	THR	3.4
1	C	200	ILE	3.3
1	B	302	HIS	3.3
1	C	194	ALA	3.3
1	D	50	LEU	3.3
1	D	56	ASP	3.3
1	C	59	ILE	3.3
1	F	49	MET	3.2
1	C	229	ASP	3.2
1	C	223	PHE	3.2
1	E	223	PHE	3.1
1	G	46	SER	3.1
1	C	280	THR	3.1
1	J	223	PHE	3.1
1	D	261	VAL	3.1
1	D	249	ILE	3.1
1	L	49	MET	3.1
1	I	226	THR	3.0
1	D	134	PHE	3.0
1	D	279	ARG	3.0
1	H	50	LEU	3.0
1	L	50	LEU	3.0
1	J	276	MET	3.0
1	D	194	ALA	3.0
1	F	301	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	232	LEU	2.9
1	E	67	LEU	2.9
1	E	45	THR	2.9
1	L	154	TYR	2.9
1	D	169	THR	2.9
1	J	222	ARG	2.9
1	L	222	ARG	2.9
1	A	50	LEU	2.9
1	E	302	HIS	2.9
1	B	154	TYR	2.9
1	J	154	TYR	2.9
1	C	219	PHE	2.8
1	F	191	ALA	2.8
1	L	278	GLY	2.8
1	C	225	THR	2.8
1	D	45	THR	2.8
1	C	249	ILE	2.8
1	H	302	HIS	2.8
1	G	191	ALA	2.8
1	C	243	THR	2.8
1	D	43	ILE	2.8
1	E	234	ALA	2.8
1	C	287	LEU	2.8
1	C	224	THR	2.8
1	C	298	ARG	2.7
1	B	49	MET	2.7
1	F	278	GLY	2.7
1	D	227	LEU	2.7
1	C	43	ILE	2.7
1	A	191	ALA	2.7
1	C	3	PHE	2.7
1	C	191	ALA	2.7
1	K	154	TYR	2.7
1	K	146	GLY	2.7
1	F	50	LEU	2.7
1	F	57	LEU	2.7
1	J	45	THR	2.7
1	G	302	HIS	2.7
1	B	155	ASP	2.7
1	C	196	THR	2.6
1	C	242	LEU	2.6
1	D	235	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	232	LEU	2.6
1	E	117	CYS	2.6
1	C	195	GLY	2.6
1	J	226	THR	2.6
1	D	232	LEU	2.6
1	C	134	PHE	2.6
1	E	294	PHE	2.6
1	G	54	TYR	2.6
1	H	154	TYR	2.6
1	D	49	MET	2.6
1	C	274	ASN	2.6
1	D	225	THR	2.6
1	C	247	VAL	2.5
1	D	190	THR	2.5
1	D	193	ALA	2.5
1	C	230	PHE	2.5
1	D	181	PHE	2.5
1	K	300	CYS	2.5
1	K	48	ASP	2.5
1	C	211	ALA	2.5
1	K	301	PRO	2.5
1	D	42	VAL	2.5
1	E	145	CYS	2.5
1	K	118	TYR	2.5
1	C	226	THR	2.5
1	I	286	LEU	2.5
1	E	120	GLY	2.5
1	C	281	ILE	2.5
1	B	48	ASP	2.4
1	K	145	CYS	2.4
1	L	24	THR	2.4
1	C	262	LEU	2.4
1	C	282	LEU	2.4
1	B	78	ILE	2.4
1	D	77	VAL	2.4
1	F	3	PHE	2.4
1	C	297	VAL	2.4
1	L	73	VAL	2.4
1	D	222	ARG	2.4
1	D	265	CYS	2.4
1	F	45	THR	2.4
1	D	57	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	221	ASN	2.4
1	E	221	ASN	2.4
1	K	119	ASN	2.4
1	D	46	SER	2.4
1	C	168	PRO	2.4
1	D	64	HIS	2.4
1	E	78	ILE	2.3
1	F	73	VAL	2.3
1	C	198	THR	2.3
1	E	128	CYS	2.3
1	C	193	ALA	2.3
1	D	58	LEU	2.3
1	D	262	LEU	2.3
1	D	219	PHE	2.3
1	D	78	ILE	2.3
1	J	224	THR	2.3
1	C	208	LEU	2.3
1	D	118	TYR	2.3
1	J	278	GLY	2.3
1	H	223	PHE	2.3
1	C	279	ARG	2.3
1	E	49	MET	2.3
1	J	50	LEU	2.3
1	J	242	LEU	2.3
1	C	244	GLN	2.2
1	C	259	ILE	2.2
1	D	198	THR	2.2
1	C	205	LEU	2.2
1	B	277	ASN	2.2
1	C	213	ILE	2.2
1	D	233	VAL	2.2
1	D	165	MET	2.2
1	C	284	SER	2.2
1	D	86	VAL	2.2
1	C	255	ALA	2.2
1	D	282	LEU	2.2
1	E	141	LEU	2.2
1	C	1	SER	2.2
1	D	54	TYR	2.2
1	G	154	TYR	2.2
1	D	226	THR	2.2
1	I	59	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	69	GLN	2.1
1	H	215	GLY	2.1
1	C	167	LEU	2.1
1	C	209	TYR	2.1
1	E	118	TYR	2.1
1	I	276	MET	2.1
1	C	140	PHE	2.1
1	A	64	HIS	2.1
1	C	212	VAL	2.1
1	D	170	GLY	2.1
1	D	171	VAL	2.1
1	J	285	ALA	2.1
1	C	286	LEU	2.1
1	D	287	LEU	2.1
1	J	227	LEU	2.1
1	D	142	ASN	2.1
1	H	47	GLU	2.1
1	C	237	TYR	2.1
1	F	154	TYR	2.1
1	D	281	ILE	2.1
1	D	298	ARG	2.1
1	L	294	PHE	2.1
1	C	260	ALA	2.1
1	D	220	LEU	2.1
1	G	50	LEU	2.1
1	C	128	CYS	2.1
1	H	51	ASN	2.1
1	D	237	TYR	2.1
1	J	279	ARG	2.1
1	A	71	GLY	2.1
1	C	215	GLY	2.1
1	K	78	ILE	2.1
1	C	233	VAL	2.1
1	C	210	ALA	2.1
1	E	46	SER	2.1
1	J	211	ALA	2.1
1	I	235	MET	2.0
1	K	49	MET	2.0
1	D	138	GLY	2.0
1	J	118	TYR	2.0
1	D	59	ILE	2.0
1	C	291	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	276	MET	2.0
1	B	234	ALA	2.0
1	D	285	ALA	2.0
1	L	191	ALA	2.0
1	J	277	ASN	2.0
1	C	227	LEU	2.0
1	C	272	LEU	2.0
1	G	57	LEU	2.0
1	D	25	THR	2.0
1	D	280	THR	2.0
1	C	109	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	L	401	1/1	0.69	0.21	83,83,83,83	0
3	PEG	F	402	7/7	0.83	0.13	43,57,65,67	0
2	NA	A	401	1/1	0.84	0.10	55,55,55,55	0
3	PEG	I	401	7/7	0.85	0.14	42,51,57,59	0
3	PEG	L	402	7/7	0.85	0.14	47,53,58,60	0
3	PEG	G	402	7/7	0.86	0.14	38,43,48,49	0
3	PEG	A	402	7/7	0.87	0.14	51,56,65,66	0
2	NA	F	401	1/1	0.89	0.07	54,54,54,54	0
2	NA	K	401	1/1	0.93	0.11	56,56,56,56	0
2	NA	G	401	1/1	0.94	0.08	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.