



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:17 PM UTC

PDB ID : 9EOX / pdb_00009eox
Title : SARS-CoV2 major protease in covalent complex with a soluble inhibitor.
Authors : Moche, M.; Lennerstrand, J.; Nyman, T.; Strandback, E.; Akaberi, D.
Deposited on : 2024-03-15
Resolution : 2.54 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

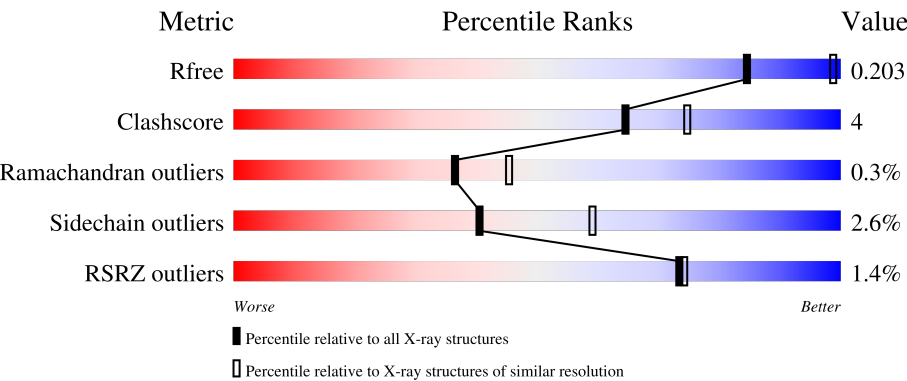
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	% 90%10%
1	B	306	2% 90%10%
1	C	306	2% 87%12%.
1	D	306	2% 86%14%
1	E	306	% 90%9%.

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Mol	Chain	Length	Quality of chain
1	F	306	% 88% 11%
2	G	4	75% 25%
2	H	4	50% 25% 25%
2	I	4	25% 75%
2	J	4	25% 50% 25%
2	K	4	25% 50% 25%
2	L	4	50% 25% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14634 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	0	0
			2367	1499	402	444	22			
1	B	306	Total	C	N	O	S	0	2	0
			2387	1510	407	448	22			
1	C	305	Total	C	N	O	S	0	0	0
			2358	1494	400	442	22			
1	D	306	Total	C	N	O	S	0	0	0
			2361	1496	399	444	22			
1	E	305	Total	C	N	O	S	0	0	0
			2358	1494	400	442	22			
1	F	305	Total	C	N	O	S	0	1	0
			2360	1495	398	445	22			

- Molecule 2 is a protein called Soluble inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			45	33	7	5			
2	H	4	Total	C	N	O	0	0	0
			45	33	7	5			
2	I	4	Total	C	N	O	0	0	0
			45	33	7	5			
2	J	4	Total	C	N	O	0	0	0
			45	33	7	5			
2	K	4	Total	C	N	O	0	0	0
			45	33	7	5			
2	L	4	Total	C	N	O	0	0	0
			45	33	7	5			

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

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

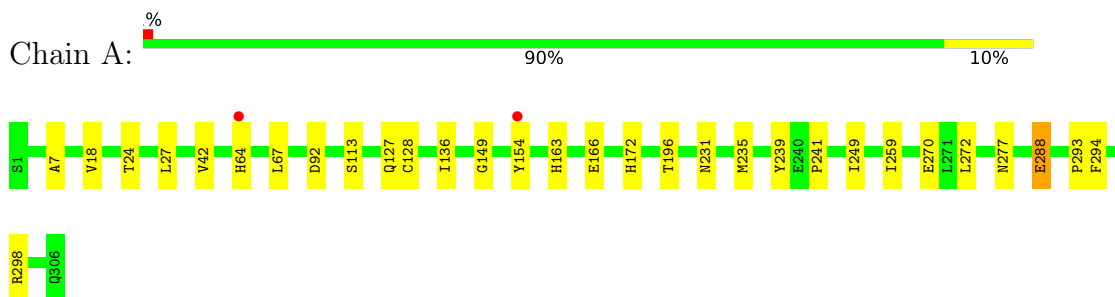
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	32	Total 32	O 32	0	0
4	C	27	Total 27	O 27	0	0
4	D	27	Total 27	O 27	0	0
4	E	31	Total 31	O 31	0	0
4	F	29	Total 29	O 29	0	0
4	G	2	Total 2	O 2	0	0
4	J	2	Total 2	O 2	0	0
4	K	2	Total 2	O 2	0	0

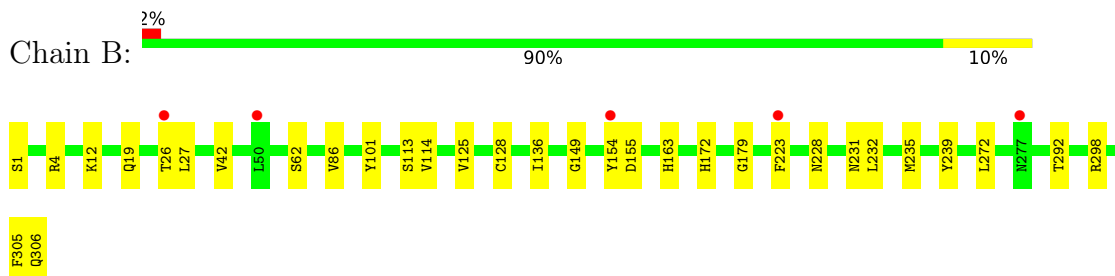
3 Residue-property plots [i](#)

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.

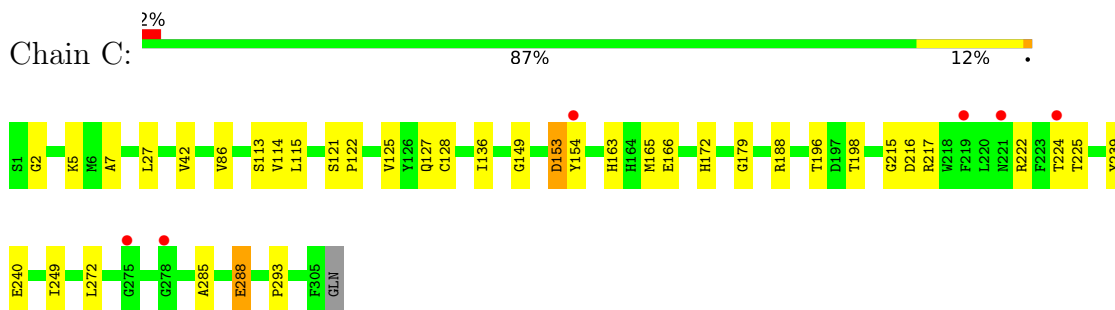
- Molecule 1: 3C-like proteinase nsp5



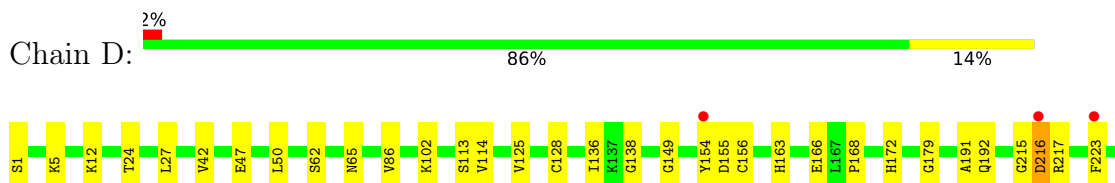
- Molecule 1: 3C-like proteinase nsp5

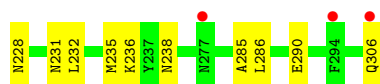


- Molecule 1: 3C-like proteinase nsp5

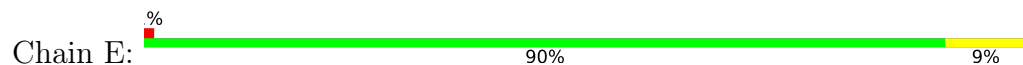


- Molecule 1: 3C-like proteinase nsp5

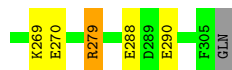
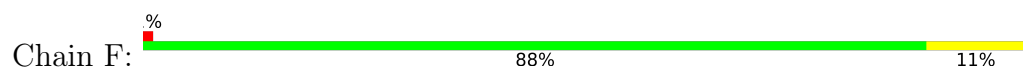




- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



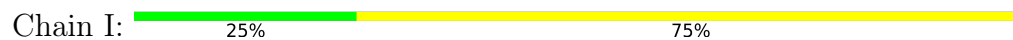
- Molecule 2: Soluble inhibitor



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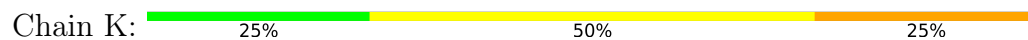


- Molecule 2: Soluble inhibitor





- Molecule 2: Soluble inhibitor



- Molecule 2: Soluble inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.46Å 85.05Å 93.90Å 79.50° 87.62° 84.14°	Depositor
Resolution (Å)	46.39 – 2.54 46.39 – 2.54	Depositor EDS
% Data completeness (in resolution range)	60.0 (46.39-2.54) 59.1 (46.39-2.54)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.189 , 0.231 (Not available) , 0.203	Depositor DCC
R_{free} test set	2051 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14634	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 6.02% 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: DNE, A1IM4, N9P, K, 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	0.54	0/2420	0.91	2/3289 (0.1%)
1	B	0.53	0/2440	0.90	0/3315
1	C	0.54	0/2411	0.92	1/3277 (0.0%)
1	D	0.54	0/2414	0.90	1/3282 (0.0%)
1	E	0.54	0/2411	0.90	0/3277
1	F	0.54	0/2413	0.93	1/3281 (0.0%)
All	All	0.54	0/14509	0.91	5/19721 (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	B	0	1
2	G	0	1
2	H	0	2
2	I	0	1
2	J	0	2
2	K	0	2
2	L	0	2
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	TYR	CA-CB-CG	6.67	125.90	113.90
1	D	216	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	153	ASP	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ASP	CA-CB-CG	5.02	117.62	112.60
1	F	110	GLN	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	ARG	Sidechain
2	G	3	A1IM3	Peptide
2	H	2	DNE	Peptide
2	H	3	A1IM3	Peptide
2	I	3	A1IM3	Peptide
2	J	2	DNE	Peptide
2	J	3	A1IM3	Peptide
2	K	2	DNE	Peptide
2	K	3	A1IM3	Peptide
2	L	2	DNE	Peptide
2	L	3	A1IM3	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	2367	0	2313	16	0
1	B	2387	0	2330	18	0
1	C	2358	0	2305	25	0
1	D	2361	0	2302	26	0
1	E	2358	0	2305	17	0
1	F	2360	0	2297	19	0
2	G	45	0	11	0	0
2	H	45	0	10	1	0
2	I	45	0	11	3	0
2	J	45	0	10	2	0
2	K	45	0	10	2	0
2	L	45	0	10	0	0
3	A	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	19	0	0	3	0
4	B	32	0	0	2	0
4	C	27	0	0	2	0
4	D	27	0	0	3	0
4	E	31	0	0	1	0
4	F	29	0	0	1	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
All	All	14634	0	13914	111	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 4.

All (111) 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:19:GLN:HE21	1:B:26:THR:HG21	1.40	0.86
1:D:192:GLN:O	4:D:501:HOH:O	1.99	0.80
1:A:231:ASN:O	1:A:235:MET:HG2	1.84	0.78
1:B:223:PHE:O	4:B:501:HOH:O	2.02	0.77
1:F:231:ASN:O	1:F:235:MET:HG2	1.88	0.73
1:D:223:PHE:O	4:D:502:HOH:O	2.07	0.72
1:E:298:ARG:NH1	4:E:501:HOH:O	2.21	0.72
1:A:24:THR:HG21	1:D:50:LEU:HD22	1.70	0.71
1:E:166:GLU:OE2	1:F:1:SER:HA	1.90	0.70
1:D:102:LYS:HD2	1:D:156:CYS:SG	2.33	0.68
1:C:166:GLU:OE2	1:D:1:SER:HA	1.95	0.67
1:A:294:PHE:CE2	1:A:298:ARG:HD3	2.32	0.65
1:F:100:LYS:HD2	1:F:155:ASP:OD1	1.98	0.64
1:A:64:HIS:HB2	4:A:514:HOH:O	1.98	0.64
1:C:215:GLY:O	1:C:217:ARG:HG3	1.98	0.63
1:C:2:GLY:HA3	1:D:138:GLY:O	2.01	0.61
1:B:292:THR:HG22	4:B:504:HOH:O	2.00	0.61
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.83	0.60
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.83	0.59
1:F:86:VAL:HG13	1:F:179:GLY:HA2	1.84	0.59
1:B:19:GLN:HE21	1:B:26:THR:CG2	2.15	0.58
1:F:233:VAL:HG21	1:F:269:LYS:HD2	1.87	0.57
1:C:288:GLU:HG3	4:C:523:HOH:O	2.05	0.56
1:D:155:ASP:HB3	1:D:306:GLN:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD13	1:D:191:ALA:HB1	1.87	0.56
1:F:226:THR:HG22	1:F:229:ASP:OD2	2.06	0.56
1:B:155:ASP:HB3	1:B:306:GLN:HG2	1.88	0.55
1:F:67:LEU:HD12	1:F:67:LEU:N	2.22	0.55
1:B:101:TYR:O	1:C:222:ARG:HB2	2.07	0.55
1:D:168:PRO:HD2	4:D:501:HOH:O	2.06	0.54
1:A:166:GLU:OE2	1:B:1:SER:HA	2.08	0.54
1:A:249:ILE:HG22	1:A:293:PRO:HG2	1.90	0.54
1:C:165:MET:SD	2:I:2:DNE:HE2	2.48	0.53
1:E:1:SER:N	1:F:140:PHE:O	2.37	0.53
1:F:226:THR:CG2	1:F:229:ASP:OD2	2.56	0.53
1:D:65:ASN:HD21	1:E:72:ASN:HA	1.73	0.53
1:E:249:ILE:HG22	1:E:293:PRO:HG2	1.91	0.53
1:E:115:LEU:HD11	1:E:122:PRO:HB3	1.93	0.51
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.92	0.50
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.94	0.50
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.94	0.50
1:A:18:VAL:HA	4:A:505:HOH:O	2.12	0.49
1:D:27:LEU:HD21	1:D:42:VAL:HB	1.94	0.49
1:D:5:LYS:HE2	1:D:290:GLU:HB2	1.93	0.49
1:B:298:ARG:HD2	1:B:305:PHE:HZ	1.77	0.49
1:C:224:THR:HG22	1:C:225:THR:N	2.28	0.49
1:D:215:GLY:O	1:D:217:ARG:HG3	2.11	0.49
1:F:1:SER:HB3	4:F:517:HOH:O	2.12	0.49
1:C:288:GLU:CG	4:C:523:HOH:O	2.60	0.49
1:F:66:PHE:C	1:F:67:LEU:HD12	2.37	0.49
1:F:27:LEU:HD21	1:F:42:VAL:HB	1.96	0.47
1:C:27:LEU:HD21	1:C:42:VAL:HB	1.94	0.47
1:B:231:ASN:O	1:B:235:MET:HG2	2.15	0.46
1:B:298:ARG:HD2	1:B:305:PHE:CZ	2.51	0.46
1:F:67:LEU:N	1:F:67:LEU:CD1	2.79	0.46
1:A:288:GLU:HG2	4:A:512:HOH:O	2.15	0.46
1:C:224:THR:HG22	1:C:225:THR:H	1.81	0.46
1:C:239:TYR:CZ	1:C:272:LEU:HD21	2.51	0.46
1:E:66:PHE:C	1:E:67:LEU:HD23	2.41	0.46
1:C:285:ALA:HB2	1:D:286:LEU:HG	1.97	0.46
2:H:3:A1IM3:O	2:H:3:A1IM3:N	2.47	0.45
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.97	0.45
1:F:243:THR:HG22	1:F:244:GLN:N	2.31	0.45
1:A:239:TYR:CZ	1:A:272:LEU:HD21	2.52	0.45
1:D:232:LEU:O	1:D:236:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLU:HB2	2:K:4:N9P:CE2	2.46	0.45
1:F:218:TRP:CE2	1:F:279:ARG:HD2	2.52	0.45
1:A:235:MET:HE1	1:A:241:PRO:HA	1.99	0.44
1:D:24:THR:C	1:E:67:LEU:HD12	2.43	0.44
1:F:243:THR:HG22	1:F:244:GLN:H	1.82	0.44
1:C:166:GLU:HB2	2:I:4:N9P:CE2	2.47	0.44
1:C:249:ILE:HG22	1:C:293:PRO:HG2	1.99	0.43
1:C:215:GLY:O	1:C:216:ASP:C	2.62	0.43
1:E:7:ALA:HA	1:E:127:GLN:NE2	2.33	0.43
1:A:7:ALA:HA	1:A:127:GLN:NE2	2.33	0.43
1:F:5:LYS:HE2	1:F:290:GLU:HB2	1.99	0.43
2:J:3:A1IM3:O	2:J:3:A1IM3:N	2.51	0.43
1:C:285:ALA:HB3	1:D:285:ALA:HB3	2.01	0.42
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.54	0.42
1:D:231:ASN:O	1:D:235:MET:HG2	2.19	0.42
1:C:114:VAL:O	1:C:125:VAL:HA	2.20	0.42
1:D:166:GLU:HB2	2:J:4:N9P:CE2	2.49	0.42
1:C:7:ALA:HA	1:C:127:GLN:NE2	2.34	0.42
1:B:12:LYS:NZ	1:B:306:GLN:HG3	2.35	0.42
1:D:163:HIS:CE1	1:D:172:HIS:HB3	2.54	0.42
1:C:188:ARG:N	2:I:2:DNE:HE1	2.34	0.42
1:C:113:SER:O	1:C:149:GLY:HA2	2.20	0.42
1:D:228:ASN:O	1:D:232:LEU:HG	2.20	0.42
1:E:228:ASN:O	1:E:232:LEU:HG	2.20	0.42
1:E:121:SER:HA	1:E:122:PRO:HD3	1.95	0.41
1:A:294:PHE:CZ	1:A:298:ARG:HD3	2.55	0.41
1:C:198:THR:OG1	1:C:240:GLU:OE2	2.31	0.41
1:D:114:VAL:O	1:D:125:VAL:HA	2.20	0.41
1:E:239:TYR:CZ	1:E:272:LEU:HD21	2.55	0.41
1:F:113:SER:O	1:F:149:GLY:HA2	2.19	0.41
1:E:49:MET:HE2	2:K:2:DNE:HD2	2.02	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.20	0.41
1:B:239:TYR:CZ	1:B:272:LEU:HD21	2.56	0.41
1:B:228:ASN:O	1:B:232:LEU:HG	2.20	0.41
1:C:121:SER:HA	1:C:122:PRO:HD3	1.93	0.41
1:E:114:VAL:O	1:E:125:VAL:HA	2.21	0.41
1:F:228:ASN:O	1:F:232:LEU:HG	2.21	0.41
1:B:114:VAL:O	1:B:125:VAL:HA	2.21	0.40
1:D:86:VAL:HG23	1:D:179:GLY:HA2	2.03	0.40
1:D:215:GLY:O	1:D:216:ASP:C	2.64	0.40
1:E:113:SER:O	1:E:149:GLY:HA2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:O	1:B:149:GLY:HA2	2.21	0.40
1:D:113:SER:O	1:D:149:GLY:HA2	2.21	0.40
1:C:163:HIS:CE1	1:C:172:HIS:HB3	2.57	0.40
1:A:163:HIS:CE1	1:A:172:HIS:HB3	2.56	0.40
1:D:12:LYS:NZ	1:D:306:GLN:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/306 (22%)	67 (100%)	0	0	100	100
1	B	306/306 (100%)	295 (96%)	10 (3%)	1 (0%)	36	45
1	C	303/306 (99%)	291 (96%)	11 (4%)	1 (0%)	36	45
1	D	304/306 (99%)	292 (96%)	11 (4%)	1 (0%)	36	45
1	E	303/306 (99%)	292 (96%)	10 (3%)	1 (0%)	36	45
1	F	304/306 (99%)	293 (96%)	10 (3%)	1 (0%)	36	45
All	All	1587/1836 (86%)	1530 (96%)	52 (3%)	5 (0%)	36	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	154	TYR
1	B	154	TYR
1	C	154	TYR
1	E	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	263/263 (100%)	256 (97%)	7 (3%)	39	58
1	B	265/263 (101%)	262 (99%)	3 (1%)	65	79
1	C	262/263 (100%)	256 (98%)	6 (2%)	44	62
1	D	262/263 (100%)	257 (98%)	5 (2%)	50	69
1	E	214/263 (81%)	206 (96%)	8 (4%)	30	45
1	F	262/263 (100%)	252 (96%)	10 (4%)	29	44
All	All	1528/1578 (97%)	1489 (97%)	39 (3%)	40	59

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	CYS
1	A	136	ILE
1	A	196	THR
1	A	259	ILE
1	A	270	GLU
1	A	277	ASN
1	A	288	GLU
1	B	62	SER
1	B	128	CYS
1	B	136	ILE
1	C	5	LYS
1	C	128	CYS
1	C	136	ILE
1	C	153	ASP
1	C	196	THR
1	C	288	GLU
1	D	47	GLU
1	D	62	SER
1	D	128	CYS
1	D	136	ILE
1	D	238	ASN
1	E	1	SER

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Mol	Chain	Res	Type
1	E	5	LYS
1	E	47	GLU
1	E	67	LEU
1	E	128	CYS
1	E	136	ILE
1	E	196	THR
1	E	288	GLU
1	F	47	GLU
1	F	67	LEU
1	F	75	LEU
1	F	90	LYS
1	F	128	CYS
1	F	136	ILE
1	F	240	GLU
1	F	270	GLU
1	F	279	ARG
1	F	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	119	ASN
1	A	127	GLN
1	A	180	ASN
1	A	274	ASN
1	A	277	ASN
1	B	19	GLN
1	B	180	ASN
1	B	189	GLN
1	B	238	ASN
1	B	244	GLN
1	C	119	ASN
1	C	127	GLN
1	D	69	GLN
1	D	74	GLN
1	D	180	ASN
1	D	244	GLN
1	D	274	ASN
1	E	119	ASN
1	E	127	GLN
1	F	69	GLN

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Mol	Chain	Res	Type
1	F	180	ASN
1	F	244	GLN
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	DNE	G	2	2	6,7,8	0.55	0	2,7,9	0.45	0
2	DNE	H	2	2	6,7,8	0.46	0	2,7,9	0.20	0
2	N9P	I	4	2	11,12,12	0.62	0	11,15,15	0.62	0
2	A1IM3	I	3	2	16,16,17	0.43	0	18,21,23	0.70	0
2	A1IM3	J	3	2	16,16,17	0.66	0	18,21,23	0.58	0
2	A1IM3	L	3	2	16,16,17	0.69	0	18,21,23	0.85	1 (5%)
2	DNE	I	2	2	6,7,8	0.55	0	2,7,9	0.32	0
2	A1IM3	K	3	2	16,16,17	0.45	0	18,21,23	0.69	0
2	DNE	J	2	2	6,7,8	0.51	0	2,7,9	0.24	0
2	A1IM3	H	3	2	16,16,17	0.57	0	18,21,23	0.63	0
2	DNE	K	2	2	6,7,8	0.54	0	2,7,9	0.41	0
2	N9P	G	4	2	11,12,12	0.72	0	11,15,15	0.58	0
2	N9P	J	4	2	11,12,12	0.66	0	11,15,15	0.63	0
2	N9P	L	4	2	11,12,12	0.66	0	11,15,15	0.64	0
2	A1IM3	G	3	2	16,16,17	0.51	0	18,21,23	0.67	0
2	N9P	K	4	2	11,12,12	0.63	0	11,15,15	0.64	0
2	DNE	L	2	2	6,7,8	0.54	0	2,7,9	0.21	0
2	N9P	H	4	2	11,12,12	0.80	0	11,15,15	0.40	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	-	2/5/6/8	-
2	DNE	H	2	2	-	2/5/6/8	-
2	N9P	I	4	2	-	2/8/8/8	0/1/1/1
2	A1IM3	I	3	2	-	4/7/7/8	0/2/2/2
2	A1IM3	J	3	2	-	4/7/7/8	0/2/2/2
2	A1IM3	L	3	2	-	4/7/7/8	0/2/2/2
2	DNE	I	2	2	-	2/5/6/8	-
2	A1IM3	K	3	2	-	4/7/7/8	0/2/2/2
2	DNE	J	2	2	-	2/5/6/8	-
2	A1IM3	H	3	2	-	3/7/7/8	0/2/2/2
2	DNE	K	2	2	-	4/5/6/8	-
2	N9P	G	4	2	-	2/8/8/8	0/1/1/1
2	N9P	J	4	2	-	3/8/8/8	0/1/1/1
2	N9P	L	4	2	-	2/8/8/8	0/1/1/1
2	A1IM3	G	3	2	-	4/7/7/8	0/2/2/2
2	N9P	K	4	2	-	3/8/8/8	0/1/1/1
2	DNE	L	2	2	-	3/5/6/8	-
2	N9P	H	4	2	-	2/8/8/8	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	A1IM3	CA-CB-CG	-2.19	107.73	110.82

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	DNE	C-CA-CB-CG
2	I	2	DNE	C-CA-CB-CG
2	K	2	DNE	N-CA-CB-CG
2	K	2	DNE	C-CA-CB-CG
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	G	3	A1IM3	C-CA-CB-N
2	G	3	A1IM3	C-CA-CB-CG
2	H	3	A1IM3	C-CA-CB-N
2	I	3	A1IM3	C-CA-CB-N
2	J	3	A1IM3	C-CA-CB-N
2	K	3	A1IM3	CA-CB-CG-CD
2	K	3	A1IM3	C-CA-CB-N
2	L	3	A1IM3	C-CA-CB-N
2	L	3	A1IM3	C-CA-CB-CG
2	G	4	N9P	O-C-CA-N
2	H	4	N9P	O-C-CA-N
2	I	4	N9P	O-C-CA-N
2	J	4	N9P	O-C-CA-N
2	J	4	N9P	N-CA-CB-CG
2	K	4	N9P	O-C-CA-N
2	L	4	N9P	O-C-CA-N
2	J	4	N9P	OXT-C-CA-N
2	K	4	N9P	OXT-C-CA-N
2	L	4	N9P	OXT-C-CA-N
2	G	4	N9P	OXT-C-CA-N
2	H	4	N9P	OXT-C-CA-N
2	I	4	N9P	OXT-C-CA-N
2	G	2	DNE	CA-CB-CG-CD
2	I	2	DNE	CA-CB-CG-CD
2	K	4	N9P	N-CA-CB-CG
2	H	2	DNE	CE-CD-CG-CB
2	L	2	DNE	CE-CD-CG-CB
2	J	2	DNE	CE-CD-CG-CB
2	H	3	A1IM3	C-CA-CB-CG
2	I	3	A1IM3	C-CA-CB-CG
2	I	3	A1IM3	N-CB-CG-CD
2	J	3	A1IM3	N-CB-CG-CD
2	K	3	A1IM3	N-CB-CG-CD
2	G	2	DNE	C-CA-CB-CG
2	J	2	DNE	C-CA-CB-CG
2	G	3	A1IM3	O-C-CA-CB
2	G	3	A1IM3	N-CB-CG-CD
2	L	3	A1IM3	N-CB-CG-CD
2	K	2	DNE	CE-CD-CG-CB
2	J	3	A1IM3	C-CA-CB-CG
2	I	3	A1IM3	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	H	3	A1IM3	N-CB-CG-CD
2	J	3	A1IM3	CA-CB-CG-CD
2	K	3	A1IM3	O-C-CA-CB
2	L	3	A1IM3	O-C-CA-CB
2	K	2	DNE	CA-CB-CG-CD

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	N9P	1	0
2	J	3	A1IM3	1	0
2	I	2	DNE	2	0
2	H	3	A1IM3	1	0
2	K	2	DNE	1	0
2	J	4	N9P	1	0
2	K	4	N9P	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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%)	0.01	2 (0%) 84 86	18, 34, 56, 79	0
1	B	306/306 (100%)	-0.11	5 (1%) 70 71	12, 29, 53, 78	2 (0%)
1	C	305/306 (99%)	0.05	6 (1%) 65 65	17, 31, 64, 87	0
1	D	306/306 (100%)	-0.03	6 (1%) 65 65	16, 31, 59, 81	0
1	E	305/306 (99%)	-0.12	3 (0%) 79 80	17, 28, 56, 76	0
1	F	305/306 (99%)	-0.07	4 (1%) 75 75	16, 28, 54, 80	1 (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%)	-0.05	26 (1%) 73 74	12, 30, 58, 87	3 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	154	TYR	3.7
1	D	216	ASP	3.6
1	A	154	TYR	3.5
1	C	154	TYR	3.3
1	E	154	TYR	3.2
1	D	306	GLN	3.0
1	B	154	TYR	2.9
1	F	222	ARG	2.8
1	D	223	PHE	2.7
1	C	278	GLY	2.7
1	C	221	ASN	2.6
1	C	275	GLY	2.5
1	E	235	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	195	GLY	2.4
1	A	64	HIS	2.3
1	B	50	LEU	2.3
1	C	219	PHE	2.3
1	C	224	THR	2.2
1	E	228	ASN	2.2
1	F	223	PHE	2.2
1	B	26	THR	2.1
1	D	154	TYR	2.1
1	D	277	ASN	2.1
1	D	294	PHE	2.0
1	B	223	PHE	2.0
1	B	277	ASN	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	DNE	I	2	8/9	0.87	0.15	40,43,50,52	0
2	DNE	K	2	8/9	0.87	0.12	24,25,28,36	0
2	DNE	L	2	8/9	0.89	0.13	30,33,35,43	0
2	DNE	H	2	8/9	0.90	0.13	29,32,35,42	0
2	DNE	G	2	8/9	0.90	0.13	28,31,39,42	0
2	A1IM3	H	3	15/16	0.90	0.12	28,32,42,42	0
2	A1IM3	J	3	15/16	0.90	0.10	28,32,34,34	0
2	N9P	H	4	12/12	0.90	0.10	28,31,35,36	0
2	A1IM3	L	3	15/16	0.91	0.09	25,27,30,31	0
2	DNE	J	2	8/9	0.91	0.11	28,32,34,41	0
2	N9P	I	4	12/12	0.92	0.09	26,28,35,37	0
2	N9P	J	4	12/12	0.92	0.08	23,26,27,29	0
2	N9P	L	4	12/12	0.93	0.08	27,29,33,37	0
2	A1IM3	I	3	15/16	0.94	0.07	30,31,35,37	0
2	N9P	G	4	12/12	0.94	0.09	24,25,26,26	0
2	N9P	K	4	12/12	0.95	0.07	28,31,33,33	0
2	A1IM3	K	3	15/16	0.95	0.08	20,21,27,32	0
2	A1IM3	G	3	15/16	0.97	0.06	19,20,26,27	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	E	401	1/1	0.77	0.09	64,64,64,64	0
3	K	A	401	1/1	0.87	0.09	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.