



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2024 – 07:21 pm BST

PDB ID : 9EOX
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

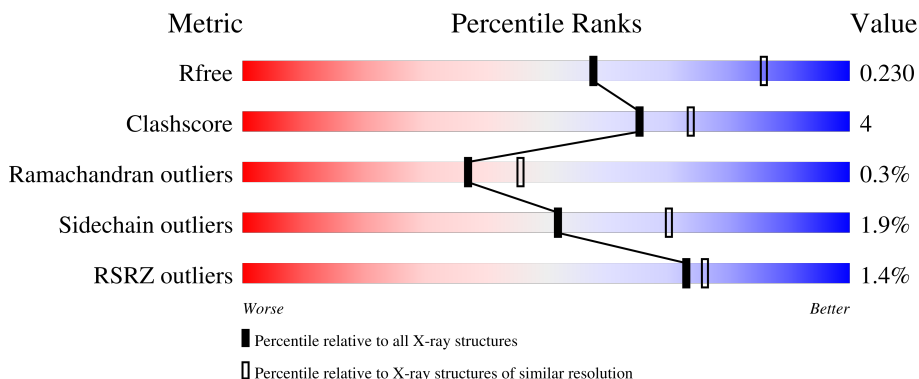
1 Overall quality at a glance

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.



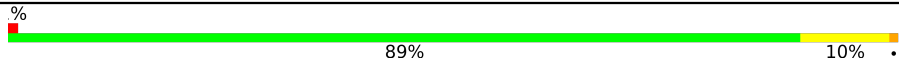


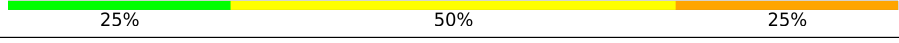
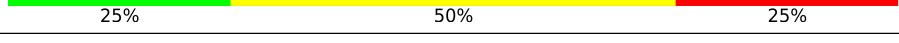

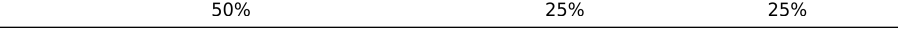
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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	91% 8%
1	B	306	90% 10%
1	C	306	88% 11%
1	D	306	87% 13%
1	E	306	89% 10%

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Mol	Chain	Length	Quality of chain
1	F	306	 <p>% 89% 10%</p>
2	G	4	 <p>75% 25%</p>
2	H	4	 <p>50% 25% 25%</p>
2	I	4	 <p>25% 50% 25%</p>
2	J	4	 <p>25% 50% 25%</p>
2	K	4	 <p>25% 25% 50%</p>
2	L	4	 <p>50% 25% 25%</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	306	Total 2367	C 1499	N 402	O 444	S 22	0	0	0
1	B	306	Total 2387	C 1510	N 407	O 448	S 22	0	2	0
1	C	305	Total 2358	C 1494	N 400	O 442	S 22	0	0	0
1	D	306	Total 2361	C 1496	N 399	O 444	S 22	0	0	0
1	E	305	Total 2358	C 1494	N 400	O 442	S 22	0	0	0
1	F	305	Total 2360	C 1495	N 398	O 445	S 22	0	1	0

- Molecule 2 is a protein called Soluble inhibitor.

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

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

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

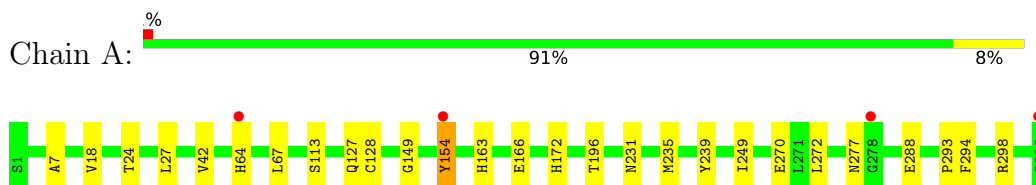
- Molecule 4 is water.

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

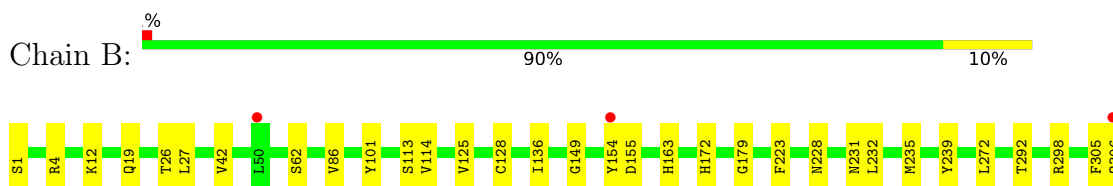
3 Residue-property plots [i](#)

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.

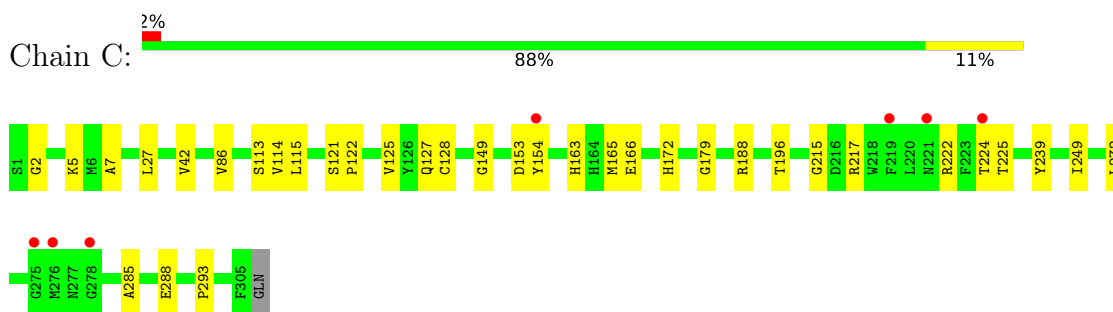
- Molecule 1: 3C-like proteinase nsp5



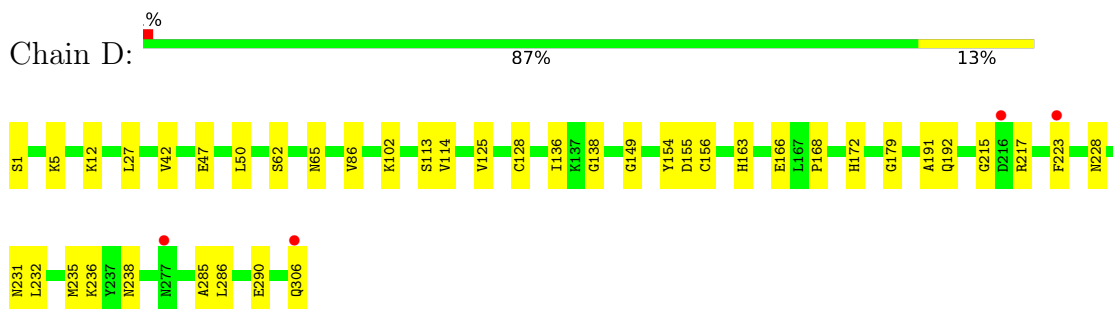
- Molecule 1: 3C-like proteinase nsp5



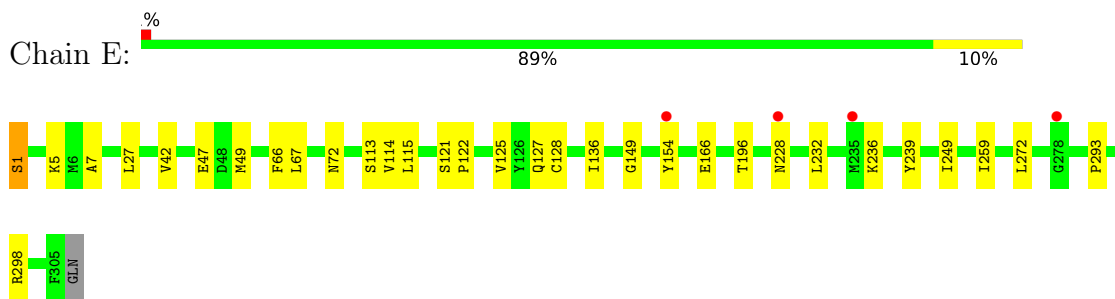
- Molecule 1: 3C-like proteinase nsp5



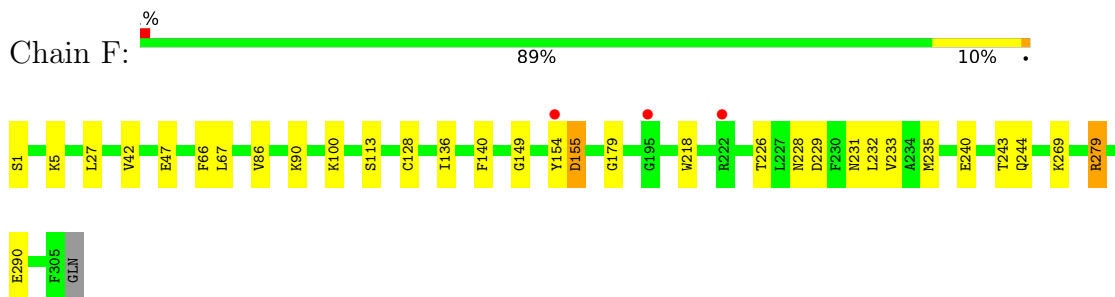
- Molecule 1: 3C-like proteinase nsp5



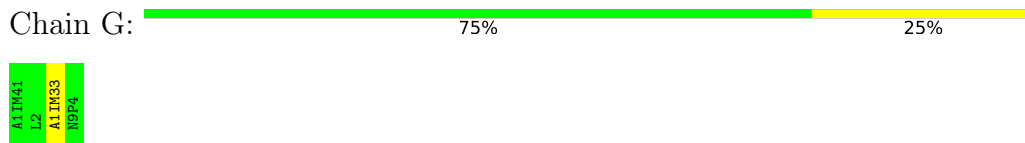
- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



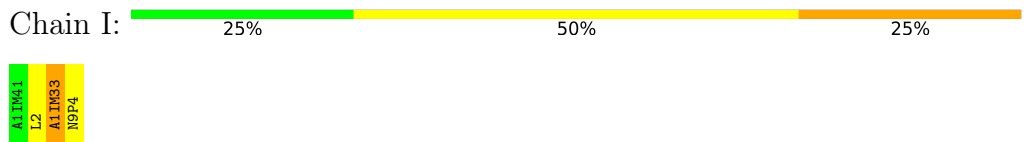
- Molecule 2: Soluble inhibitor



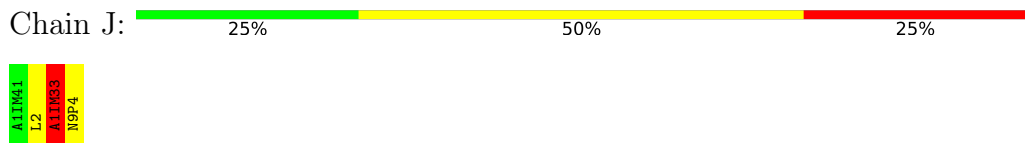
- Molecule 2: Soluble inhibitor



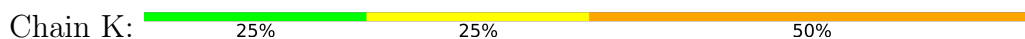
- Molecule 2: Soluble inhibitor



- Molecule 2: Soluble inhibitor



- Molecule 2: Soluble inhibitor





- Molecule 2: Soluble inhibitor

Chain L: 50% 25% 25%



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) 60.3 (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)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.189 , 0.231 0.193 , 0.230	Depositor DCC
R_{free} test set	3422 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: A1IM3, N9P, K, A1IM4, DNE

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	0.37	0/2420	0.68	1/3289 (0.0%)
1	B	0.37	0/2440	0.66	0/3315
1	C	0.37	0/2411	0.67	0/3277
1	D	0.38	0/2414	0.65	0/3282
1	E	0.37	0/2411	0.65	0/3277
1	F	0.37	0/2413	0.69	1/3281 (0.0%)
All	All	0.37	0/14509	0.67	2/19721 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	TYR	CA-CB-CG	6.58	125.90	113.40
1	F	155	ASP	CB-CG-OD1	6.51	124.16	118.30

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 [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	2367	0	2313	15	0
1	B	2387	0	2330	18	0
1	C	2358	0	2305	23	0
1	D	2361	0	2302	24	0
1	E	2358	0	2305	16	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	106	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 (106) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1:SER:N	1:F:140:PHE:O	2.37	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: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: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
1:E:166:GLU:HB2	2:K:4:N9P:CE2	2.46	0.45
1:F:66:PHE:C	1:F:67:LEU:HD12	2.37	0.45
1:F:218:TRP:CE2	1:F:279:ARG:HD2	2.52	0.45
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:E:7:ALA:HA	1:E:127:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:49:MET:HE2	2:K:2:DNE:HD2	2.01	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: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:66:PHE:C	1:E:67:LEU:HD23	2.41	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:E:113:SER:O	1:E:149:GLY:HA2	2.20	0.40
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	304/306 (99%)	292 (96%)	11 (4%)	1 (0%)	37	46
1	B	306/306 (100%)	295 (96%)	10 (3%)	1 (0%)	37	46
1	C	303/306 (99%)	291 (96%)	11 (4%)	1 (0%)	37	46
1	D	304/306 (99%)	292 (96%)	11 (4%)	1 (0%)	37	46
1	E	303/306 (99%)	292 (96%)	10 (3%)	1 (0%)	37	46
1	F	304/306 (99%)	293 (96%)	10 (3%)	1 (0%)	37	46
All	All	1824/1836 (99%)	1755 (96%)	63 (4%)	6 (0%)	37	46

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	259 (98%)	4 (2%)	60	76
1	B	265/263 (101%)	262 (99%)	3 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	262/263 (100%)	258 (98%)	4 (2%)	60	76
1	D	262/263 (100%)	257 (98%)	5 (2%)	52	70
1	E	262/263 (100%)	254 (97%)	8 (3%)	35	50
1	F	262/263 (100%)	256 (98%)	6 (2%)	45	63
All	All	1576/1578 (100%)	1546 (98%)	30 (2%)	52	70

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	CYS
1	A	196	THR
1	A	270	GLU
1	A	277	ASN
1	B	62	SER
1	B	128	CYS
1	B	136	ILE
1	C	5	LYS
1	C	128	CYS
1	C	153	ASP
1	C	196	THR
1	D	47	GLU
1	D	62	SER
1	D	128	CYS
1	D	136	ILE
1	D	238	ASN
1	E	1	SER
1	E	5	LYS
1	E	47	GLU
1	E	128	CYS
1	E	136	ILE
1	E	196	THR
1	E	236	LYS
1	E	259	ILE
1	F	47	GLU
1	F	90	LYS
1	F	128	CYS
1	F	136	ILE
1	F	240	GLU
1	F	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	127	GLN
1	A	274	ASN
1	A	277	ASN
1	B	19	GLN
1	B	189	GLN
1	C	127	GLN
1	D	189	GLN
1	D	274	ASN
1	E	74	GLN
1	E	110	GLN
1	E	127	GLN
1	F	277	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1IM3	H	3	2	15,16,17	0.67	0	14,21,23	0.99	1 (7%)
2	A1IM3	I	3	2	15,16,17	0.64	0	14,21,23	1.06	1 (7%)
2	N9P	L	4	2	11,12,12	0.64	0	14,15,15	0.68	0
2	DNE	I	2	2	6,7,8	0.54	0	2,7,9	0.32	0
2	A1IM3	K	3	2	15,16,17	0.68	0	14,21,23	1.08	1 (7%)
2	N9P	K	4	2	11,12,12	0.61	0	14,15,15	0.71	0
2	DNE	H	2	2	6,7,8	0.45	0	2,7,9	0.22	0
2	DNE	L	2	2	6,7,8	0.53	0	2,7,9	0.23	0
2	A1IM3	G	3	2	15,16,17	0.70	0	14,21,23	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	N9P	G	4	2	11,12,12	0.70	0	14,15,15	0.71	0
2	N9P	I	4	2	11,12,12	0.60	0	14,15,15	0.79	0
2	N9P	J	4	2	11,12,12	0.64	0	14,15,15	0.73	0
2	DNE	G	2	2	6,7,8	0.53	0	2,7,9	0.48	0
2	A1IM3	J	3	2	15,16,17	0.72	0	14,21,23	0.95	1 (7%)
2	N9P	H	4	2	11,12,12	0.78	0	14,15,15	0.56	0
2	A1IM3	L	3	2	15,16,17	0.78	0	14,21,23	1.21	2 (14%)
2	DNE	K	2	2	6,7,8	0.53	0	2,7,9	0.44	0
2	DNE	J	2	2	6,7,8	0.50	0	2,7,9	0.26	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	A1IM3	H	3	2	-	3/6/7/8	0/2/2/2
2	A1IM3	I	3	2	-	4/6/7/8	0/2/2/2
2	N9P	L	4	2	-	2/8/8/8	0/1/1/1
2	DNE	I	2	2	-	2/5/6/8	-
2	A1IM3	K	3	2	-	4/6/7/8	0/2/2/2
2	N9P	K	4	2	-	3/8/8/8	0/1/1/1
2	DNE	H	2	2	-	2/5/6/8	-
2	DNE	L	2	2	-	3/5/6/8	-
2	A1IM3	G	3	2	-	4/6/7/8	0/2/2/2
2	N9P	G	4	2	-	2/8/8/8	0/1/1/1
2	N9P	I	4	2	-	2/8/8/8	0/1/1/1
2	N9P	J	4	2	-	3/8/8/8	0/1/1/1
2	DNE	G	2	2	-	2/5/6/8	-
2	A1IM3	J	3	2	-	4/6/7/8	0/2/2/2
2	N9P	H	4	2	-	2/8/8/8	0/1/1/1
2	A1IM3	L	3	2	-	3/6/7/8	0/2/2/2
2	DNE	K	2	2	-	4/5/6/8	-
2	DNE	J	2	2	-	2/5/6/8	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	A1IM3	CT2-CH2-CZ2	-2.30	116.77	120.08
2	I	3	A1IM3	CT2-CH2-CZ2	-2.18	116.94	120.08
2	L	3	A1IM3	CA-CB-CG	-2.13	107.73	110.81
2	H	3	A1IM3	CT2-CH2-CZ2	-2.11	117.04	120.08
2	J	3	A1IM3	CT2-CH2-CZ2	-2.07	117.11	120.08
2	L	3	A1IM3	CT2-CH2-CZ2	-2.06	117.12	120.08

There are no chirality outliers.

All (51) 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
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	H	3	A1IM3	C-CA-CB-CG
2	I	3	A1IM3	C-CA-CB-N
2	I	3	A1IM3	C-CA-CB-CG
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

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

There are no ring outliers.

7 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

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%)	-0.10	4 (1%) 74 77	18, 34, 56, 79	0
1	B	306/306 (100%)	-0.21	3 (0%) 79 82	12, 29, 53, 78	2 (0%)
1	C	305/306 (99%)	-0.05	7 (2%) 61 65	17, 31, 64, 87	0
1	D	306/306 (100%)	-0.13	4 (1%) 74 77	16, 31, 59, 81	0
1	E	305/306 (99%)	-0.22	4 (1%) 74 77	17, 28, 56, 76	0
1	F	305/306 (99%)	-0.18	3 (0%) 79 82	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%)	-0.15	25 (1%) 73 76	12, 30, 58, 87	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	216	ASP	3.6
1	F	154	TYR	3.6
1	A	154	TYR	3.4
1	E	154	TYR	3.2
1	C	154	TYR	3.2
1	F	222	ARG	3.2
1	D	306	GLN	3.0
1	B	154	TYR	2.8
1	D	223	PHE	2.7
1	C	221	ASN	2.7
1	E	228	ASN	2.5
1	F	195	GLY	2.4
1	C	275	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	235	MET	2.3
1	C	219	PHE	2.2
1	C	278	GLY	2.2
1	A	64	HIS	2.2
1	A	306	GLN	2.2
1	E	278	GLY	2.1
1	B	50	LEU	2.1
1	B	306	GLN	2.1
1	D	277	ASN	2.1
1	C	276	MET	2.0
1	A	278	GLY	2.0
1	C	224	THR	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	0.86	0.15	40,43,50,52	0
2	DNE	K	2	8/9	0.88	0.12	24,25,28,36	0
2	DNE	H	2	8/9	0.89	0.13	29,32,35,42	0
2	DNE	L	2	8/9	0.89	0.13	30,33,35,43	0
2	N9P	H	4	12/12	0.89	0.11	28,31,35,36	0
2	A1IM3	J	3	15/16	0.90	0.10	28,32,34,34	0
2	DNE	G	2	8/9	0.90	0.13	28,31,39,42	0
2	A1IM3	L	3	15/16	0.91	0.09	25,27,30,31	0
2	A1IM3	H	3	15/16	0.91	0.11	28,32,42,42	0
2	DNE	J	2	8/9	0.92	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	0.92	0.09	27,29,33,37	0
2	A1IM3	I	3	15/16	0.94	0.07	30,31,35,37	0
2	N9P	K	4	12/12	0.94	0.08	28,31,33,33	0
2	N9P	G	4	12/12	0.94	0.08	24,25,26,26	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	K	E	401	1/1	0.76	0.09	64,64,64,64	0
3	K	A	401	1/1	0.85	0.10	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.