



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:17 PM UTC

PDB ID : 8DRY / pdb_00008dry
Title : Product structure of SARS-CoV-2 Mpro C145A mutant 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 : 2.49 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

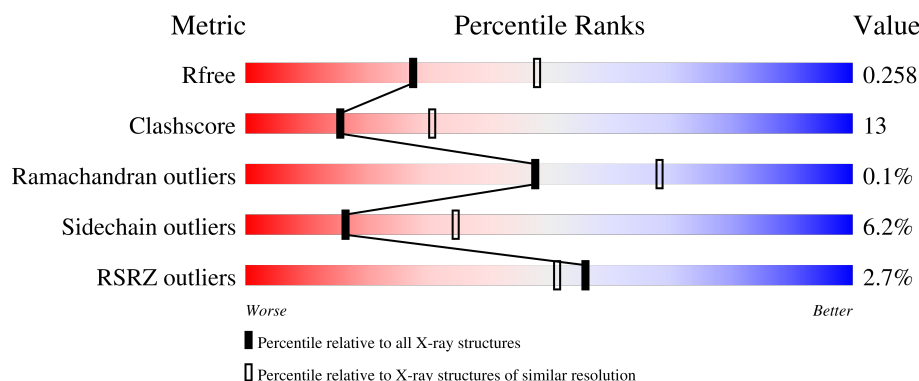
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 9% .
1	B	306	86% 13% .
1	C	306	3% 82% 18%
1	D	306	% 77% 22% .
1	E	306	84% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	306	% 82% 16% .
1	G	306	2% 81% 17% ..
1	H	306	3% 75% 23% ..
1	I	306	8% 78% 21% .
1	J	306	12% 75% 24% .
1	K	306	83% 15% ..
1	L	306	% 85% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28308 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 Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2342	1484	400	437	21			
1	B	303	Total	C	N	O	S	0	1	0
			2354	1491	403	439	21			
1	C	306	Total	C	N	O	S	0	0	0
			2366	1497	404	444	21			
1	D	306	Total	C	N	O	S	0	0	0
			2367	1500	404	442	21			
1	E	303	Total	C	N	O	S	0	1	0
			2350	1489	403	437	21			
1	F	302	Total	C	N	O	S	0	0	0
			2339	1482	399	437	21			
1	G	302	Total	C	N	O	S	0	0	0
			2328	1474	399	434	21			
1	H	302	Total	C	N	O	S	0	1	0
			2340	1482	399	438	21			
1	I	306	Total	C	N	O	S	0	0	0
			2352	1490	399	442	21			
1	J	306	Total	C	N	O	S	0	0	0
			2329	1474	398	437	20			
1	K	303	Total	C	N	O	S	0	0	0
			2329	1474	400	434	21			
1	L	302	Total	C	N	O	S	0	0	0
			2339	1482	399	437	21			

There are 12 discrepancies between the modelled and reference sequences:

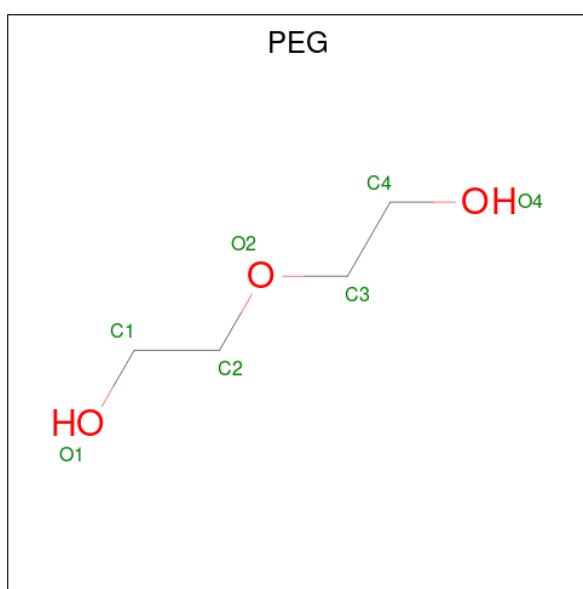
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	145	ALA	CYS	engineered mutation	UNP P0DTD1
F	145	ALA	CYS	engineered mutation	UNP P0DTD1
G	145	ALA	CYS	engineered mutation	UNP P0DTD1
H	145	ALA	CYS	engineered mutation	UNP P0DTD1
I	145	ALA	CYS	engineered mutation	UNP P0DTD1
J	145	ALA	CYS	engineered mutation	UNP P0DTD1
K	145	ALA	CYS	engineered mutation	UNP P0DTD1
L	145	ALA	CYS	engineered mutation	UNP P0DTD1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	28	Total	O	0	0
			28	28		
3	C	13	Total	O	0	0
			13	13		

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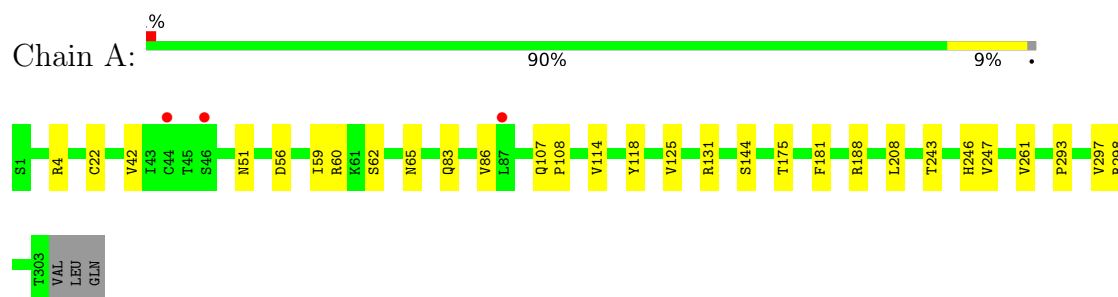
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	6	Total 6	O 6	0	0
3	E	20	Total 20	O 20	0	0
3	F	17	Total 17	O 17	0	0
3	G	12	Total 12	O 12	0	0
3	H	5	Total 5	O 5	0	0
3	I	1	Total 1	O 1	0	0
3	J	2	Total 2	O 2	0	0
3	K	15	Total 15	O 15	0	0
3	L	17	Total 17	O 17	0	0

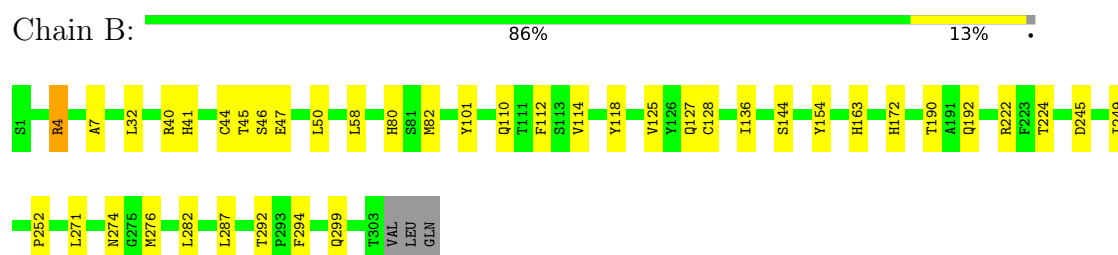
3 Residue-property plots [i](#)

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.

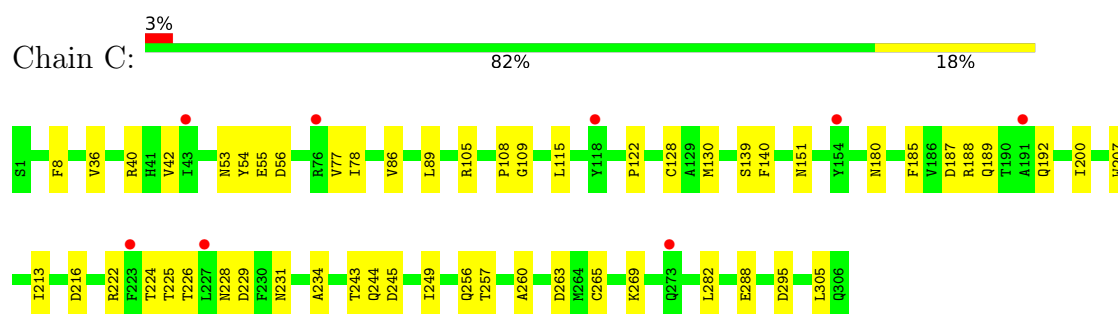
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site



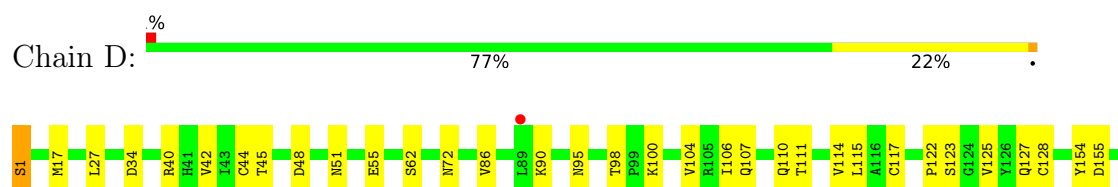
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

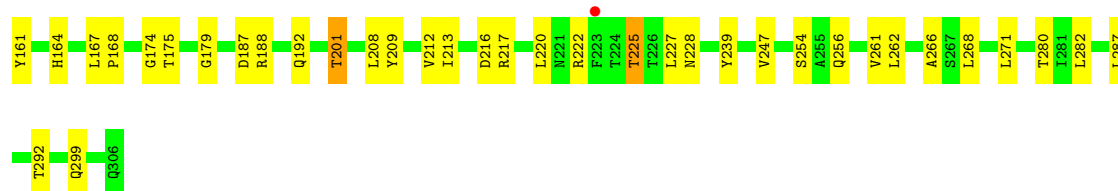


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site



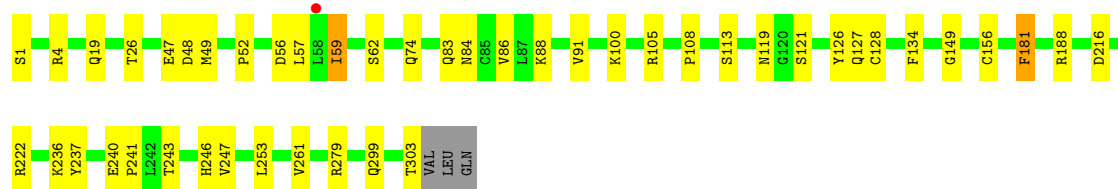
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site





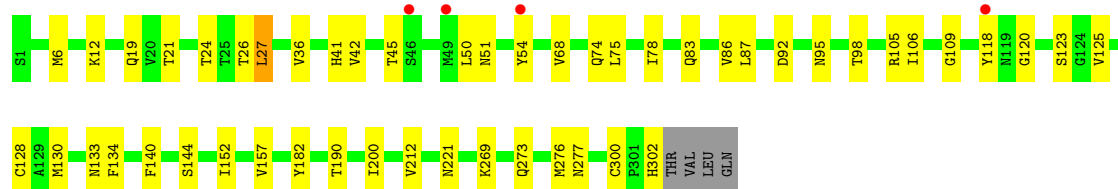
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

Chain E: 84% 14% ..



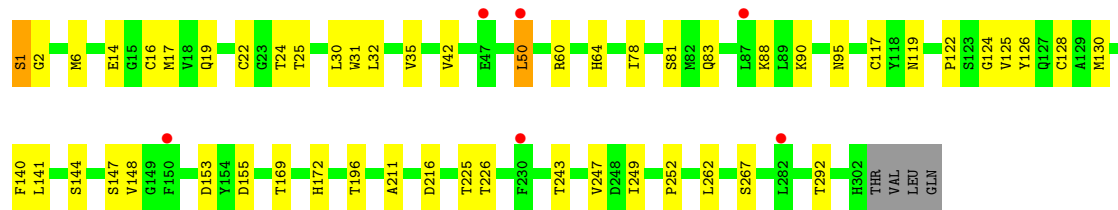
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

Chain F: 82% 16% .



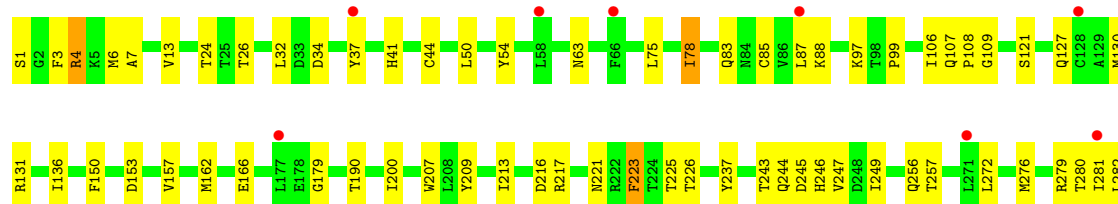
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

Chain G: 81% 17% ..



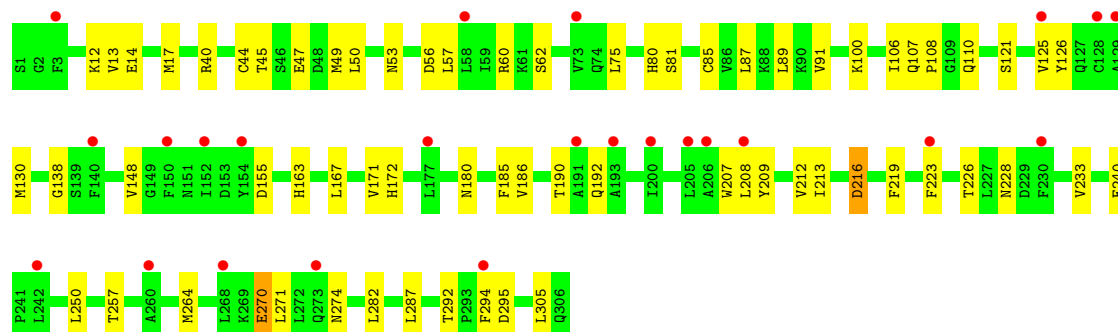
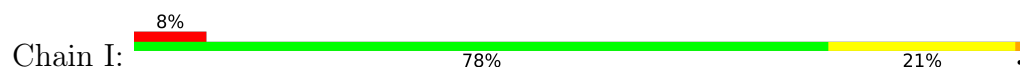
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

Chain H: 75% 23% ..

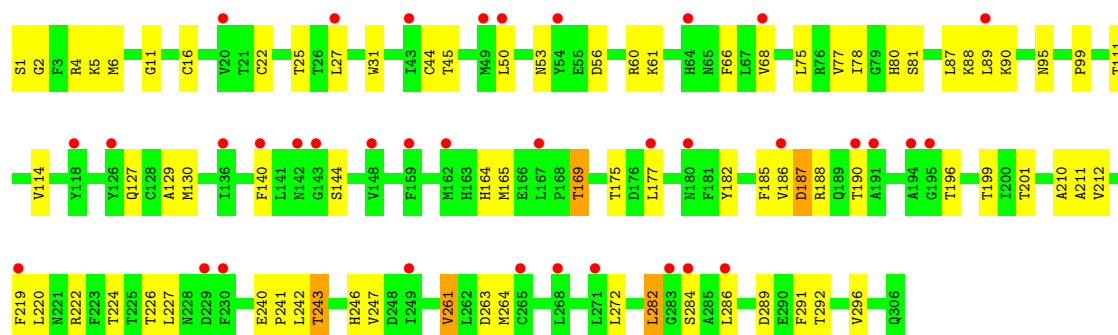
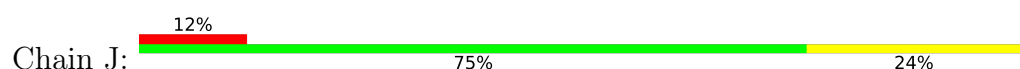




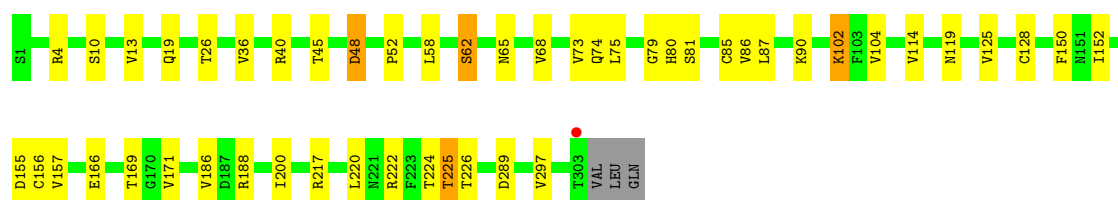
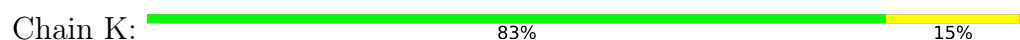
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site



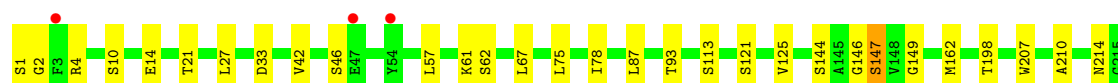
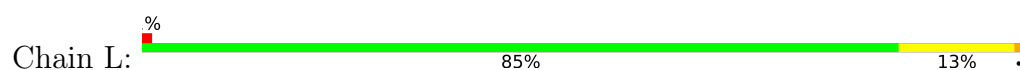
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site

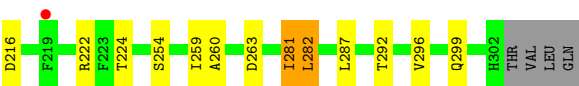


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site



- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp12-nsp13 (C12) cut site





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.33Å 107.92Å 277.25Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	65.23 – 2.49 65.23 – 2.49	Depositor EDS
% Data completeness (in resolution range)	72.5 (65.23-2.49) 72.5 (65.23-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.264 (Not available) , 0.258	Depositor DCC
R_{free} test set	2007 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28308	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 23.60 % 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 4.5167e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/2396	0.72	0/3259
1	B	0.54	0/2411	0.75	0/3278
1	C	0.44	0/2420	0.64	0/3290
1	D	0.42	0/2421	0.61	0/3292
1	E	0.48	0/2407	0.67	0/3273
1	F	0.43	0/2393	0.62	0/3254
1	G	0.39	0/2381	0.58	0/3238
1	H	0.45	0/2397	0.68	0/3261
1	I	0.35	0/2406	0.55	0/3273
1	J	0.39	0/2382	0.57	0/3244
1	K	0.46	0/2382	0.68	0/3240
1	L	0.45	0/2393	0.65	1/3254 (0.0%)
All	All	0.45	0/28789	0.65	1/39156 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	33	ASP	CB-CA-C	-6.19	109.42	116.54

There are no chirality outliers.

There are no planarity outliers.

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	2342	0	2290	18	0
1	B	2354	0	2307	22	0
1	C	2366	0	2306	28	0
1	D	2367	0	2318	32	0
1	E	2350	0	2303	21	0
1	F	2339	0	2287	24	0
1	G	2328	0	2276	27	0
1	H	2340	0	2282	40	0
1	I	2352	0	2283	34	0
1	J	2329	0	2242	39	0
1	K	2329	0	2272	26	0
1	L	2339	0	2287	19	0
2	B	7	0	10	0	0
2	E	7	0	10	0	0
3	A	23	0	0	1	0
3	B	28	0	0	2	0
3	C	13	0	0	0	0
3	D	6	0	0	0	0
3	E	20	0	0	2	0
3	F	17	0	0	2	0
3	G	12	0	0	1	0
3	H	5	0	0	1	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	15	0	0	1	0
3	L	17	0	0	1	0
All	All	28308	0	27473	312	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 13.

All (312) 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:H:109:GLY:HA2	1:H:200:ILE:HD13	1.57	0.86
1:J:188:ARG:HG3	1:J:190:THR:H	1.40	0.85
1:G:124:GLY:HA3	1:H:6:MET:HE3	1.63	0.80
1:J:140:PHE:HD2	1:J:144:SER:HB2	1.48	0.79
1:A:243:THR:H	1:A:246:HIS:HD2	1.30	0.77
1:I:56:ASP:HB3	1:I:60:ARG:HH22	1.49	0.77
1:G:1:SER:HB3	1:H:166:GLU:OE2	1.85	0.76
1:A:56:ASP:OD2	1:A:60:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:ILE:HG12	1:K:157:VAL:HG22	1.71	0.72
1:H:3:PHE:CZ	1:H:296:VAL:HG22	2.25	0.71
1:E:4:ARG:H	1:E:299:GLN:HE22	1.36	0.71
1:I:167:LEU:HD11	1:I:185:PHE:HE2	1.57	0.70
1:C:185:PHE:HA	1:C:192:GLN:HE22	1.55	0.70
1:J:60:ARG:HG3	1:J:61:LYS:HD3	1.73	0.69
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.56	0.69
1:I:219:PHE:HB2	1:I:271:LEU:HD11	1.75	0.68
1:D:34:ASP:OD2	1:D:90:LYS:HE3	1.95	0.66
1:J:240:GLU:HG3	1:J:241:PRO:HD2	1.77	0.65
1:H:63:ASN:ND2	1:H:78:ILE:O	2.30	0.65
1:B:224:THR:N	3:B:501:HOH:O	2.25	0.65
1:B:45:THR:HG23	1:B:47:GLU:OE1	1.97	0.64
1:A:243:THR:H	1:A:246:HIS:CD2	2.13	0.64
1:E:127:GLN:HG2	3:E:513:HOH:O	1.97	0.64
1:C:260:ALA:HB3	1:C:263:ASP:HB2	1.81	0.63
1:F:109:GLY:HA2	1:F:200:ILE:HD13	1.82	0.62
1:D:40:ARG:NE	1:D:187:ASP:OD2	2.26	0.62
1:G:14:GLU:HG2	1:G:122:PRO:HG2	1.81	0.61
1:J:164:HIS:C	1:J:165:MET:HG3	2.23	0.61
1:J:219:PHE:CE1	1:J:264:MET:HE1	2.35	0.61
1:J:5:LYS:HE3	1:J:291:PHE:CE1	2.26	0.61
1:H:276:MET:HE1	1:H:281:ILE:HG13	1.82	0.61
1:G:155:ASP:OD1	1:G:155:ASP:N	2.31	0.61
1:I:53:ASN:O	1:I:57:LEU:HD12	2.01	0.61
1:I:207:TRP:CZ3	1:I:287:LEU:HA	2.36	0.60
1:D:100:LYS:HE3	1:D:155:ASP:OD2	2.02	0.60
1:H:281:ILE:C	1:H:283:GLY:H	2.09	0.60
1:C:139:SER:OG	1:D:299:GLN:NE2	2.34	0.59
1:E:243:THR:H	1:E:246:HIS:CD2	2.20	0.59
1:I:126:TYR:HD2	1:J:6:MET:HG3	1.68	0.59
1:J:87:LEU:HD22	1:J:88:LYS:H	1.66	0.59
1:A:118:TYR:CE1	1:A:144:SER:HB3	2.37	0.59
1:J:165:MET:HE1	1:J:187:ASP:CA	2.24	0.59
1:C:8:PHE:HE2	1:C:151:ASN:HD22	1.51	0.58
1:K:222:ARG:NH2	3:K:402:HOH:O	2.37	0.58
1:I:223:PHE:HE1	1:I:270:GLU:OE2	1.86	0.57
1:L:4:ARG:O	1:L:299:GLN:NE2	2.32	0.57
1:D:217:ARG:HH22	1:E:47:GLU:HA	1.70	0.57
1:K:45:THR:HG23	1:K:48:ASP:H	1.70	0.57
1:C:55:GLU:CD	1:C:55:GLU:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:LEU:HB3	1:I:264:MET:HE2	1.87	0.57
1:D:247:VAL:HG22	1:D:261:VAL:HG11	1.87	0.56
1:J:247:VAL:HG13	1:J:261:VAL:HG11	1.87	0.56
1:G:1:SER:OG	1:G:2:GLY:N	2.37	0.56
1:J:68:VAL:HG23	1:J:75:LEU:HB2	1.88	0.56
1:L:144:SER:O	1:L:147:SER:OG	2.22	0.56
1:H:7:ALA:HA	1:H:127:GLN:NE2	2.21	0.55
1:J:243:THR:HG23	1:J:246:HIS:H	1.71	0.55
1:E:56:ASP:O	1:E:59:ILE:HG22	2.06	0.55
1:I:44:CYS:HB2	1:I:49:MET:HE1	1.88	0.55
1:B:292:THR:HG22	1:B:294:PHE:N	2.21	0.55
1:G:148:VAL:HG22	3:G:402:HOH:O	2.06	0.54
1:D:17:MET:HG3	1:D:117:CYS:SG	2.48	0.54
1:G:141:LEU:CD2	1:H:301:PRO:HD2	2.37	0.54
1:F:269:LYS:O	1:F:273:GLN:HG2	2.08	0.54
1:B:41:HIS:CG	1:C:305:LEU:HD13	2.43	0.54
1:E:108:PRO:HG3	1:E:134:PHE:CE1	2.43	0.54
1:D:51:ASN:HA	1:D:188:ARG:HH11	1.73	0.54
1:F:118:TYR:CE1	1:F:144:SER:HB3	2.43	0.54
1:I:208:LEU:O	1:I:212:VAL:HG23	2.08	0.54
1:H:245:ASP:O	1:H:249:ILE:HD12	2.07	0.53
1:I:108:PRO:HA	1:I:130:MET:HG2	1.90	0.53
1:J:66:PHE:CE1	1:J:77:VAL:HG11	2.44	0.53
1:J:210:ALA:HB2	1:J:296:VAL:HG13	1.90	0.53
1:K:166:GLU:OE2	1:L:1:SER:HB3	2.08	0.53
1:J:66:PHE:HE1	1:J:77:VAL:HG11	1.72	0.53
1:K:169:THR:HG23	1:K:171:VAL:HG22	1.90	0.53
1:B:271:LEU:HD13	1:B:287:LEU:HD21	1.91	0.53
1:I:40:ARG:HD3	1:I:85:CYS:HA	1.90	0.53
1:L:1:SER:OG	1:L:2:GLY:N	2.41	0.53
1:H:3:PHE:HA	1:H:299:GLN:OE1	2.08	0.53
1:G:35:VAL:HG11	1:G:88:LYS:HE3	1.89	0.52
1:G:243:THR:O	1:G:247:VAL:HG23	2.09	0.52
1:F:21:THR:HG23	1:F:26:THR:OG1	2.10	0.52
1:F:12:LYS:NZ	3:F:401:HOH:O	2.43	0.52
1:H:41:HIS:HA	1:H:54:TYR:HE2	1.75	0.52
1:J:5:LYS:HG2	1:J:127:GLN:HB3	1.91	0.52
1:J:16:CYS:SG	1:J:99:PRO:HD3	2.50	0.52
1:J:140:PHE:CD2	1:J:144:SER:HB2	2.38	0.52
1:A:107:GLN:HG3	1:A:108:PRO:HD2	1.92	0.51
1:B:50:LEU:HD23	3:B:511:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:ARG:HD3	1:K:85:CYS:HA	1.93	0.51
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.74	0.51
1:I:56:ASP:HB3	1:I:60:ARG:NH2	2.22	0.51
1:H:249:ILE:HG22	1:H:293:PRO:HB2	1.92	0.51
1:K:166:GLU:CD	1:L:1:SER:HB3	2.36	0.51
1:G:19:GLN:HG3	1:G:119:ASN:HA	1.92	0.51
1:A:247:VAL:HG22	1:A:261:VAL:HG11	1.93	0.50
1:D:201:THR:HG23	1:D:239:TYR:HD2	1.75	0.50
1:F:106:ILE:HD12	1:F:130:MET:HB2	1.93	0.50
1:B:190:THR:O	1:B:192:GLN:HG3	2.11	0.50
1:B:245:ASP:O	1:B:249:ILE:HG12	2.11	0.50
1:F:50:LEU:HD23	1:F:51:ASN:H	1.77	0.50
1:G:211:ALA:HB1	1:G:216:ASP:HB3	1.93	0.50
1:J:130:MET:HE1	1:J:182:TYR:CB	2.40	0.50
1:L:10:SER:OG	1:L:14:GLU:OE2	2.20	0.50
1:K:200:ILE:HG13	1:K:289:ASP:OD2	2.11	0.50
1:H:279:ARG:NH2	1:H:280:THR:HG22	2.27	0.50
1:H:243:THR:HG23	1:H:246:HIS:CE1	2.47	0.50
1:I:163:HIS:HE1	1:I:172:HIS:HB3	1.76	0.50
1:G:78:ILE:HG12	1:G:90:LYS:HB3	1.94	0.50
1:K:58:LEU:HD11	1:K:80:HIS:CD2	2.47	0.50
1:L:2:GLY:N	1:L:214:ASN:HD21	2.10	0.50
1:L:254:SER:OG	1:L:259:ILE:O	2.26	0.50
1:B:40:ARG:HD2	1:B:82:MET:CE	2.40	0.49
1:B:292:THR:HG22	1:B:294:PHE:H	1.76	0.49
1:B:4:ARG:H	1:B:299:GLN:NE2	1.99	0.49
1:H:83:GLN:OE1	1:H:88:LYS:NZ	2.35	0.49
1:C:36:VAL:HB	1:C:89:LEU:HB2	1.95	0.49
1:K:217:ARG:HB3	1:K:220:LEU:HD12	1.95	0.49
1:E:240:GLU:HG3	1:E:241:PRO:HD2	1.94	0.48
1:J:53:ASN:HB3	1:J:56:ASP:OD1	2.13	0.48
1:G:17:MET:HE2	1:G:117:CYS:SG	2.54	0.48
1:E:113:SER:O	1:E:149:GLY:HA2	2.13	0.48
1:G:16:CYS:HB2	1:G:30:LEU:HD12	1.95	0.48
1:E:236:LYS:HG2	1:E:237:TYR:CD2	2.48	0.48
1:D:86:VAL:HG13	1:D:179:GLY:HA2	1.95	0.48
1:H:130:MET:HB2	1:H:130:MET:HE2	1.62	0.48
1:H:34:ASP:OD1	1:H:34:ASP:N	2.46	0.48
1:D:45:THR:HG22	1:D:48:ASP:OD1	2.13	0.48
1:B:112:PHE:HZ	1:B:136:ILE:HG21	1.78	0.48
1:I:186:VAL:O	1:I:192:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:THR:HG22	1:K:225:THR:N	2.29	0.48
1:L:57:LEU:O	1:L:61:LYS:HG2	2.14	0.48
1:G:144:SER:O	1:G:147:SER:OG	2.31	0.48
1:J:211:ALA:HA	1:J:282:LEU:HD21	1.95	0.48
1:C:213:ILE:HD13	1:C:256:GLN:OE1	2.14	0.47
1:F:68:VAL:HG12	1:F:75:LEU:HD12	1.95	0.47
1:B:58:LEU:HD11	1:B:80:HIS:HD2	1.80	0.47
1:E:84:ASN:OD1	3:E:501:HOH:O	2.20	0.47
1:E:126:TYR:CE2	1:F:6:MET:HE2	2.49	0.47
1:K:114:VAL:O	1:K:125:VAL:HA	2.14	0.47
1:H:97:LYS:O	1:H:99:PRO:HD3	2.15	0.47
1:J:22:CYS:HB2	1:J:66:PHE:HB3	1.97	0.47
1:J:227:LEU:HD21	1:J:242:LEU:HD23	1.96	0.47
1:K:62:SER:H	1:K:65:ASN:ND2	2.10	0.47
1:C:108:PRO:HA	1:C:130:MET:HG2	1.97	0.47
1:I:17:MET:CE	1:I:148:VAL:HG22	2.45	0.47
1:C:207:TRP:CD2	1:C:288:GLU:HB2	2.50	0.47
1:H:209:TYR:CD1	1:H:257:THR:HG21	2.50	0.47
1:I:292:THR:HG22	1:I:294:PHE:N	2.30	0.46
1:L:281:ILE:O	1:L:282:LEU:C	2.58	0.46
1:D:55:GLU:OE1	1:D:55:GLU:N	2.42	0.46
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.15	0.46
1:J:61:LYS:HD3	1:J:61:LYS:N	2.30	0.46
1:F:83:GLN:HB3	1:F:86:VAL:HG23	1.97	0.46
1:F:27:LEU:HD11	1:F:42:VAL:HB	1.98	0.46
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.98	0.46
1:K:224:THR:HG22	1:K:225:THR:O	2.16	0.46
1:A:56:ASP:O	1:A:59:ILE:HG12	2.16	0.46
1:E:279[B]:ARG:HE	1:E:279[B]:ARG:HB2	1.55	0.46
1:F:24:THR:HG22	1:F:45:THR:HG23	1.98	0.46
1:J:31:TRP:CE2	1:J:95:ASN:HB2	2.51	0.46
1:F:152:ILE:HD12	1:F:157:VAL:HG22	1.98	0.45
1:K:225:THR:OG1	1:K:226:THR:N	2.48	0.45
1:D:164:HIS:CD2	1:D:175:THR:HG23	2.52	0.45
1:E:247:VAL:HG13	1:E:261:VAL:HG11	1.98	0.45
1:I:14:GLU:OE2	1:J:11:GLY:N	2.50	0.45
1:A:62:SER:H	1:A:65:ASN:ND2	2.13	0.45
1:F:133:ASN:O	1:F:134:PHE:HB2	2.16	0.45
1:G:128:CYS:SG	1:H:4:ARG:NH1	2.90	0.45
1:H:13:VAL:HG21	1:H:150:PHE:CD2	2.51	0.45
1:H:85:CYS:HB2	1:H:179:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:CYS:HB3	1:G:42:VAL:HG22	1.98	0.45
1:I:216:ASP:OD1	1:I:216:ASP:N	2.48	0.45
1:K:13:VAL:HG21	1:K:150:PHE:CD1	2.51	0.45
1:L:207:TRP:HZ3	1:L:287:LEU:HD23	1.81	0.45
1:F:118:TYR:HB3	3:F:403:HOH:O	2.16	0.45
1:K:52:PRO:O	1:K:188:ARG:NH1	2.49	0.45
1:L:210:ALA:HB2	1:L:296:VAL:HG13	1.98	0.45
1:H:136:ILE:O	1:H:136:ILE:HG13	2.14	0.45
1:K:4:ARG:HH11	1:K:4:ARG:HB3	1.82	0.45
1:D:114:VAL:O	1:D:125:VAL:HA	2.17	0.45
1:H:256:GLN:HA	1:H:302:HIS:NE2	2.32	0.45
1:H:106:ILE:C	1:H:106:ILE:HD12	2.42	0.45
1:I:294:PHE:N	1:I:294:PHE:CD1	2.85	0.45
1:K:36:VAL:HG21	1:K:68:VAL:HG11	1.99	0.45
1:A:22:CYS:HB3	1:A:42:VAL:O	2.17	0.45
1:B:7:ALA:HA	1:B:127:GLN:OE1	2.16	0.44
1:I:209:TYR:CD1	1:I:257:THR:HG21	2.53	0.44
1:J:66:PHE:CZ	1:J:80:HIS:HB3	2.51	0.44
1:L:113:SER:O	1:L:149:GLY:HA2	2.17	0.44
1:C:207:TRP:CE2	1:C:288:GLU:HB2	2.52	0.44
1:G:225:THR:O	1:G:262:LEU:HD13	2.17	0.44
1:C:225:THR:HG22	1:C:226:THR:O	2.17	0.44
1:L:27:LEU:HD21	1:L:42:VAL:HB	2.00	0.44
1:C:185:PHE:HA	1:C:192:GLN:NE2	2.27	0.44
1:F:78:ILE:HD11	1:F:92:ASP:HA	1.99	0.44
1:A:83:GLN:O	1:A:86:VAL:HG22	2.17	0.44
1:C:53:ASN:O	1:C:54:TYR:C	2.60	0.44
1:C:140:PHE:O	1:D:1:SER:N	2.49	0.44
1:D:287:LEU:HD12	1:D:287:LEU:H	1.82	0.44
1:G:249:ILE:O	1:G:252:PRO:HD2	2.18	0.44
1:J:111:THR:HG22	1:J:129:ALA:CB	2.47	0.44
1:H:75:LEU:HD23	1:H:75:LEU:HA	1.86	0.44
1:H:221[B]:ASN:ND2	1:H:223:PHE:H	2.16	0.44
1:F:41:HIS:HA	1:F:54:TYR:HE1	1.83	0.44
1:J:87:LEU:HD13	1:J:89:LEU:N	2.31	0.44
1:K:58:LEU:HD11	1:K:80:HIS:HD2	1.82	0.44
1:I:107:GLN:H	1:I:110:GLN:NE2	2.16	0.43
1:A:293:PRO:O	1:A:297:VAL:HG23	2.18	0.43
1:J:222:ARG:H	1:J:222:ARG:HD3	1.83	0.43
1:K:102:LYS:HB3	1:K:102:LYS:HE2	1.57	0.43
1:C:243:THR:HG22	1:C:245:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LEU:HA	1:D:282:LEU:HD23	1.68	0.43
1:F:19:GLN:HB2	1:F:120:GLY:HA3	2.00	0.43
1:G:126:TYR:HD2	1:H:6:MET:HG2	1.83	0.43
1:H:244:GLN:O	1:H:247:VAL:HB	2.18	0.43
1:J:169:THR:O	1:J:169:THR:OG1	2.31	0.43
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.82	0.43
1:G:140:PHE:HB2	1:G:172:HIS:CD2	2.54	0.43
1:I:87:LEU:HD23	1:I:89:LEU:CD1	2.47	0.43
1:I:167:LEU:HD11	1:I:185:PHE:CE2	2.46	0.43
1:I:207:TRP:HZ3	1:I:287:LEU:HA	1.82	0.43
1:C:105:ARG:NH1	1:C:180:ASN:HB3	2.33	0.43
1:C:249:ILE:H	1:C:249:ILE:HG13	1.64	0.43
1:K:19:GLN:OE1	1:K:119:ASN:HB3	2.18	0.43
1:B:32:LEU:HD13	1:B:101:TYR:CD2	2.53	0.43
1:B:249:ILE:O	1:B:252:PRO:HD2	2.19	0.43
1:A:114:VAL:O	1:A:125:VAL:HA	2.18	0.43
1:B:114:VAL:O	1:B:125:VAL:HA	2.19	0.43
1:G:83:GLN:HB2	1:G:88:LYS:HG3	1.99	0.43
1:H:13:VAL:HG22	1:H:157:VAL:HG11	2.01	0.43
1:J:187:ASP:OD1	1:J:187:ASP:N	2.49	0.43
1:H:131:ARG:HE	1:H:131:ARG:HB3	1.53	0.43
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.80	0.43
1:C:231:ASN:HA	1:C:234:ALA:HB3	2.00	0.43
1:D:228:ASN:OD1	1:D:228:ASN:N	2.50	0.43
1:G:141:LEU:HD12	1:H:1:SER:H1	1.80	0.43
1:K:52:PRO:HD2	1:K:188:ARG:HH11	1.83	0.43
1:F:95:ASN:HB3	1:F:98:THR:OG1	2.18	0.42
1:F:276:MET:O	1:F:277:ASN:C	2.62	0.42
1:D:268:LEU:HA	1:D:271:LEU:HD23	2.01	0.42
1:E:83:GLN:HB2	1:E:88:LYS:HZ3	1.83	0.42
1:I:45:THR:HG23	1:I:47:GLU:H	1.84	0.42
1:E:126:TYR:HD2	1:F:6:MET:HG2	1.84	0.42
1:C:282:LEU:HA	1:C:282:LEU:HD23	1.78	0.42
1:D:167:LEU:HB3	1:D:168:PRO:HD2	2.00	0.42
1:H:237:TYR:HD2	1:H:272:LEU:HG	1.85	0.42
1:L:62:SER:OG	3:L:401:HOH:O	2.21	0.42
1:C:222:ARG:CD	1:C:222:ARG:H	2.33	0.42
1:F:87:LEU:HD23	1:F:87:LEU:HA	1.81	0.42
1:H:37:TYR:O	1:H:162:MET:HE1	2.18	0.42
1:I:106:ILE:H	1:I:106:ILE:HG12	1.67	0.42
1:L:260:ALA:O	1:L:263:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG22	1:A:181:PHE:HA	2.02	0.42
1:E:4:ARG:N	1:E:299:GLN:HE22	2.11	0.42
1:K:188:ARG:NH1	1:K:188:ARG:HG2	2.35	0.42
1:C:243:THR:HG22	1:C:244:GLN:N	2.35	0.42
1:D:115:LEU:HD21	1:D:122:PRO:HB3	2.01	0.42
1:E:52:PRO:HD2	1:E:188:ARG:HE	1.85	0.42
1:E:105:ARG:NH2	1:E:181:PHE:O	2.52	0.42
1:G:125:VAL:HG12	1:H:7:ALA:O	2.20	0.42
1:D:107:GLN:H	1:D:110:GLN:NE2	2.16	0.42
1:D:111:THR:HG23	1:D:292:THR:HG23	2.02	0.42
1:F:140:PHE:HD1	1:F:144:SER:HB2	1.84	0.42
1:H:127:GLN:HG2	3:H:401:HOH:O	2.19	0.42
1:I:138:GLY:HA2	1:J:4:ARG:HD2	2.02	0.42
1:J:68:VAL:CG2	1:J:75:LEU:HB2	2.49	0.41
1:B:118:TYR:CZ	1:B:144:SER:HB3	2.55	0.41
1:D:27:LEU:HD21	1:D:42:VAL:HB	2.01	0.41
1:D:225:THR:HG23	1:D:266:ALA:HB2	2.01	0.41
1:I:75:LEU:HD13	1:I:91:VAL:HG11	2.02	0.41
1:F:105:ARG:HG3	1:F:182:TYR:CE1	2.56	0.41
1:I:62:SER:HA	1:I:80:HIS:HE1	1.86	0.41
1:I:209:TYR:O	1:I:213:ILE:HD12	2.20	0.41
1:A:4:ARG:HA	3:A:403:HOH:O	2.21	0.41
1:B:276:MET:HE3	1:B:276:MET:HB3	1.87	0.41
1:I:226:THR:HG23	1:I:228:ASN:H	1.85	0.41
1:K:74:GLN:HG2	1:K:75:LEU:H	1.85	0.41
1:C:40:ARG:C	1:C:42:VAL:N	2.79	0.41
1:C:265:CYS:O	1:C:269:LYS:N	2.49	0.41
1:G:130:MET:HE2	1:G:130:MET:HB2	1.79	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.76	0.41
1:B:163:HIS:CE1	1:B:172:HIS:HB3	2.55	0.41
1:D:187:ASP:N	1:D:187:ASP:OD1	2.51	0.41
1:G:50:LEU:H	1:G:50:LEU:HG	1.62	0.41
1:H:207:TRP:CZ3	1:H:287:LEU:HA	2.56	0.41
1:J:68:VAL:HG11	1:J:89:LEU:HD11	2.02	0.41
1:L:146:GLY:O	1:L:162:MET:HE2	2.21	0.41
1:C:77:VAL:O	1:C:78:ILE:HD13	2.21	0.41
1:H:293:PRO:O	1:H:297:VAL:HG23	2.21	0.41
1:J:111:THR:HG23	1:J:292:THR:HG23	2.03	0.41
1:L:21:THR:HB	1:L:67:LEU:HB2	2.01	0.41
1:L:222:ARG:NH1	1:L:222:ARG:HG2	2.35	0.41
1:D:209:TYR:O	1:D:212:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLN:HB2	1:E:119:ASN:C	2.46	0.41
1:E:253:LEU:HD23	1:E:253:LEU:HA	1.91	0.41
1:G:31:TRP:CD2	1:G:95:ASN:HB2	2.57	0.41
1:E:100:LYS:HD3	1:E:156:CYS:HB2	2.03	0.40
1:H:107:GLN:HB3	1:H:108:PRO:HD2	2.03	0.40
1:I:185:PHE:HD1	1:I:185:PHE:N	2.20	0.40
1:A:131:ARG:HE	1:A:131:ARG:HB3	1.55	0.40
1:D:213:ILE:HD13	1:D:256:GLN:NE2	2.36	0.40
1:J:1:SER:OG	1:J:2:GLY:N	2.55	0.40
1:D:227:LEU:CD1	1:D:262:LEU:HD21	2.50	0.40
1:K:79:GLY:O	1:K:90:LYS:N	2.54	0.40
1:C:109:GLY:HA2	1:C:200:ILE:HD13	2.04	0.40
1:D:161:TYR:CE1	1:D:174:GLY:HA3	2.56	0.40
1:J:78:ILE:HB	1:J:90:LYS:HG2	2.04	0.40
1:A:51:ASN:HD22	1:A:188:ARG:HD2	1.87	0.40
1:C:54:TYR:O	1:C:55:GLU:C	2.64	0.40
1:I:12:LYS:HA	1:I:12:LYS:HD3	1.91	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	301/306 (98%)	289 (96%)	12 (4%)	0	100	100
1	B	302/306 (99%)	289 (96%)	13 (4%)	0	100	100
1	C	304/306 (99%)	285 (94%)	19 (6%)	0	100	100
1	D	304/306 (99%)	291 (96%)	12 (4%)	1 (0%)	36	55
1	E	302/306 (99%)	283 (94%)	19 (6%)	0	100	100
1	F	300/306 (98%)	277 (92%)	23 (8%)	0	100	100
1	G	300/306 (98%)	288 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	301/306 (98%)	282 (94%)	18 (6%)	1 (0%)	36	55
1	I	304/306 (99%)	286 (94%)	18 (6%)	0	100	100
1	J	304/306 (99%)	283 (93%)	21 (7%)	0	100	100
1	K	301/306 (98%)	290 (96%)	11 (4%)	0	100	100
1	L	300/306 (98%)	283 (94%)	17 (6%)	0	100	100
All	All	3623/3672 (99%)	3426 (95%)	195 (5%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	282	LEU
1	D	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	25/263 (10%)	25 (100%)	0	100	100
1	B	197/263 (75%)	189 (96%)	8 (4%)	27	53
1	C	261/263 (99%)	249 (95%)	12 (5%)	24	48
1	D	262/263 (100%)	245 (94%)	17 (6%)	15	32
1	E	260/263 (99%)	244 (94%)	16 (6%)	16	34
1	F	259/263 (98%)	248 (96%)	11 (4%)	26	52
1	G	257/263 (98%)	242 (94%)	15 (6%)	18	38
1	H	259/263 (98%)	242 (93%)	17 (7%)	15	32
1	I	258/263 (98%)	239 (93%)	19 (7%)	13	27
1	J	252/263 (96%)	224 (89%)	28 (11%)	6	12
1	K	256/263 (97%)	240 (94%)	16 (6%)	16	34
1	L	259/263 (98%)	245 (95%)	14 (5%)	20	41
All	All	2805/3156 (89%)	2632 (94%)	173 (6%)	16	34

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	ARG
1	B	44	CYS
1	B	46	SER
1	B	110	GLN
1	B	128	CYS
1	B	154	TYR
1	B	222	ARG
1	B	274	ASN
1	C	56	ASP
1	C	86	VAL
1	C	128	CYS
1	C	187	ASP
1	C	188	ARG
1	C	189	GLN
1	C	216	ASP
1	C	224	THR
1	C	228	ASN
1	C	229	ASP
1	C	257	THR
1	C	295	ASP
1	D	1	SER
1	D	44	CYS
1	D	62	SER
1	D	72	ASN
1	D	104	VAL
1	D	106	ILE
1	D	123	SER
1	D	128	CYS
1	D	192	GLN
1	D	201	THR
1	D	208	LEU
1	D	216	ASP
1	D	220	LEU
1	D	222	ARG
1	D	225	THR
1	D	254	SER
1	D	280	THR
1	E	1	SER
1	E	26	THR
1	E	48	ASP
1	E	49	MET
1	E	57	LEU

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Mol	Chain	Res	Type
1	E	59	ILE
1	E	62	SER
1	E	74	GLN
1	E	86	VAL
1	E	91	VAL
1	E	121	SER
1	E	128	CYS
1	E	181	PHE
1	E	216	ASP
1	E	222	ARG
1	E	303	THR
1	F	27	LEU
1	F	36	VAL
1	F	74	GLN
1	F	123	SER
1	F	125	VAL
1	F	128	CYS
1	F	190	THR
1	F	212	VAL
1	F	221	ASN
1	F	300	CYS
1	F	302	HIS
1	G	1	SER
1	G	6	MET
1	G	24	THR
1	G	25	THR
1	G	32	LEU
1	G	50	LEU
1	G	60	ARG
1	G	64	HIS
1	G	81	SER
1	G	153	ASP
1	G	169	THR
1	G	196	THR
1	G	226	THR
1	G	267	SER
1	G	292	THR
1	H	4	ARG
1	H	24	THR
1	H	26	THR
1	H	32	LEU
1	H	44	CYS

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Mol	Chain	Res	Type
1	H	50	LEU
1	H	78	ILE
1	H	87	LEU
1	H	121	SER
1	H	153	ASP
1	H	190	THR
1	H	213	ILE
1	H	216	ASP
1	H	217	ARG
1	H	223	PHE
1	H	225	THR
1	H	226	THR
1	I	13	VAL
1	I	50	LEU
1	I	81	SER
1	I	100	LYS
1	I	121	SER
1	I	125	VAL
1	I	155	ASP
1	I	171	VAL
1	I	180	ASN
1	I	190	THR
1	I	216	ASP
1	I	233	VAL
1	I	240	GLU
1	I	250	LEU
1	I	270	GLU
1	I	274	ASN
1	I	282	LEU
1	I	295	ASP
1	I	305	LEU
1	J	25	THR
1	J	27	LEU
1	J	44	CYS
1	J	45	THR
1	J	50	LEU
1	J	81	SER
1	J	114	VAL
1	J	169	THR
1	J	175	THR
1	J	177	LEU
1	J	185	PHE

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Mol	Chain	Res	Type
1	J	186	VAL
1	J	187	ASP
1	J	196	THR
1	J	199	THR
1	J	201	THR
1	J	212	VAL
1	J	220	LEU
1	J	224	THR
1	J	226	THR
1	J	243	THR
1	J	261	VAL
1	J	263	ASP
1	J	272	LEU
1	J	282	LEU
1	J	284	SER
1	J	286	LEU
1	J	289	ASP
1	K	10	SER
1	K	26	THR
1	K	48	ASP
1	K	62	SER
1	K	73	VAL
1	K	81	SER
1	K	86	VAL
1	K	87	LEU
1	K	102	LYS
1	K	104	VAL
1	K	128	CYS
1	K	155	ASP
1	K	156	CYS
1	K	186	VAL
1	K	225	THR
1	K	297	VAL
1	L	46	SER
1	L	75	LEU
1	L	78	ILE
1	L	87	LEU
1	L	93	THR
1	L	121	SER
1	L	125	VAL
1	L	147	SER
1	L	198	THR

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Mol	Chain	Res	Type
1	L	216	ASP
1	L	224	THR
1	L	281	ILE
1	L	282	LEU
1	L	292	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	110	GLN
1	B	164	HIS
1	B	299	GLN
1	C	19	GLN
1	C	80	HIS
1	C	107	GLN
1	C	142	ASN
1	C	151	ASN
1	C	163	HIS
1	C	164	HIS
1	C	192	GLN
1	C	214	ASN
1	C	228	ASN
1	D	74	GLN
1	D	84	ASN
1	D	95	ASN
1	D	110	GLN
1	D	127	GLN
1	D	142	ASN
1	D	172	HIS
1	D	180	ASN
1	D	277	ASN
1	D	299	GLN
1	D	302	HIS
1	E	142	ASN
1	E	189	GLN
1	E	246	HIS
1	E	299	GLN
1	F	19	GLN
1	F	63	ASN
1	F	64	HIS
1	F	69	GLN
1	F	119	ASN

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Mol	Chain	Res	Type
1	F	164	HIS
1	G	19	GLN
1	G	41	HIS
1	G	72	ASN
1	G	80	HIS
1	G	127	GLN
1	G	180	ASN
1	G	244	GLN
1	G	277	ASN
1	H	127	GLN
1	H	142	ASN
1	H	214	ASN
1	H	273	GLN
1	H	274	ASN
1	I	53	ASN
1	I	80	HIS
1	I	110	GLN
1	I	163	HIS
1	I	172	HIS
1	I	221	ASN
1	I	246	HIS
1	I	274	ASN
1	I	299	GLN
1	J	41	HIS
1	J	63	ASN
1	J	110	GLN
1	J	238	ASN
1	J	244	GLN
1	J	273	GLN
1	J	274	ASN
1	K	65	ASN
1	K	69	GLN
1	K	110	GLN
1	K	142	ASN
1	K	164	HIS
1	K	299	GLN
1	L	41	HIS
1	L	53	ASN
1	L	80	HIS
1	L	110	GLN
1	L	119	ASN
1	L	189	GLN

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Mol	Chain	Res	Type
1	L	214	ASN
1	L	273	GLN
1	L	274	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 ⓘ

2 ligands 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	PEG	B	401	-	6,6,6	0.25	0	5,5,5	0.24	0
2	PEG	E	401	-	6,6,6	0.35	0	5,5,5	0.20	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	PEG	B	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	E	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	PEG	O2-C3-C4-O4
2	B	401	PEG	O1-C1-C2-O2
2	E	401	PEG	C1-C2-O2-C3
2	B	401	PEG	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/306 (99%)	-0.16	3 (0%) 79 76	23, 38, 77, 131	0
1	B	303/306 (99%)	-0.25	0 100 100	21, 37, 64, 114	1 (0%)
1	C	306/306 (100%)	0.18	8 (2%) 57 52	28, 54, 98, 144	0
1	D	306/306 (100%)	0.03	2 (0%) 84 81	30, 52, 102, 129	0
1	E	303/306 (99%)	-0.21	1 (0%) 90 87	24, 42, 76, 145	1 (0%)
1	F	302/306 (98%)	0.03	4 (1%) 75 71	28, 48, 91, 149	0
1	G	302/306 (98%)	0.17	6 (1%) 65 61	38, 60, 94, 123	0
1	H	302/306 (98%)	0.27	8 (2%) 57 52	42, 65, 102, 122	1 (0%)
1	I	306/306 (100%)	0.75	24 (7%) 19 17	44, 84, 127, 156	0
1	J	306/306 (100%)	0.91	36 (11%) 9 7	35, 86, 130, 181	0
1	K	303/306 (99%)	-0.14	1 (0%) 90 87	28, 44, 76, 110	0
1	L	302/306 (98%)	0.05	4 (1%) 75 71	31, 50, 88, 155	0
All	All	3644/3672 (99%)	0.14	97 (2%) 56 51	21, 53, 109, 181	3 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	208	LEU	4.8
1	I	154	TYR	4.5
1	J	20	VAL	4.5
1	J	126	TYR	4.0
1	I	268	LEU	3.9
1	J	148	VAL	3.7
1	I	294	PHE	3.7
1	C	223	PHE	3.6
1	J	140	PHE	3.6
1	J	118	TYR	3.5
1	J	89	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	143	GLY	3.5
1	J	230	PHE	3.5
1	F	54	TYR	3.4
1	C	191	ALA	3.3
1	I	193	ALA	3.3
1	J	27	LEU	3.2
1	J	191	ALA	3.1
1	I	205	LEU	3.1
1	H	37	TYR	3.1
1	L	47	GLU	3.1
1	I	242	LEU	3.1
1	J	194	ALA	3.0
1	I	58	LEU	2.9
1	I	177	LEU	2.8
1	L	219	PHE	2.8
1	J	49	MET	2.7
1	L	3	PHE	2.7
1	J	136	ILE	2.7
1	L	54	TYR	2.7
1	H	87	LEU	2.7
1	J	268	LEU	2.7
1	I	191	ALA	2.7
1	F	46	SER	2.6
1	A	44	CYS	2.6
1	H	66	PHE	2.6
1	J	162	MET	2.6
1	C	76	ARG	2.6
1	E	58	LEU	2.5
1	J	249	ILE	2.5
1	C	227	LEU	2.5
1	I	3	PHE	2.5
1	J	284	SER	2.5
1	C	43	ILE	2.4
1	F	118	TYR	2.4
1	J	186	VAL	2.4
1	G	282	LEU	2.4
1	H	177	LEU	2.4
1	I	125	VAL	2.4
1	J	159	PHE	2.4
1	I	230	PHE	2.3
1	H	58	LEU	2.3
1	J	43	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	271	LEU	2.3
1	H	128	CYS	2.3
1	I	223	PHE	2.3
1	K	303	THR	2.3
1	J	177	LEU	2.3
1	J	54	TYR	2.3
1	J	142	ASN	2.3
1	J	283	GLY	2.3
1	I	73	VAL	2.3
1	A	87	LEU	2.2
1	I	273	GLN	2.2
1	J	64	HIS	2.2
1	J	195	GLY	2.2
1	J	286	LEU	2.2
1	G	230	PHE	2.2
1	J	219	PHE	2.2
1	G	87	LEU	2.1
1	J	167	LEU	2.1
1	I	128	CYS	2.1
1	J	229	ASP	2.1
1	J	180	ASN	2.1
1	D	89	LEU	2.1
1	G	50	LEU	2.1
1	H	271	LEU	2.1
1	H	281	ILE	2.1
1	C	118	TYR	2.1
1	D	223	PHE	2.1
1	I	129	ALA	2.1
1	I	260	ALA	2.1
1	C	154	TYR	2.1
1	A	46	SER	2.1
1	G	150	PHE	2.1
1	I	140	PHE	2.1
1	J	68	VAL	2.1
1	J	50	LEU	2.1
1	J	265	CYS	2.1
1	C	273	GLN	2.0
1	I	150	PHE	2.0
1	I	206	ALA	2.0
1	G	47	GLU	2.0
1	J	190	THR	2.0
1	I	152	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	200	ILE	2.0
1	F	49	MET	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($\text{\AA}^2$)	Q<0.9
2	PEG	E	401	7/7	0.71	0.16	46,50,54,57	0
2	PEG	B	401	7/7	0.81	0.13	44,47,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.