



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:16 AM UTC

PDB ID : 8DRU / pdb_00008dru
Title : Product structure of SARS-CoV-2 Mpro C145A mutant in complex with nsp7-nsp8 (C7) 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 : 2.31 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

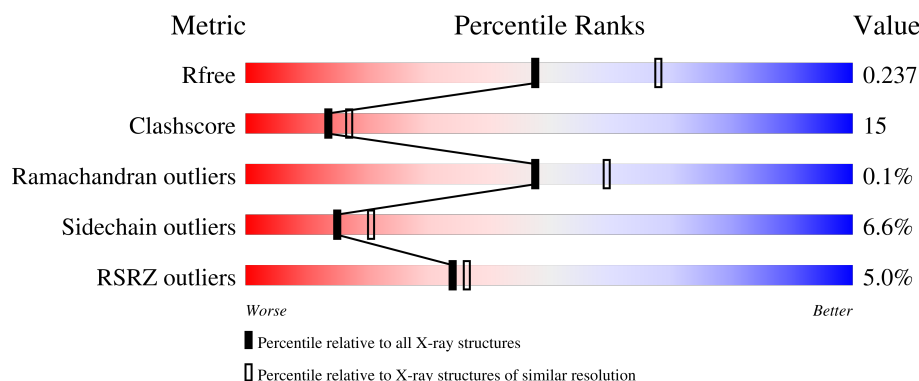
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	9% 69% 28% .
1	B	306	82% 17% .
1	C	306	5% 70% 28% .
1	D	306	8% 70% 26% .
1	E	306	2% 73% 25% .

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Mol	Chain	Length	Quality of chain
1	F	306	4% 62% 33% 5%
1	G	306	7% 67% 28% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16871 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.

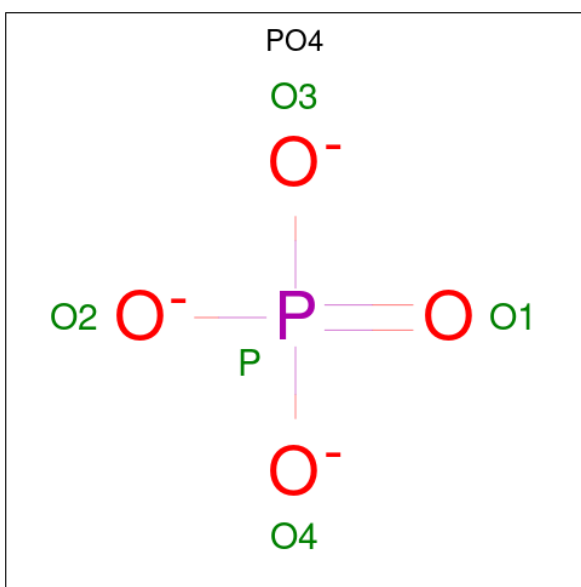
- Molecule 1 is a protein called Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2334	1471	398	444	21			
1	B	306	Total	C	N	O	S	0	0	0
			2367	1497	406	443	21			
1	C	306	Total	C	N	O	S	0	2	0
			2377	1501	410	445	21			
1	D	306	Total	C	N	O	S	0	0	0
			2356	1489	404	443	20			
1	E	306	Total	C	N	O	S	0	0	0
			2358	1490	403	444	21			
1	F	306	Total	C	N	O	S	0	1	0
			2342	1478	401	442	21			
1	G	306	Total	C	N	O	S	0	2	0
			2364	1494	403	446	21			

There are 7 discrepancies between the modelled and reference sequences:

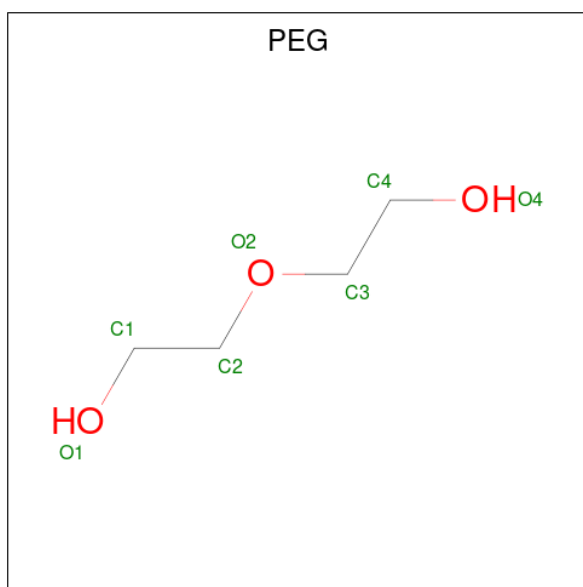
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1
E	145	ALA	CYS	engineered mutation	UNP P0DTD1
F	145	ALA	CYS	engineered mutation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

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



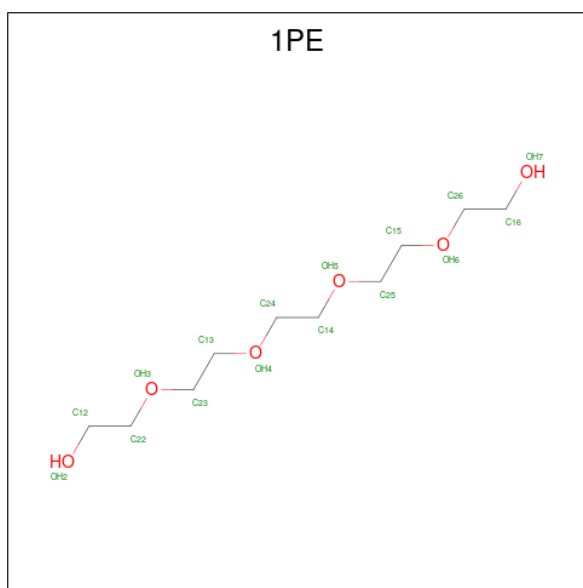
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			14	8	6		
4	G	1	Total	C	O	0	0
			16	10	6		

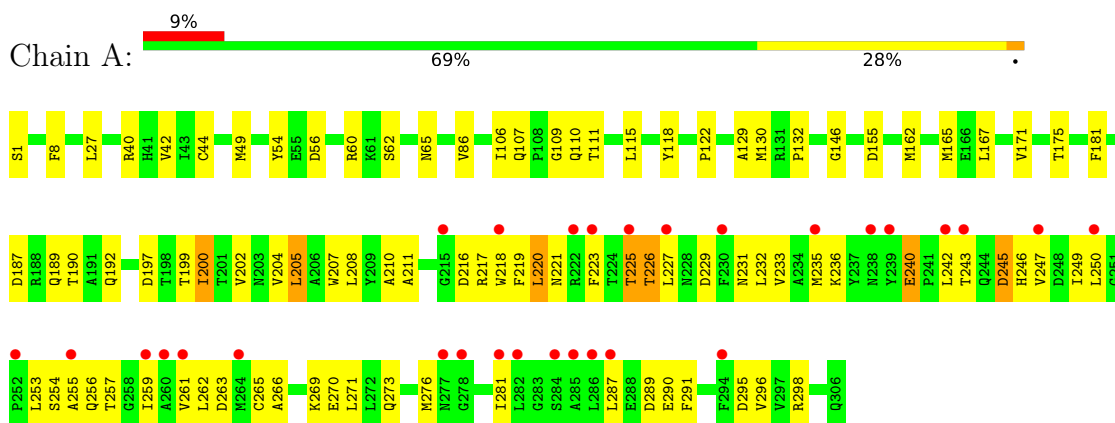
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	48	Total	O	0	0
			48	48		
5	C	49	Total	O	0	0
			49	49		
5	D	18	Total	O	0	0
			18	18		
5	E	18	Total	O	0	0
			18	18		
5	F	12	Total	O	0	0
			12	12		
5	G	19	Total	O	0	0
			19	19		

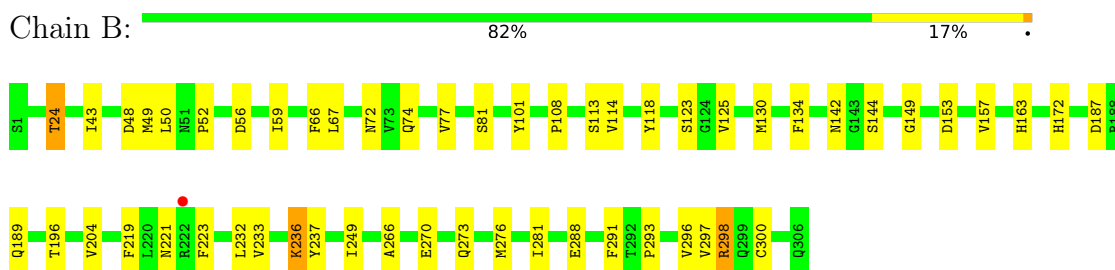
3 Residue-property plots [i](#)

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.

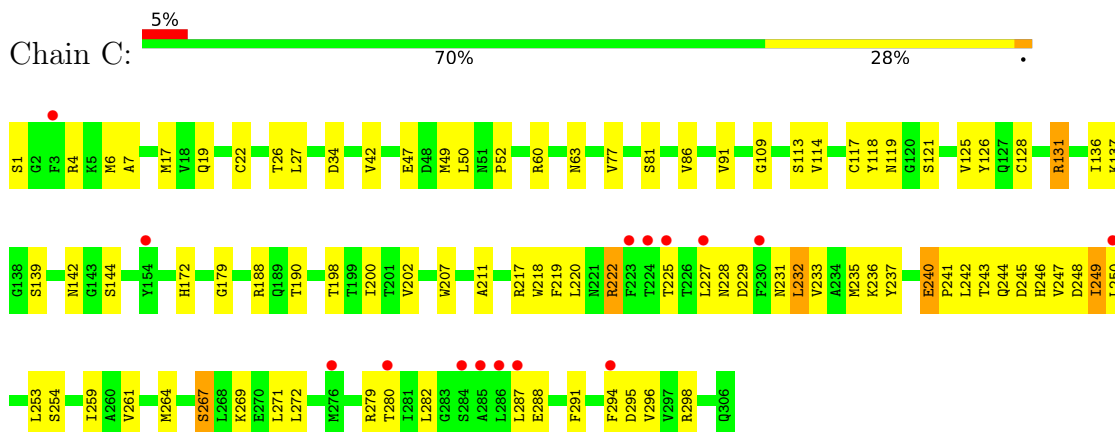
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



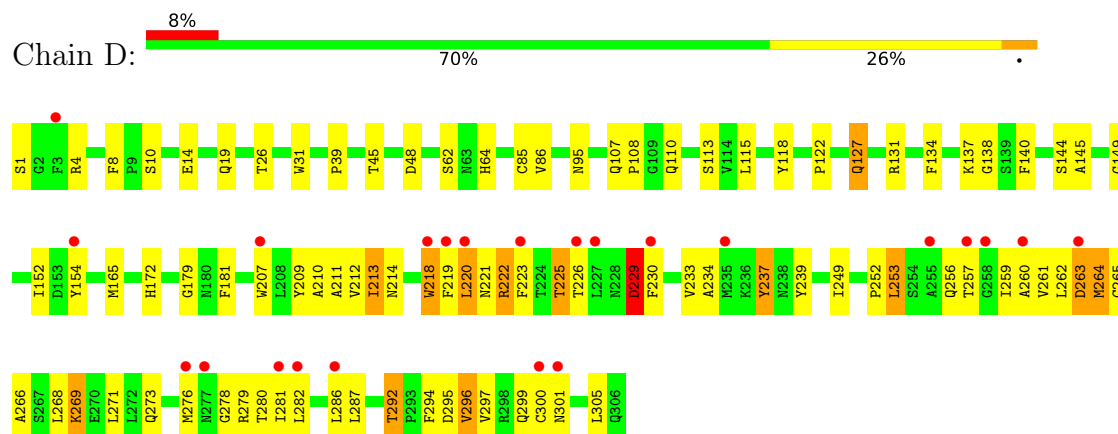
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



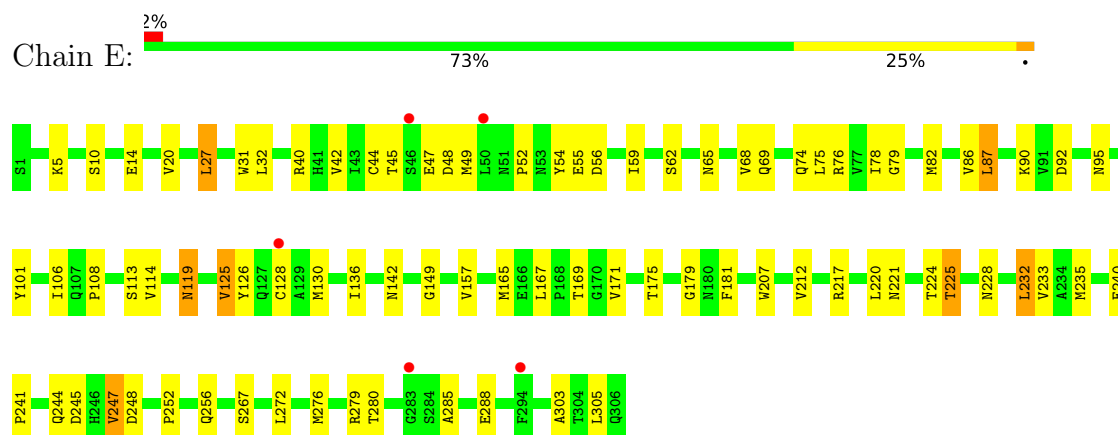
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



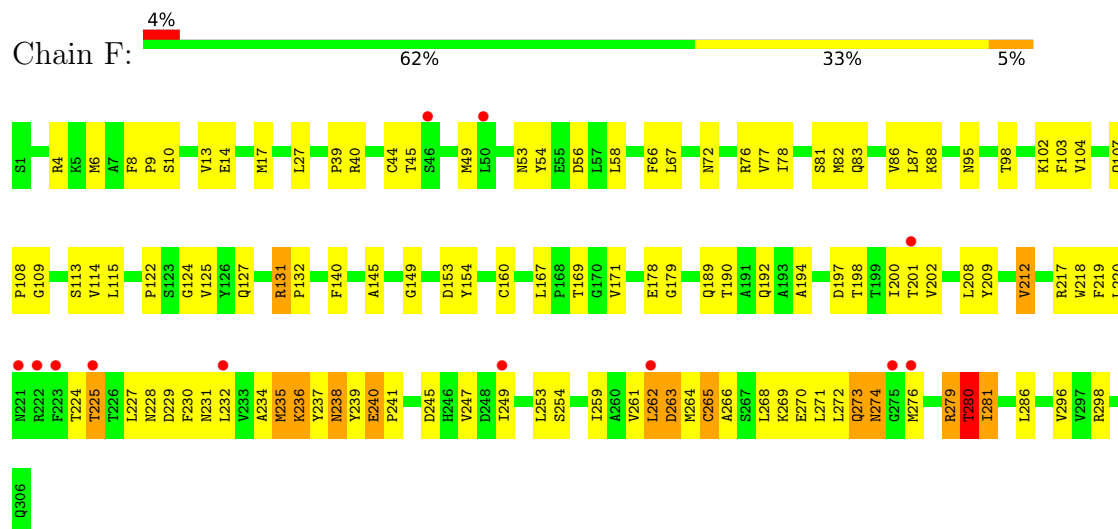
- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site

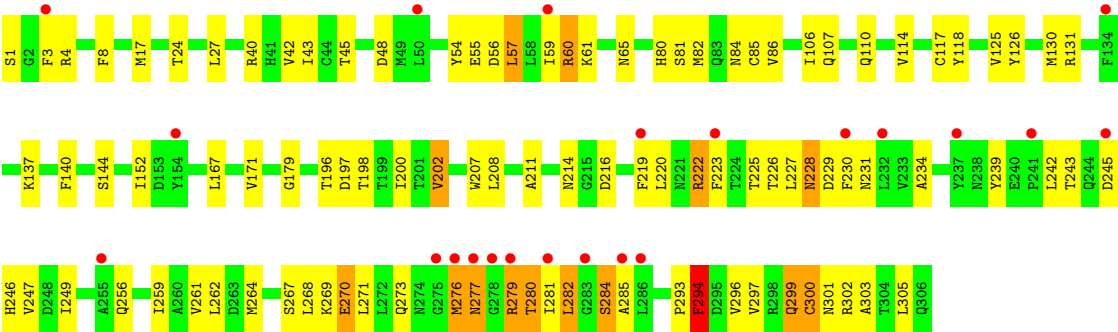


- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



- Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.11Å 174.89Å 96.33Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	46.22 – 2.31 46.22 – 2.31	Depositor EDS
% Data completeness (in resolution range)	70.3 (46.22-2.31) 70.3 (46.22-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.237 0.190 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16871	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: 1PE, PO4, 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	0.58	0/2383	0.89	2/3243 (0.1%)
1	B	0.46	2/2419 (0.1%)	0.61	0/3287
1	C	0.59	0/2434	0.85	1/3306 (0.0%)
1	D	0.55	1/2408 (0.0%)	0.87	2/3274 (0.1%)
1	E	0.44	0/2409	0.65	0/3274
1	F	0.61	2/2395 (0.1%)	0.96	7/3259 (0.2%)
1	G	0.62	3/2422 (0.1%)	0.90	4/3294 (0.1%)
All	All	0.55	8/16870 (0.0%)	0.83	16/22937 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	293	PRO	C-N	8.03	1.46	1.33
1	B	297	VAL	C-N	7.85	1.44	1.34
1	D	299	GLN	C-N	-6.12	1.25	1.33
1	F	280	THR	C-N	5.66	1.40	1.33
1	B	298	ARG	C-N	-5.62	1.25	1.33
1	F	279	ARG	C-N	5.60	1.41	1.33
1	G	294	PHE	C-N	-5.45	1.25	1.33
1	G	55	GLU	C-O	5.40	1.30	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	60	ARG	N-CA-C	-7.24	104.44	113.28
1	A	254	SER	N-CA-C	-6.60	104.09	111.28
1	D	226	THR	N-CA-C	-6.04	101.55	110.48
1	D	229	ASP	CA-CB-CG	5.87	118.47	112.60
1	G	276	MET	N-CA-C	-5.80	106.06	113.02
1	A	245	ASP	N-CA-C	-5.44	105.35	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	MET	N-CA-C	-5.41	105.79	112.38
1	C	222	ARG	N-CA-CB	-5.35	102.44	110.73
1	F	154	TYR	CB-CA-C	-5.24	110.10	117.23
1	F	236	LYS	N-CA-C	-5.18	106.81	113.23
1	F	40	ARG	CA-C-N	-5.14	112.02	122.31
1	F	40	ARG	C-N-CA	-5.14	112.02	122.31
1	F	265	CYS	N-CA-C	-5.05	105.22	111.33
1	G	57	LEU	N-CA-C	-5.05	105.78	111.28
1	F	279	ARG	O-C-N	5.04	128.85	122.65
1	G	293	PRO	O-C-N	5.01	128.95	122.24

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	2334	0	2265	85	0
1	B	2367	0	2319	32	0
1	C	2377	0	2335	74	0
1	D	2356	0	2287	75	0
1	E	2358	0	2305	59	0
1	F	2342	0	2274	92	0
1	G	2364	0	2298	83	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
3	A	28	0	40	6	0
3	B	14	0	20	0	0
3	C	21	0	30	1	0
3	D	7	0	10	0	0
3	E	7	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	14	0	20	3	0
3	G	7	0	10	0	0
4	E	14	0	17	1	0
4	G	16	0	22	0	0
5	A	41	0	0	1	0
5	B	48	0	0	0	0
5	C	49	0	0	1	0
5	D	18	0	0	2	0
5	E	18	0	0	0	0
5	F	12	0	0	0	1
5	G	19	0	0	1	0
All	All	16871	0	16262	479	1

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 15.

All (479) 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:G:40:ARG:HH11	1:G:82:MET:CE	1.63	1.11
1:C:27:LEU:HD21	1:C:42:VAL:HB	1.34	1.03
1:A:217:ARG:HB3	1:A:220:LEU:HD12	1.32	1.03
1:G:40:ARG:HD2	1:G:82:MET:HE3	1.37	1.01
1:G:40:ARG:NH1	1:G:82:MET:CE	2.26	0.97
1:G:106:ILE:HD11	1:G:130:MET:CE	1.99	0.93
1:D:257:THR:HG22	1:D:259:ILE:HG12	1.50	0.92
1:A:236:LYS:HA	1:D:222:ARG:HG2	1.52	0.90
1:G:40:ARG:HH11	1:G:82:MET:HE2	1.36	0.90
1:G:214:ASN:HD21	1:G:301:ASN:H	1.21	0.87
1:F:240:GLU:HG2	1:F:241:PRO:HD2	1.58	0.85
1:C:250:LEU:HD11	1:C:261:VAL:HG13	1.57	0.85
1:G:247:VAL:HG13	1:G:261:VAL:HG21	1.59	0.83
1:A:243:THR:HG23	1:A:246:HIS:H	1.41	0.83
1:G:27:LEU:HD21	1:G:42:VAL:HB	1.63	0.80
1:G:40:ARG:HD3	1:G:85:CYS:HA	1.63	0.80
1:D:220:LEU:HB3	1:D:222:ARG:HD3	1.63	0.79
1:B:196:THR:HG22	1:C:217:ARG:HH12	1.47	0.79
1:G:106:ILE:HD11	1:G:130:MET:HE1	1.64	0.79
1:A:220:LEU:HD23	1:A:221:ASN:H	1.48	0.79
1:A:220:LEU:HD21	1:A:259:ILE:HD13	1.65	0.79
1:G:40:ARG:CD	1:G:82:MET:HE3	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:ILE:CD1	1:G:130:MET:CE	2.61	0.78
1:A:255:ALA:C	1:A:257:THR:H	1.90	0.78
1:F:54:TYR:HB3	1:F:82:MET:HE1	1.67	0.77
1:F:86:VAL:HG13	1:F:179:GLY:HA2	1.67	0.77
1:A:247:VAL:HG22	1:A:261:VAL:HG11	1.68	0.75
1:D:131:ARG:HD3	1:D:137:LYS:HE2	1.68	0.75
1:D:218:TRP:CZ2	1:D:281:ILE:HG13	2.20	0.75
1:F:229:ASP:HA	1:F:232:LEU:HG	1.70	0.74
1:F:225:THR:HG23	1:F:266:ALA:HA	1.70	0.74
1:F:298:ARG:HG2	3:F:402:PEG:H41	1.68	0.73
1:G:56:ASP:OD1	1:G:57:LEU:N	2.22	0.73
1:G:40:ARG:NH1	1:G:82:MET:HE2	1.97	0.73
1:G:54:TYR:HB2	1:G:82:MET:HE1	1.70	0.73
1:G:40:ARG:HH11	1:G:82:MET:HE3	1.51	0.72
1:A:210:ALA:HB2	1:A:296:VAL:HG13	1.71	0.71
1:E:126:TYR:CE2	1:E:128:CYS:SG	2.83	0.71
1:F:240:GLU:CG	1:F:241:PRO:HD2	2.20	0.71
1:A:243:THR:HG22	1:A:246:HIS:CG	2.26	0.71
1:E:305:LEU:HD12	1:F:49:MET:HG2	1.72	0.70
1:A:269:LYS:HE3	1:A:273:GLN:HG2	1.73	0.70
1:D:230:PHE:CD2	1:D:265:CYS:HB3	2.25	0.70
1:A:107:GLN:H	1:A:110:GLN:NE2	1.90	0.70
1:D:230:PHE:HZ	1:D:268:LEU:HD23	1.57	0.69
1:D:212:VAL:HG11	1:D:259:ILE:HG13	1.72	0.69
1:F:247:VAL:HG22	1:F:261:VAL:HG11	1.75	0.69
1:F:201:THR:HG22	1:F:239:TYR:HD2	1.57	0.69
1:D:229:ASP:OD1	1:D:230:PHE:N	2.26	0.68
1:F:247:VAL:HG13	1:F:261:VAL:HG21	1.76	0.67
1:G:8:PHE:HB3	1:G:152:ILE:HD12	1.76	0.67
1:G:106:ILE:HD11	1:G:130:MET:HE3	1.75	0.67
1:F:109:GLY:HA2	1:F:200:ILE:HD13	1.76	0.67
1:A:262:LEU:HD22	1:A:262:LEU:H	1.60	0.67
1:A:107:GLN:H	1:A:110:GLN:HE21	1.42	0.67
1:B:288:GLU:HG2	1:B:291:PHE:HD2	1.61	0.66
1:G:230:PHE:HZ	1:G:268:LEU:HD23	1.60	0.66
1:D:234:ALA:HB1	1:D:239:TYR:HB2	1.77	0.66
1:C:288:GLU:HG2	1:C:291:PHE:HD2	1.59	0.66
1:F:268:LEU:HA	1:F:271:LEU:HG	1.77	0.66
1:C:233:VAL:O	1:C:237:TYR:HD2	1.79	0.66
1:C:225:THR:HG21	1:C:269:LYS:NZ	2.11	0.66
1:C:202:VAL:HG23	1:C:250:LEU:HD23	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:MET:HG3	1:C:117:CYS:SG	2.36	0.65
1:A:243:THR:CG2	1:A:246:HIS:H	2.08	0.65
1:A:271:LEU:HD22	1:A:276:MET:HG2	1.78	0.65
1:C:217:ARG:HG3	1:C:220:LEU:HD12	1.78	0.64
1:C:231:ASN:O	1:C:235:MET:HG2	1.99	0.63
1:F:261:VAL:HG12	1:F:265:CYS:SG	2.39	0.63
1:A:227:LEU:HD11	1:A:242:LEU:HB3	1.80	0.63
1:C:27:LEU:CD2	1:C:42:VAL:HB	2.20	0.63
1:F:217:ARG:HG2	1:F:220:LEU:HD13	1.81	0.63
1:A:255:ALA:C	1:A:257:THR:N	2.56	0.62
1:G:54:TYR:HA	1:G:57:LEU:HD12	1.81	0.62
1:D:209:TYR:OH	1:D:261:VAL:HA	2.00	0.62
1:F:279:ARG:HA	1:F:279:ARG:HH11	1.65	0.62
1:D:115:LEU:HD11	1:D:122:PRO:HB3	1.81	0.62
1:D:110:GLN:NE2	5:D:502:HOH:O	2.31	0.61
1:D:286:LEU:HD21	1:G:285:ALA:HB3	1.81	0.61
1:G:86:VAL:HG13	1:G:179:GLY:HA2	1.82	0.61
1:A:165:MET:HB3	1:D:305:LEU:HD23	1.82	0.61
1:E:126:TYR:HE2	1:E:128:CYS:SG	2.22	0.61
1:A:243:THR:O	1:A:246:HIS:HB2	2.00	0.61
1:F:234:ALA:O	1:F:237:TYR:N	2.33	0.61
1:A:210:ALA:HB2	1:A:296:VAL:CG1	2.30	0.61
1:E:142:ASN:H	3:E:402:PEG:H11	1.65	0.61
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.83	0.61
1:D:253:LEU:HA	1:D:256:GLN:HG2	1.82	0.60
1:C:202:VAL:HG21	1:C:249:ILE:HD11	1.83	0.60
1:C:246:HIS:O	1:C:249:ILE:HG12	2.01	0.60
1:A:243:THR:HG22	1:A:246:HIS:ND1	2.16	0.60
1:A:298:ARG:HD3	3:A:402:PEG:H41	1.83	0.60
1:B:49:MET:HB3	1:B:189:GLN:HG3	1.83	0.59
1:C:233:VAL:HG21	1:C:269:LYS:HE2	1.85	0.59
1:G:294:PHE:CD1	1:G:294:PHE:C	2.80	0.59
1:D:1:SER:N	1:G:140:PHE:O	2.36	0.59
1:E:49:MET:HG3	1:G:305:LEU:HD12	1.84	0.59
1:F:39:PRO:HG2	1:F:145:ALA:HB1	1.84	0.59
1:E:40:ARG:HH11	1:E:82:MET:HE1	1.68	0.59
1:B:130:MET:HE2	1:B:134:PHE:C	2.28	0.58
1:A:225:THR:HG23	1:A:229:ASP:HB2	1.85	0.58
1:E:45:THR:HG22	1:E:48:ASP:CG	2.29	0.58
1:C:217:ARG:HG3	1:C:220:LEU:CD1	2.34	0.58
1:C:288:GLU:HG2	1:C:291:PHE:CD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:TRP:CD1	1:F:219:PHE:N	2.72	0.57
1:C:245:ASP:O	1:C:249:ILE:HG23	2.03	0.57
1:C:247:VAL:HG13	1:C:261:VAL:HG21	1.85	0.57
1:D:292:THR:HG23	1:D:294:PHE:H	1.70	0.57
1:F:227:LEU:HD12	1:F:228:ASN:H	1.68	0.57
1:A:255:ALA:O	1:A:257:THR:N	2.37	0.57
1:F:202:VAL:HG21	1:F:249:ILE:HD11	1.87	0.57
1:G:106:ILE:CD1	1:G:130:MET:HE3	2.33	0.57
1:D:218:TRP:H	1:D:218:TRP:CD1	2.21	0.57
1:E:303:ALA:O	1:F:189:GLN:HG2	2.04	0.57
1:C:294:PHE:CZ	1:C:298:ARG:HD3	2.40	0.57
1:D:165:MET:HE2	1:D:181:PHE:CE1	2.40	0.57
1:B:249:ILE:CG2	1:B:293:PRO:HG2	2.35	0.56
1:A:199:THR:O	1:A:240:GLU:HB3	2.05	0.56
1:E:119:ASN:N	1:E:119:ASN:HD22	2.03	0.56
1:E:27:LEU:HD11	1:E:42:VAL:HB	1.86	0.56
1:C:235:MET:HE1	1:C:241:PRO:HG3	1.86	0.56
1:F:232:LEU:HD23	1:F:232:LEU:N	2.20	0.56
1:C:52:PRO:HD2	1:C:188[B]:ARG:HG2	1.86	0.56
1:C:225:THR:CB	1:C:269:LYS:HZ1	2.19	0.55
1:F:274:ASN:ND2	1:F:274:ASN:H	2.02	0.55
1:C:217:ARG:CG	1:C:220:LEU:HD12	2.37	0.55
1:D:213:ILE:HG22	1:D:257:THR:HG23	1.89	0.55
1:C:225:THR:HG21	1:C:269:LYS:HZ1	1.70	0.55
1:E:252:PRO:O	1:E:256:GLN:HG3	2.07	0.55
1:D:286:LEU:HD11	1:G:285:ALA:HB3	1.88	0.55
1:F:107:GLN:HG2	1:F:108:PRO:HD2	1.89	0.55
1:F:224:THR:HG23	1:F:262:LEU:HB3	1.88	0.54
1:A:132:PRO:HD2	1:A:197:ASP:OD1	2.07	0.54
1:A:155:ASP:OD1	1:A:155:ASP:N	2.41	0.54
1:D:230:PHE:HE2	1:D:265:CYS:HA	1.72	0.54
1:G:56:ASP:OD1	1:G:57:LEU:HG	2.08	0.54
1:C:1:SER:N	1:F:140:PHE:O	2.41	0.54
1:D:292:THR:HG22	1:D:295:ASP:CG	2.33	0.54
1:D:211:ALA:HA	1:D:282:LEU:HD11	1.89	0.54
1:F:103:PHE:H	3:F:403:PEG:H31	1.72	0.54
1:E:217:ARG:CG	1:E:220:LEU:HD23	2.37	0.54
1:G:106:ILE:CD1	1:G:130:MET:SD	2.96	0.54
1:D:230:PHE:CE2	1:D:265:CYS:HA	2.42	0.53
1:F:95:ASN:HB3	1:F:98:THR:OG1	2.08	0.53
1:G:230:PHE:CZ	1:G:268:LEU:HD23	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:N	1:A:65:ASN:OD1	2.39	0.53
1:E:142:ASN:N	3:E:402:PEG:H11	2.24	0.53
1:F:234:ALA:HB1	1:F:239:TYR:HB2	1.90	0.53
1:G:40:ARG:HD2	1:G:82:MET:CE	2.26	0.53
1:A:8:PHE:HZ	3:A:405:PEG:H42	1.73	0.53
1:C:240:GLU:HG2	1:C:241:PRO:CD	2.38	0.53
1:F:209:TYR:O	1:F:212:VAL:HG22	2.08	0.53
1:D:225:THR:HG21	1:D:265:CYS:HB2	1.90	0.53
1:E:5:LYS:NZ	1:E:288:GLU:OE1	2.41	0.53
1:A:109:GLY:HA2	1:A:200:ILE:HD12	1.90	0.53
1:B:249:ILE:HG22	1:B:293:PRO:HG2	1.91	0.53
1:F:53:ASN:HB3	1:F:56:ASP:OD2	2.09	0.52
1:A:221:ASN:HB2	1:A:263:ASP:HB3	1.90	0.52
1:D:118:TYR:CE2	1:D:144:SER:HB3	2.44	0.52
1:F:254:SER:HB2	1:F:259:ILE:O	2.10	0.52
1:C:86:VAL:HG13	1:C:179:GLY:HA2	1.92	0.52
1:F:227:LEU:HD12	1:F:228:ASN:OD1	2.09	0.52
1:D:210:ALA:HB2	1:D:296:VAL:HG13	1.92	0.52
1:A:217:ARG:O	1:A:220:LEU:HB2	2.10	0.52
1:D:230:PHE:HD2	1:D:265:CYS:HB3	1.75	0.52
1:E:52:PRO:HG2	1:E:54:TYR:CE2	2.45	0.52
1:C:229:ASP:O	1:C:233:VAL:HG23	2.10	0.51
1:E:221:ASN:HD21	1:E:267:SER:HA	1.75	0.51
1:A:231:ASN:ND2	1:A:242:LEU:H	2.07	0.51
1:E:86:VAL:HG13	1:E:179:GLY:HA2	1.93	0.51
1:A:44:CYS:SG	1:A:54:TYR:CE1	3.04	0.51
1:F:114:VAL:O	1:F:125:VAL:HA	2.11	0.51
1:A:253:LEU:O	1:A:257:THR:OG1	2.26	0.51
1:D:268:LEU:HA	1:D:271:LEU:HB3	1.92	0.51
1:F:201:THR:HG22	1:F:239:TYR:CD2	2.43	0.51
1:A:146:GLY:HA2	1:A:162:MET:HE2	1.92	0.51
1:D:229:ASP:O	1:D:233:VAL:HG23	2.11	0.51
1:F:218:TRP:CD1	1:F:218:TRP:C	2.88	0.51
1:C:294:PHE:CE1	1:C:298:ARG:HD3	2.46	0.51
1:F:208:LEU:O	1:F:212:VAL:HG13	2.10	0.51
1:G:234:ALA:HB1	1:G:239:TYR:HB2	1.92	0.51
1:E:169:THR:OG1	1:E:171:VAL:HG22	2.11	0.50
1:F:169:THR:HG23	1:F:171:VAL:HG22	1.92	0.50
1:A:262:LEU:HD22	1:A:262:LEU:N	2.25	0.50
1:D:8:PHE:HB3	1:D:152:ILE:HD12	1.92	0.50
1:D:269:LYS:O	1:D:273:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ARG:HD2	1:G:126:TYR:CD1	2.47	0.50
1:D:108:PRO:HG3	1:D:134:PHE:CE1	2.47	0.50
1:D:213:ILE:HG13	1:D:214:ASN:N	2.26	0.49
1:A:217:ARG:HB3	1:A:220:LEU:CD1	2.24	0.49
1:D:209:TYR:O	1:D:213:ILE:HG23	2.12	0.49
1:D:137:LYS:O	1:G:4:ARG:HD2	2.11	0.49
1:G:40:ARG:NH1	1:G:82:MET:HE1	2.22	0.49
1:F:234:ALA:C	1:F:237:TYR:H	2.21	0.49
1:F:132:PRO:HD2	1:F:197:ASP:OD1	2.12	0.49
1:B:66:PHE:HB2	1:B:77:VAL:HG21	1.95	0.49
1:B:288:GLU:HG2	1:B:291:PHE:CD2	2.44	0.49
1:D:218:TRP:CZ3	1:D:276:MET:HB3	2.46	0.49
1:D:221:ASN:OD1	1:D:266:ALA:HB3	2.12	0.49
1:F:58:LEU:HD22	1:F:82:MET:HE3	1.94	0.49
1:C:218:TRP:HH2	1:C:280:THR:C	2.21	0.49
1:D:221:ASN:CG	1:D:221:ASN:O	2.56	0.49
1:D:62:SER:HB2	1:D:64:HIS:CE1	2.47	0.49
1:F:66:PHE:HB2	1:F:77:VAL:HG21	1.95	0.49
1:G:277:ASN:OD1	1:G:279:ARG:HB2	2.13	0.49
1:A:167:LEU:HD12	1:A:171:VAL:HG23	1.95	0.48
1:G:17:MET:HG3	1:G:117:CYS:SG	2.52	0.48
1:D:268:LEU:O	1:D:269:LYS:C	2.54	0.48
1:D:292:THR:HG23	1:D:294:PHE:N	2.28	0.48
1:F:240:GLU:HG2	1:F:241:PRO:CD	2.38	0.48
1:F:227:LEU:HD12	1:F:228:ASN:N	2.27	0.48
1:D:221:ASN:O	1:D:222:ARG:C	2.57	0.48
1:F:268:LEU:HA	1:F:271:LEU:CG	2.42	0.48
1:A:175:THR:HG22	1:A:181:PHE:HA	1.96	0.48
1:D:249:ILE:O	1:D:252:PRO:HD2	2.12	0.48
1:E:221:ASN:ND2	1:E:267:SER:HA	2.29	0.48
1:A:187:ASP:OD1	1:A:187:ASP:N	2.46	0.48
1:F:83:GLN:HB2	1:F:88:LYS:HE2	1.95	0.48
1:F:263:ASP:N	1:F:263:ASP:OD1	2.46	0.48
1:A:111:THR:HG22	1:A:129:ALA:HB2	1.96	0.48
1:D:209:TYR:OH	1:D:260:ALA:C	2.57	0.48
1:D:257:THR:CG2	1:D:259:ILE:HG12	2.34	0.48
1:B:67:LEU:HD13	1:B:74:GLN:HE21	1.79	0.48
1:C:34:ASP:HB2	1:C:91:VAL:O	2.13	0.48
1:F:10:SER:OG	1:F:14:GLU:OE2	2.31	0.48
1:C:240:GLU:HG2	1:C:241:PRO:HD3	1.95	0.48
1:F:234:ALA:HA	1:F:237:TYR:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLN:HG3	1:C:26:THR:CG2	2.43	0.47
1:F:237:TYR:C	1:F:238:ASN:CG	2.81	0.47
1:G:211:ALA:HA	1:G:282:LEU:HG	1.96	0.47
1:B:266:ALA:O	1:B:270:GLU:HG2	2.14	0.47
1:D:45:THR:H	1:D:48:ASP:HB2	1.79	0.47
1:E:56:ASP:O	1:E:59:ILE:HG12	2.14	0.47
1:F:10:SER:O	1:F:14:GLU:HG3	2.14	0.47
1:G:225:THR:O	1:G:262:LEU:HD22	2.14	0.47
1:G:279:ARG:HB2	1:G:279:ARG:HE	1.52	0.47
1:A:40:ARG:HH21	1:A:187:ASP:CG	2.22	0.47
1:B:113:SER:O	1:B:149:GLY:HA2	2.15	0.47
1:A:204:VAL:O	1:A:208:LEU:HG	2.14	0.47
1:C:225:THR:HG23	1:C:229:ASP:HB2	1.96	0.47
1:E:279:ARG:HG3	1:E:280:THR:H	1.79	0.47
1:E:165:MET:HB3	1:G:305:LEU:HD23	1.96	0.47
1:A:226:THR:O	1:A:227:LEU:C	2.57	0.47
1:C:22:CYS:HB3	1:C:42:VAL:O	2.14	0.47
1:C:118:TYR:CE1	1:C:144:SER:HB3	2.50	0.47
1:D:19:GLN:HE21	1:D:26:THR:HG21	1.79	0.47
1:C:109:GLY:HA2	1:C:200:ILE:HD13	1.97	0.47
1:D:140:PHE:O	1:G:1:SER:N	2.48	0.47
1:D:266:ALA:HA	1:D:269:LYS:HE3	1.97	0.47
1:F:268:LEU:HA	1:F:271:LEU:CD1	2.45	0.47
1:G:245:ASP:O	1:G:249:ILE:HD12	2.15	0.47
1:A:221:ASN:CB	1:A:263:ASP:HB3	2.45	0.47
1:G:219:PHE:HB2	1:G:271:LEU:HD11	1.97	0.47
1:A:106:ILE:HD11	1:A:130:MET:HE2	1.97	0.47
1:B:236:LYS:HB3	1:B:236:LYS:HE3	1.55	0.47
1:D:39:PRO:HG2	1:D:145:ALA:HB1	1.97	0.47
1:C:225:THR:CG2	1:C:269:LYS:HZ1	2.28	0.47
1:A:221:ASN:CG	1:A:263:ASP:HB3	2.41	0.46
1:C:6:MET:CE	1:F:124:GLY:HA3	2.45	0.46
1:C:228:ASN:O	1:C:232:LEU:HD22	2.15	0.46
1:D:297:VAL:HA	1:D:300:CYS:SG	2.56	0.46
1:A:233:VAL:HG11	1:A:269:LYS:HD2	1.97	0.46
1:C:50:LEU:HD22	1:C:190:THR:HG22	1.97	0.46
1:D:138:GLY:O	1:D:172:HIS:HE1	1.98	0.46
1:E:276:MET:HE1	1:E:285:ALA:HA	1.98	0.46
1:G:280:THR:HA	1:G:284:SER:O	2.15	0.46
1:G:202:VAL:HG21	1:G:246:HIS:CD2	2.50	0.46
1:G:65:ASN:N	1:G:65:ASN:HD22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:LEU:HD23	1:G:282:LEU:HA	1.76	0.46
1:A:221:ASN:ND2	1:A:223:PHE:H	2.13	0.46
1:F:261:VAL:O	1:F:265:CYS:SG	2.70	0.46
1:G:297:VAL:HA	1:G:300[C]:CYS:SG	2.55	0.46
1:E:276:MET:HE3	1:E:280:THR:HA	1.98	0.46
1:D:223:PHE:HD1	1:D:223:PHE:H	1.64	0.46
1:F:115:LEU:HD11	1:F:122:PRO:HB3	1.98	0.46
1:F:273:GLN:H	1:F:273:GLN:HG2	1.39	0.46
1:B:56:ASP:O	1:B:59:ILE:HG22	2.16	0.46
1:C:4:ARG:NH2	1:F:127:GLN:O	2.49	0.46
1:A:44:CYS:SG	1:A:54:TYR:HE1	2.38	0.45
1:C:225:THR:HG21	1:C:269:LYS:HZ3	1.82	0.45
1:E:20:VAL:HG12	1:E:42:VAL:HG21	1.97	0.45
1:A:221:ASN:ND2	1:A:223:PHE:O	2.37	0.45
1:F:274:ASN:ND2	1:F:274:ASN:N	2.64	0.45
1:D:214:ASN:ND2	1:D:301:ASN:OD1	2.50	0.45
1:E:82:MET:HB2	1:E:87:LEU:HD12	1.99	0.45
1:B:232:LEU:O	1:B:236:LYS:HG3	2.16	0.45
1:E:31:TRP:CE2	1:E:95:ASN:HB2	2.52	0.45
1:F:201:THR:CG2	1:F:239:TYR:HB3	2.47	0.45
1:G:270:GLU:HA	1:G:273:GLN:HG2	1.97	0.45
1:A:246:HIS:O	1:A:250:LEU:HD22	2.16	0.45
1:B:196:THR:HG23	1:C:217:ARG:HH22	1.82	0.45
1:C:136:ILE:HG13	1:C:172:HIS:HB2	1.98	0.45
1:C:243:THR:O	1:C:246:HIS:HB2	2.17	0.45
1:E:40:ARG:HA	1:E:87:LEU:HD13	1.97	0.45
1:A:56:ASP:O	1:A:60:ARG:HG3	2.17	0.45
1:C:131:ARG:HD3	1:C:137:LYS:HE2	1.99	0.45
1:C:27:LEU:HG	1:C:42:VAL:HG23	1.99	0.45
1:E:31:TRP:CD2	1:E:95:ASN:HB2	2.51	0.45
1:E:165:MET:HE3	1:G:303:ALA:HB1	1.99	0.45
1:E:245:ASP:O	1:E:248:ASP:N	2.49	0.45
1:F:131:ARG:HE	1:F:131:ARG:HB3	1.51	0.45
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.79	0.44
1:A:287:LEU:H	1:A:287:LEU:HD22	1.82	0.44
1:G:249:ILE:HD12	1:G:249:ILE:H	1.80	0.44
1:G:114:VAL:O	1:G:125:VAL:HA	2.18	0.44
1:A:281:ILE:HD13	1:A:281:ILE:HA	1.72	0.44
1:F:231:ASN:O	1:F:235:MET:HG3	2.18	0.44
1:F:268:LEU:CA	1:F:271:LEU:HG	2.47	0.44
1:G:242:LEU:HD23	1:G:242:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:O	1:E:125:VAL:HA	2.17	0.44
1:B:296:VAL:O	1:B:300:CYS:HB2	2.17	0.44
1:C:7:ALA:HB1	1:C:113:SER:HB3	1.99	0.44
1:C:27:LEU:C	1:C:27:LEU:HD12	2.43	0.44
1:C:218:TRP:CH2	1:C:279:ARG:HB3	2.53	0.44
1:F:76:ARG:HD2	1:F:78:ILE:HD11	1.98	0.44
1:G:60:ARG:CZ	1:G:60:ARG:HB3	2.47	0.44
1:G:211:ALA:HB1	1:G:216:ASP:HB2	1.99	0.44
1:G:227:LEU:O	1:G:228:ASN:C	2.60	0.44
1:A:207:TRP:O	1:A:210:ALA:HB3	2.17	0.44
1:B:221:ASN:ND2	1:B:270:GLU:HG3	2.33	0.44
1:G:167:LEU:HA	1:G:167:LEU:HD23	1.78	0.44
1:G:230:PHE:O	1:G:231:ASN:C	2.59	0.44
1:A:270:GLU:O	1:A:273:GLN:HG3	2.17	0.44
1:F:227:LEU:C	1:F:229:ASP:H	2.24	0.44
1:B:219:PHE:CE2	1:B:281:ILE:HG12	2.52	0.44
1:D:234:ALA:HB1	1:D:239:TYR:CB	2.45	0.44
1:E:86:VAL:HG13	1:E:179:GLY:CA	2.48	0.44
1:E:228:ASN:O	1:E:232:LEU:HD23	2.18	0.44
1:A:109:GLY:HA2	1:A:200:ILE:HG21	1.99	0.43
1:C:63:ASN:HB3	1:C:77:VAL:O	2.18	0.43
1:C:211:ALA:HA	1:C:282:LEU:HD21	1.99	0.43
3:C:402:PEG:H21	3:C:402:PEG:H41	1.45	0.43
1:D:86:VAL:HG13	1:D:179:GLY:HA2	2.00	0.43
1:D:113:SER:O	1:D:149:GLY:HA2	2.18	0.43
1:E:74:GLN:C	1:E:75:LEU:HD23	2.43	0.43
1:E:113:SER:O	1:E:149:GLY:HA2	2.18	0.43
1:F:86:VAL:HG13	1:F:179:GLY:CA	2.44	0.43
1:A:269:LYS:CE	1:A:273:GLN:HG2	2.45	0.43
1:E:224:THR:OG1	1:E:225:THR:N	2.51	0.43
1:C:49:MET:HA	1:C:52:PRO:HG3	2.00	0.43
1:C:219:PHE:O	1:C:267:SER:HB3	2.18	0.43
1:E:74:GLN:OE1	1:E:74:GLN:N	2.33	0.43
1:G:84:ASN:HB3	1:G:179:GLY:O	2.19	0.43
1:A:245:ASP:O	1:A:249:ILE:HG13	2.17	0.43
1:C:269:LYS:HB2	1:C:269:LYS:HE3	1.73	0.43
1:D:278:GLY:O	1:D:279:ARG:HB2	2.18	0.43
1:G:270:GLU:O	1:G:271:LEU:C	2.61	0.43
1:A:111:THR:HG21	1:A:290:GLU:O	2.18	0.43
1:A:247:VAL:HG13	1:A:261:VAL:HG21	2.01	0.43
1:C:139:SER:HB3	1:F:6:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:SER:O	1:D:14:GLU:HG3	2.18	0.43
1:G:56:ASP:O	1:G:59:ILE:HG22	2.19	0.43
1:B:187:ASP:OD1	1:B:187:ASP:N	2.52	0.43
1:C:227:LEU:HG	1:C:228:ASN:N	2.33	0.43
1:C:264:MET:O	1:C:264:MET:HE3	2.19	0.43
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.83	0.43
1:E:55:GLU:O	1:E:59:ILE:HG23	2.19	0.43
1:F:103:PHE:H	3:F:403:PEG:C3	2.31	0.43
1:G:3:PHE:CD1	1:G:299[B]:GLN:HG3	2.54	0.43
1:G:27:LEU:HG	1:G:42:VAL:HG23	2.01	0.43
1:A:8:PHE:CZ	3:A:402:PEG:H22	2.54	0.43
1:A:291:PHE:HB2	5:A:513:HOH:O	2.18	0.43
1:B:72:ASN:H	1:B:72:ASN:HD22	1.66	0.43
1:B:108:PRO:HA	1:B:130:MET:HG2	2.01	0.43
1:C:126:TYR:CD2	1:F:4:ARG:HD2	2.54	0.43
1:F:224:THR:O	1:F:225:THR:C	2.60	0.43
1:G:45:THR:HA	5:G:509:HOH:O	2.17	0.43
1:A:130:MET:HE2	1:A:130:MET:HB2	1.79	0.43
1:B:163:HIS:HE1	1:B:172:HIS:HB3	1.84	0.43
1:F:167:LEU:CD1	1:F:194:ALA:HB2	2.49	0.43
1:A:218:TRP:O	1:A:219:PHE:CB	2.67	0.43
3:A:404:PEG:H12	3:A:404:PEG:H31	1.90	0.43
1:C:225:THR:CG2	1:C:229:ASP:HB2	2.49	0.43
1:D:85:CYS:HB2	1:D:179:GLY:O	2.18	0.43
1:A:262:LEU:H	1:A:262:LEU:CD2	2.31	0.42
1:C:126:TYR:CD1	1:F:6:MET:HG2	2.54	0.42
1:C:218:TRP:CD1	1:C:219:PHE:N	2.87	0.42
1:F:44:CYS:HB2	1:F:49:MET:HE3	2.01	0.42
1:G:107:GLN:O	1:G:110:GLN:HG3	2.18	0.42
1:G:137:LYS:HG2	1:G:171:VAL:HG12	2.01	0.42
1:F:102:LYS:HE2	1:F:102:LYS:HB2	1.85	0.42
1:F:230:PHE:O	1:F:231:ASN:C	2.61	0.42
1:C:244:GLN:HG3	1:C:248:ASP:OD2	2.19	0.42
1:D:237:TYR:N	1:D:237:TYR:CD1	2.88	0.42
1:F:13:VAL:HG12	1:F:17:MET:HE2	2.01	0.42
1:F:113:SER:O	1:F:149:GLY:HA2	2.18	0.42
1:G:259:ILE:HG21	1:G:264:MET:HE2	2.01	0.42
1:C:237:TYR:CD2	1:C:272:LEU:HD13	2.53	0.42
1:E:136:ILE:HD13	1:E:136:ILE:HG21	1.75	0.42
1:E:272:LEU:HD23	1:E:272:LEU:HA	1.81	0.42
1:A:250:LEU:HD22	1:A:250:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:O	1:B:237:TYR:HD1	2.02	0.42
1:E:54:TYR:N	2:E:401:PO4:O1	2.47	0.42
1:G:118:TYR:CE2	1:G:144:SER:HB3	2.54	0.42
1:A:190:THR:O	1:A:192:GLN:HG3	2.19	0.42
1:B:276:MET:HE1	1:B:281:ILE:HD12	2.02	0.42
1:E:175:THR:HG22	1:E:181:PHE:HA	2.02	0.42
4:E:403:1PE:H121	4:E:403:1PE:H232	1.67	0.42
1:F:87:LEU:HD23	1:F:87:LEU:HA	1.86	0.42
1:F:264:MET:O	1:F:265:CYS:C	2.61	0.42
1:D:263:ASP:OD1	1:D:264:MET:N	2.52	0.42
1:E:62:SER:H	1:E:65:ASN:HD22	1.67	0.42
1:E:167:LEU:HD12	1:E:171:VAL:HG23	2.01	0.42
1:G:86:VAL:HG13	1:G:179:GLY:CA	2.49	0.42
1:D:107:GLN:H	1:D:110:GLN:HG3	1.84	0.42
1:B:101:TYR:HA	1:B:157:VAL:O	2.18	0.42
1:C:242:LEU:HD23	1:C:242:LEU:HA	1.78	0.42
1:D:207:TRP:CZ3	1:D:287:LEU:HA	2.55	0.42
1:F:279:ARG:HA	1:F:279:ARG:HD2	1.88	0.42
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.84	0.42
1:B:221:ASN:ND2	1:B:223:PHE:HD2	2.18	0.42
1:C:253:LEU:HD23	1:C:253:LEU:HA	1.88	0.42
1:F:218:TRP:CH2	1:F:279:ARG:HB3	2.55	0.42
1:A:261:VAL:O	1:A:265:CYS:SG	2.71	0.41
1:B:114:VAL:O	1:B:125:VAL:HA	2.19	0.41
1:F:190:THR:O	1:F:192:GLN:HG3	2.20	0.41
1:F:269:LYS:O	1:F:272:LEU:HB2	2.20	0.41
1:A:49:MET:HB3	1:A:189:GLN:HG3	2.01	0.41
1:A:210:ALA:CB	1:A:296:VAL:HG13	2.46	0.41
1:A:231:ASN:HD21	1:A:242:LEU:H	1.65	0.41
1:C:4:ARG:O	1:C:6:MET:HG3	2.19	0.41
1:G:222:ARG:HD2	1:G:222:ARG:HA	1.40	0.41
1:B:24:THR:HB	1:F:45:THR:HB	2.02	0.41
1:C:19:GLN:HG2	5:C:523:HOH:O	2.19	0.41
1:F:8:PHE:O	1:F:9:PRO:C	2.63	0.41
1:F:218:TRP:HH2	1:F:280:THR:C	2.28	0.41
1:F:227:LEU:C	1:F:229:ASP:N	2.78	0.41
1:C:220:LEU:HD22	1:C:259:ILE:HD13	2.01	0.41
1:E:40:ARG:HH11	1:E:82:MET:CE	2.32	0.41
1:E:20:VAL:HG22	1:E:68:VAL:HG22	2.03	0.41
1:E:76:ARG:HB2	1:E:92:ASP:CG	2.46	0.41
1:F:104:VAL:O	1:F:160:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:O	1:A:211:ALA:C	2.63	0.41
1:D:295:ASP:HB3	5:D:512:HOH:O	2.21	0.41
1:E:10:SER:O	1:E:14:GLU:HG3	2.20	0.41
1:E:207:TRP:CD2	1:E:288:GLU:HB2	2.55	0.41
1:F:218:TRP:CZ2	1:F:281:ILE:HG12	2.56	0.41
1:F:270:GLU:O	1:F:271:LEU:C	2.63	0.41
1:G:8:PHE:CB	1:G:152:ILE:HD12	2.49	0.41
1:A:27:LEU:HD11	1:A:42:VAL:HB	2.03	0.41
1:D:269:LYS:HE3	1:D:269:LYS:HB3	1.84	0.41
1:E:235:MET:HE2	1:E:241:PRO:HG3	2.02	0.41
1:G:4:ARG:H	1:G:299[B]:GLN:CD	2.28	0.41
1:G:243:THR:HG23	1:G:246:HIS:ND1	2.35	0.41
1:A:200:ILE:HG13	1:A:289:ASP:HB2	2.02	0.41
1:B:48:ASP:O	1:B:52:PRO:HB3	2.21	0.41
1:B:118:TYR:CE2	1:B:144:SER:HB3	2.55	0.41
1:C:114:VAL:O	1:C:125:VAL:HA	2.21	0.41
1:E:32:LEU:HD13	1:E:101:TYR:CE2	2.56	0.41
1:A:118:TYR:CG	3:A:404:PEG:H11	2.55	0.41
1:B:236:LYS:O	1:C:222:ARG:NH1	2.54	0.41
1:C:207:TRP:HZ3	1:C:287:LEU:HD23	1.86	0.41
1:E:79:GLY:HA3	1:E:90:LYS:HB3	2.03	0.41
1:E:130:MET:HE3	1:E:130:MET:HB2	1.98	0.41
1:F:234:ALA:C	1:F:236:LYS:N	2.77	0.41
1:A:8:PHE:CE1	3:A:402:PEG:H22	2.56	0.41
1:B:273:GLN:H	1:B:273:GLN:HG2	1.74	0.41
1:E:244:GLN:O	1:E:247:VAL:HG22	2.21	0.41
1:A:243:THR:HG23	1:A:245:ASP:N	2.36	0.40
1:D:31:TRP:CE2	1:D:95:ASN:HB2	2.56	0.40
1:G:43:ILE:HD13	1:G:57:LEU:HB2	2.02	0.40
1:G:80:HIS:ND1	1:G:80:HIS:N	2.69	0.40
1:G:262:LEU:HD23	1:G:262:LEU:HA	1.91	0.40
1:D:264:MET:HE3	1:D:264:MET:HB2	1.54	0.40
1:E:108:PRO:HA	1:E:130:MET:HG2	2.03	0.40
1:G:243:THR:HG1	1:G:246:HIS:H	1.65	0.40
1:D:223:PHE:CD1	1:D:223:PHE:N	2.89	0.40
1:G:3:PHE:HZ	1:G:296:VAL:HA	1.85	0.40
1:E:217:ARG:HA	1:E:220:LEU:HD23	2.04	0.40
1:F:67:LEU:HA	1:F:67:LEU:HD23	1.69	0.40
1:G:207:TRP:CZ2	1:G:281:ILE:O	2.75	0.40
1:A:235:MET:HE2	1:D:222:ARG:O	2.21	0.40
1:A:266:ALA:O	1:A:269:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:CYS:HB3	1:E:48:ASP:HB2	2.03	0.40
1:E:74:GLN:O	1:E:75:LEU:HD23	2.22	0.40
1:G:40:ARG:O	1:G:43:ILE:HG13	2.21	0.40
1:G:131:ARG:HB3	1:G:197:ASP:OD1	2.21	0.40
1:G:225:THR:HG23	1:G:229:ASP:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:512:HOH:O	5:F:512:HOH:O[2_555]	2.11	0.09

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%)	289 (95%)	14 (5%)	1 (0%)	36	45
1	B	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	C	306/306 (100%)	292 (95%)	14 (5%)	0	100	100
1	D	304/306 (99%)	293 (96%)	10 (3%)	1 (0%)	36	45
1	E	304/306 (99%)	291 (96%)	13 (4%)	0	100	100
1	F	305/306 (100%)	289 (95%)	16 (5%)	0	100	100
1	G	306/306 (100%)	286 (94%)	20 (6%)	0	100	100
All	All	2133/2142 (100%)	2039 (96%)	92 (4%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLN

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Mol	Chain	Res	Type
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	255/262 (97%)	244 (96%)	11 (4%)	26	38
1	B	261/262 (100%)	251 (96%)	10 (4%)	29	43
1	C	263/262 (100%)	246 (94%)	17 (6%)	15	21
1	D	257/262 (98%)	240 (93%)	17 (7%)	15	21
1	E	260/262 (99%)	245 (94%)	15 (6%)	18	25
1	F	256/262 (98%)	234 (91%)	22 (9%)	10	12
1	G	260/262 (99%)	230 (88%)	30 (12%)	5	6
All	All	1812/1834 (99%)	1690 (93%)	122 (7%)	15	20

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	86	VAL
1	A	200	ILE
1	A	202	VAL
1	A	205	LEU
1	A	216	ASP
1	A	220	LEU
1	A	225	THR
1	A	226	THR
1	A	240	GLU
1	A	295	ASP
1	B	24	THR
1	B	43	ILE
1	B	50	LEU
1	B	81	SER
1	B	123	SER

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Mol	Chain	Res	Type
1	B	142	ASN
1	B	153	ASP
1	B	204	VAL
1	B	236	LYS
1	B	298	ARG
1	C	47	GLU
1	C	60	ARG
1	C	81	SER
1	C	121	SER
1	C	128	CYS
1	C	131	ARG
1	C	142	ASN
1	C	198	THR
1	C	232	LEU
1	C	236	LYS
1	C	240	GLU
1	C	249	ILE
1	C	254	SER
1	C	267	SER
1	C	271	LEU
1	C	295	ASP
1	C	296	VAL
1	D	127	GLN
1	D	213	ILE
1	D	218	TRP
1	D	219	PHE
1	D	220	LEU
1	D	222	ARG
1	D	225	THR
1	D	229	ASP
1	D	237	TYR
1	D	253	LEU
1	D	262	LEU
1	D	263	ASP
1	D	264	MET
1	D	269	LYS
1	D	280	THR
1	D	292	THR
1	D	296	VAL
1	E	27	LEU
1	E	47	GLU
1	E	69	GLN

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Mol	Chain	Res	Type
1	E	78	ILE
1	E	87	LEU
1	E	106	ILE
1	E	119	ASN
1	E	125	VAL
1	E	157	VAL
1	E	212	VAL
1	E	225	THR
1	E	232	LEU
1	E	233	VAL
1	E	240	GLU
1	E	247	VAL
1	F	27	LEU
1	F	72	ASN
1	F	81	SER
1	F	131	ARG
1	F	153	ASP
1	F	178	GLU
1	F	198	THR
1	F	212	VAL
1	F	225	THR
1	F	238	ASN
1	F	240	GLU
1	F	245	ASP
1	F	253	LEU
1	F	262	LEU
1	F	263	ASP
1	F	273	GLN
1	F	274	ASN
1	F	276	MET
1	F	280	THR
1	F	281	ILE
1	F	286	LEU
1	F	296	VAL
1	G	24	THR
1	G	48	ASP
1	G	61	LYS
1	G	81	SER
1	G	196	THR
1	G	198	THR
1	G	200	ILE
1	G	202	VAL

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Mol	Chain	Res	Type
1	G	208	LEU
1	G	220	LEU
1	G	222	ARG
1	G	223	PHE
1	G	226	THR
1	G	228	ASN
1	G	256	GLN
1	G	267	SER
1	G	269	LYS
1	G	270	GLU
1	G	276	MET
1	G	277	ASN
1	G	279	ARG
1	G	280	THR
1	G	282	LEU
1	G	284	SER
1	G	294	PHE
1	G	299[A]	GLN
1	G	299[B]	GLN
1	G	300[A]	CYS
1	G	300[C]	CYS
1	G	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	110	GLN
1	A	180	ASN
1	A	231	ASN
1	A	256	GLN
1	B	64	HIS
1	B	69	GLN
1	B	72	ASN
1	B	74	GLN
1	B	110	GLN
1	B	119	ASN
1	B	164	HIS
1	B	221	ASN
1	C	19	GLN
1	C	74	GLN
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	127	GLN
1	C	189	GLN
1	C	228	ASN
1	C	273	GLN
1	D	19	GLN
1	D	72	ASN
1	D	107	GLN
1	D	127	GLN
1	D	142	ASN
1	D	180	ASN
1	E	65	ASN
1	E	119	ASN
1	E	163	HIS
1	E	221	ASN
1	F	110	GLN
1	F	164	HIS
1	F	244	GLN
1	F	273	GLN
1	F	274	ASN
1	G	19	GLN
1	G	64	HIS
1	G	84	ASN
1	G	189	GLN
1	G	214	ASN
1	G	273	GLN

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

24 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$
4	1PE	E	403	-	12,12,15	0.33	0	11,11,14	0.27	0
2	PO4	A	401	-	4,4,4	0.77	0	6,6,6	0.79	0
2	PO4	B	402	-	4,4,4	0.77	0	6,6,6	0.47	0
3	PEG	A	404	-	6,6,6	0.38	0	5,5,5	0.15	0
3	PEG	C	404	-	6,6,6	0.09	0	5,5,5	0.12	0
2	PO4	C	401	-	4,4,4	0.56	0	6,6,6	1.11	0
3	PEG	A	405	-	6,6,6	0.37	0	5,5,5	0.14	0
3	PEG	E	402	-	6,6,6	0.20	0	5,5,5	0.11	0
3	PEG	B	404	-	6,6,6	0.12	0	5,5,5	0.08	0
2	PO4	G	401	-	4,4,4	0.73	0	6,6,6	0.46	0
3	PEG	B	403	-	6,6,6	0.29	0	5,5,5	0.14	0
2	PO4	E	401	-	4,4,4	0.70	0	6,6,6	0.99	0
3	PEG	C	402	-	6,6,6	0.10	0	5,5,5	0.11	0
3	PEG	C	403	-	6,6,6	0.10	0	5,5,5	0.08	0
3	PEG	F	403	-	6,6,6	0.09	0	5,5,5	0.11	0
3	PEG	F	402	-	6,6,6	0.09	0	5,5,5	0.09	0
3	PEG	A	403	-	6,6,6	0.38	0	5,5,5	0.15	0
3	PEG	D	402	-	6,6,6	0.09	0	5,5,5	0.08	0
3	PEG	G	402	-	6,6,6	0.21	0	5,5,5	0.07	0
4	1PE	G	403	-	15,15,15	0.14	0	14,14,14	0.12	0
2	PO4	B	401	-	4,4,4	0.80	0	6,6,6	0.84	0
2	PO4	D	401	-	4,4,4	0.66	0	6,6,6	0.70	0
3	PEG	A	402	-	6,6,6	0.19	0	5,5,5	0.22	0
2	PO4	F	401	-	4,4,4	0.73	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	G	402	-	-	3/4/4/4	-
3	PEG	C	402	-	-	4/4/4/4	-
4	1PE	G	403	-	-	8/13/13/13	-
4	1PE	E	403	-	-	6/10/10/13	-
3	PEG	C	403	-	-	2/4/4/4	-
3	PEG	E	402	-	-	3/4/4/4	-
3	PEG	B	404	-	-	2/4/4/4	-
3	PEG	F	402	-	-	0/4/4/4	-
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
3	PEG	A	404	-	-	2/4/4/4	-
3	PEG	C	404	-	-	1/4/4/4	-
3	PEG	A	403	-	-	3/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	A	405	-	-	4/4/4/4	-
3	PEG	B	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	403	1PE	OH5-C14-C24-OH4
3	A	405	PEG	O1-C1-C2-O2
3	C	404	PEG	O2-C3-C4-O4
4	G	403	1PE	OH2-C12-C22-OH3
3	C	402	PEG	C4-C3-O2-C2
4	E	403	1PE	OH4-C13-C23-OH3
3	A	402	PEG	O2-C3-C4-O4
3	A	403	PEG	O2-C3-C4-O4
3	A	405	PEG	O2-C3-C4-O4
3	C	402	PEG	O1-C1-C2-O2
3	C	402	PEG	O2-C3-C4-O4
3	C	403	PEG	O2-C3-C4-O4
4	E	403	1PE	OH6-C15-C25-OH5
3	B	403	PEG	O2-C3-C4-O4
3	G	402	PEG	O2-C3-C4-O4
3	A	404	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	A	403	PEG	O1-C1-C2-O2
3	D	402	PEG	O2-C3-C4-O4
3	E	402	PEG	O2-C3-C4-O4
4	G	403	1PE	OH4-C13-C23-OH3
4	E	403	1PE	C12-C22-OH3-C23
3	A	402	PEG	C4-C3-O2-C2
3	A	405	PEG	C4-C3-O2-C2
4	G	403	1PE	C24-C14-OH5-C25
3	A	402	PEG	C1-C2-O2-C3
3	F	403	PEG	C4-C3-O2-C2
3	D	402	PEG	C4-C3-O2-C2
3	C	403	PEG	C1-C2-O2-C3
3	D	402	PEG	C1-C2-O2-C3
4	G	403	1PE	C14-C24-OH4-C13
4	G	403	1PE	C23-C13-OH4-C24
3	A	404	PEG	O2-C3-C4-O4
3	G	402	PEG	C1-C2-O2-C3
3	B	404	PEG	O2-C3-C4-O4
3	B	404	PEG	C4-C3-O2-C2
3	A	403	PEG	C4-C3-O2-C2
4	G	403	1PE	C13-C23-OH3-C22
4	E	403	1PE	C14-C24-OH4-C13
3	A	405	PEG	C1-C2-O2-C3
3	G	402	PEG	C4-C3-O2-C2
3	E	402	PEG	C4-C3-O2-C2
4	E	403	1PE	OH2-C12-C22-OH3
3	E	402	PEG	C1-C2-O2-C3
3	C	402	PEG	C1-C2-O2-C3
4	E	403	1PE	C13-C23-OH3-C22
3	B	403	PEG	C4-C3-O2-C2
4	G	403	1PE	C12-C22-OH3-C23

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	1PE	1	0
3	A	404	PEG	2	0
3	A	405	PEG	1	0
3	E	402	PEG	2	0
2	E	401	PO4	1	0
3	C	402	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	403	PEG	2	0
3	F	402	PEG	1	0
3	A	402	PEG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/306 (100%)	0.24	29 (9%) 14 16	28, 51, 122, 149	0
1	B	306/306 (100%)	-0.33	1 (0%) 90 90	31, 47, 77, 128	0
1	C	306/306 (100%)	0.11	15 (4%) 35 37	28, 48, 110, 138	2 (0%)
1	D	306/306 (100%)	0.28	23 (7%) 20 23	33, 60, 117, 163	0
1	E	306/306 (100%)	0.17	5 (1%) 70 72	35, 63, 104, 148	0
1	F	306/306 (100%)	0.44	12 (3%) 43 46	32, 64, 136, 158	1 (0%)
1	G	306/306 (100%)	0.49	22 (7%) 21 24	36, 67, 111, 161	2 (0%)
All	All	2142/2142 (100%)	0.20	107 (4%) 34 36	28, 58, 115, 163	5 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	4.6
1	G	286	LEU	4.6
1	D	257	THR	4.4
1	C	227	LEU	4.2
1	A	286	LEU	4.0
1	D	220	LEU	3.9
1	A	238	ASN	3.6
1	F	223	PHE	3.5
1	E	128	CYS	3.4
1	G	278	GLY	3.4
1	C	224	THR	3.3
1	F	276	MET	3.3
1	A	294	PHE	3.2
1	G	281	ILE	3.2
1	D	230	PHE	3.1
1	G	275	GLY	3.1
1	D	255	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	300	CYS	3.0
1	C	154	TYR	3.0
1	E	294	PHE	2.9
1	A	285	ALA	2.9
1	C	285	ALA	2.9
1	A	250	LEU	2.9
1	A	282	LEU	2.9
1	A	255	ALA	2.9
1	A	222	ARG	2.8
1	F	232	LEU	2.8
1	G	232	LEU	2.8
1	F	225	THR	2.7
1	C	286	LEU	2.7
1	C	276	MET	2.7
1	D	219	PHE	2.7
1	A	261	VAL	2.7
1	F	262	LEU	2.6
1	G	255	ALA	2.6
1	D	3	PHE	2.6
1	A	284	SER	2.6
1	G	50	LEU	2.6
1	G	219	PHE	2.6
1	D	154	TYR	2.6
1	G	154	TYR	2.6
1	C	250	LEU	2.5
1	G	276	MET	2.5
1	G	241	PRO	2.5
1	A	230	PHE	2.5
1	G	283	GLY	2.5
1	A	225	THR	2.5
1	A	223	PHE	2.5
1	C	223	PHE	2.5
1	F	46	SER	2.5
1	G	223	PHE	2.5
1	A	281	ILE	2.5
1	D	263	ASP	2.5
1	A	278	GLY	2.5
1	E	46	SER	2.4
1	G	59	ILE	2.4
1	D	227	LEU	2.4
1	D	286	LEU	2.4
1	D	276	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	50	LEU	2.4
1	D	301	ASN	2.4
1	F	222	ARG	2.4
1	G	277	ASN	2.4
1	G	279	ARG	2.4
1	D	277	ASN	2.4
1	F	221	ASN	2.4
1	D	260	ALA	2.4
1	D	235	MET	2.4
1	E	50	LEU	2.4
1	D	218	TRP	2.4
1	F	275	GLY	2.3
1	D	223	PHE	2.3
1	G	134	PHE	2.3
1	A	218	TRP	2.3
1	E	283	GLY	2.3
1	C	225	THR	2.3
1	F	249	ILE	2.3
1	C	3	PHE	2.3
1	G	3	PHE	2.3
1	A	242	LEU	2.3
1	D	282	LEU	2.3
1	C	280	THR	2.3
1	A	259	ILE	2.3
1	A	215	GLY	2.2
1	A	243	THR	2.2
1	A	277	ASN	2.2
1	A	260	ALA	2.2
1	A	239	TYR	2.2
1	A	264	MET	2.2
1	C	284	SER	2.2
1	F	201	THR	2.2
1	G	245	ASP	2.1
1	A	227	LEU	2.1
1	D	207	TRP	2.1
1	C	294	PHE	2.1
1	D	258	GLY	2.1
1	G	237	TYR	2.1
1	A	287	LEU	2.1
1	A	252	PRO	2.1
1	C	230	PHE	2.1
1	D	226	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	MET	2.0
1	G	285	ALA	2.0
1	C	287	LEU	2.0
1	B	222	ARG	2.0
1	G	230	PHE	2.0
1	D	281	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	G	401	5/5	0.75	0.10	103,103,122,125	0
2	PO4	E	401	5/5	0.76	0.13	90,97,105,107	0
3	PEG	A	405	7/7	0.78	0.17	63,70,74,76	0
3	PEG	F	403	7/7	0.78	0.16	72,72,78,84	0
3	PEG	C	403	7/7	0.79	0.17	63,72,81,84	0
3	PEG	F	402	7/7	0.80	0.17	63,67,79,80	0
3	PEG	B	404	7/7	0.81	0.19	66,74,86,86	0
3	PEG	B	403	7/7	0.82	0.16	66,70,73,79	0
2	PO4	D	401	5/5	0.83	0.10	72,94,101,110	0
3	PEG	A	403	7/7	0.84	0.13	56,60,68,75	0
3	PEG	C	404	7/7	0.84	0.13	60,67,74,77	0
3	PEG	C	402	7/7	0.85	0.15	56,66,69,70	0
3	PEG	D	402	7/7	0.86	0.12	61,64,78,88	0
3	PEG	G	402	7/7	0.87	0.13	65,68,74,79	0
2	PO4	C	401	5/5	0.88	0.09	64,64,84,87	0
3	PEG	A	404	7/7	0.88	0.14	54,61,65,66	0
4	1PE	E	403	14/16	0.88	0.14	47,66,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	F	401	5/5	0.89	0.09	68,68,79,88	0
4	1PE	G	403	16/16	0.89	0.13	55,59,68,70	0
3	PEG	E	402	7/7	0.91	0.11	52,60,66,74	0
3	PEG	A	402	7/7	0.91	0.12	53,56,66,75	0
2	PO4	A	401	5/5	0.93	0.07	46,58,68,68	0
2	PO4	B	402	5/5	0.95	0.10	58,59,65,79	0
2	PO4	B	401	5/5	0.95	0.11	57,61,65,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.