Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 03:29 PM EDT

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

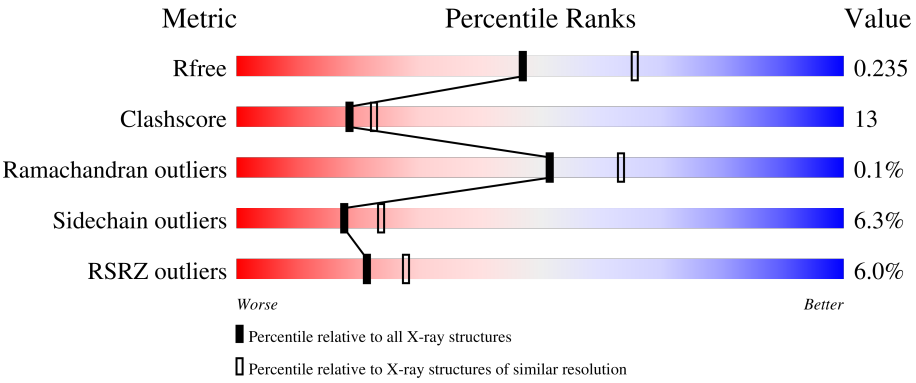
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 <=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% 71% 27%
1	B	306	2% 85% 14%
1	C	306	4% 72% 26%
1	D	306	8% 71% 25% 5%
1	E	306	4% 76% 23%

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Mol	Chain	Length	Quality of chain
1	F	306	8% 67% 30%
1	G	306	8% 70% 26%

2 Entry composition (i)

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.

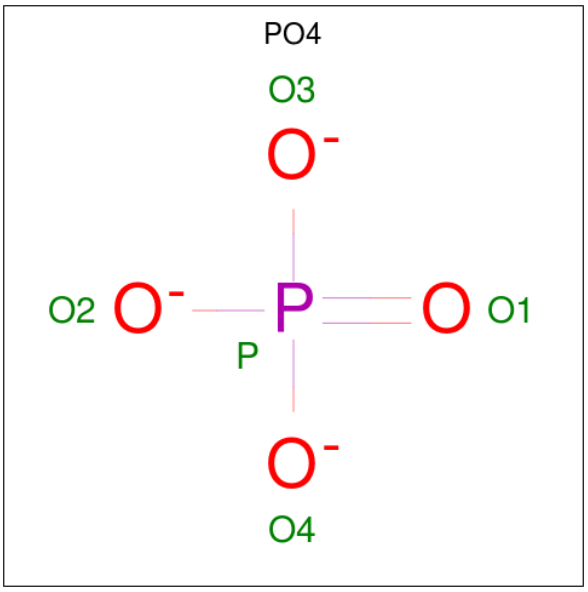
- Molecule 1 is a protein called Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site.

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:

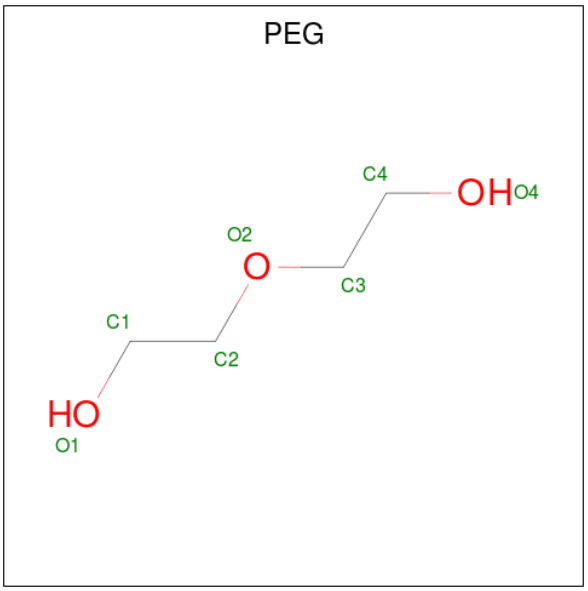
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1
E	145	ALA	CYS	engineered mutation	UNP P0DTD1
F	145	ALA	CYS	engineered mutation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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



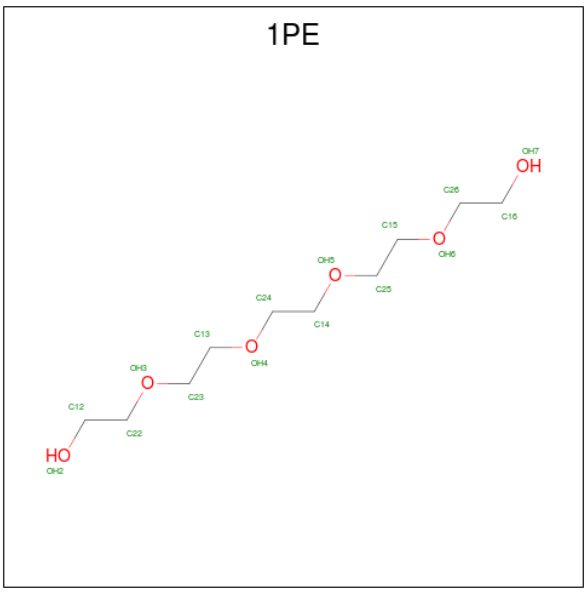
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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 (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

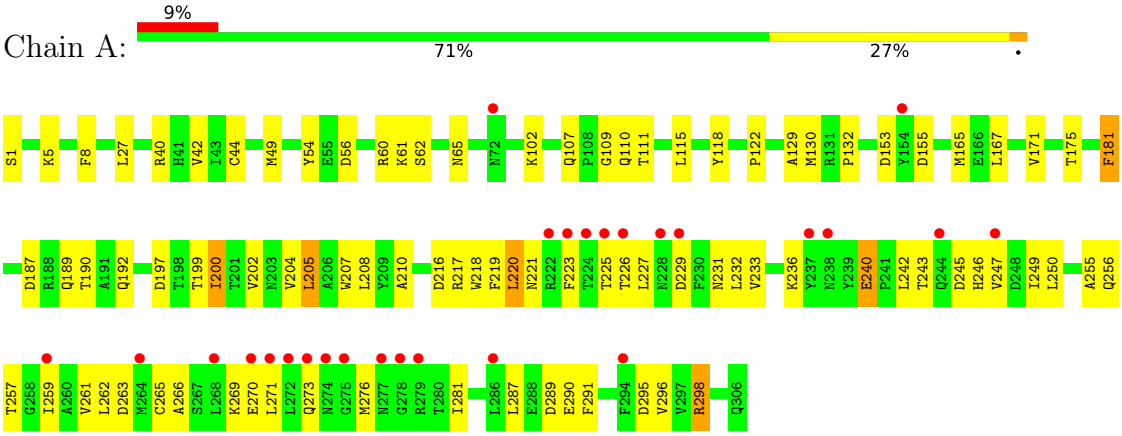
- Molecule 5 is water.

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

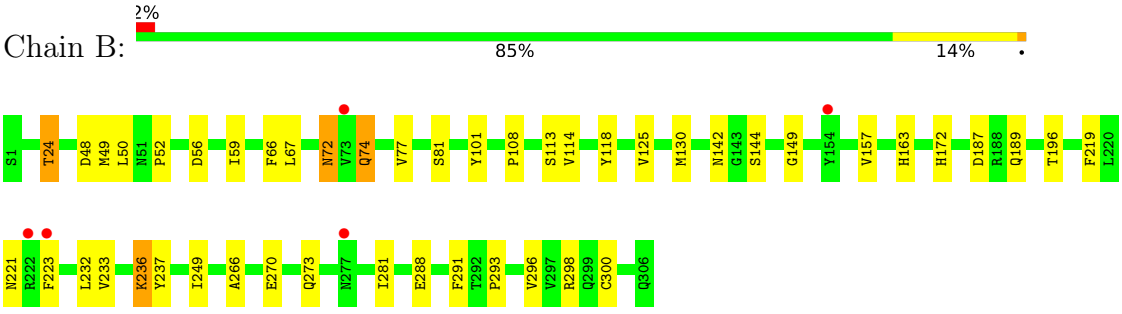
3 Residue-property plots (i)

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.

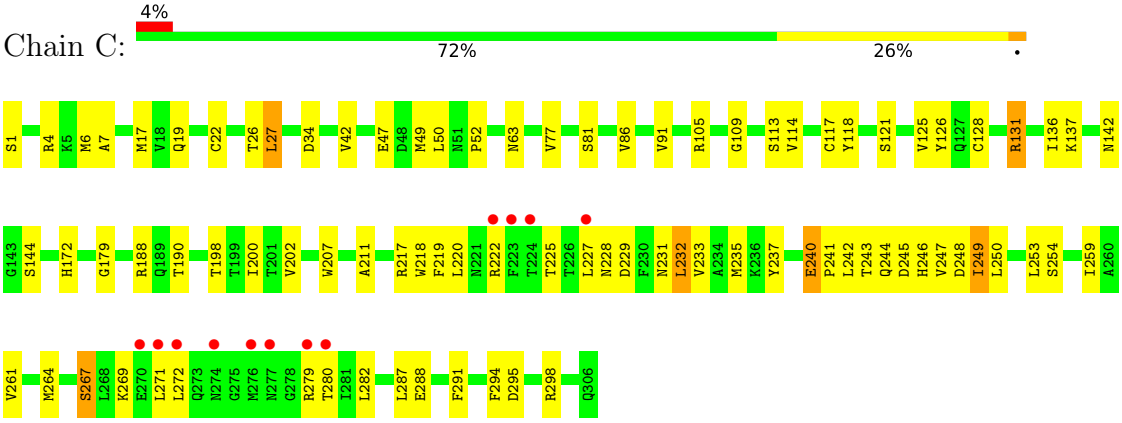
• Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



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

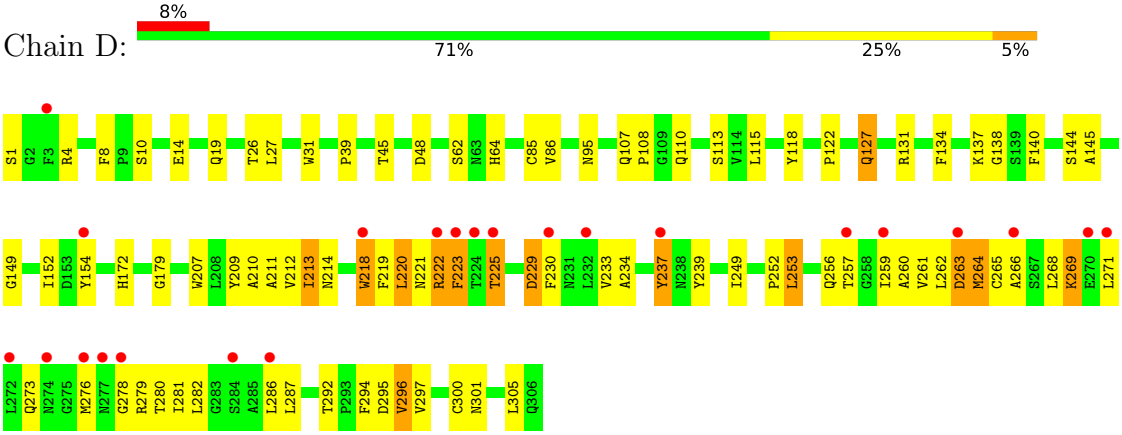


• Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site



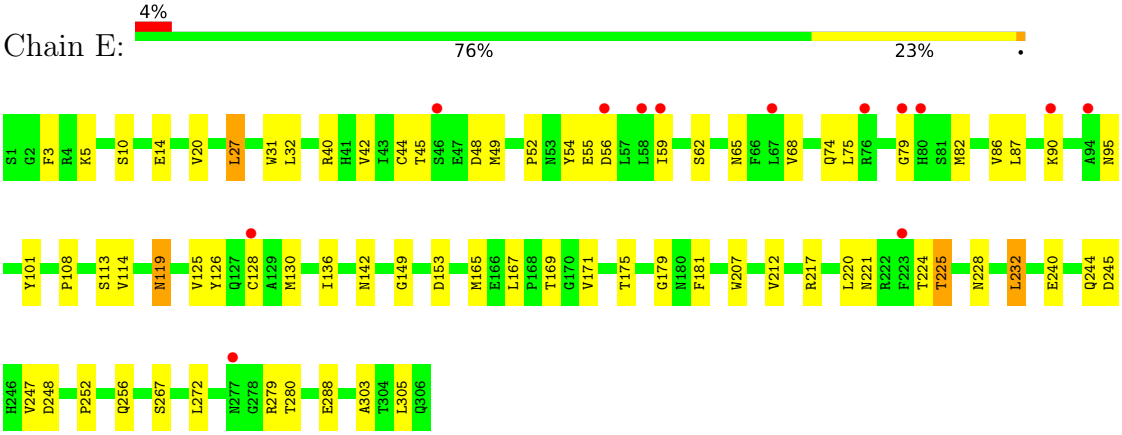
• Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site

Chain D:



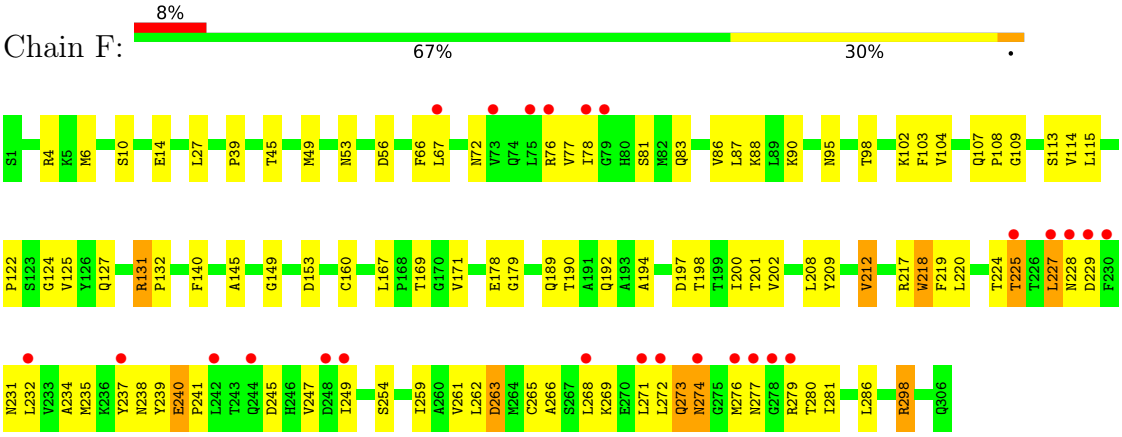
• Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site

Chain E:



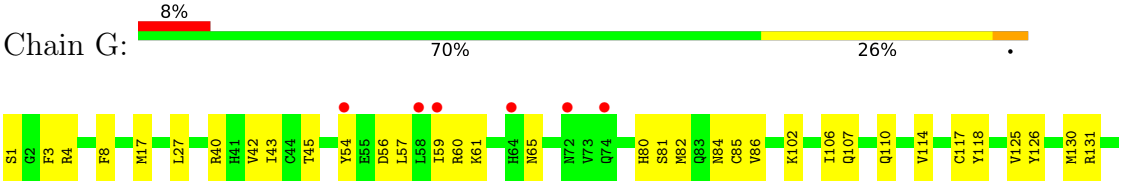
• Molecule 1: Fusion protein of 3C-like proteinase nsp5 and nsp7-nsp8 (C7) cut site

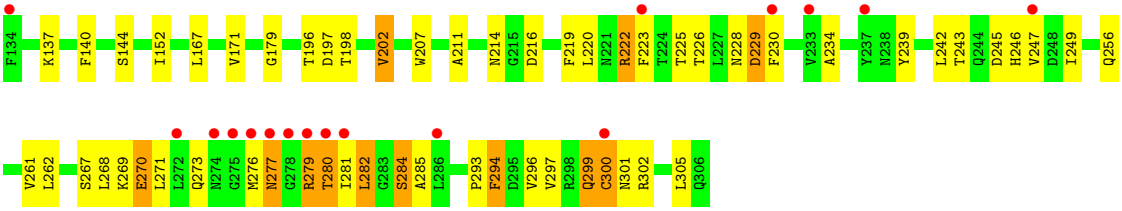
Chain F:



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

Chain G:




F134
K137
F140
S144
I152
L167
V171
G179
T196
D197
T198
V202
W207
A211
N214
G215
D216
F219
L220
N221
R222
F223
T224
T225
T226
L227
N228
D229
F230
V233
A234
Y237
N238
Y239
L242
T243
Q244
D245
H246
V247
D248
I249
Q256
V261
L262
S267
L268
K269
E270
L271
L272
Q273
N274
G275
M276
N277
G278
R279
T280
I281
L282
G283
S284
A285
L286
P293
F294
D295
V296
V297
R298
Q299
C300
N301
R302
L305
Q306

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.237 0.189 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (2.47%)	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 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, PEG, 1PE

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	0.51	0/2383	0.70	0/3243
1	B	0.47	0/2419	0.64	0/3287
1	C	0.50	0/2434	0.69	0/3306
1	D	0.49	0/2408	0.68	0/3274
1	E	0.46	0/2409	0.63	0/3274
1	F	0.48	0/2395	0.69	0/3259
1	G	0.50	1/2422 (0.0%)	0.69	0/3294
All	All	0.49	1/16870 (0.0%)	0.67	0/22937

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	293	PRO	C-N	5.27	1.46	1.34

There are no bond angle outliers.

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	80	0
1	B	2367	0	2319	30	0
1	C	2377	0	2335	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2356	0	2287	72	0
1	E	2358	0	2305	51	0
1	F	2342	0	2274	78	0
1	G	2364	0	2298	73	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
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	433	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 13.

All (433) 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:106:ILE:HD11	1:G:130:MET:HE1	1.43	1.01
1:G:40:ARG:HH11	1:G:82:MET:HE2	1.25	0.98
1:G:40:ARG:NH1	1:G:82:MET:CE	2.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:106:ILE:CD1	1:G:130:MET:CE	2.61	0.78
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:HD2	1:G:82:MET:HE3	1.69	0.73
1:A:255:ALA:C	1:A:257:THR:H	1.90	0.73
1:C:225:THR:HG21	1:C:269:LYS:HZ1	1.53	0.73
1:A:210:ALA:HB2	1:A:296:VAL:HG13	1.71	0.71
1:G:40:ARG:NH1	1:G:82:MET:HE1	2.03	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:G:106:ILE:CD1	1:G:130:MET:HE1	2.20	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:202:VAL:HG23	1:C:250:LEU:HD23	1.76	0.65
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:225:THR:HG21	1:C:269:LYS:NZ	2.11	0.64
1:C:217:ARG:HG3	1:C:220:LEU:HD12	1.78	0.64
1:G:40:ARG:HD2	1:G:82:MET:CE	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:225:THR:HG23	1:A:229:ASP:HB2	1.85	0.58
1:A:255:ALA:C	1:A:257:THR:N	2.56	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
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: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: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: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: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: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:G:294:PHE:CD1	1:G:294:PHE:C	2.80	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:45:THR:HG22	1:E:48:ASP:CG	2.29	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
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: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: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:C:225:THR:CB	1:C:269:LYS:HZ2	2.24	0.51
1:D:229:ASP:O	1:D:233:VAL:HG23	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:292:THR:HG22	1:D:295:ASP:CG	2.33	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: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: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: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: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
1:C:19:GLN:HG3	1:C:26:THR:CG2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:209:TYR:HH	1:D:260:ALA:C	2.18	0.47
1:E:165:MET:HB3	1:G:305:LEU:HD23	1.96	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: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:A:261:VAL:O	1:A:265:CYS:SG	2.71	0.47
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: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:F:218:TRP:CD1	1:F:218:TRP:C	2.88	0.46
1:G:65:ASN:N	1:G:65:ASN:HD22	2.13	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:CYS:SG	1:A:54:TYR:HE1	2.38	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: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:F:234:ALA:C	1:F:237:TYR:H	2.21	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
1:C:218:TRP:HH2	1:C:280:THR:C	2.21	0.44
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:O	1:A:273:GLN:HG3	2.17	0.44
1:B:219:PHE:CE2	1:B:281:ILE:HG12	2.52	0.44
1:D:268:LEU:O	1:D:269:LYS:C	2.54	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:D:221:ASN:O	1:D:222:ARG:C	2.57	0.43
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: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:D:221:ASN:O	1:D:221:ASN:CG	2.56	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:209:TYR:OH	1:D:260:ALA:C	2.57	0.43
1:D:278:GLY:O	1:D:279:ARG:HB2	2.18	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:CD2	1:F:4:ARG:HD2	2.54	0.43
1:G:45:THR:HA	5:G:509:HOH:O	2.17	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:40:ARG:HH21	1:A:187:ASP:CG	2.22	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:E:40:ARG:HH11	1:E:82:MET:CE	2.32	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:A:226:THR:O	1:A:227:LEU:C	2.57	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:113:SER:O	1:F:149:GLY:HA2	2.18	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
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: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:G:54:TYR:HB2	1:G:82:MET:HE3	2.00	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:A:130:MET:HE2	1:A:130:MET:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:221:ASN:CG	1:A:263:ASP:HB3	2.41	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: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:C:220:LEU:HD22	1:C:259:ILE:HD13	2.01	0.41
1:E:20:VAL:HG22	1:E:68:VAL:HG22	2.03	0.41
1:F:104:VAL:O	1:F:160:CYS:HA	2.21	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: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: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: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:F:227:LEU:C	1:F:229:ASP:H	2.24	0.41
1:A:243:THR:HG23	1:A:245:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:108:PRO:HA	1:E:130:MET:HG2	2.03	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:G:54:TYR:CB	1:G:82:MET:HE3	2.51	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:266:ALA:O	1:A:269:LYS:HB3	2.22	0.40
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%)	41	50
1	B	304/306 (99%)	299 (98%)	5 (2%)	0	100	100
1	C	306/306 (100%)	292 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	304/306 (99%)	293 (96%)	10 (3%)	1 (0%)	41 50
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%)	51 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	D	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	255/262 (97%)	241 (94%)	14 (6%)	21 29
1	B	261/262 (100%)	253 (97%)	8 (3%)	40 55
1	C	263/262 (100%)	246 (94%)	17 (6%)	17 22
1	D	257/262 (98%)	239 (93%)	18 (7%)	15 19
1	E	260/262 (99%)	252 (97%)	8 (3%)	40 55
1	F	256/262 (98%)	233 (91%)	23 (9%)	9 11
1	G	260/262 (99%)	232 (89%)	28 (11%)	6 7
All	All	1812/1834 (99%)	1696 (94%)	116 (6%)	18 23

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	LYS
1	A	61	LYS
1	A	102	LYS

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Mol	Chain	Res	Type
1	A	153	ASP
1	A	181	PHE
1	A	200	ILE
1	A	202	VAL
1	A	205	LEU
1	A	216	ASP
1	A	220	LEU
1	A	240	GLU
1	A	295	ASP
1	A	298	ARG
1	B	24	THR
1	B	50	LEU
1	B	72	ASN
1	B	74	GLN
1	B	81	SER
1	B	142	ASN
1	B	236	LYS
1	B	298	ARG
1	C	27	LEU
1	C	47	GLU
1	C	81	SER
1	C	105	ARG
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	240	GLU
1	C	249	ILE
1	C	254	SER
1	C	264	MET
1	C	267	SER
1	C	271	LEU
1	C	295	ASP
1	D	27	LEU
1	D	127	GLN
1	D	213	ILE
1	D	218	TRP
1	D	219	PHE
1	D	220	LEU
1	D	222	ARG

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Mol	Chain	Res	Type
1	D	223	PHE
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	296	VAL
1	E	3	PHE
1	E	27	LEU
1	E	119	ASN
1	E	153	ASP
1	E	212	VAL
1	E	225	THR
1	E	232	LEU
1	E	240	GLU
1	F	27	LEU
1	F	72	ASN
1	F	81	SER
1	F	90	LYS
1	F	131	ARG
1	F	153	ASP
1	F	178	GLU
1	F	198	THR
1	F	212	VAL
1	F	218	TRP
1	F	225	THR
1	F	227	LEU
1	F	238	ASN
1	F	240	GLU
1	F	245	ASP
1	F	263	ASP
1	F	273	GLN
1	F	274	ASN
1	F	276	MET
1	F	277	ASN
1	F	280	THR
1	F	286	LEU
1	F	298	ARG

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Mol	Chain	Res	Type
1	G	61	LYS
1	G	81	SER
1	G	102	LYS
1	G	196	THR
1	G	198	THR
1	G	202	VAL
1	G	220	LEU
1	G	222	ARG
1	G	223	PHE
1	G	226	THR
1	G	228	ASN
1	G	229	ASP
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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	110	GLN
1	A	231	ASN
1	A	256	GLN
1	B	69	GLN
1	B	72	ASN
1	B	164	HIS
1	B	221	ASN
1	C	19	GLN
1	C	69	GLN

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Mol	Chain	Res	Type
1	C	74	GLN
1	C	189	GLN
1	C	273	GLN
1	D	19	GLN
1	D	127	GLN
1	D	164	HIS
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	273	GLN
1	F	274	ASN
1	G	19	GLN
1	G	189	GLN
1	G	214	ASN
1	G	301	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 monosaccharides 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	$\#\|Z\| > 2$
2	PO4	C	401	-	4,4,4	0.51	0	6,6,6	1.06	0
3	PEG	C	403	-	6,6,6	0.10	0	5,5,5	0.08	0
2	PO4	B	401	-	4,4,4	0.76	0	6,6,6	0.80	0
3	PEG	A	404	-	6,6,6	0.38	0	5,5,5	0.16	0
3	PEG	E	402	-	6,6,6	0.20	0	5,5,5	0.11	0
4	1PE	G	403	-	15,15,15	0.14	0	14,14,14	0.13	0
4	1PE	E	403	-	12,12,15	0.34	0	11,11,14	0.27	0
3	PEG	B	404	-	6,6,6	0.12	0	5,5,5	0.08	0
3	PEG	B	403	-	6,6,6	0.28	0	5,5,5	0.14	0
3	PEG	C	402	-	6,6,6	0.10	0	5,5,5	0.11	0
2	PO4	G	401	-	4,4,4	0.69	0	6,6,6	0.42	0
3	PEG	A	402	-	6,6,6	0.18	0	5,5,5	0.22	0
2	PO4	F	401	-	4,4,4	0.68	0	6,6,6	0.42	0
3	PEG	F	403	-	6,6,6	0.09	0	5,5,5	0.11	0
2	PO4	D	401	-	4,4,4	0.61	0	6,6,6	0.66	0
2	PO4	E	401	-	4,4,4	0.66	0	6,6,6	0.95	0
3	PEG	F	402	-	6,6,6	0.09	0	5,5,5	0.09	0
3	PEG	G	402	-	6,6,6	0.21	0	5,5,5	0.07	0
3	PEG	C	404	-	6,6,6	0.09	0	5,5,5	0.12	0
2	PO4	A	401	-	4,4,4	0.71	0	6,6,6	0.76	0
3	PEG	A	403	-	6,6,6	0.38	0	5,5,5	0.15	0
2	PO4	B	402	-	4,4,4	0.73	0	6,6,6	0.44	0
3	PEG	A	405	-	6,6,6	0.37	0	5,5,5	0.15	0
3	PEG	D	402	-	6,6,6	0.09	0	5,5,5	0.08	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	B	403	-	-	2/4/4/4	-
3	PEG	C	402	-	-	4/4/4/4	-
3	PEG	C	403	-	-	2/4/4/4	-
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	G	402	-	-	3/4/4/4	-
3	PEG	C	404	-	-	1/4/4/4	-
3	PEG	A	404	-	-	2/4/4/4	-
3	PEG	E	402	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	G	403	-	-	8/13/13/13	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	A	403	-	-	3/4/4/4	-
3	PEG	A	405	-	-	4/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
4	1PE	E	403	-	-	6/10/10/13	-
3	PEG	F	402	-	-	0/4/4/4	-
3	PEG	B	404	-	-	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
3	A	405	PEG	O1-C1-C2-O2
3	C	404	PEG	O2-C3-C4-O4
4	G	403	1PE	OH2-C12-C22-OH3
4	G	403	1PE	OH5-C14-C24-OH4
3	C	402	PEG	C4-C3-O2-C2
3	A	402	PEG	O2-C3-C4-O4
3	A	405	PEG	O2-C3-C4-O4
3	C	402	PEG	O1-C1-C2-O2
4	E	403	1PE	OH4-C13-C23-OH3
3	A	403	PEG	O2-C3-C4-O4
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	A	404	PEG	C1-C2-O2-C3
3	G	402	PEG	O2-C3-C4-O4
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

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

There are no ring outliers.

9 monomers are involved in 14 short contacts:

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

5.7 Other polymers

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, 95^{th} 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%)	0.27	27 (8%)	10	14	28, 51, 122, 149	0
1	B	306/306 (100%)	-0.19	5 (1%)	72	78	31, 47, 77, 128	0
1	C	306/306 (100%)	0.09	12 (3%)	39	46	29, 48, 110, 138	0
1	D	306/306 (100%)	0.17	23 (7%)	14	19	33, 60, 117, 163	0
1	E	306/306 (100%)	0.14	13 (4%)	36	43	35, 63, 104, 148	0
1	F	306/306 (100%)	0.30	25 (8%)	11	15	39, 64, 136, 158	0
1	G	306/306 (100%)	0.28	23 (7%)	14	19	37, 67, 111, 161	0
All	All	2142/2142 (100%)	0.15	128 (5%)	21	28	28, 58, 115, 163	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	276	MET	7.5
1	A	247	VAL	7.1
1	G	278	GLY	5.7
1	G	275	GLY	5.1
1	A	223	PHE	5.1
1	C	270	GLU	4.8
1	A	273	GLN	4.7
1	G	286	LEU	4.6
1	A	222	ARG	4.5
1	G	59	ILE	4.5
1	B	222	ARG	4.5
1	C	276	MET	4.4
1	G	276	MET	4.4
1	F	227	LEU	4.3
1	G	230	PHE	4.3
1	F	75	LEU	4.0
1	F	225	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	237	TYR	3.9
1	D	271	LEU	3.8
1	E	56	ASP	3.8
1	F	230	PHE	3.8
1	A	286	LEU	3.8
1	D	257	THR	3.8
1	D	223	PHE	3.7
1	D	274	ASN	3.7
1	G	64	HIS	3.7
1	A	274	ASN	3.7
1	F	272	LEU	3.6
1	A	277	ASN	3.6
1	F	73	VAL	3.5
1	G	58	LEU	3.5
1	D	222	ARG	3.5
1	A	154	TYR	3.5
1	E	59	ILE	3.5
1	D	232	LEU	3.4
1	E	277	ASN	3.4
1	D	224	THR	3.3
1	C	223	PHE	3.3
1	G	237	TYR	3.3
1	F	271	LEU	3.3
1	F	76	ARG	3.3
1	E	79	GLY	3.3
1	F	278	GLY	3.2
1	F	232	LEU	3.2
1	G	272	LEU	3.2
1	G	277	ASN	3.2
1	B	223	PHE	3.1
1	A	272	LEU	3.1
1	C	272	LEU	3.1
1	F	78	ILE	3.1
1	D	270	GLU	3.1
1	C	227	LEU	3.0
1	D	237	TYR	3.0
1	A	226	THR	3.0
1	D	263	ASP	3.0
1	F	244	GLN	2.9
1	A	271	LEU	2.9
1	G	281	ILE	2.9
1	E	58	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	238	ASN	2.9
1	A	279	ARG	2.9
1	D	277	ASN	2.8
1	F	228	ASN	2.8
1	C	224	THR	2.8
1	D	225	THR	2.8
1	F	277	ASN	2.8
1	A	224	THR	2.8
1	F	237	TYR	2.8
1	F	242	LEU	2.7
1	D	278	GLY	2.7
1	G	247	VAL	2.7
1	D	276	MET	2.7
1	A	278	GLY	2.7
1	A	259	ILE	2.6
1	A	294	PHE	2.6
1	E	67	LEU	2.6
1	F	249	ILE	2.6
1	D	286	LEU	2.6
1	E	128	CYS	2.6
1	F	279	ARG	2.6
1	D	230	PHE	2.5
1	G	279	ARG	2.5
1	A	229	ASP	2.5
1	A	275	GLY	2.5
1	C	274	ASN	2.4
1	D	284	SER	2.4
1	D	266	ALA	2.4
1	F	79	GLY	2.4
1	D	154	TYR	2.4
1	C	277	ASN	2.4
1	A	244	GLN	2.4
1	F	274	ASN	2.4
1	C	279	ARG	2.4
1	D	272	LEU	2.4
1	G	74	GLN	2.4
1	C	271	LEU	2.3
1	C	280	THR	2.3
1	E	80	HIS	2.3
1	G	134	PHE	2.3
1	F	248	ASP	2.3
1	C	222	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	233	VAL	2.2
1	A	225	THR	2.2
1	F	268	LEU	2.2
1	E	46	SER	2.2
1	D	259	ILE	2.2
1	E	94	ALA	2.2
1	D	218	TRP	2.2
1	E	76	ARG	2.2
1	A	228	ASN	2.2
1	G	280	THR	2.2
1	E	223	PHE	2.1
1	E	90	LYS	2.1
1	G	54	TYR	2.1
1	G	223	PHE	2.1
1	F	229	ASP	2.1
1	B	277	ASN	2.1
1	A	270	GLU	2.1
1	A	264	MET	2.1
1	A	72	ASN	2.1
1	D	3	PHE	2.1
1	A	268	LEU	2.0
1	B	73	VAL	2.0
1	B	154	TYR	2.0
1	G	300[A]	CYS	2.0
1	G	72	ASN	2.0
1	G	274	ASN	2.0
1	F	67	LEU	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 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, 95^{th} 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	PEG	B	404	7/7	0.55	0.29	66,74,86,86	0
3	PEG	A	403	7/7	0.81	0.25	56,60,68,75	0
3	PEG	F	403	7/7	0.81	0.22	72,72,78,84	0
2	PO4	G	401	5/5	0.82	0.23	103,103,122,125	0
3	PEG	B	403	7/7	0.82	0.20	66,70,73,79	0
3	PEG	F	402	7/7	0.84	0.18	63,67,79,80	0
2	PO4	E	401	5/5	0.85	0.13	90,97,105,107	0
3	PEG	C	403	7/7	0.85	0.20	63,72,81,84	0
3	PEG	D	402	7/7	0.88	0.15	61,64,78,88	0
3	PEG	A	405	7/7	0.88	0.17	63,70,74,76	0
3	PEG	C	404	7/7	0.88	0.32	60,67,74,77	0
3	PEG	C	402	7/7	0.89	0.12	56,66,69,70	0
3	PEG	G	402	7/7	0.89	0.16	65,68,74,79	0
3	PEG	A	402	7/7	0.90	0.15	53,56,66,75	0
3	PEG	A	404	7/7	0.90	0.16	54,61,65,66	0
3	PEG	E	402	7/7	0.91	0.23	52,60,66,74	0
4	1PE	G	403	16/16	0.91	0.16	55,59,68,70	0
4	1PE	E	403	14/16	0.92	0.14	47,66,72,77	0
2	PO4	D	401	5/5	0.93	0.12	72,94,101,110	0
2	PO4	F	401	5/5	0.95	0.11	68,68,79,88	0
2	PO4	C	401	5/5	0.95	0.10	64,64,84,87	0
2	PO4	B	402	5/5	0.97	0.16	58,59,65,79	0
2	PO4	A	401	5/5	0.97	0.11	46,58,68,68	0
2	PO4	B	401	5/5	0.98	0.10	57,61,65,74	0

6.5 Other polymers (i)

There are no such residues in this entry.