Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 12:38 PM JST

PDB ID	:	7W64
Title	:	Crystal structure of minor pilin TcpB from Vibrio cholerae complexed with N-terminal peptide fragment of TcpF
Authors	:	Oki, H.; Kawahara, K.; Iimori, M.; Imoto, Y.; Maruno, T.; Uchiyama, S.; Muroga, Y.; Yoshida, A.; Yoshida, T.; Ohkubo, T.; Matsuda, S.; Iida, T.; Nakamura, S.
Deposited on	:	2021-12-01
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

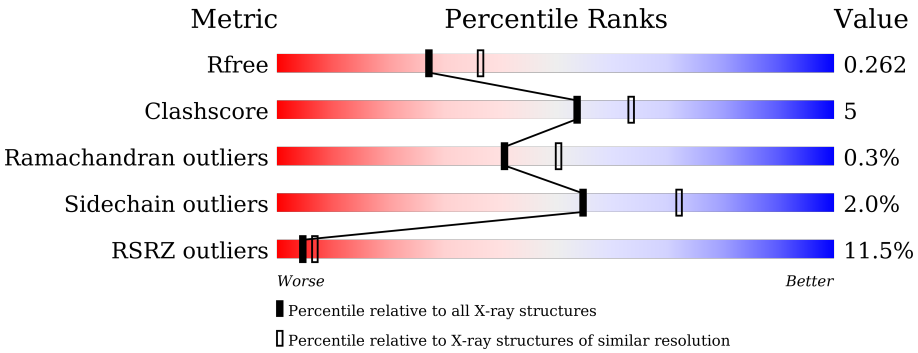
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	397	20% 86% 12%
1	B	397	8% 90% 9%
1	C	397	6% 83% 16%
1	D	397	15% 84% 13%
1	E	397	8% 89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	397	12% 84% 15%
2	G	15	67% 7% 27%
2	H	15	60% 13% 27%
2	I	15	67% 7% 27%
2	J	15	53% 13% 7% 27%
2	K	15	33% 67% 7% 27%
2	L	15	7% 73% 27%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19163 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 Toxin-coregulated pilus biosynthesis protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3020	1889	513	610	8			
1	B	395	Total	C	N	O	S	0	0	0
			3053	1911	517	616	9			
1	C	395	Total	C	N	O	S	0	0	0
			3053	1911	517	616	9			
1	D	391	Total	C	N	O	S	0	0	0
			3020	1889	513	610	8			
1	E	395	Total	C	N	O	S	0	0	0
			3053	1911	517	616	9			
1	F	395	Total	C	N	O	S	0	0	0
			3053	1911	517	616	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q9AGX1
A	28	GLY	-	expression tag	UNP Q9AGX1
B	27	GLY	-	expression tag	UNP Q9AGX1
B	28	GLY	-	expression tag	UNP Q9AGX1
C	27	GLY	-	expression tag	UNP Q9AGX1
C	28	GLY	-	expression tag	UNP Q9AGX1
D	27	GLY	-	expression tag	UNP Q9AGX1
D	28	GLY	-	expression tag	UNP Q9AGX1
E	27	GLY	-	expression tag	UNP Q9AGX1
E	28	GLY	-	expression tag	UNP Q9AGX1
F	27	GLY	-	expression tag	UNP Q9AGX1
F	28	GLY	-	expression tag	UNP Q9AGX1

- Molecule 2 is a protein called TcpF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	11	Total	C	N	O	0	0	0
			86	52	13	21			
2	H	11	Total	C	N	O	0	0	0
			86	52	13	21			
2	I	11	Total	C	N	O	0	0	0
			86	52	13	21			
2	J	11	Total	C	N	O	0	0	0
			86	52	13	21			
2	K	11	Total	C	N	O	0	0	0
			86	52	13	21			
2	L	11	Total	C	N	O	0	0	0
			86	52	13	21			

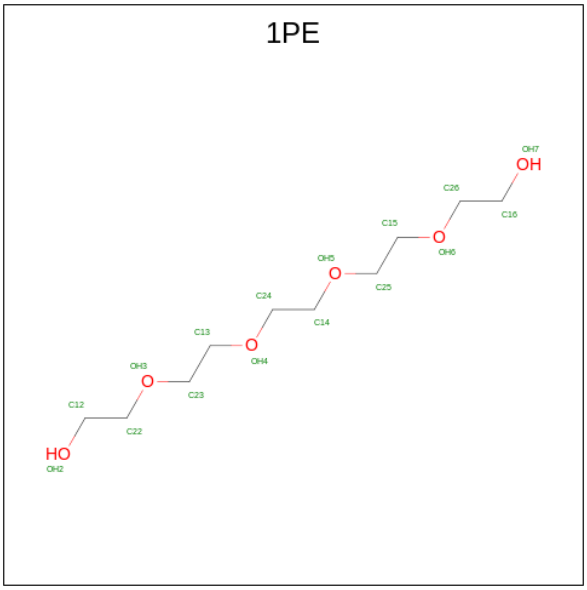
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	3	Total	Ca	0	0
			3	3		
3	C	2	Total	Ca	0	0
			2	2		
3	D	1	Total	Ca	0	0
			1	1		
3	E	3	Total	Ca	0	0
			3	3		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	I	1	Total	Cl	0	0
			1	1		
4	L	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 16 10 6	0	0

- Molecule 6 is water.

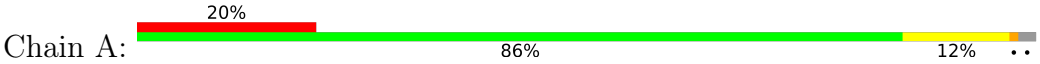
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	76	Total O 76 76	0	0
6	B	103	Total O 103 103	0	0
6	C	66	Total O 66 66	0	0
6	D	20	Total O 20 20	0	0
6	E	55	Total O 55 55	0	0
6	F	35	Total O 35 35	0	0
6	G	2	Total O 2 2	0	0
6	H	5	Total O 5 5	0	0

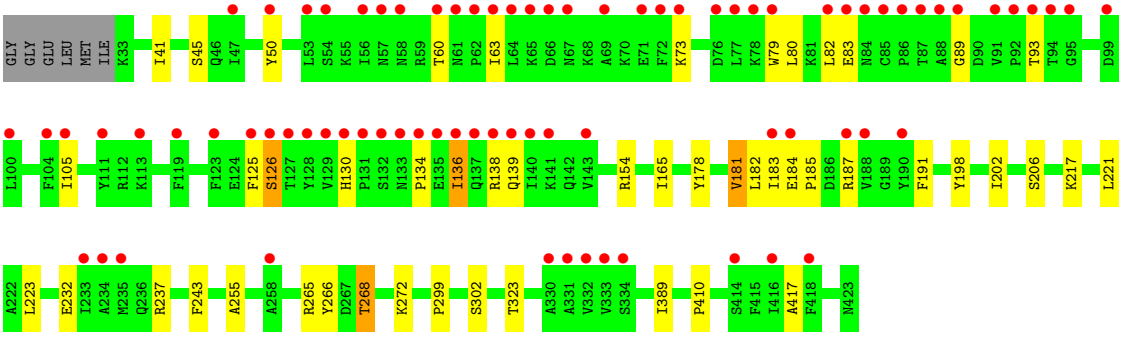
3 Residue-property plots (i)

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: Toxin-coregulated pilus biosynthesis protein B

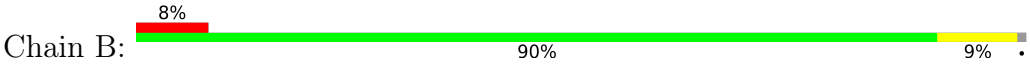
Chain A:

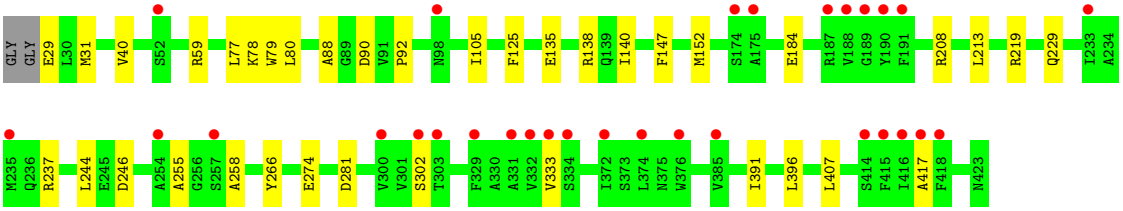




• Molecule 1: Toxin-coregulated pilus biosynthesis protein B

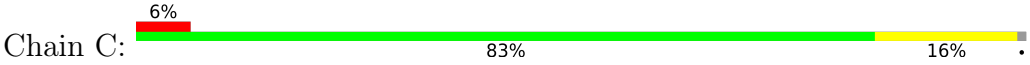
Chain B:

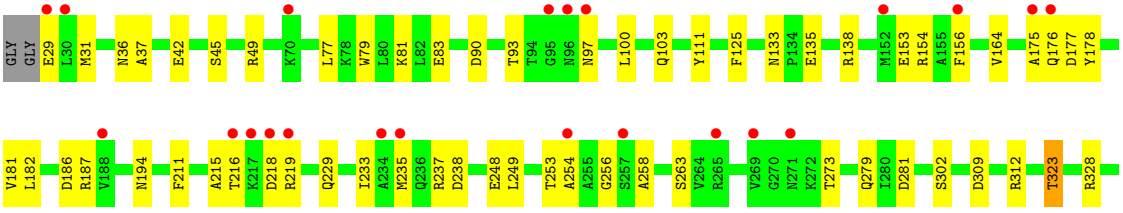


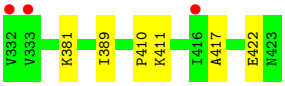


• Molecule 1: Toxin-coregulated pilus biosynthesis protein B

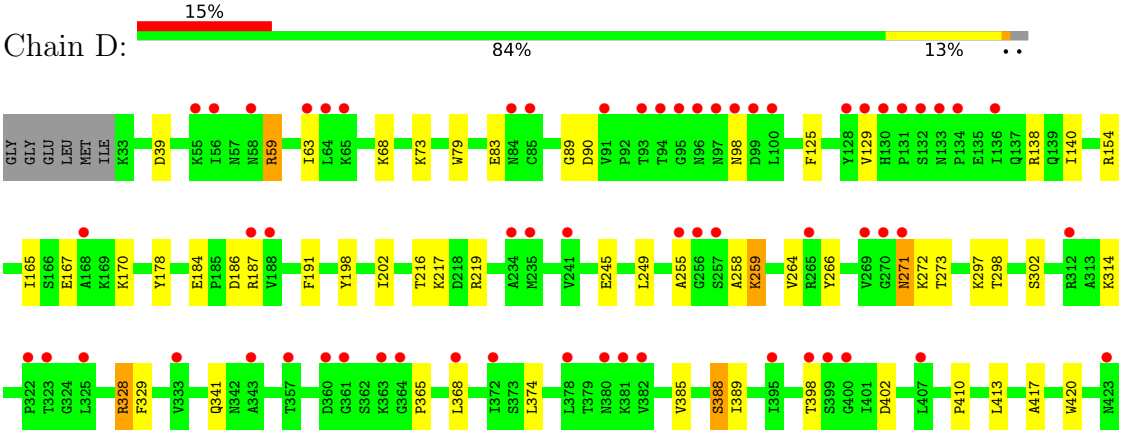
Chain C:



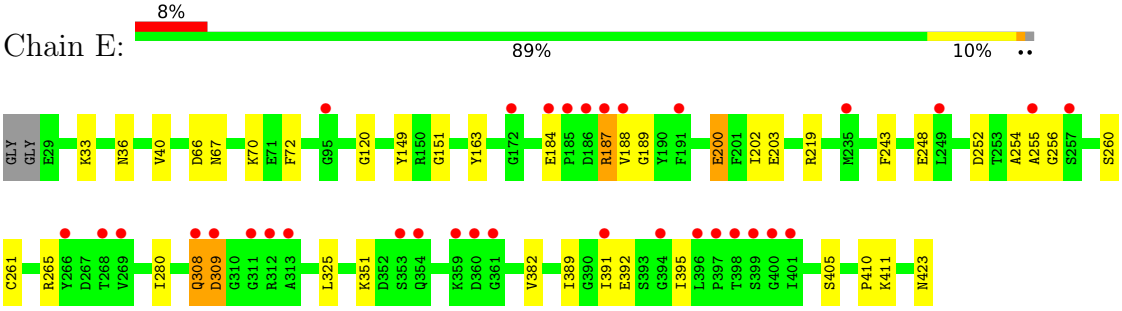




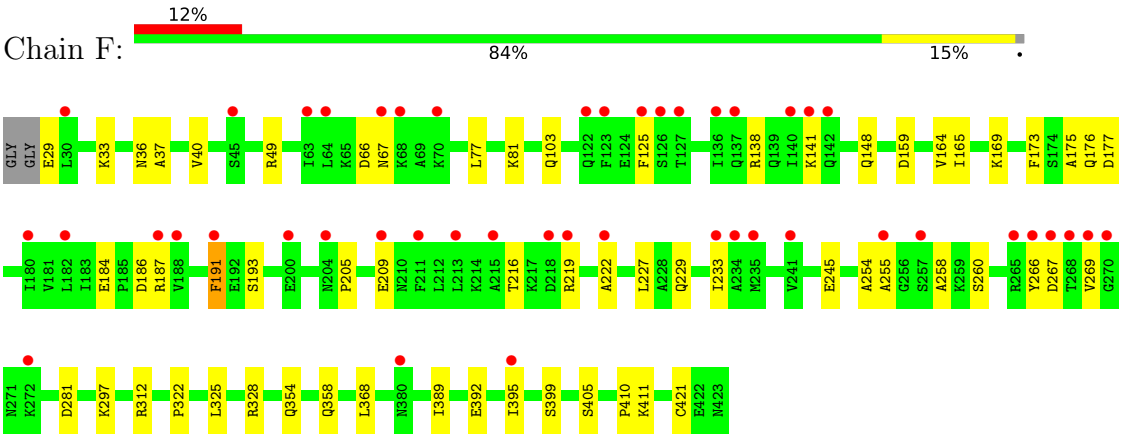
• Molecule 1: Toxin-coregulated pilus biosynthesis protein B



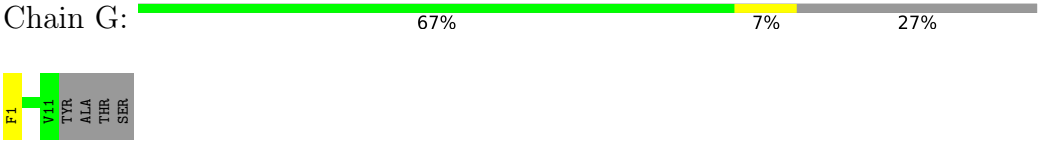
• Molecule 1: Toxin-coregulated pilus biosynthesis protein B



• Molecule 1: Toxin-coregulated pilus biosynthesis protein B



• Molecule 2: TcpF



• Molecule 2: TcpF

Chain H:

• Molecule 2: TcpF

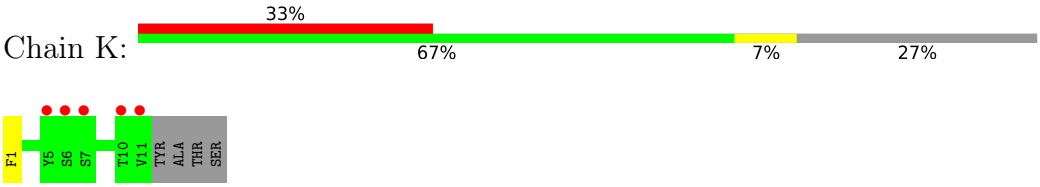
Chain I:

• Molecule 2: TcpF

Chain J:

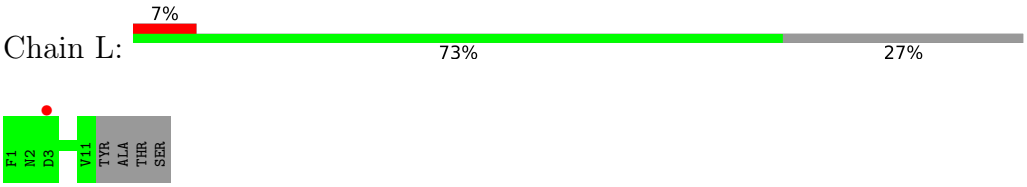
• Molecule 2: TcpF

Chain K:



• Molecule 2: TcpF

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.88Å 128.56Å 327.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.20 – 2.30 48.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.20-2.30) 98.8 (48.77-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
R, R_{free}	0.222 , 0.264 0.220 , 0.262	Depositor DCC
R_{free} test set	13805 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19163	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CL, CA, 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	0.49	0/3075	0.67	0/4157
1	B	0.54	0/3108	0.66	0/4201
1	C	0.50	0/3108	0.66	0/4201
1	D	0.42	0/3075	0.63	0/4157
1	E	0.49	0/3108	0.64	0/4201
1	F	0.45	0/3108	0.62	0/4201
2	G	0.55	0/87	0.57	0/118
2	H	0.48	0/87	0.63	0/118
2	I	0.45	0/87	0.54	0/118
2	J	0.36	0/87	0.51	0/118
2	K	0.34	0/87	0.55	0/118
2	L	0.41	0/87	0.54	0/118
All	All	0.48	0/19104	0.64	0/25826

There are no bond length outliers.

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	3020	0	2933	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3053	0	2970	22	0
1	C	3053	0	2970	45	0
1	D	3020	0	2933	38	0
1	E	3053	0	2972	27	0
1	F	3053	0	2970	40	0
2	G	86	0	74	1	0
2	H	86	0	74	2	0
2	I	86	0	74	1	0
2	J	86	0	74	3	0
2	K	86	0	74	1	0
2	L	86	0	74	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	1	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	B	16	0	22	1	0
6	A	76	0	0	2	0
6	B	103	0	0	3	0
6	C	66	0	0	6	0
6	D	20	0	0	0	0
6	E	55	0	0	0	0
6	F	35	0	0	4	0
6	G	2	0	0	0	0
6	H	5	0	0	1	0
All	All	19163	0	18214	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (196) 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:D:255:ALA:HB1	1:D:259:LYS:HE2	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:NH2	1:F:354:GLN:HG3	2.01	0.76
1:A:237:ARG:HA	1:C:235:MET:HE3	1.71	0.73
1:F:229:GLN:HB3	1:F:233:ILE:HG13	1.71	0.72
1:C:29:GLU:HG3	1:C:31:MET:HG3	1.72	0.70
1:D:271:ASN:O	1:D:271:ASN:ND2	2.28	0.67
1:F:184:GLU:OE2	1:F:191:PHE:HE1	1.79	0.66
1:C:176:GLN:O	1:C:176:GLN:HG3	1.95	0.66
1:A:389:ILE:HG13	1:A:410:PRO:HG3	1.80	0.64
1:D:83:GLU:HA	1:D:89:GLY:H	1.63	0.62
1:B:255:ALA:HB3	1:B:258:ALA:HB3	1.81	0.62
1:A:130:HIS:ND1	1:A:136:ILE:O	2.33	0.61
1:A:184:GLU:HG3	1:A:191:PHE:HE1	1.66	0.60
1:F:205:PRO:O	1:F:209:GLU:HG2	2.02	0.59
1:E:309:ASP:OD1	1:E:411:LYS:CE	2.50	0.59
1:F:193:SER:HB3	1:F:219:ARG:NH1	2.17	0.58
1:D:328:ARG:HG2	1:D:420:TRP:CZ2	2.38	0.58
1:E:254:ALA:C	1:E:256:GLY:H	2.05	0.58
1:C:36:ASN:ND2	6:C:607:HOH:O	2.37	0.58
1:B:135:GLU:HG2	6:B:608:HOH:O	2.04	0.58
1:E:184:GLU:OE2	1:E:219:ARG:HG2	2.04	0.58
1:A:232:GLU:OE2	1:B:237:ARG:NE	2.27	0.57
1:E:391:ILE:O	1:E:405:SER:OG	2.21	0.57
1:A:125:PHE:CG	1:A:138:ARG:HD2	2.39	0.57
1:C:49:ARG:NH2	1:C:103:GLN:O	2.38	0.57
1:A:82:LEU:HD22	1:A:93:THR:HG22	1.87	0.57
1:C:153:GLU:HB3	1:C:156:PHE:CD2	2.39	0.57
1:D:365:PRO:HG2	2:J:8:THR:HG22	1.85	0.57
1:B:80:LEU:HD23	1:B:105:ILE:HD13	1.86	0.57
1:C:125:PHE:CG	1:C:138:ARG:HD2	2.40	0.57
1:A:83:GLU:HG2	1:A:93:THR:HG23	1.86	0.57
1:D:39:ASP:OD1	1:F:169:LYS:NZ	2.38	0.56
1:A:265:ARG:CG	1:A:266:TYR:N	2.68	0.56
1:F:175:ALA:HB2	1:F:227:LEU:HD23	1.88	0.56
2:J:2:ASN:HD22	2:J:2:ASN:H	1.54	0.56
1:A:237:ARG:HA	1:C:235:MET:CE	2.35	0.56
1:C:79:TRP:HA	1:C:90:ASP:HB2	1.87	0.56
1:E:187:ARG:NE	1:E:187:ARG:HA	2.19	0.56
1:A:136:ILE:O	1:A:136:ILE:HG13	2.05	0.56
1:A:184:GLU:HG3	1:A:191:PHE:CE1	2.42	0.55
2:J:2:ASN:HD22	2:J:2:ASN:N	2.04	0.54
1:D:63:ILE:O	1:D:138:ARG:NH1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:PHE:N	4:G:101:CL:CL	2.62	0.54
1:C:229:GLN:HB3	1:C:233:ILE:HG13	1.89	0.54
1:C:175:ALA:HA	1:C:178:TYR:CE1	2.43	0.53
1:F:125:PHE:O	1:F:141:LYS:NZ	2.41	0.53
1:D:59:ARG:HH11	1:D:59:ARG:HB2	1.73	0.53
1:B:213:LEU:HA	5:B:504:1PE:H131	1.89	0.53
1:F:267:ASP:OD1	1:F:269:VAL:HG22	2.09	0.52
2:H:1:PHE:HA	6:H:101:HOH:O	2.10	0.52
1:A:181:VAL:HG23	1:A:183:ILE:HG23	1.91	0.52
1:E:260:SER:HB2	1:E:280:ILE:HD13	1.91	0.52
1:F:193:SER:HB3	1:F:219:ARG:HH12	1.73	0.52
1:F:49:ARG:NH2	1:F:103:GLN:O	2.43	0.52
1:A:187:ARG:N	1:A:187:ARG:CD	2.73	0.51
1:C:323:THR:HG21	6:C:655:HOH:O	2.11	0.51
1:D:374:LEU:O	1:E:351:LYS:HE2	2.10	0.51
1:C:154:ARG:NH1	1:C:215:ALA:O	2.43	0.51
1:A:198:TYR:O	1:A:202:ILE:HG12	2.11	0.51
1:D:59:ARG:HB2	1:D:59:ARG:NH1	2.26	0.51
1:D:198:TYR:O	1:D:202:ILE:HG12	2.10	0.51
1:A:243:PHE:CE2	1:C:249:LEU:HD11	2.47	0.50
1:B:184:GLU:OE2	1:B:219:ARG:NE	2.42	0.50
1:F:255:ALA:HB3	1:F:258:ALA:HB3	1.92	0.50
1:A:130:HIS:CD2	1:A:134:PRO:HA	2.46	0.50
1:B:208:ARG:NH1	6:B:604:HOH:O	2.24	0.50
1:F:186:ASP:OD1	1:F:187:ARG:N	2.44	0.50
1:A:178:TYR:OH	1:A:223:LEU:HD21	2.12	0.50
1:A:299:PRO:HB3	6:A:674:HOH:O	2.11	0.50
1:A:73:LYS:HB3	1:A:79:TRP:CE2	2.46	0.50
1:D:154:ARG:NH1	1:D:216:THR:O	2.45	0.50
1:C:256:GLY:HA2	6:C:612:HOH:O	2.10	0.49
1:F:193:SER:CB	1:F:219:ARG:NH1	2.75	0.49
1:C:216:THR:OG1	1:C:218:ASP:OD1	2.30	0.49
1:F:322:PRO:HG2	1:F:325:LEU:HD12	1.95	0.49
1:A:187:ARG:N	1:A:187:ARG:HD3	2.28	0.49
1:B:78:LYS:NZ	1:B:88:ALA:O	2.45	0.49
1:D:266:TYR:CE1	1:F:255:ALA:HB2	2.48	0.48
1:D:374:LEU:HD21	1:D:413:LEU:HD21	1.95	0.48
1:A:266:TYR:CE2	1:A:268:THR:HA	2.48	0.48
1:E:309:ASP:OD1	1:E:411:LYS:HE3	2.14	0.48
1:D:273:THR:O	1:F:281:ASP:HB2	2.13	0.48
1:C:37:ALA:HB1	1:C:164:VAL:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:LEU:CD2	1:E:423:ASN:HB3	2.44	0.48
1:F:125:PHE:CG	1:F:138:ARG:HD2	2.49	0.48
1:A:130:HIS:NE2	1:A:134:PRO:HA	2.29	0.47
1:F:66:ASP:OD1	1:F:67:ASN:N	2.40	0.47
1:F:389:ILE:HG13	1:F:410:PRO:HG3	1.96	0.47
1:C:410:PRO:HA	6:C:625:HOH:O	2.15	0.47
1:C:186:ASP:OD2	6:C:601:HOH:O	2.21	0.47
1:C:302:SER:HA	1:C:417:ALA:O	2.14	0.47
1:E:248:GLU:HB3	1:E:261:CYS:HB3	1.96	0.47
1:A:182:LEU:HD23	1:A:221:LEU:HA	1.97	0.46
1:D:73:LYS:HB3	1:D:79:TRP:NE1	2.30	0.46
1:D:184:GLU:OE2	1:D:219:ARG:NH1	2.48	0.46
1:E:254:ALA:C	1:E:256:GLY:N	2.69	0.46
1:F:175:ALA:O	1:F:177:ASP:N	2.48	0.46
1:A:255:ALA:HB2	1:B:266:TYR:CD1	2.50	0.46
1:C:248:GLU:HG2	1:C:263:SER:HB3	1.96	0.46
1:C:83:GLU:OE2	1:C:93:THR:OG1	2.33	0.46
1:E:248:GLU:OE2	1:E:265:ARG:NH2	2.47	0.46
1:D:79:TRP:HA	1:D:90:ASP:HB2	1.97	0.46
1:F:77:LEU:O	1:F:81:LYS:HG3	2.16	0.46
1:E:254:ALA:HB3	1:F:266:TYR:CD2	2.50	0.46
1:C:328:ARG:NH1	1:C:422:GLU:OE2	2.49	0.46
1:D:138:ARG:HH11	1:D:138:ARG:HG2	1.81	0.46
1:C:42:GLU:OE1	1:C:111:TYR:OH	2.32	0.46
1:C:182:LEU:HG	1:C:211:PHE:CZ	2.51	0.46
1:D:73:LYS:HB3	1:D:79:TRP:CE2	2.52	0.45
1:A:80:LEU:HD23	1:A:105:ILE:HD13	1.97	0.45
2:H:10:THR:HG22	2:I:10:THR:HG22	1.98	0.45
1:C:389:ILE:HG13	1:C:410:PRO:HG3	1.98	0.45
1:D:264:VAL:HG11	1:F:260:SER:HB2	1.99	0.45
1:A:154:ARG:HD3	1:A:221:LEU:HD22	1.98	0.45
1:E:66:ASP:OD1	1:E:67:ASN:N	2.45	0.45
1:E:33:LYS:HE2	1:E:163:TYR:HE1	1.82	0.45
1:F:410:PRO:HA	6:F:606:HOH:O	2.17	0.45
1:F:29:GLU:O	1:F:33:LYS:HG3	2.17	0.45
1:F:37:ALA:HB1	1:F:164:VAL:HA	1.99	0.44
1:F:358:GLN:NE2	6:F:612:HOH:O	2.51	0.44
1:C:186:ASP:OD1	1:C:187:ARG:N	2.47	0.44
1:D:125:PHE:CE1	1:D:140:ILE:HG12	2.52	0.44
1:A:126:SER:HB3	1:A:139:GLN:HE21	1.83	0.44
1:A:165:ILE:HB	1:A:178:TYR:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:HG23	1:A:136:ILE:HG22	1.98	0.44
1:B:29:GLU:HG3	1:B:31:MET:H	1.83	0.43
1:B:140:ILE:HG22	1:B:229:GLN:HG3	2.00	0.43
1:A:265:ARG:HG2	1:A:266:TYR:N	2.34	0.43
1:B:391:ILE:HG21	1:B:407:LEU:HD11	1.99	0.43
1:E:70:LYS:HZ1	1:E:188:VAL:HG11	1.84	0.43
1:C:187:ARG:H	1:C:187:ARG:HD2	1.83	0.43
1:D:165:ILE:HD12	1:D:178:TYR:CD2	2.53	0.43
1:D:167:GLU:OE1	1:D:170:LYS:NZ	2.52	0.43
1:F:297:LYS:HA	1:F:421:CYS:O	2.19	0.43
1:A:50:TYR:OH	1:A:63:ILE:HB	2.18	0.43
1:B:302:SER:HA	1:B:417:ALA:O	2.19	0.43
1:F:328:ARG:NH2	6:F:613:HOH:O	2.51	0.43
1:A:83:GLU:HA	1:A:89:GLY:H	1.82	0.43
1:C:194:ASN:OD1	1:C:219:ARG:NH1	2.52	0.43
1:F:184:GLU:OE2	1:F:191:PHE:CE1	2.67	0.43
1:D:271:ASN:N	1:D:271:ASN:HD22	2.16	0.43
1:F:392:GLU:HG3	1:F:395:ILE:HD12	2.00	0.43
1:E:202:ILE:HG13	1:E:203:GLU:HG3	2.01	0.42
1:F:173:PHE:O	6:F:601:HOH:O	2.21	0.42
1:B:59:ARG:HD3	1:B:92:PRO:HB2	2.01	0.42
1:D:328:ARG:HG3	1:D:329:PHE:H	1.84	0.42
1:B:79:TRP:HA	1:B:90:ASP:HB2	2.01	0.42
1:B:125:PHE:CG	1:B:138:ARG:HD2	2.54	0.42
1:C:411:LYS:HB3	1:C:411:LYS:HE2	1.85	0.42
1:E:309:ASP:OD1	1:E:411:LYS:NZ	2.50	0.42
1:F:36:ASN:O	1:F:40:VAL:HG23	2.19	0.42
1:A:266:TYR:HB3	1:C:254:ALA:HB3	2.01	0.42
1:C:77:LEU:O	1:C:81:LYS:HG3	2.19	0.42
1:D:186:ASP:CG	1:D:187:ARG:H	2.22	0.42
1:D:368:LEU:HD13	1:F:368:LEU:HB2	2.01	0.42
1:D:389:ILE:HG13	1:D:410:PRO:HG3	2.00	0.42
1:C:133:ASN:OD1	1:C:135:GLU:HB2	2.19	0.42
1:E:252:ASP:O	1:F:245:GLU:HG2	2.20	0.42
1:E:411:LYS:HE2	1:E:411:LYS:HB3	1.86	0.42
1:D:272:LYS:HA	1:F:281:ASP:OD2	2.19	0.42
1:B:281:ASP:HB2	1:C:273:THR:O	2.19	0.42
1:B:77:LEU:HD13	1:B:105:ILE:HD12	2.01	0.41
1:C:187:ARG:N	1:C:187:ARG:HD2	2.35	0.41
1:D:341:GLN:HG2	1:D:402:ASP:OD2	2.20	0.41
1:A:184:GLU:CG	1:A:191:PHE:CE1	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLU:CD	6:B:606:HOH:O	2.58	0.41
1:E:72:PHE:CZ	1:E:120:GLY:HA3	2.55	0.41
1:A:272:LYS:HG3	1:C:281:ASP:HB3	2.02	0.41
1:D:73:LYS:HB3	1:D:79:TRP:CD1	2.55	0.41
1:C:381:LYS:HB3	1:C:381:LYS:HE3	1.80	0.41
1:A:41:ILE:HD13	1:A:41:ILE:HA	1.85	0.41
1:A:45:SER:O	6:A:601:HOH:O	2.22	0.41
1:C:177:ASP:OD1	1:C:177:ASP:N	2.52	0.41
1:D:302:SER:HA	1:D:417:ALA:O	2.21	0.41
1:D:388:SER:OG	2:K:1:PHE:N	2.38	0.41
1:E:389:ILE:HG13	1:E:410:PRO:HG3	2.01	0.41
1:A:302:SER:HA	1:A:417:ALA:O	2.21	0.41
1:D:245:GLU:OE2	1:F:254:ALA:HB2	2.21	0.41
1:B:244:LEU:HD12	1:C:238:ASP:HB3	2.02	0.41
1:C:175:ALA:HA	1:C:178:TYR:HE1	1.85	0.41
1:E:200:GLU:O	1:E:200:GLU:HG3	2.19	0.41
1:B:391:ILE:HD11	1:B:396:LEU:HD11	2.03	0.41
1:B:40:VAL:HG13	1:B:147:PHE:CE2	2.56	0.40
1:C:279:GLN:HB2	6:C:632:HOH:O	2.20	0.40
1:E:392:GLU:HG3	1:E:395:ILE:HD12	2.03	0.40
1:C:49:ARG:NH1	1:C:238:ASP:OD2	2.54	0.40
1:C:100:LEU:HD11	1:C:237:ARG:HH22	1.86	0.40
1:D:186:ASP:OD2	1:D:191:PHE:HB3	2.21	0.40
1:F:148:GLN:HA	1:F:222:ALA:HA	2.04	0.40
1:D:314:LYS:HB3	1:D:385:VAL:HB	2.02	0.40
1:E:36:ASN:O	1:E:40:VAL:HG23	2.22	0.40
1:E:149:TYR:CZ	1:E:151:GLY:HA3	2.56	0.40
1:C:154:ARG:HH11	1:C:215:ALA:HB1	1.85	0.40
1:C:253:THR:HG22	1:C:258:ALA:O	2.21	0.40
1:D:249:LEU:HD11	1:E:243:PHE:CE2	2.57	0.40
1:F:411:LYS:HE2	1:F:411:LYS:HB3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	389/397 (98%)	374 (96%)	14 (4%)	1 (0%)	41 50
1	B	393/397 (99%)	381 (97%)	12 (3%)	0	100 100
1	C	393/397 (99%)	380 (97%)	13 (3%)	0	100 100
1	D	389/397 (98%)	373 (96%)	15 (4%)	1 (0%)	41 50
1	E	393/397 (99%)	375 (95%)	14 (4%)	4 (1%)	15 17
1	F	393/397 (99%)	381 (97%)	11 (3%)	1 (0%)	41 50
2	G	9/15 (60%)	9 (100%)	0	0	100 100
2	H	9/15 (60%)	9 (100%)	0	0	100 100
2	I	9/15 (60%)	8 (89%)	1 (11%)	0	100 100
2	J	9/15 (60%)	9 (100%)	0	0	100 100
2	K	9/15 (60%)	9 (100%)	0	0	100 100
2	L	9/15 (60%)	9 (100%)	0	0	100 100
All	All	2404/2472 (97%)	2317 (96%)	80 (3%)	7 (0%)	41 50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	258	ALA
1	E	308	GLN
1	E	309	ASP
1	F	176	GLN
1	E	255	ALA
1	A	185	PRO
1	E	189	GLY

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	330/334 (99%)	323 (98%)	7 (2%)	53 70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	334/334 (100%)	331 (99%)	3 (1%)	78 89
1	C	334/334 (100%)	328 (98%)	6 (2%)	59 75
1	D	330/334 (99%)	318 (96%)	12 (4%)	35 49
1	E	334/334 (100%)	330 (99%)	4 (1%)	71 84
1	F	334/334 (100%)	327 (98%)	7 (2%)	53 70
2	G	11/14 (79%)	11 (100%)	0	100 100
2	H	11/14 (79%)	11 (100%)	0	100 100
2	I	11/14 (79%)	11 (100%)	0	100 100
2	J	11/14 (79%)	9 (82%)	2 (18%)	1 1
2	K	11/14 (79%)	11 (100%)	0	100 100
2	L	11/14 (79%)	11 (100%)	0	100 100
All	All	2062/2088 (99%)	2021 (98%)	41 (2%)	55 72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	136	ILE
1	A	181	VAL
1	A	206	SER
1	A	217	LYS
1	A	268	THR
1	A	323	THR
1	B	152	MET
1	B	246	ASP
1	B	333	VAL
1	C	45	SER
1	C	97	ASN
1	C	181	VAL
1	C	309	ASP
1	C	312	ARG
1	C	323	THR
1	D	59	ARG
1	D	68	LYS
1	D	98	ASN
1	D	129	VAL
1	D	217	LYS
1	D	259	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	271	ASN
1	D	297	LYS
1	D	298	THR
1	D	328	ARG
1	D	388	SER
1	D	398	THR
1	E	187	ARG
1	E	200	GLU
1	E	308	GLN
1	E	382	VAL
1	F	159	ASP
1	F	165	ILE
1	F	191	PHE
1	F	216	THR
1	F	312	ARG
1	F	399	SER
1	F	405	SER
2	J	2	ASN
2	J	11	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	B	148	GLN
1	C	176	GLN
1	D	271	ASN
2	J	2	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 (i)

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
5	1PE	B	504	-	15,15,15	0.53	0	14,14,14	0.50	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
5	1PE	B	504	-	-	9/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	1PE	OH6-C15-C25-OH5
5	B	504	1PE	OH4-C13-C23-OH3
5	B	504	1PE	OH5-C14-C24-OH4
5	B	504	1PE	C15-C25-OH5-C14
5	B	504	1PE	C16-C26-OH6-C15
5	B	504	1PE	C24-C14-OH5-C25
5	B	504	1PE	C23-C13-OH4-C24
5	B	504	1PE	OH7-C16-C26-OH6
5	B	504	1PE	C14-C24-OH4-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	1PE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	391/397 (98%)	1.11	79 (20%) 1 1	34, 61, 112, 130	0
1	B	395/397 (99%)	0.57	30 (7%) 13 18	35, 54, 82, 111	0
1	C	395/397 (99%)	0.49	25 (6%) 20 25	34, 59, 91, 105	0
1	D	391/397 (98%)	0.92	61 (15%) 2 2	49, 77, 105, 117	0
1	E	395/397 (99%)	0.49	33 (8%) 11 15	46, 62, 93, 104	0
1	F	395/397 (99%)	0.69	46 (11%) 4 6	47, 71, 97, 115	0
2	G	11/15 (73%)	-0.27	0 100 100	46, 51, 66, 69	0
2	H	11/15 (73%)	-0.01	0 100 100	43, 53, 61, 67	0
2	I	11/15 (73%)	-0.20	0 100 100	45, 51, 68, 71	0
2	J	11/15 (73%)	0.90	0 100 100	72, 82, 87, 90	0
2	K	11/15 (73%)	2.07	5 (45%) 0 0	91, 98, 105, 106	0
2	L	11/15 (73%)	0.88	1 (9%) 9 12	63, 75, 93, 94	0
All	All	2428/2472 (98%)	0.71	280 (11%) 4 7	34, 63, 100, 130	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	GLN	8.8
1	A	129	VAL	8.6
1	A	63	ILE	7.9
1	A	128	TYR	7.8
1	A	188	VAL	7.3
1	F	188	VAL	7.2
1	F	269	VAL	6.7
1	A	91	VAL	6.6
1	A	61	ASN	6.1
1	B	187	ARG	6.1
1	D	129	VAL	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	95	GLY	6.1
1	A	60	THR	6.1
1	A	127	THR	5.8
1	B	188	VAL	5.7
1	D	131	PRO	5.7
1	D	97	ASN	5.6
1	F	213	LEU	5.6
1	A	136	ILE	5.5
1	D	357	THR	5.4
1	A	72	PHE	5.4
1	C	188	VAL	5.3
1	A	134	PRO	5.3
1	A	123	PHE	5.2
1	E	188	VAL	5.1
1	A	143	VAL	5.1
1	F	266	TYR	5.1
1	A	140	ILE	5.1
1	D	100	LEU	5.1
1	D	380	ASN	5.1
1	D	136	ILE	5.0
1	C	257	SER	5.0
1	A	82	LEU	5.0
1	A	65	LYS	5.0
1	A	130	HIS	4.9
1	A	125	PHE	4.9
1	D	188	VAL	4.9
1	A	92	PRO	4.9
1	E	312	ARG	4.9
1	C	29	GLU	4.8
1	C	175	ALA	4.7
1	A	100	LEU	4.7
1	A	126	SER	4.7
1	A	133	ASN	4.7
2	K	6	SER	4.6
1	D	64	LEU	4.6
1	A	64	LEU	4.6
2	K	5	TYR	4.5
1	A	99	ASP	4.4
1	F	219	ARG	4.4
1	D	256	GLY	4.4
1	D	94	THR	4.3
1	D	381	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	134	PRO	4.2
1	A	77	LEU	4.1
1	D	98	ASN	4.1
1	E	269	VAL	4.1
1	D	325	LEU	4.1
1	B	254	ALA	4.1
1	D	128	TYR	4.0
1	D	398	THR	4.0
1	F	63	ILE	3.9
1	C	216	THR	3.9
1	F	234	ALA	3.9
1	A	113	LYS	3.8
1	E	311	GLY	3.8
1	A	84	ASN	3.8
1	B	332	VAL	3.8
1	A	78	LYS	3.8
1	A	85	CYS	3.8
1	D	91	VAL	3.7
1	C	176	GLN	3.7
1	E	255	ALA	3.7
1	A	95	GLY	3.7
1	E	95	GLY	3.7
1	D	378	LEU	3.7
1	A	135	GLU	3.6
1	D	269	VAL	3.7
1	F	268	THR	3.6
1	E	391	ILE	3.6
1	A	79	TRP	3.6
1	E	313	ALA	3.6
1	D	96	ASN	3.6
1	E	401	ILE	3.6
1	D	399	SER	3.5
1	B	416	ILE	3.5
1	F	67	ASN	3.5
1	A	53	LEU	3.5
1	E	398	THR	3.4
1	A	332	VAL	3.4
1	D	130	HIS	3.4
1	D	343	ALA	3.4
1	D	58	ASN	3.4
1	B	189	GLY	3.4
1	B	233	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	58	ASN	3.4
1	A	56	ILE	3.4
1	A	119	PHE	3.4
1	A	87	THR	3.3
1	E	400	GLY	3.3
1	E	308	GLN	3.3
1	C	156	PHE	3.3
1	A	62	PRO	3.3
1	E	359	LYS	3.3
1	F	218	ASP	3.2
1	E	353	SER	3.2
1	F	265	ARG	3.2
1	A	86	PRO	3.1
1	B	98	ASN	3.1
1	E	184	GLU	3.1
1	B	415	PHE	3.1
1	C	332	VAL	3.1
1	B	417	ALA	3.1
1	F	187	ARG	3.1
1	F	191	PHE	3.1
1	C	269	VAL	3.1
1	C	254	ALA	3.0
1	B	333	VAL	3.0
1	E	399	SER	3.0
1	D	99	ASP	3.0
1	F	241	VAL	3.0
1	F	141	LYS	3.0
1	E	394	GLY	3.0
1	D	132	SER	3.0
1	F	257	SER	3.0
1	A	333	VAL	3.0
1	B	418	PHE	2.9
1	A	67	ASN	2.9
1	A	54	SER	2.9
1	A	141	LYS	2.9
1	F	222	ALA	2.9
1	A	132	SER	2.8
1	D	56	ILE	2.8
1	F	30	LEU	2.8
1	F	272	LYS	2.8
1	F	233	ILE	2.8
1	B	190	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	219	ARG	2.8
1	A	83	GLU	2.8
1	B	376	TRP	2.8
1	D	395	ILE	2.7
1	C	218	ASP	2.7
1	D	400	GLY	2.7
1	C	97	ASN	2.7
1	D	241	VAL	2.7
1	D	407	LEU	2.7
1	E	396	LEU	2.7
1	D	323	THR	2.7
1	C	265	ARG	2.7
1	D	360	ASP	2.7
1	D	361	GLY	2.7
1	B	331	ALA	2.7
1	E	186	ASP	2.7
1	F	182	LEU	2.7
1	E	187	ARG	2.7
1	E	361	GLY	2.7
1	A	139	GLN	2.6
1	D	234	ALA	2.6
1	F	127	THR	2.6
1	A	57	ASN	2.6
1	D	255	ALA	2.6
1	F	180	ILE	2.6
1	F	64	LEU	2.6
1	F	125	PHE	2.6
1	A	138	ARG	2.6
1	A	187	ARG	2.6
1	A	47	ILE	2.6
1	A	183	ILE	2.6
1	D	84	ASN	2.6
1	F	136	ILE	2.6
1	F	140	ILE	2.6
1	C	30	LEU	2.5
1	A	94	THR	2.5
1	A	235	MET	2.5
1	B	191	PHE	2.5
2	K	11	VAL	2.5
1	D	271	ASN	2.5
1	A	88	ALA	2.5
1	A	258	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	234	ALA	2.5
1	D	368	LEU	2.5
1	F	123	PHE	2.5
1	B	174	SER	2.5
1	D	63	ILE	2.5
1	A	131	PRO	2.5
1	E	235	MET	2.4
1	C	217	LYS	2.4
1	F	211	PHE	2.4
1	F	200	GLU	2.4
1	B	334	SER	2.4
1	F	255	ALA	2.4
1	D	322	PRO	2.4
1	E	191	PHE	2.4
1	D	265	ARG	2.4
1	A	93	THR	2.4
1	A	73	LYS	2.4
1	F	395	ILE	2.4
1	A	76	ASP	2.4
1	E	309	ASP	2.4
1	E	397	PRO	2.4
1	B	303	THR	2.4
1	F	137	GLN	2.4
1	A	414	SER	2.4
1	D	363	LYS	2.3
1	A	69	ALA	2.3
1	B	300	VAL	2.3
1	B	385	VAL	2.3
1	D	382	VAL	2.3
1	A	50	TYR	2.3
1	A	104	PHE	2.3
1	F	122	GLN	2.3
1	F	142	GLN	2.3
1	D	93	THR	2.3
1	C	95	GLY	2.3
1	E	185	PRO	2.3
1	C	271	ASN	2.3
1	A	111	TYR	2.3
1	F	126	SER	2.3
1	D	85	CYS	2.3
1	E	172	GLY	2.3
1	D	312	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	68	LYS	2.3
1	A	190	TYR	2.2
1	E	266	TYR	2.2
1	A	184	GLU	2.2
1	A	234	ALA	2.2
1	F	70	LYS	2.2
1	D	423	ASN	2.2
1	F	380	ASN	2.2
2	K	10	THR	2.2
1	B	302	SER	2.2
1	A	71	GLU	2.2
1	D	187	ARG	2.2
1	F	267	ASP	2.2
1	D	133	ASN	2.2
1	D	55	LYS	2.2
1	F	215	ALA	2.2
1	A	105	ILE	2.2
1	B	374	LEU	2.2
1	C	152	MET	2.2
1	A	334	SER	2.1
1	B	414	SER	2.1
1	A	89	GLY	2.1
1	F	235	MET	2.1
1	A	418	PHE	2.1
1	B	372	ILE	2.1
1	E	249	LEU	2.1
2	K	7	SER	2.1
1	C	235	MET	2.1
1	C	333	VAL	2.1
1	B	329	PHE	2.1
1	A	416	ILE	2.1
1	A	66	ASP	2.1
1	E	360	ASP	2.1
2	L	3	ASP	2.1
1	D	168	ALA	2.1
1	D	270	GLY	2.1
1	D	65	LYS	2.1
1	E	257	SER	2.1
1	D	372	ILE	2.1
1	E	268	THR	2.1
1	D	257	SER	2.1
1	F	209	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	233	ILE	2.0
1	B	235	MET	2.0
1	C	96	ASN	2.0
1	F	204	ASN	2.0
1	A	331	ALA	2.0
1	B	175	ALA	2.0
1	B	257	SER	2.0
1	D	333	VAL	2.0
1	C	70	LYS	2.0
1	C	416	ILE	2.0
1	D	235	MET	2.0
1	D	364	GLY	2.0
1	E	354	GLN	2.0
1	F	270	GLY	2.0
1	B	52	SER	2.0
1	F	45	SER	2.0
1	A	330	ALA	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	CA	B	503	1/1	0.78	0.33	88,88,88,88	0
3	CA	D	501	1/1	0.80	0.11	85,85,85,85	0
3	CA	B	502	1/1	0.84	0.12	59,59,59,59	0
4	CL	D	502	1/1	0.84	0.13	86,86,86,86	0
3	CA	E	502	1/1	0.86	0.19	69,69,69,69	0
5	1PE	B	504	16/16	0.89	0.17	54,64,71,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	502	1/1	0.90	0.24	85,85,85,85	0
4	CL	E	504	1/1	0.90	0.07	95,95,95,95	0
3	CA	E	503	1/1	0.90	0.22	102,102,102,102	0
4	CL	L	101	1/1	0.92	0.13	66,66,66,66	0
3	CA	B	501	1/1	0.93	0.28	67,67,67,67	0
4	CL	I	101	1/1	0.94	0.17	53,53,53,53	0
3	CA	F	501	1/1	0.95	0.21	82,82,82,82	0
3	CA	E	501	1/1	0.95	0.25	73,73,73,73	0
4	CL	A	502	1/1	0.97	0.10	54,54,54,54	0
3	CA	A	501	1/1	0.97	0.07	66,66,66,66	0
4	CL	G	101	1/1	0.98	0.07	54,54,54,54	0
3	CA	C	501	1/1	0.98	0.27	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.