



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 AM UTC

PDB ID : 7W64 / pdb_00007w64
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 ⓘ 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

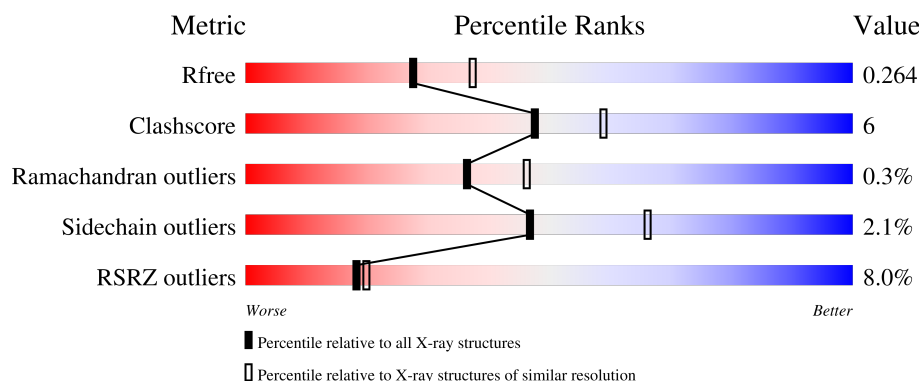
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	397	11% 85% 12% ..
1	B	397	2% 90% 10% .
1	C	397	5% 83% 17% .
1	D	397	15% 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	E	397	7% 88% 11% ..
1	F	397	7% 83% 16% .
2	G	15	67% 7% 27%
2	H	15	7% 60% 13% 27%
2	I	15	7% 60% 13% 27%
2	J	15	33% 53% 13% 7% 27%
2	K	15	27% 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			

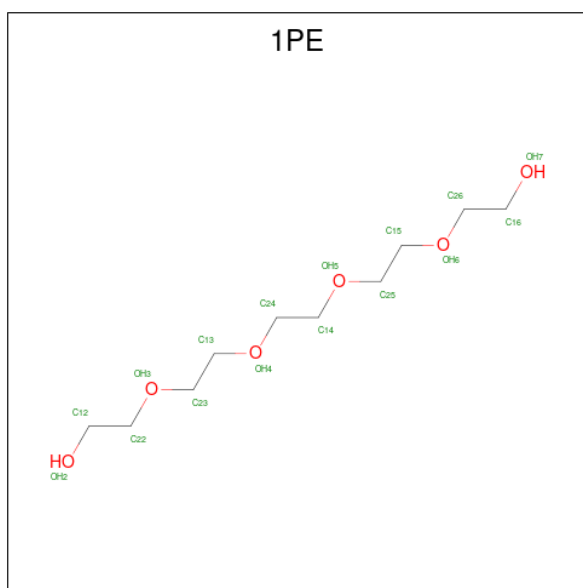
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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 (CCD ID: 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 (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

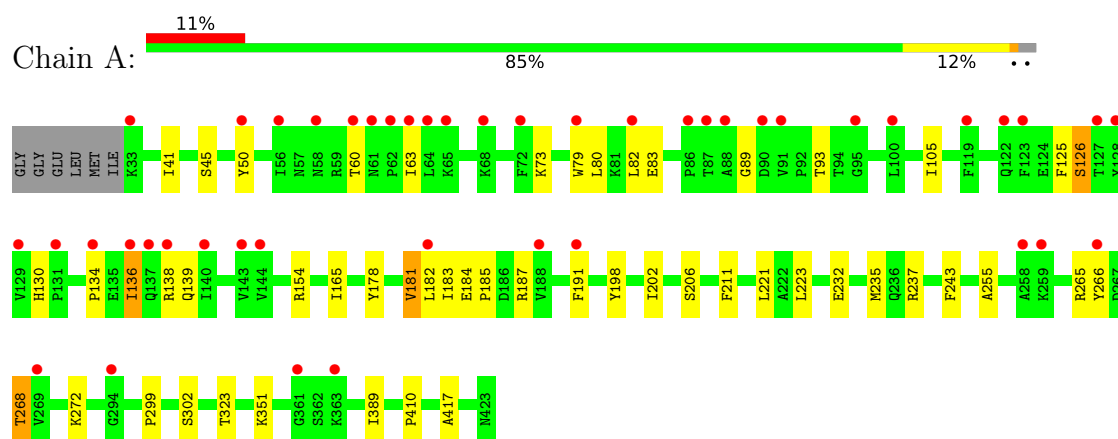
- Molecule 6 is water.

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

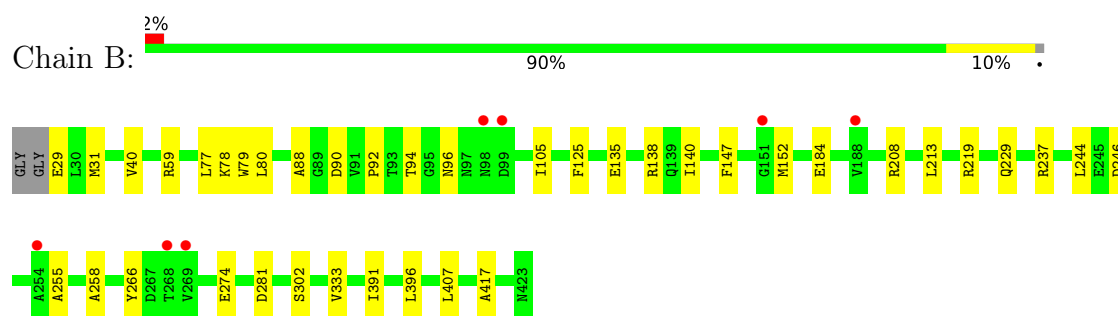
3 Residue-property plots [i](#)

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.

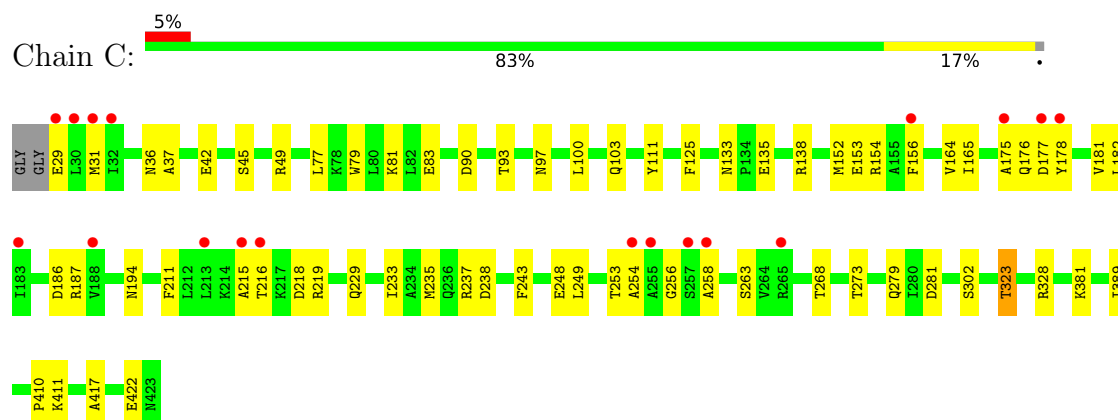
- Molecule 1: Toxin-coregulated pilus biosynthesis protein B



- Molecule 1: Toxin-coregulated pilus biosynthesis protein B



- Molecule 1: Toxin-coregulated pilus biosynthesis protein B



Chain D:

15% 83% 14%

GLY
GLY
GLU
LEU
MET
ILE
K33
D39
R59
I63
L64
K68
K73
W79
E83
F86
T87
A88
G89
D90
V91
P92
T93
N98
D99
L100
Q101
F125
V129
H130
P131
P134
E135
I136
Q137
R138
Q139
I140
M152
F153
R154
I165
S166
E167
V170

Y178
E184
F185
D186
R187
V188
G189
Y190
F191
Y198
I202
T216
K217
D218
R219
M235
F243
L244
E245
L249
A255
G256
S257
A258
K259
V264
R265
Y266
D267
T268
V269
G270
N271
K272
T273
K297
T298
S302
F307
G311
R312
A313
K314
T315
I316
C321
G324
R328
F329
G340
Q341
R342
A343
S346
S353
T357
Q358
K359
S362
K363
G364
R366
A367
L368
I372
S373
L374
N375
W376
T377
L378
T379
N380
K381
V382
W383
D384
V385
T386
A387
S388
I389
G390
I391
I395
T398
I401
D402
S403
G404
S405
L406
I407

Chain E:

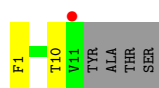
7% 88% 11%

GLY GLY E29 L30 M31 I32 K33 N36 V40 D66 N67 K70 F71 F72 G95 L100 G120 V129 Y149 H150 G151 Y163 E184 P185 D186 R187 V188 G189 Y190 F191 E200 F201 I202 E203 R219 F243 E248 D252 T253 A254 A255 G256 S257 A258 R259 S260 C261 R265 I280 F307 Q308 D309 A313 L325 F336 K344 F345 K351 D352 S353 Q354 G355 T356 T357 Q358 K359 D360 G361 P365 H366 A367 L368 L369 V392 I389 G390 I391 E392 I395 S405 L406 L407 P410 K411 N423

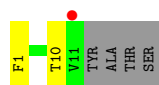
Chain F:

Chain G:

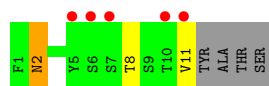
● Molecule 2: TcpF



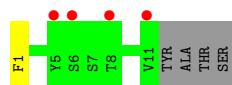
● Molecule 2: TcpF



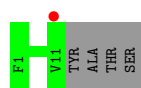
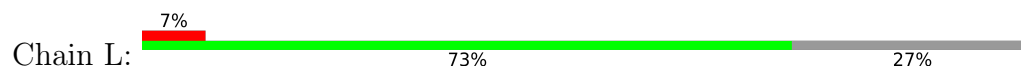
● Molecule 2: TcpF



● Molecule 2: TcpF



● Molecule 2: TcpF



4 Data and refinement statistics

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 37.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.20-2.30) 98.7 (37.20-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
R, R_{free}	0.222 , 0.264 0.221 , 0.264	Depositor DCC
R_{free} test set	13808 reflections (9.78%)	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)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 1PE, CL

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	0.46	0/3075	0.68	0/4157
1	B	0.51	0/3108	0.67	0/4201
1	C	0.45	0/3108	0.63	0/4201
1	D	0.41	0/3075	0.61	0/4157
1	E	0.46	0/3108	0.65	0/4201
1	F	0.41	0/3108	0.60	0/4201
2	G	0.40	0/87	0.52	0/118
2	H	0.36	0/87	0.68	0/118
2	I	0.34	0/87	0.54	0/118
2	J	0.27	0/87	0.49	0/118
2	K	0.29	0/87	0.51	0/118
2	L	0.30	0/87	0.41	0/118
All	All	0.45	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3020	0	2933	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3053	0	2970	23	0
1	C	3053	0	2970	47	0
1	D	3020	0	2933	42	0
1	E	3053	0	2972	28	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	2	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	1	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	7	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	208	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 6.

All (208) 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

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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: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:237:ARG:HA	1:C:235:MET:HE2	1.79	0.64
1:A:389:ILE:HG13	1:A:410:PRO:HG3	1.80	0.64
1:E:254:ALA:C	1:E:256:GLY:H	2.05	0.63
1:C:235:MET:HE3	1:C:243:PHE:CD1	2.35	0.62
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: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	0.55
2:G:1:PHE:N	4:G:101:CL:CL	2.62	0.55
1:A:184:GLU:HG3	1:A:191:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LYS:HZ2	1:E:188:VAL:HG11	1.71	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
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
2:I:1:PHE:N	4:I:101:CL:CL	2.78	0.52
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:E:254:ALA:C	1:E:256:GLY:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:186:ASP:CG	1:D:187:ARG:H	2.22	0.47
1:D:235:MET:HE2	1:D:243:PHE:CE2	2.50	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: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:B:274:GLU:CD	6:B:606:HOH:O	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:94:THR:C	1:B:96:ASN:H	2.26	0.44
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:C:152:MET:HE3	1:C:152:MET:HB2	1.82	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:A:351:LYS:NZ	6:C:604:HOH:O	2.50	0.43
1:B:391:ILE:HG21	1:B:407:LEU:HD11	1.99	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:D:271:ASN:C	1:D:271:ASN:HD22	2.24	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:216:THR:OG1	1:D:218:ASP:OD1	2.26	0.43
1:D:271:ASN:HD22	1:D:271:ASN:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:29:GLU:OE2	1:E:31:MET:HE2	2.21	0.41
1:A:211:PHE:CD1	1:A:211:PHE:C	2.98	0.41
1:A:235:MET:HE2	1:A:243:PHE:CZ	2.55	0.41
1:C:381:LYS:HB3	1:C:381:LYS:HE3	1.80	0.41
1:D:93:THR:HG1	1:D:101:GLN:CD	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	46
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%)	36	46
1	E	393/397 (99%)	375 (95%)	14 (4%)	4 (1%)	12	15
1	F	393/397 (99%)	381 (97%)	11 (3%)	1 (0%)	36	46
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%)	36	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	258	ALA
1	E	308	GLN

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Mol	Chain	Res	Type
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 ⓘ

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%)	324 (98%)	6 (2%)	51	70
1	B	334/334 (100%)	331 (99%)	3 (1%)	70	84
1	C	334/334 (100%)	328 (98%)	6 (2%)	51	70
1	D	330/334 (99%)	318 (96%)	12 (4%)	31	47
1	E	334/334 (100%)	330 (99%)	4 (1%)	63	79
1	F	334/334 (100%)	324 (97%)	10 (3%)	36	53
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%)	2	2
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%)	2019 (98%)	43 (2%)	47	66

All (43) 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	268	THR

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Mol	Chain	Res	Type
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	165	ILE
1	C	181	VAL
1	C	268	THR
1	C	323	THR
1	D	59	ARG
1	D	68	LYS
1	D	98	ASN
1	D	100	LEU
1	D	129	VAL
1	D	170	LYS
1	D	259	LYS
1	D	271	ASN
1	D	297	LYS
1	D	298	THR
1	D	388	SER
1	D	398	THR
1	E	129	VAL
1	E	200	GLU
1	E	308	GLN
1	E	382	VAL
1	F	32	ILE
1	F	129	VAL
1	F	143	VAL
1	F	159	ASP
1	F	165	ILE
1	F	191	PHE
1	F	199	GLU
1	F	216	THR
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	137	GLN
1	A	139	GLN
1	A	194	ASN
1	A	236	GLN
1	B	148	GLN
1	B	229	GLN
1	B	326	ASN
1	B	358	GLN
1	C	58	ASN
1	C	101	GLN
1	C	122	GLN
1	C	176	GLN
1	C	326	ASN
1	C	342	ASN
1	C	358	GLN
1	D	137	GLN
1	D	210	ASN
1	D	271	ASN
1	E	194	ASN
1	E	326	ASN
1	E	342	ASN
1	E	358	GLN
1	F	358	GLN
2	J	2	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.54	0	14,14,14	0.49	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	-	-	10/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) 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	C24-C14-OH5-C25
5	B	504	1PE	C16-C26-OH6-C15
5	B	504	1PE	C23-C13-OH4-C24
5	B	504	1PE	OH7-C16-C26-OH6
5	B	504	1PE	C14-C24-OH4-C13
5	B	504	1PE	C25-C15-OH6-C26

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 [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	391/397 (98%)	0.77	45 (11%) 9 10	34, 61, 112, 130	0
1	B	395/397 (99%)	0.37	7 (1%) 67 69	35, 54, 82, 111	0
1	C	395/397 (99%)	0.51	18 (4%) 37 39	34, 59, 91, 105	0
1	D	391/397 (98%)	1.08	59 (15%) 5 6	49, 77, 105, 117	0
1	E	395/397 (99%)	0.68	27 (6%) 23 25	46, 62, 93, 104	0
1	F	395/397 (99%)	0.85	27 (6%) 23 25	47, 71, 97, 115	0
2	G	11/15 (73%)	0.29	0 100 100	46, 51, 66, 69	0
2	H	11/15 (73%)	0.51	1 (9%) 15 16	43, 53, 61, 67	0
2	I	11/15 (73%)	0.43	1 (9%) 15 16	45, 51, 68, 71	0
2	J	11/15 (73%)	1.88	5 (45%) 0 0	72, 82, 87, 90	0
2	K	11/15 (73%)	1.98	4 (36%) 1 1	91, 98, 105, 106	0
2	L	11/15 (73%)	1.67	1 (9%) 15 16	63, 75, 93, 94	0
All	All	2428/2472 (98%)	0.72	195 (8%) 18 20	34, 63, 100, 130	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	11	VAL	5.2
2	K	11	VAL	4.8
2	J	11	VAL	4.6
1	A	100	LEU	4.2
1	C	188	VAL	4.1
1	C	178	TYR	4.1
1	B	254	ALA	4.0
1	D	188	VAL	4.0
1	A	61	ASN	4.0
1	A	188	VAL	3.9
1	C	175	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	313	ALA	3.7
1	A	63	ILE	3.6
1	C	30	LEU	3.6
1	D	129	VAL	3.6
1	D	100	LEU	3.6
1	E	255	ALA	3.6
1	A	128	TYR	3.6
1	D	406	LEU	3.5
1	D	88	ALA	3.5
1	F	30	LEU	3.4
1	A	72	PHE	3.4
1	B	269	VAL	3.4
1	A	258	ALA	3.4
1	A	361	GLY	3.4
1	F	213	LEU	3.4
2	K	5	TYR	3.4
1	D	395	ILE	3.3
1	A	91	VAL	3.3
1	A	136	ILE	3.3
1	A	88	ALA	3.3
1	D	378	LEU	3.3
1	D	382	VAL	3.3
1	A	140	ILE	3.2
2	K	6	SER	3.2
1	E	186	ASP	3.1
1	F	175	ALA	3.1
1	A	137	GLN	3.1
1	F	256	GLY	3.1
1	D	377	THR	3.0
1	D	383	TRP	3.0
1	E	258	ALA	3.0
1	F	185	PRO	3.0
1	A	56	ILE	3.0
1	A	123	PHE	3.0
1	A	64	LEU	3.0
1	A	129	VAL	3.0
1	E	391	ILE	3.0
1	D	268	THR	3.0
1	D	269	VAL	2.9
1	D	385	VAL	2.9
1	C	29	GLU	2.9
1	D	404	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	329	PHE	2.9
1	E	185	PRO	2.9
1	A	127	THR	2.8
1	A	363	LYS	2.8
1	A	95	GLY	2.8
1	C	258	ALA	2.8
1	F	188	VAL	2.8
1	B	188	VAL	2.8
2	H	11	VAL	2.8
2	J	5	TYR	2.8
1	C	255	ALA	2.8
1	D	307	PHE	2.8
1	E	188	VAL	2.8
1	F	268	THR	2.7
1	D	91	VAL	2.7
1	D	33	LYS	2.7
1	F	216	THR	2.7
1	C	32	ILE	2.7
1	C	31	MET	2.7
1	A	82	LEU	2.7
1	F	178	TYR	2.6
1	F	211	PHE	2.6
1	D	357	THR	2.6
2	K	8	THR	2.6
1	D	256	GLY	2.6
1	A	131	PRO	2.6
1	F	391	ILE	2.6
1	A	65	LYS	2.6
1	E	313	ALA	2.6
1	E	191	PHE	2.6
1	A	87	THR	2.6
1	A	86	PRO	2.6
1	F	369	LEU	2.6
1	A	143	VAL	2.6
1	D	189	GLY	2.6
1	C	183	ILE	2.6
1	D	401	ILE	2.6
1	D	343	ALA	2.5
1	D	364	GLY	2.5
1	D	389	ILE	2.5
1	E	353	SER	2.5
1	D	407	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	58	ASN	2.5
1	F	254	ALA	2.5
1	F	290	PHE	2.5
1	F	266	TYR	2.5
1	C	254	ALA	2.5
1	D	368	LEU	2.5
1	D	87	THR	2.4
1	D	265	ARG	2.4
1	F	191	PHE	2.4
2	J	7	SER	2.4
1	D	376	TRP	2.4
1	D	420	TRP	2.4
1	E	357	THR	2.4
2	J	6	SER	2.4
1	F	56	ILE	2.4
2	I	11	VAL	2.4
1	A	79	TRP	2.4
1	D	374	LEU	2.4
1	A	62	PRO	2.4
1	C	215	ALA	2.4
1	D	311	GLY	2.4
1	E	254	ALA	2.4
1	A	33	LYS	2.4
1	E	369	LEU	2.4
1	D	258	ALA	2.3
1	C	216	THR	2.3
1	D	362	SER	2.3
1	C	265	ARG	2.3
1	F	182	LEU	2.3
1	A	90	ASP	2.3
1	A	266	TYR	2.3
1	C	156	PHE	2.3
1	E	184	GLU	2.3
1	E	344	ASN	2.3
1	A	191	PHE	2.3
1	C	213	LEU	2.3
1	D	380	ASN	2.3
1	D	324	GLY	2.3
1	D	266	TYR	2.3
1	D	367	ALA	2.3
1	E	367	ALA	2.3
1	D	398	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	257	SER	2.3
1	E	407	LEU	2.2
1	C	177	ASP	2.2
1	E	95	GLY	2.2
1	A	50	TYR	2.2
1	D	353	SER	2.2
1	D	359	LYS	2.2
1	A	294	GLY	2.2
1	E	361	GLY	2.2
1	D	316	ILE	2.2
1	D	134	PRO	2.2
1	B	268	THR	2.2
1	A	182	LEU	2.2
1	D	136	ILE	2.2
1	D	372	ILE	2.2
1	F	129	VAL	2.2
1	E	336	PHE	2.2
1	A	68	LYS	2.2
1	A	259	LYS	2.2
1	E	355	GLY	2.2
1	D	387	ALA	2.2
1	F	255	ALA	2.2
1	D	152	MET	2.1
1	A	119	PHE	2.1
1	A	134	PRO	2.1
1	F	354	GLN	2.1
1	D	340	GLY	2.1
1	D	346	SER	2.1
1	D	417	ALA	2.1
1	F	100	LEU	2.1
1	A	122	GLN	2.1
1	D	131	PRO	2.1
1	E	365	PRO	2.1
1	D	321	CYS	2.1
1	A	60	THR	2.1
1	E	100	LEU	2.1
1	B	98	ASN	2.1
1	E	352	ASP	2.1
1	A	144	VAL	2.1
2	J	10	THR	2.1
1	D	64	LEU	2.1
1	A	269	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLY	2.1
1	E	345	PHE	2.1
1	A	138	ARG	2.1
1	D	257	SER	2.0
1	B	99	ASP	2.0
1	F	218	ASP	2.0
1	D	391	ILE	2.0
1	F	395	ILE	2.0
1	D	86	PRO	2.0
1	E	307	PHE	2.0
1	E	359	LYS	2.0
1	D	379	THR	2.0
1	F	127	THR	2.0
1	F	258	ALA	2.0
1	F	64	LEU	2.0
1	E	389	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
3	CA	E	503	1/1	0.72	0.10	102,102,102,102	0
3	CA	B	503	1/1	0.78	0.17	88,88,88,88	0
3	CA	D	501	1/1	0.85	0.10	85,85,85,85	0
4	CL	D	502	1/1	0.85	0.15	86,86,86,86	0
3	CA	B	502	1/1	0.86	0.10	59,59,59,59	0
3	CA	E	502	1/1	0.86	0.14	69,69,69,69	0
5	1PE	B	504	16/16	0.86	0.13	54,64,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	I	101	1/1	0.93	0.09	53,53,53,53	0
4	CL	E	504	1/1	0.93	0.09	95,95,95,95	0
3	CA	C	502	1/1	0.94	0.13	85,85,85,85	0
4	CL	L	101	1/1	0.94	0.18	66,66,66,66	0
3	CA	E	501	1/1	0.94	0.16	73,73,73,73	0
3	CA	B	501	1/1	0.95	0.18	67,67,67,67	0
3	CA	F	501	1/1	0.96	0.12	82,82,82,82	0
4	CL	A	502	1/1	0.97	0.09	54,54,54,54	0
3	CA	C	501	1/1	0.97	0.10	65,65,65,65	0
4	CL	G	101	1/1	0.98	0.06	54,54,54,54	0
3	CA	A	501	1/1	0.98	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.