



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:57 PM GMT

PDB ID : 2BMC
Title : AURORA-2 T287D T288D COMPLEXED WITH PHA-680632
Authors : Cameron, A.D.; Izzo, G.; Sagliano, A.; Rusconi, L.; Storici, P.; Fancelli, D.; Berta, D.; Bindi, S.; Catana, C.; Forte, B.; Giordano, P.; Mantegani, S.; Meroni, M.; Moll, J.; Pittala, V.; Severino, D.; Tonani, R.; Varasi, M.; Vulpetti, A.; Vianello, P.
Deposited on : 2005-03-11
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

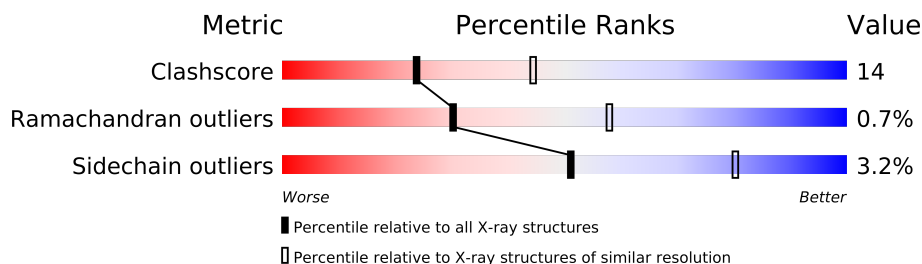
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	
1	F	306	

2 Entry composition i

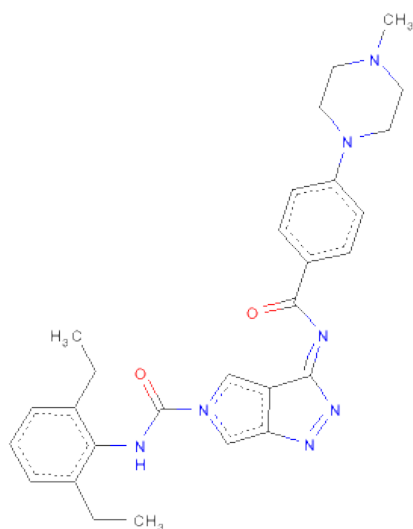
There are 3 unique types of molecules in this entry. The entry contains 13094 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SERINE THREONINE-PROTEIN KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	B	258	Total	C	N	O	S	0	0	0
			2125	1367	373	379	6			
1	C	257	Total	C	N	O	S	0	0	0
			2116	1362	371	377	6			
1	D	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	E	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	F	257	Total	C	N	O	S	0	0	0
			2116	1361	371	378	6			

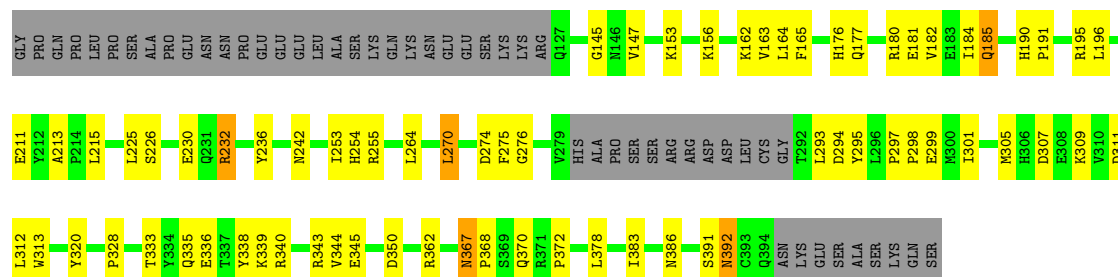
- Molecule 2 is (3E)-N-(2,6-DIETHYLPHENYL)-3-{[4-(4-METHYLPYPERAZIN-1-YL)BENZYL]IMINO}PYRROLO[3,4-C]PYRAZOLE-5(3H)-CARBOXAMIDE (three-letter code: MPY) (formula: C₂₈H₃₁N₇O₂).



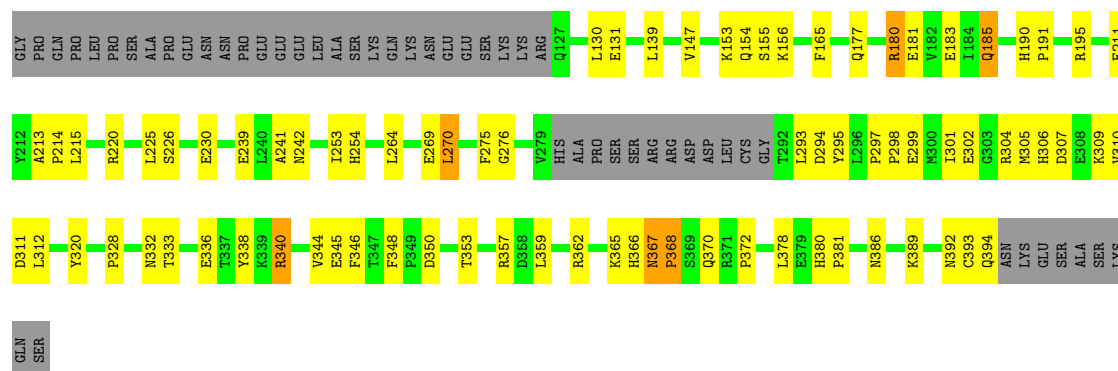
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	28	7	2		
2	B	1	Total	C	N	O	0	0
			37	28	7	2		
2	C	1	Total	C	N	O	0	0
			37	28	7	2		
2	D	1	Total	C	N	O	0	0
			37	28	7	2		
2	E	1	Total	C	N	O	0	0
			37	28	7	2		
2	F	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 3 is water.

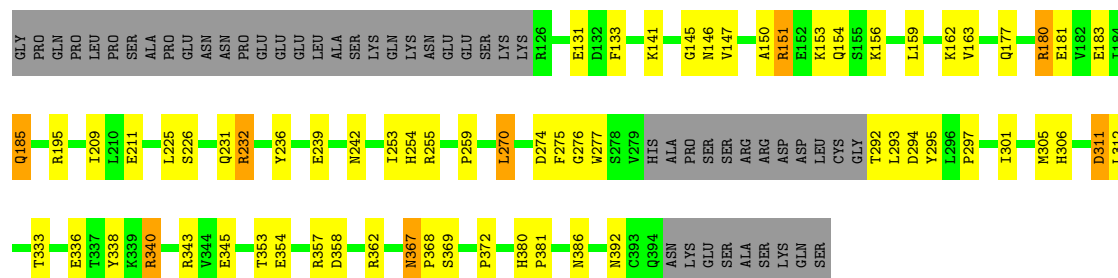
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	37	Total	O	0	0
			37	37		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		
3	E	29	Total	O	0	0
			29	29		
3	F	37	Total	O	0	0
			37	37		

Chain D: 

- Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

Chain E: 

- Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

Chain F: 

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 101.22Å 101.49Å 115.73° 92.40° 101.54°	Depositor
Resolution (Å)	29.95 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (29.95-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13094	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPY

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	0.35	0/2157	0.60	0/2915
1	B	0.34	0/2177	0.61	0/2940
1	C	0.35	0/2168	0.62	0/2928
1	D	0.33	0/2157	0.59	0/2915
1	E	0.32	0/2157	0.60	0/2915
1	F	0.34	0/2168	0.62	0/2929
All	All	0.34	0/12984	0.61	0/17542

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2105	0	2107	51	0
1	B	2125	0	2133	62	0
1	C	2116	0	2125	58	0
1	D	2105	0	2107	70	0
1	E	2105	0	2107	94	0
1	F	2116	0	2120	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	37	0	31	2	0
2	B	37	0	31	2	0
2	C	37	0	31	3	0
2	D	37	0	31	2	0
2	E	37	0	31	1	0
2	F	37	0	31	1	0
3	A	45	0	0	0	0
3	B	37	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
3	E	29	0	0	2	0
3	F	37	0	0	0	0
All	All	13094	0	12885	369	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (369) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:151:ARG:HD3	1:F:156:LYS:HA	1.50	0.93
1:E:348:PHE:CE2	1:E:357:ARG:HA	2.15	0.81
1:C:253:ILE:HG21	1:C:308:GLU:HG2	1.63	0.80
1:B:367:ASN:HD22	1:B:370:GLN:HG3	1.46	0.80
1:E:333:THR:OG1	1:E:336:GLU:HG3	1.83	0.78
1:D:153:LYS:O	1:D:156:LYS:HE3	1.85	0.77
1:F:185:GLN:HG3	1:F:275:PHE:CD2	2.19	0.76
1:F:131:GLU:O	1:F:153:LYS:HE2	1.85	0.76
1:E:346:PHE:HE1	1:E:348:PHE:CE1	2.04	0.75
1:E:340:ARG:HB3	1:E:340:ARG:HH11	1.51	0.75
1:B:362:ARG:NH2	1:F:343:ARG:HB3	2.02	0.75
1:D:242:ASN:HD21	1:D:392:ASN:H	1.35	0.75
1:B:367:ASN:HD22	1:B:370:GLN:CG	2.00	0.74
1:F:242:ASN:HD21	1:F:392:ASN:H	1.36	0.74
1:E:348:PHE:HE2	1:E:357:ARG:HA	1.52	0.73
1:B:162:LYS:HE2	1:B:164:LEU:HD21	1.70	0.72
1:C:378:LEU:HD22	1:C:391:SER:HB2	1.72	0.71
1:D:242:ASN:ND2	1:D:392:ASN:H	1.90	0.69
1:D:254:HIS:HE1	1:D:274:ASP:OD1	1.76	0.69
1:F:254:HIS:HD2	1:F:255:ARG:O	1.77	0.68
1:C:254:HIS:HD2	1:C:255:ARG:O	1.78	0.67
1:E:348:PHE:CD2	1:E:357:ARG:HG2	2.30	0.67
1:E:253:ILE:HD13	1:E:307:ASP:HB2	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:298:PRO:O	1:E:302:GLU:HG3	1.95	0.66
1:E:297:PRO:HB2	1:E:299:GLU:OE2	1.96	0.66
1:F:232:ARG:HB2	1:F:232:ARG:HH11	1.61	0.66
1:F:367:ASN:HD22	1:F:368:PRO:HD2	1.60	0.66
1:E:305:MET:HG3	1:E:306:HIS:H	1.60	0.66
1:E:242:ASN:ND2	1:E:392:ASN:H	1.94	0.65
1:B:232:ARG:HH11	1:B:232:ARG:HB2	1.61	0.65
1:E:353:THR:O	1:E:357:ARG:HG3	1.97	0.65
1:E:367:ASN:HB3	1:E:370:GLN:HG2	1.78	0.64
1:A:339:LYS:HD3	1:A:343:ARG:HH21	1.62	0.64
1:E:338:TYR:CE2	1:F:305:MET:HG3	2.33	0.64
1:D:309:LYS:HA	1:D:312:LEU:HD12	1.80	0.64
1:F:353:THR:O	1:F:357:ARG:HG3	1.98	0.64
1:F:141:LYS:HD2	1:F:146:ASN:OD1	1.98	0.63
1:D:232:ARG:HH11	1:D:232:ARG:HB2	1.62	0.63
1:B:254:HIS:HE1	1:B:274:ASP:OD1	1.82	0.63
1:A:185:GLN:HG3	1:A:275:PHE:CD2	2.34	0.63
1:F:147:VAL:HG22	1:F:162:LYS:HG3	1.81	0.62
1:E:367:ASN:HB3	1:E:370:GLN:CG	2.30	0.62
1:B:232:ARG:HD2	1:B:236:TYR:CZ	2.34	0.62
1:E:346:PHE:HE1	1:E:348:PHE:HE1	1.48	0.62
1:B:370:GLN:NE2	1:E:370:GLN:NE2	2.48	0.61
1:C:358:ASP:O	1:C:362:ARG:HG2	2.01	0.61
1:F:231:GLN:NE2	1:F:386:ASN:HD22	1.98	0.61
1:B:370:GLN:NE2	1:E:370:GLN:HE22	1.99	0.61
1:B:362:ARG:HG3	1:B:362:ARG:HH11	1.65	0.60
1:C:254:HIS:HE1	1:C:274:ASP:OD1	1.84	0.60
1:B:340:ARG:NH1	1:B:345:GLU:O	2.34	0.60
1:D:253:ILE:HD13	1:D:307:ASP:HB2	1.81	0.60
1:B:339:LYS:HD3	1:B:343:ARG:HH21	1.67	0.60
1:B:225:LEU:O	1:B:226:SER:HB2	2.02	0.60
1:F:253:ILE:HG22	1:F:254:HIS:N	2.17	0.60
1:C:151:ARG:NH1	1:C:158:ILE:HD11	2.17	0.60
1:E:242:ASN:HD21	1:E:392:ASN:H	1.46	0.60
1:E:253:ILE:HG21	1:E:307:ASP:HB3	1.83	0.59
1:B:152:GLU:OE1	1:B:154:GLN:HB2	2.01	0.59
1:F:367:ASN:HD22	1:F:368:PRO:CD	2.14	0.59
1:E:153:LYS:O	1:E:156:LYS:HE3	2.01	0.59
1:E:340:ARG:HB3	1:E:340:ARG:NH1	2.15	0.59
1:E:309:LYS:HD3	1:E:312:LEU:HD12	1.83	0.59
1:E:215:LEU:HB2	1:E:264:LEU:HB2	1.85	0.59
1:A:242:ASN:HD21	1:A:392:ASN:H	1.50	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:312:LEU:HD13	1:F:372:PRO:O	2.01	0.59
1:D:215:LEU:HB2	1:D:264:LEU:HB2	1.84	0.58
1:B:334:TYR:O	1:B:338:TYR:HD1	1.87	0.58
1:A:293:LEU:HD11	1:B:338:TYR:CE1	2.38	0.58
1:F:151:ARG:HH11	1:F:151:ARG:CB	2.17	0.58
1:E:305:MET:HB3	1:F:338:TYR:CZ	2.38	0.58
1:A:340:ARG:NH1	1:A:345:GLU:O	2.37	0.58
1:D:182:VAL:HG13	1:D:196:LEU:HD21	1.86	0.58
1:A:338:TYR:CE1	1:B:293:LEU:HD11	2.39	0.57
1:A:177:GLN:HG2	1:A:181:GLU:OE2	2.04	0.57
1:B:190:HIS:CG	1:B:191:PRO:HD2	2.40	0.57
1:A:343:ARG:HB3	1:E:362:ARG:NH2	2.19	0.57
1:A:312:LEU:HD13	1:A:372:PRO:O	2.05	0.57
1:C:338:TYR:CZ	1:D:305:MET:HB3	2.40	0.57
1:B:353:THR:O	1:B:357:ARG:HG3	2.05	0.57
1:C:301:ILE:HD11	1:D:338:TYR:HA	1.87	0.57
1:E:346:PHE:CE1	1:E:348:PHE:HE1	2.22	0.57
1:D:344:VAL:O	1:D:344:VAL:HG12	2.04	0.57
1:F:293:LEU:HD22	1:F:301:ILE:HG21	1.87	0.56
1:E:309:LYS:HA	1:E:312:LEU:HD12	1.87	0.56
1:F:151:ARG:HB3	1:F:151:ARG:HH11	1.70	0.56
1:A:242:ASN:ND2	1:A:392:ASN:H	2.03	0.56
1:C:255:ARG:CZ	1:C:276:GLY:HA2	2.36	0.56
1:D:333:THR:HG23	1:D:336:GLU:OE2	2.05	0.56
1:C:312:LEU:HD13	1:C:372:PRO:O	2.06	0.56
1:A:270:LEU:C	1:A:270:LEU:HD23	2.27	0.56
1:E:362:ARG:HH11	1:E:362:ARG:HG3	1.71	0.56
1:D:270:LEU:HD23	1:D:270:LEU:O	2.06	0.56
1:D:190:HIS:CG	1:D:191:PRO:HD2	2.41	0.56
1:E:190:HIS:CG	1:E:191:PRO:HD2	2.41	0.56
1:D:362:ARG:HH11	1:D:362:ARG:HG3	1.71	0.55
1:D:335:GLN:H	1:D:335:GLN:CD	2.09	0.55
1:C:185:GLN:HG3	1:C:277:TRP:CD1	2.41	0.55
1:A:246:TYR:CD1	1:A:246:TYR:C	2.79	0.55
1:C:225:LEU:O	1:C:226:SER:HB2	2.07	0.55
1:A:338:TYR:CZ	1:B:293:LEU:HD11	2.41	0.55
1:A:232:ARG:HD2	1:A:236:TYR:CZ	2.42	0.55
1:E:312:LEU:HD13	1:E:372:PRO:O	2.06	0.55
1:D:230:GLU:HB3	1:D:386:ASN:ND2	2.22	0.55
1:F:232:ARG:HD2	1:F:236:TYR:CZ	2.42	0.54
1:E:346:PHE:CE1	1:E:348:PHE:CE1	2.90	0.54
1:D:253:ILE:HG22	1:D:254:HIS:N	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:293:LEU:O	1:F:295:TYR:N	2.40	0.54
1:E:298:PRO:HA	1:E:301:ILE:HG22	1.90	0.54
1:E:241:ALA:HB3	1:E:378:LEU:HD21	1.89	0.54
1:B:131:GLU:OE1	1:B:131:GLU:N	2.36	0.54
1:D:340:ARG:NH1	1:D:345:GLU:O	2.41	0.54
1:A:225:LEU:O	1:A:226:SER:HB2	2.06	0.54
1:D:242:ASN:HD21	1:D:392:ASN:N	2.05	0.54
1:F:195:ARG:HB3	1:F:211:GLU:HB2	1.89	0.54
1:E:338:TYR:CD2	1:F:305:MET:HG3	2.43	0.54
1:E:155:SER:O	1:E:156:LYS:HB2	2.07	0.54
1:E:367:ASN:O	1:E:370:GLN:HB2	2.08	0.54
1:A:190:HIS:CG	1:A:191:PRO:HD2	2.43	0.54
1:F:358:ASP:O	1:F:362:ARG:HG2	2.08	0.54
1:E:393:CYS:O	1:E:394:GLN:HB2	2.07	0.53
1:F:311:ASP:N	1:F:311:ASP:OD1	2.36	0.53
1:C:177:GLN:HG2	1:C:181:GLU:OE2	2.08	0.53
1:D:230:GLU:HB3	1:D:386:ASN:HD22	1.73	0.53
1:B:339:LYS:O	1:B:343:ARG:HG3	2.09	0.53
1:C:228:PHE:CG	1:C:232:ARG:HD2	2.43	0.53
1:C:335:GLN:HG3	1:C:339:LYS:HE3	1.90	0.53
1:A:181:GLU:OE1	1:A:275:PHE:O	2.27	0.53
1:A:312:LEU:HD21	1:A:374:LEU:HD23	1.91	0.53
1:B:378:LEU:HD22	1:B:391:SER:HB2	1.90	0.53
1:B:298:PRO:O	1:B:302:GLU:HG3	2.08	0.53
1:A:298:PRO:HA	1:A:301:ILE:HG22	1.90	0.52
1:C:270:LEU:HD23	1:C:270:LEU:O	2.08	0.52
1:B:367:ASN:ND2	1:B:370:GLN:HG3	2.20	0.52
1:F:177:GLN:HG2	1:F:181:GLU:OE2	2.09	0.52
1:A:147:VAL:HG23	2:A:1395:MPY:H341	1.90	0.52
1:C:180:ARG:O	1:C:183:GLU:HB3	2.10	0.52
1:F:380:HIS:ND1	1:F:381:PRO:HD2	2.24	0.52
1:E:366:HIS:O	1:E:368:PRO:HD3	2.09	0.52
1:C:147:VAL:HG23	2:C:1394:MPY:H341	1.91	0.52
1:E:293:LEU:HD22	1:E:301:ILE:CD1	2.39	0.52
1:E:185:GLN:HG3	1:E:275:PHE:CD2	2.45	0.51
1:A:344:VAL:HG21	1:A:366:HIS:HB2	1.92	0.51
1:C:152:GLU:OE1	1:C:154:GLN:HB2	2.11	0.51
1:F:362:ARG:HH11	1:F:362:ARG:HG3	1.76	0.51
1:D:340:ARG:HB3	1:D:340:ARG:HH11	1.75	0.51
1:E:332:ASN:HB2	1:E:336:GLU:OE1	2.11	0.50
1:C:293:LEU:HD13	1:C:301:ILE:HD11	1.93	0.50
1:A:232:ARG:HH11	1:A:232:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:ILE:O	1:A:304:ARG:HG2	2.11	0.50
1:E:305:MET:HG3	1:E:306:HIS:N	2.25	0.50
1:D:367:ASN:HD22	1:D:368:PRO:N	2.09	0.50
1:E:253:ILE:HG22	1:E:254:HIS:N	2.26	0.50
1:E:344:VAL:HG12	1:E:344:VAL:O	2.10	0.50
1:D:232:ARG:HD2	1:D:236:TYR:CZ	2.47	0.50
1:A:340:ARG:HH11	1:A:340:ARG:HB3	1.76	0.50
1:B:362:ARG:NH1	1:B:362:ARG:HG3	2.26	0.50
1:B:185:GLN:HG3	1:B:275:PHE:CD2	2.47	0.50
1:B:232:ARG:HH11	1:B:232:ARG:CB	2.24	0.50
1:B:195:ARG:HB3	1:B:211:GLU:HB2	1.94	0.50
1:F:180:ARG:O	1:F:183:GLU:HB3	2.12	0.50
1:F:225:LEU:O	1:F:226:SER:HB2	2.11	0.50
1:A:185:GLN:HG3	1:A:275:PHE:HD2	1.77	0.49
1:D:270:LEU:HD23	1:D:270:LEU:C	2.33	0.49
1:A:301:ILE:HG23	1:A:302:GLU:N	2.27	0.49
1:A:353:THR:O	1:A:357:ARG:HG3	2.12	0.49
1:C:301:ILE:HG12	1:D:338:TYR:HD1	1.77	0.49
1:D:367:ASN:C	1:D:367:ASN:HD22	2.15	0.49
1:C:334:TYR:CE1	1:D:293:LEU:HD11	2.47	0.49
1:C:298:PRO:O	1:C:301:ILE:HG22	2.12	0.49
1:B:312:LEU:HD13	1:B:372:PRO:O	2.13	0.49
1:A:302:GLU:HA	1:A:305:MET:HG2	1.95	0.48
1:A:253:ILE:HG22	1:A:254:HIS:N	2.28	0.48
1:B:340:ARG:HD2	1:B:345:GLU:HG3	1.96	0.48
1:C:159:LEU:HD12	1:C:159:LEU:C	2.34	0.48
1:C:313:TRP:CG	1:D:297:PRO:HB3	2.47	0.48
1:A:195:ARG:HB3	1:A:211:GLU:HB2	1.96	0.48
1:C:297:PRO:HB3	1:D:313:TRP:CG	2.48	0.48
1:C:232:ARG:HG3	1:C:232:ARG:HH11	1.78	0.48
1:F:254:HIS:CD2	1:F:255:ARG:N	2.81	0.48
1:F:255:ARG:CZ	1:F:276:GLY:HA2	2.43	0.48
1:C:254:HIS:O	1:C:311:ASP:OD1	2.32	0.48
1:F:141:LYS:HD2	1:F:146:ASN:CG	2.33	0.48
1:A:253:ILE:CD1	1:A:308:GLU:HG2	2.43	0.48
1:E:295:TYR:CE2	1:F:259:PRO:HD3	2.49	0.48
1:B:177:GLN:HG2	1:B:181:GLU:OE2	2.14	0.48
1:E:309:LYS:HD3	1:E:312:LEU:CD1	2.43	0.48
1:D:312:LEU:HD13	1:D:372:PRO:O	2.14	0.48
1:A:340:ARG:CZ	1:E:381:PRO:HG3	2.44	0.48
1:C:195:ARG:HB3	1:C:211:GLU:HB2	1.95	0.47
1:B:224:LYS:NZ	2:B:1395:MPY:H233	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:253:ILE:HG21	1:D:307:ASP:HB3	1.96	0.47
1:A:182:VAL:HG13	1:A:196:LEU:HD21	1.96	0.47
1:D:225:LEU:O	1:D:226:SER:HB2	2.14	0.47
1:E:340:ARG:NH1	1:E:345:GLU:O	2.48	0.47
1:E:177:GLN:HG2	1:E:181:GLU:OE2	2.14	0.47
1:E:131:GLU:O	1:E:153:LYS:HD2	2.14	0.47
1:B:185:GLN:HG2	1:B:277:TRP:CD1	2.50	0.47
1:E:225:LEU:O	1:E:226:SER:HB2	2.15	0.47
1:E:195:ARG:HH11	1:E:195:ARG:HG2	1.79	0.47
1:F:340:ARG:NH1	1:F:345:GLU:O	2.48	0.47
1:C:332:ASN:HB2	1:C:336:GLU:OE2	2.15	0.47
1:D:254:HIS:CE1	1:D:274:ASP:OD1	2.62	0.47
1:B:381:PRO:HG3	1:F:340:ARG:CZ	2.45	0.47
1:D:367:ASN:C	1:D:367:ASN:ND2	2.68	0.46
1:E:195:ARG:HG2	1:E:195:ARG:NH1	2.29	0.46
1:E:310:VAL:HG13	1:F:297:PRO:HG3	1.97	0.46
1:E:180:ARG:O	1:E:183:GLU:HB3	2.14	0.46
1:E:239:GLU:HB3	1:E:270:LEU:HD22	1.96	0.46
1:B:181:GLU:OE1	1:B:275:PHE:O	2.34	0.46
1:E:293:LEU:HD22	1:E:301:ILE:HD12	1.96	0.46
1:D:165:PHE:CD1	1:D:165:PHE:N	2.83	0.46
1:F:147:VAL:HG23	2:F:1395:MPY:H341	1.97	0.46
1:D:145:GLY:HA3	1:D:163:VAL:O	2.15	0.46
1:C:179:ARG:C	1:C:179:ARG:HD3	2.35	0.46
1:C:333:THR:HG23	1:C:336:GLU:OE2	2.16	0.46
1:B:240:LEU:HG	1:B:270:LEU:HD11	1.97	0.46
1:F:185:GLN:HG3	1:F:275:PHE:HD2	1.79	0.46
1:C:141:LYS:HD2	1:C:146:ASN:OD1	2.15	0.46
1:B:147:VAL:HG23	2:B:1395:MPY:H341	1.97	0.46
1:C:254:HIS:CE1	1:C:274:ASP:OD1	2.67	0.45
1:F:367:ASN:HD22	1:F:368:PRO:N	2.14	0.45
1:D:336:GLU:O	1:D:340:ARG:HG2	2.15	0.45
1:A:298:PRO:O	1:A:301:ILE:HG22	2.16	0.45
1:E:320:TYR:CD2	1:E:328:PRO:HD3	2.51	0.45
1:A:147:VAL:CG2	2:A:1395:MPY:H341	2.44	0.45
1:E:270:LEU:C	1:E:270:LEU:HD23	2.37	0.45
1:D:162:LYS:HE2	1:D:164:LEU:HD21	1.99	0.45
1:C:145:GLY:HA3	1:C:163:VAL:O	2.17	0.45
1:E:139:LEU:HA	1:E:139:LEU:HD23	1.80	0.45
1:D:181:GLU:OE1	1:D:275:PHE:O	2.35	0.45
1:A:335:GLN:CD	1:A:335:GLN:H	2.19	0.45
1:F:181:GLU:OE1	1:F:275:PHE:O	2.34	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:259:PRO:HD3	1:D:295:TYR:CE2	2.52	0.45
1:B:344:VAL:O	1:B:344:VAL:HG12	2.17	0.45
1:C:253:ILE:CG2	1:C:308:GLU:HG2	2.39	0.45
1:C:181:GLU:CD	1:C:255:ARG:HH22	2.20	0.45
1:B:332:ASN:HB2	1:B:336:GLU:OE1	2.17	0.45
1:E:338:TYR:HE1	1:F:301:ILE:O	2.00	0.45
1:B:339:LYS:HD3	1:B:343:ARG:NH2	2.32	0.45
1:D:230:GLU:CB	1:D:386:ASN:HD22	2.30	0.45
1:D:378:LEU:HD22	1:D:391:SER:HB2	1.97	0.45
1:A:313:TRP:CG	1:B:297:PRO:HB3	2.52	0.45
1:A:259:PRO:HD2	1:A:260:GLU:OE1	2.17	0.45
1:A:301:ILE:CG2	1:A:302:GLU:N	2.80	0.44
1:E:195:ARG:HB3	1:E:211:GLU:HB2	1.99	0.44
1:B:311:ASP:N	1:B:311:ASP:OD1	2.50	0.44
1:F:274:ASP:OD1	1:F:274:ASP:C	2.56	0.44
1:C:309:LYS:HD3	1:C:312:LEU:HD12	2.00	0.44
1:A:240:LEU:HD23	1:A:270:LEU:HD21	1.98	0.44
1:D:362:ARG:NH1	1:D:362:ARG:HG3	2.33	0.44
1:B:302:GLU:HA	1:B:305:MET:HG2	1.99	0.44
1:E:185:GLN:HG3	1:E:275:PHE:HD2	1.80	0.44
1:F:239:GLU:OE1	1:F:270:LEU:HD22	2.18	0.44
1:C:147:VAL:CG2	2:C:1394:MPY:H341	2.46	0.44
1:F:145:GLY:HA3	1:F:163:VAL:O	2.17	0.44
1:A:392:ASN:C	1:A:392:ASN:HD22	2.21	0.44
1:E:336:GLU:O	1:E:340:ARG:HG2	2.17	0.44
1:C:254:HIS:CD2	1:C:255:ARG:N	2.86	0.44
1:D:333:THR:OG1	1:D:336:GLU:HG3	2.18	0.44
1:C:270:LEU:HD23	1:C:270:LEU:C	2.38	0.44
1:E:230:GLU:CB	1:E:386:ASN:HD22	2.29	0.44
1:A:392:ASN:ND2	1:A:392:ASN:C	2.71	0.44
1:D:185:GLN:HB3	1:D:185:GLN:HE21	1.59	0.44
1:D:185:GLN:HG3	1:D:275:PHE:CD2	2.52	0.44
1:F:150:ALA:HB3	1:F:159:LEU:HD12	1.98	0.44
1:E:389:LYS:HE2	3:E:2007:HOH:O	2.17	0.44
1:E:367:ASN:CB	1:E:370:GLN:HG2	2.48	0.44
1:E:362:ARG:HG3	1:E:362:ARG:NH1	2.32	0.44
1:E:380:HIS:HA	1:E:381:PRO:HD3	1.91	0.44
1:C:340:ARG:NH1	1:C:345:GLU:O	2.51	0.44
1:E:165:PHE:CD1	1:E:165:PHE:N	2.86	0.44
1:E:367:ASN:C	1:E:367:ASN:ND2	2.70	0.43
1:E:253:ILE:CG2	1:E:254:HIS:N	2.81	0.43
1:A:297:PRO:HB3	1:B:313:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:270:LEU:HD23	1:B:270:LEU:O	2.18	0.43
1:D:147:VAL:HG23	2:D:1395:MPY:H341	2.00	0.43
1:E:254:HIS:O	1:E:311:ASP:OD1	2.36	0.43
1:F:133:PHE:HZ	1:F:209:ILE:HD13	1.83	0.43
1:E:301:ILE:HG12	1:F:338:TYR:HD2	1.84	0.43
1:D:177:GLN:HG2	1:D:181:GLU:OE2	2.19	0.43
1:D:339:LYS:HD3	1:D:343:ARG:HH21	1.83	0.43
1:C:215:LEU:HD12	1:C:265:GLY:O	2.18	0.43
1:D:367:ASN:HD22	1:D:368:PRO:CD	2.32	0.43
1:E:359:LEU:HD13	1:E:380:HIS:CD2	2.54	0.43
1:D:367:ASN:O	1:D:370:GLN:HB2	2.18	0.43
1:E:213:ALA:HA	1:E:214:PRO:HD2	1.87	0.43
1:D:242:ASN:HD22	1:D:242:ASN:HA	1.64	0.43
1:C:151:ARG:HH12	1:C:158:ILE:HD11	1.83	0.43
1:D:213:ALA:O	2:D:1395:MPY:H12	2.18	0.43
1:B:246:TYR:C	1:B:246:TYR:CD1	2.91	0.43
1:A:145:GLY:HA3	1:A:163:VAL:O	2.18	0.43
1:E:180:ARG:HG2	1:E:180:ARG:NH1	2.32	0.43
1:C:141:LYS:HD2	1:C:146:ASN:CG	2.39	0.43
1:F:333:THR:HG23	1:F:336:GLU:OE2	2.18	0.43
1:C:301:ILE:HG12	1:D:338:TYR:CD1	2.54	0.43
1:A:220:ARG:HA	1:A:220:ARG:HD3	1.85	0.43
1:B:125:LYS:HD2	1:B:126:ARG:H	1.84	0.43
1:E:181:GLU:OE1	1:E:275:PHE:O	2.37	0.42
1:F:306:HIS:CE1	1:F:369:SER:HB3	2.54	0.42
1:F:292:THR:HB	1:F:293:LEU:H	1.72	0.42
1:D:298:PRO:HA	1:D:301:ILE:HG12	2.01	0.42
1:B:134:GLU:HB2	1:B:151:ARG:HB3	2.01	0.42
1:E:147:VAL:HG23	2:E:1395:MPY:H341	2.01	0.42
1:E:365:LYS:HD3	1:E:370:GLN:HB3	2.01	0.42
1:D:215:LEU:HB2	1:D:264:LEU:CB	2.48	0.42
1:B:380:HIS:HA	1:B:381:PRO:HD3	1.92	0.42
1:C:171:LYS:O	1:D:176:HIS:CD2	2.73	0.42
1:D:195:ARG:HH11	1:D:195:ARG:HG2	1.84	0.42
1:F:185:GLN:HG2	1:F:277:TRP:CD1	2.54	0.42
1:B:232:ARG:CG	1:B:232:ARG:HH11	2.32	0.42
1:F:362:ARG:HG3	1:F:362:ARG:NH1	2.33	0.42
1:C:162:LYS:HE2	1:C:164:LEU:HD21	2.02	0.42
1:D:297:PRO:HB2	1:D:299:GLU:OE2	2.19	0.42
1:E:305:MET:HB3	1:F:338:TYR:CE2	2.53	0.42
1:E:305:MET:CB	1:F:338:TYR:CE2	3.01	0.42
1:D:195:ARG:HB3	1:D:211:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:200:PHE:CD1	1:B:200:PHE:N	2.87	0.42
1:A:159:LEU:HD12	1:A:159:LEU:C	2.40	0.42
1:B:165:PHE:N	1:B:165:PHE:CD1	2.87	0.42
1:B:232:ARG:HD2	1:B:236:TYR:CE2	2.54	0.42
1:B:254:HIS:CE1	1:B:274:ASP:OD1	2.68	0.42
1:F:195:ARG:HH11	1:F:195:ARG:HG2	1.83	0.42
1:C:215:LEU:HB2	1:C:264:LEU:HB2	2.02	0.42
1:E:338:TYR:CD1	1:F:301:ILE:HD12	2.55	0.42
1:D:190:HIS:CE1	1:D:191:PRO:HG2	2.54	0.42
1:E:180:ARG:HH11	1:E:180:ARG:HG2	1.85	0.42
1:E:320:TYR:HD2	1:E:328:PRO:HD3	1.85	0.42
1:D:185:GLN:HG3	1:D:275:PHE:HD2	1.85	0.42
1:F:159:LEU:C	1:F:159:LEU:HD12	2.40	0.42
1:F:306:HIS:CB	1:F:368:PRO:HB2	2.50	0.41
1:C:162:LYS:HB3	1:C:208:LEU:HB2	2.02	0.41
1:B:159:LEU:HD12	1:B:159:LEU:C	2.40	0.41
1:D:145:GLY:HA2	1:D:165:PHE:CE1	2.55	0.41
1:D:195:ARG:HG2	1:D:195:ARG:NH1	2.35	0.41
1:D:180:ARG:O	1:D:184:ILE:HG13	2.20	0.41
1:F:255:ARG:NH1	1:F:276:GLY:HA2	2.35	0.41
1:C:338:TYR:C	1:C:338:TYR:CD1	2.92	0.41
1:D:254:HIS:HD2	1:D:255:ARG:O	2.02	0.41
1:C:240:LEU:HG	1:C:270:LEU:HD11	2.03	0.41
1:E:269:GLU:HB2	3:E:2022:HOH:O	2.19	0.41
1:C:259:PRO:HD2	1:C:260:GLU:OE1	2.21	0.41
1:F:270:LEU:HD23	1:F:270:LEU:O	2.21	0.41
1:E:220:ARG:HA	1:E:220:ARG:HD2	1.72	0.41
1:C:213:ALA:O	2:C:1394:MPY:H12	2.20	0.41
1:B:362:ARG:HH22	1:F:343:ARG:HB3	1.78	0.41
1:A:240:LEU:CD2	1:A:270:LEU:HD21	2.50	0.41
1:C:275:PHE:O	1:C:277:TRP:N	2.51	0.41
1:B:370:GLN:CD	1:E:370:GLN:NE2	2.74	0.41
1:F:242:ASN:ND2	1:F:392:ASN:H	2.12	0.41
1:F:380:HIS:CE1	1:F:381:PRO:HD2	2.55	0.41
1:B:259:PRO:HD2	1:B:260:GLU:OE1	2.21	0.41
1:A:162:LYS:HB3	1:A:208:LEU:HB2	2.02	0.41
1:B:220:ARG:HA	1:B:220:ARG:HD3	1.97	0.41
1:A:185:GLN:HG2	1:A:277:TRP:CD1	2.56	0.41
1:E:270:LEU:O	1:E:270:LEU:HD23	2.21	0.41
1:C:179:ARG:HA	1:C:179:ARG:HD3	1.79	0.41
1:F:253:ILE:CG2	1:F:254:HIS:N	2.82	0.40
1:E:301:ILE:O	1:E:304:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:320:TYR:CD2	1:D:328:PRO:HD3	2.57	0.40
1:E:307:ASP:C	1:E:309:LYS:H	2.25	0.40
1:D:383:ILE:HA	1:D:383:ILE:HD13	1.93	0.40
1:E:380:HIS:ND1	1:E:381:PRO:HD2	2.37	0.40
1:A:293:LEU:CD1	1:B:338:TYR:CE1	3.04	0.40
1:F:253:ILE:HG22	1:F:254:HIS:H	1.87	0.40
1:C:147:VAL:HG22	1:C:162:LYS:HG3	2.02	0.40
1:B:312:LEU:HD21	1:B:374:LEU:HD23	2.04	0.40
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.89	0.40
1:A:137:ARG:HA	1:A:138:PRO:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/306 (82%)	244 (97%)	7 (3%)	1 (0%)	43	72
1	B	254/306 (83%)	246 (97%)	7 (3%)	1 (0%)	43	72
1	C	253/306 (83%)	242 (96%)	9 (4%)	2 (1%)	27	53
1	D	252/306 (82%)	243 (96%)	7 (3%)	2 (1%)	27	53
1	E	252/306 (82%)	241 (96%)	8 (3%)	3 (1%)	19	39
1	F	253/306 (83%)	241 (95%)	10 (4%)	2 (1%)	27	53
All	All	1516/1836 (83%)	1457 (96%)	48 (3%)	11 (1%)	30	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	ASP
1	E	294	ASP
1	F	294	ASP
1	C	294	ASP
1	E	154	GLN

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Mol	Chain	Res	Type
1	F	154	GLN
1	C	276	GLY
1	E	276	GLY
1	A	276	GLY
1	D	276	GLY
1	B	276	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	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	B	229/271 (84%)	220 (96%)	9 (4%)	43	74
1	C	228/271 (84%)	223 (98%)	5 (2%)	64	89
1	D	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	E	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	F	228/271 (84%)	219 (96%)	9 (4%)	43	74
All	All	1366/1626 (84%)	1322 (97%)	44 (3%)	51	80

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	232	ARG
1	A	246	TYR
1	A	270	LEU
1	A	311	ASP
1	A	367	ASN
1	A	392	ASN
1	B	180	ARG
1	B	185	GLN
1	B	232	ARG
1	B	246	TYR
1	B	270	LEU
1	B	311	ASP

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Mol	Chain	Res	Type
1	B	340	ARG
1	B	354	GLU
1	B	367	ASN
1	C	179	ARG
1	C	185	GLN
1	C	270	LEU
1	C	340	ARG
1	C	354	GLU
1	D	185	GLN
1	D	232	ARG
1	D	270	LEU
1	D	311	ASP
1	D	350	ASP
1	D	367	ASN
1	D	392	ASN
1	E	180	ARG
1	E	185	GLN
1	E	270	LEU
1	E	340	ARG
1	E	350	ASP
1	E	367	ASN
1	E	368	PRO
1	F	151	ARG
1	F	180	ARG
1	F	185	GLN
1	F	232	ARG
1	F	270	LEU
1	F	311	ASP
1	F	340	ARG
1	F	354	GLU
1	F	367	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	335	GLN
1	A	367	ASN
1	A	392	ASN
1	B	185	GLN
1	B	254	HIS
1	B	367	ASN

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Mol	Chain	Res	Type
1	B	370	GLN
1	B	392	ASN
1	C	242	ASN
1	C	254	HIS
1	C	392	ASN
1	D	185	GLN
1	D	242	ASN
1	D	254	HIS
1	D	367	ASN
1	D	386	ASN
1	D	392	ASN
1	D	394	GLN
1	E	185	GLN
1	E	231	GLN
1	E	242	ASN
1	E	367	ASN
1	E	370	GLN
1	E	392	ASN
1	F	242	ASN
1	F	254	HIS
1	F	367	ASN
1	F	386	ASN
1	F	392	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	MPY	A	1395	-	41,41,41	2.71	20 (48%)	55,58,58	4.67	19 (34%)
2	MPY	B	1395	-	41,41,41	2.68	19 (46%)	55,58,58	5.03	18 (32%)
2	MPY	C	1394	-	41,41,41	2.74	19 (46%)	55,58,58	4.93	19 (34%)
2	MPY	D	1395	-	41,41,41	2.79	21 (51%)	55,58,58	5.21	20 (36%)
2	MPY	E	1395	-	41,41,41	2.82	20 (48%)	55,58,58	4.99	18 (32%)
2	MPY	F	1395	-	41,41,41	2.65	17 (41%)	55,58,58	4.81	17 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPY	A	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	B	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	C	1394	-	-	0/19/43/43	0/3/5/5
2	MPY	D	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	E	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	F	1395	-	-	0/19/43/43	0/3/5/5

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1395	MPY	C16-N1	6.86	1.50	1.39
2	A	1395	MPY	C15-C14	6.81	1.47	1.38
2	C	1394	MPY	C15-C14	6.59	1.47	1.38
2	B	1395	MPY	C16-N1	6.51	1.49	1.39
2	F	1395	MPY	C16-N1	6.50	1.49	1.39
2	E	1395	MPY	C15-C14	6.45	1.47	1.38
2	D	1395	MPY	C15-C14	6.45	1.47	1.38
2	A	1395	MPY	C16-N1	6.45	1.49	1.39
2	F	1395	MPY	C15-C14	6.44	1.47	1.38
2	B	1395	MPY	C15-C14	6.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1394	MPY	C16-N1	6.25	1.49	1.39
2	E	1395	MPY	C16-N1	6.24	1.49	1.39
2	E	1395	MPY	C15-N1	5.98	1.48	1.39
2	C	1394	MPY	C16-C13	5.95	1.47	1.38
2	B	1395	MPY	C16-C13	5.95	1.47	1.38
2	D	1395	MPY	C16-C13	5.74	1.47	1.38
2	F	1395	MPY	C16-C13	5.69	1.47	1.38
2	E	1395	MPY	C16-C13	5.62	1.47	1.38
2	D	1395	MPY	C15-N1	5.48	1.48	1.39
2	A	1395	MPY	C16-C13	5.37	1.46	1.38
2	F	1395	MPY	C15-N1	4.93	1.47	1.39
2	A	1395	MPY	C15-N1	4.91	1.47	1.39
2	C	1394	MPY	C15-N1	4.90	1.47	1.39
2	B	1395	MPY	C15-N1	4.88	1.47	1.39
2	F	1395	MPY	C27-C28	4.71	1.47	1.40
2	E	1395	MPY	C27-C28	4.31	1.46	1.40
2	F	1395	MPY	C14-C13	-4.26	1.35	1.41
2	C	1394	MPY	C27-C28	4.15	1.46	1.40
2	D	1395	MPY	C27-C28	4.05	1.46	1.40
2	A	1395	MPY	C27-C28	4.05	1.46	1.40
2	C	1394	MPY	C18-N17	4.04	1.52	1.46
2	B	1395	MPY	C14-C13	-3.94	1.35	1.41
2	A	1395	MPY	C14-C13	-3.67	1.35	1.41
2	D	1395	MPY	C18-N17	3.66	1.52	1.46
2	B	1395	MPY	C27-C28	3.64	1.45	1.40
2	E	1395	MPY	C18-N17	3.62	1.52	1.46
2	C	1394	MPY	C22-N17	3.53	1.52	1.46
2	B	1395	MPY	C27-C29	3.46	1.45	1.40
2	A	1395	MPY	C18-N17	3.45	1.51	1.46
2	D	1395	MPY	C22-N17	3.39	1.51	1.46
2	E	1395	MPY	C22-N17	3.39	1.51	1.46
2	D	1395	MPY	C11-C24	3.38	1.46	1.39
2	A	1395	MPY	C27-C29	3.35	1.45	1.40
2	C	1394	MPY	C27-C29	3.34	1.45	1.40
2	E	1395	MPY	C13-N2	-3.32	1.34	1.38
2	E	1395	MPY	C11-C24	3.32	1.46	1.39
2	B	1395	MPY	C11-C24	3.28	1.45	1.39
2	F	1395	MPY	C27-C29	3.26	1.45	1.40
2	E	1395	MPY	C9-C7	3.23	1.44	1.39
2	A	1395	MPY	C3-N5	3.18	1.41	1.30
2	C	1394	MPY	C11-C24	3.18	1.45	1.39
2	C	1394	MPY	C14-C13	-3.12	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1395	MPY	C14-C13	-3.10	1.36	1.41
2	E	1395	MPY	C14-C13	-3.10	1.36	1.41
2	A	1395	MPY	C13-N2	-3.03	1.34	1.38
2	B	1395	MPY	C18-N17	3.02	1.51	1.46
2	E	1395	MPY	C3-N5	3.02	1.40	1.30
2	B	1395	MPY	C13-N2	-3.00	1.35	1.38
2	B	1395	MPY	C3-N5	2.97	1.40	1.30
2	D	1395	MPY	C3-N5	2.94	1.40	1.30
2	C	1394	MPY	C6-N5	2.93	1.43	1.37
2	A	1395	MPY	C6-N5	2.91	1.43	1.37
2	E	1395	MPY	C24-N17	2.91	1.46	1.38
2	C	1394	MPY	C12-C7	2.90	1.44	1.39
2	B	1395	MPY	C6-N5	2.89	1.43	1.37
2	B	1395	MPY	C9-C7	2.89	1.44	1.39
2	A	1395	MPY	C11-C24	2.87	1.45	1.39
2	E	1395	MPY	C27-C29	2.86	1.44	1.40
2	D	1395	MPY	C12-C7	2.84	1.44	1.39
2	D	1395	MPY	C21-N20	2.84	1.53	1.46
2	F	1395	MPY	C11-C24	2.82	1.45	1.39
2	D	1395	MPY	C9-C7	2.82	1.44	1.39
2	E	1395	MPY	C10-C24	2.80	1.45	1.39
2	D	1395	MPY	C13-N2	-2.78	1.35	1.38
2	E	1395	MPY	C12-C7	2.72	1.44	1.39
2	C	1394	MPY	C9-C7	2.72	1.44	1.39
2	D	1395	MPY	C6-N5	2.71	1.42	1.37
2	F	1395	MPY	C13-N2	-2.70	1.35	1.38
2	F	1395	MPY	C6-N5	2.68	1.42	1.37
2	A	1395	MPY	C22-N17	2.67	1.50	1.46
2	F	1395	MPY	C3-N5	2.66	1.39	1.30
2	C	1394	MPY	C10-C24	2.66	1.44	1.39
2	D	1395	MPY	C27-C29	2.64	1.44	1.40
2	A	1395	MPY	C24-N17	2.61	1.46	1.38
2	C	1394	MPY	C3-N5	2.60	1.39	1.30
2	F	1395	MPY	C12-C7	2.58	1.43	1.39
2	B	1395	MPY	C21-N20	2.56	1.52	1.46
2	A	1395	MPY	C9-C7	2.55	1.43	1.39
2	C	1394	MPY	C21-N20	2.55	1.52	1.46
2	E	1395	MPY	C6-N5	2.51	1.42	1.37
2	F	1395	MPY	C21-N20	2.50	1.52	1.46
2	C	1394	MPY	C24-N17	2.50	1.45	1.38
2	D	1395	MPY	C24-N17	2.49	1.45	1.38
2	D	1395	MPY	C10-C24	2.48	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1395	MPY	C7-C6	2.44	1.53	1.49
2	F	1395	MPY	C9-C7	2.43	1.43	1.39
2	B	1395	MPY	C12-C7	2.42	1.43	1.39
2	E	1395	MPY	C7-C6	2.38	1.52	1.49
2	E	1395	MPY	C21-N20	2.38	1.51	1.46
2	A	1395	MPY	C21-N20	2.37	1.51	1.46
2	B	1395	MPY	C24-N17	2.33	1.45	1.38
2	B	1395	MPY	C22-N17	2.31	1.50	1.46
2	F	1395	MPY	C22-N17	2.30	1.50	1.46
2	D	1395	MPY	C14-C3	-2.27	1.42	1.47
2	D	1395	MPY	C12-C11	2.25	1.43	1.38
2	E	1395	MPY	C14-C3	-2.23	1.42	1.47
2	A	1395	MPY	C10-C24	2.20	1.43	1.39
2	A	1395	MPY	C12-C7	2.16	1.43	1.39
2	F	1395	MPY	C10-C24	2.15	1.43	1.39
2	B	1395	MPY	C10-C24	2.14	1.43	1.39
2	C	1394	MPY	C14-C3	-2.14	1.42	1.47
2	F	1395	MPY	C24-N17	2.13	1.44	1.38
2	D	1395	MPY	C33-C29	2.10	1.43	1.39
2	A	1395	MPY	C31-C28	2.02	1.43	1.39
2	B	1395	MPY	C14-C3	-2.02	1.42	1.47
2	C	1394	MPY	C13-N2	-2.01	1.36	1.38

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1395	MPY	O26-C25-N1	33.22	122.71	116.25
2	B	1395	MPY	O26-C25-N1	31.85	122.44	116.25
2	E	1395	MPY	O26-C25-N1	31.24	122.33	116.25
2	C	1394	MPY	O26-C25-N1	30.69	122.22	116.25
2	F	1395	MPY	O26-C25-N1	30.06	122.09	116.25
2	A	1395	MPY	O26-C25-N1	28.72	121.83	116.25
2	C	1394	MPY	C16-N1-C15	12.97	113.38	108.13
2	F	1395	MPY	C16-N1-C15	12.48	113.18	108.13
2	E	1395	MPY	C16-N1-C15	12.32	113.11	108.13
2	B	1395	MPY	C16-N1-C15	11.81	112.91	108.13
2	D	1395	MPY	C16-N1-C15	11.78	112.90	108.13
2	A	1395	MPY	C16-N1-C15	11.49	112.78	108.13
2	E	1395	MPY	N5-C3-N4	-5.86	119.88	129.58
2	F	1395	MPY	N5-C3-N4	-5.56	120.39	129.58
2	D	1395	MPY	N5-C3-N4	-5.48	120.51	129.58
2	C	1394	MPY	N5-C3-N4	-5.37	120.70	129.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1395	MPY	N5-C3-N4	-5.36	120.71	129.58
2	B	1395	MPY	N5-C3-N4	-5.25	120.90	129.58
2	A	1395	MPY	C21-N20-C19	4.92	116.41	109.54
2	D	1395	MPY	C21-N20-C19	4.86	116.33	109.54
2	E	1395	MPY	C16-C13-C14	4.75	118.46	111.12
2	D	1395	MPY	C16-C13-C14	4.66	118.33	111.12
2	F	1395	MPY	C21-N20-C19	4.64	116.01	109.54
2	D	1395	MPY	C27-N30-C25	4.63	129.50	121.98
2	B	1395	MPY	C21-N20-C19	4.60	115.96	109.54
2	B	1395	MPY	C16-C13-C14	4.60	118.22	111.12
2	B	1395	MPY	C27-N30-C25	4.54	129.37	121.98
2	A	1395	MPY	C16-C13-C14	4.50	118.08	111.12
2	F	1395	MPY	C16-C13-C14	4.50	118.08	111.12
2	E	1395	MPY	C27-N30-C25	4.38	129.10	121.98
2	C	1394	MPY	C16-C13-C14	4.36	117.85	111.12
2	D	1395	MPY	C22-C21-N20	4.26	115.52	110.82
2	B	1395	MPY	C14-C13-N2	-4.23	109.03	112.68
2	A	1395	MPY	C27-N30-C25	4.23	128.85	121.98
2	C	1394	MPY	C22-C21-N20	4.22	115.48	110.82
2	D	1395	MPY	C14-C13-N2	-4.15	109.10	112.68
2	C	1394	MPY	C14-C13-N2	-4.15	109.11	112.68
2	E	1395	MPY	C6-N5-C3	4.11	128.99	123.12
2	A	1395	MPY	C14-C13-N2	-4.04	109.20	112.68
2	F	1395	MPY	C27-N30-C25	4.02	128.52	121.98
2	E	1395	MPY	C22-C21-N20	3.96	115.20	110.82
2	A	1395	MPY	C22-C21-N20	3.94	115.17	110.82
2	E	1395	MPY	C14-C13-N2	-3.85	109.36	112.68
2	C	1394	MPY	C21-N20-C19	3.72	114.73	109.54
2	B	1395	MPY	C22-C21-N20	3.68	114.89	110.82
2	F	1395	MPY	C14-C13-N2	-3.64	109.55	112.68
2	E	1395	MPY	C14-C3-N5	3.50	130.41	122.95
2	E	1395	MPY	C21-N20-C19	3.46	114.36	109.54
2	F	1395	MPY	C18-C19-N20	3.39	114.56	110.82
2	C	1394	MPY	C27-N30-C25	3.32	127.38	121.98
2	E	1395	MPY	C16-N1-C25	-3.28	118.22	125.95
2	A	1395	MPY	C16-N1-C25	-3.22	118.36	125.95
2	B	1395	MPY	C18-C19-N20	3.21	114.37	110.82
2	F	1395	MPY	C16-N1-C25	-3.20	118.41	125.95
2	A	1395	MPY	C13-N2-N4	3.16	111.10	109.23
2	F	1395	MPY	C6-N5-C3	3.13	127.58	123.12
2	D	1395	MPY	C16-N1-C25	-3.11	118.63	125.95
2	F	1395	MPY	C14-C3-N5	3.09	129.54	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1395	MPY	C6-N5-C3	3.05	127.48	123.12
2	E	1395	MPY	C15-C14-C13	-3.04	106.41	111.12
2	D	1395	MPY	C14-C3-N5	3.02	129.40	122.95
2	B	1395	MPY	C13-N2-N4	3.02	111.02	109.23
2	D	1395	MPY	C15-C14-C13	-3.02	106.45	111.12
2	A	1395	MPY	C15-C14-C13	-3.01	106.46	111.12
2	C	1394	MPY	C15-C14-C13	-3.00	106.48	111.12
2	B	1395	MPY	C15-C14-C13	-2.99	106.50	111.12
2	C	1394	MPY	C22-N17-C18	2.99	117.81	111.67
2	A	1395	MPY	C14-C3-N5	2.98	129.30	122.95
2	B	1395	MPY	C14-C3-N5	2.95	129.24	122.95
2	C	1394	MPY	C14-C3-N5	2.94	129.23	122.95
2	C	1394	MPY	C21-C22-N17	2.92	116.12	110.62
2	A	1395	MPY	C6-N5-C3	2.88	127.23	123.12
2	C	1394	MPY	C16-N1-C25	-2.79	119.37	125.95
2	B	1395	MPY	C6-N5-C3	2.79	127.10	123.12
2	D	1395	MPY	C18-C19-N20	2.71	113.81	110.82
2	C	1394	MPY	C6-N5-C3	2.70	126.98	123.12
2	F	1395	MPY	C22-C21-N20	2.69	113.79	110.82
2	D	1395	MPY	C22-N17-C18	2.63	117.09	111.67
2	F	1395	MPY	C15-C14-C13	-2.63	107.05	111.12
2	B	1395	MPY	C34-C29-C27	2.62	125.79	121.37
2	C	1394	MPY	C19-C18-N17	2.61	115.54	110.62
2	E	1395	MPY	C21-C22-N17	2.58	115.48	110.62
2	A	1395	MPY	C18-C19-N20	2.58	113.67	110.82
2	B	1395	MPY	C16-N1-C25	-2.57	119.89	125.95
2	D	1395	MPY	C19-C18-N17	2.56	115.43	110.62
2	C	1394	MPY	C34-C29-C27	2.51	125.61	121.37
2	F	1395	MPY	C34-C29-C27	2.50	125.59	121.37
2	D	1395	MPY	C13-N2-N4	2.46	110.69	109.23
2	E	1395	MPY	C19-C18-N17	2.38	115.11	110.62
2	A	1395	MPY	C34-C29-C27	2.37	125.38	121.37
2	C	1394	MPY	C12-C7-C6	2.36	124.44	120.47
2	E	1395	MPY	C13-N2-N4	2.36	110.63	109.23
2	F	1395	MPY	C13-N2-N4	2.36	110.63	109.23
2	D	1395	MPY	C12-C7-C6	2.34	124.40	120.47
2	F	1395	MPY	C14-C15-N1	-2.32	104.15	111.00
2	E	1395	MPY	C22-N17-C18	2.32	116.44	111.67
2	A	1395	MPY	C22-N17-C18	2.27	116.33	111.67
2	E	1395	MPY	C14-C15-N1	-2.26	104.32	111.00
2	D	1395	MPY	C21-C22-N17	2.24	114.83	110.62
2	E	1395	MPY	C34-C29-C27	2.23	125.14	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	1395	MPY	C32-C28-C27	2.22	125.12	121.37
2	C	1394	MPY	C14-C15-N1	-2.17	104.58	111.00
2	A	1395	MPY	C14-C15-N1	-2.17	104.60	111.00
2	D	1395	MPY	C14-C15-N1	-2.13	104.69	111.00
2	A	1395	MPY	C19-C18-N17	2.11	114.60	110.62
2	D	1395	MPY	C34-C29-C27	2.11	124.94	121.37
2	B	1395	MPY	C19-C18-N17	2.11	114.58	110.62
2	B	1395	MPY	C14-C15-N1	-2.08	104.84	111.00
2	B	1395	MPY	C29-C27-N30	2.07	122.89	119.33
2	C	1394	MPY	C29-C27-N30	2.06	122.86	119.33
2	A	1395	MPY	C29-C27-N30	2.03	122.81	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.