



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:03 AM GMT

PDB ID : 3GMJ
Title : Crystal structure of MAD MH2 domain
Authors : Wu, J.W.; Wang, C.
Deposited on : 2009-03-14
Resolution : 2.80 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>

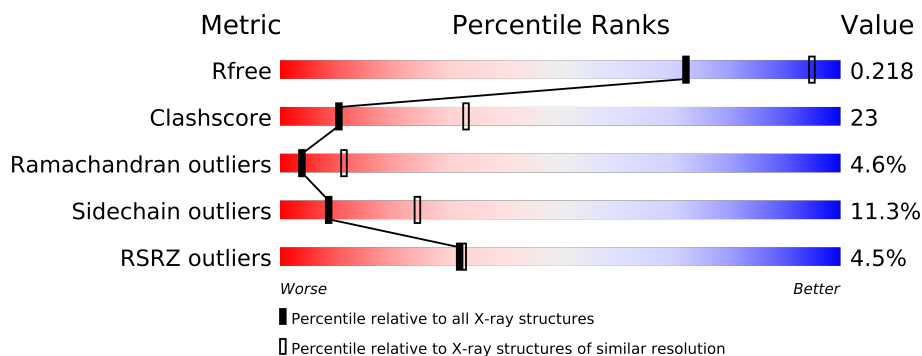
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
1	C	245	
1	D	245	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6248 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 Protein mothers against dpp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	199	Total	C	N	O	S	0	1	0
			1576	988	278	296	14			
1	B	199	Total	C	N	O	S	0	1	0
			1576	988	278	296	14			
1	A	199	Total	C	N	O	S	0	0	0
			1573	986	278	296	13			
1	C	188	Total	C	N	O	S	0	0	0
			1499	943	264	279	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	211	GLY	-	EXPRESSION TAG	UNP P42003
D	212	PRO	-	EXPRESSION TAG	UNP P42003
D	213	HIS	-	EXPRESSION TAG	UNP P42003
D	214	MET	-	EXPRESSION TAG	UNP P42003
D	353	GLN	HIS	SEE REMARK 999	UNP P42003
B	211	GLY	-	EXPRESSION TAG	UNP P42003
B	212	PRO	-	EXPRESSION TAG	UNP P42003
B	213	HIS	-	EXPRESSION TAG	UNP P42003
B	214	MET	-	EXPRESSION TAG	UNP P42003
B	353	GLN	HIS	SEE REMARK 999	UNP P42003
A	211	GLY	-	EXPRESSION TAG	UNP P42003
A	212	PRO	-	EXPRESSION TAG	UNP P42003
A	213	HIS	-	EXPRESSION TAG	UNP P42003
A	214	MET	-	EXPRESSION TAG	UNP P42003
A	353	GLN	HIS	SEE REMARK 999	UNP P42003
C	211	GLY	-	EXPRESSION TAG	UNP P42003
C	212	PRO	-	EXPRESSION TAG	UNP P42003
C	213	HIS	-	EXPRESSION TAG	UNP P42003
C	214	MET	-	EXPRESSION TAG	UNP P42003
C	353	GLN	HIS	SEE REMARK 999	UNP P42003

- Molecule 2 is water.

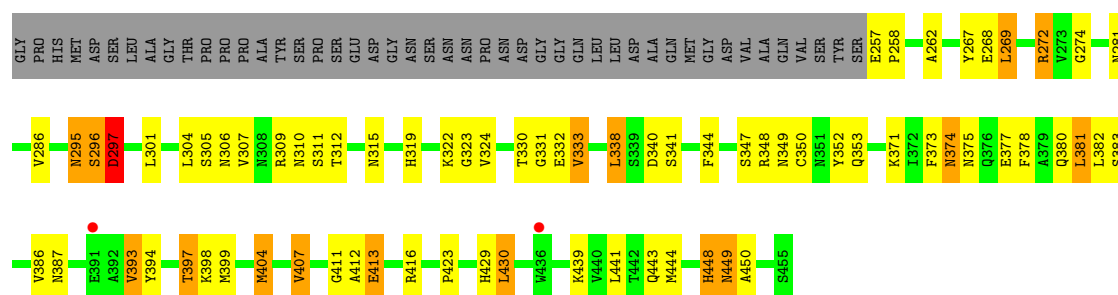
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	O 3	0	0
2	B	5	Total 5	O 5	0	0
2	C	1	Total 1	O 1	0	0
2	D	15	Total 15	O 15	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

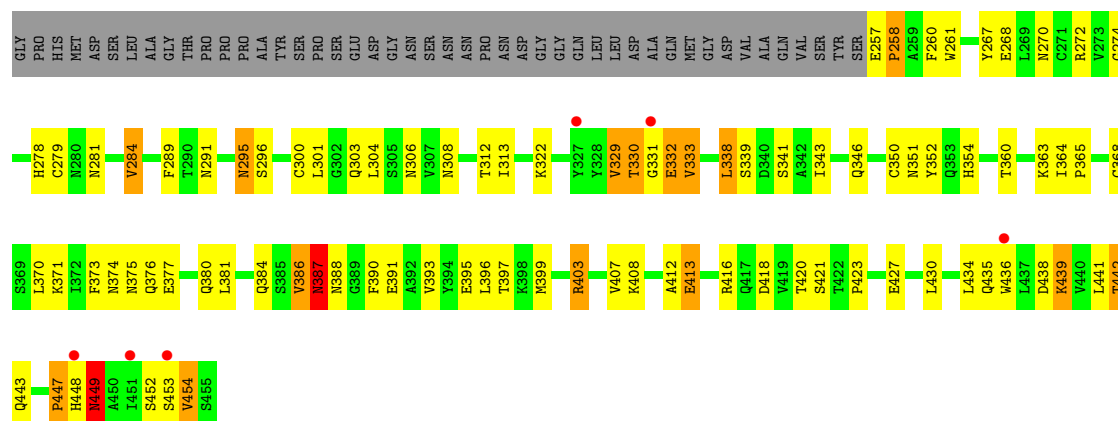
• Molecule 1: Protein mothers against dpp

Chain D:



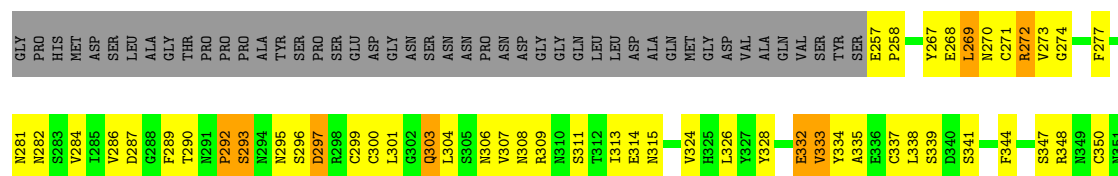
• Molecule 1: Protein mothers against dpp

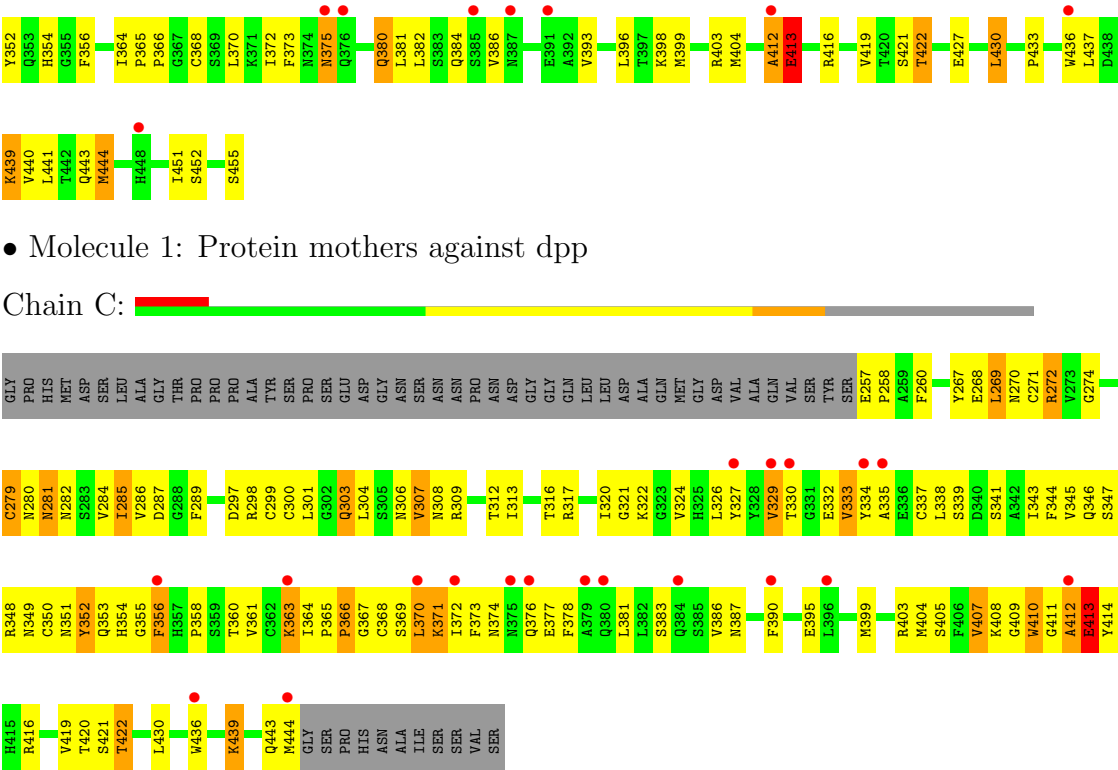
Chain B:



• Molecule 1: Protein mothers against dpp

Chain A:





● Molecule 1: Protein mothers against dpp

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	137.26Å 137.26Å 194.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.33 – 2.80 22.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (22.33-2.80) 99.9 (22.33-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.179 , 0.219 0.179 , 0.218	Depositor DCC
R_{free} test set	1701 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
Estimated twinning fraction	0.849 for k,h,-l 0.124 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.849 for k,h,-l	Depositor
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 33566 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.41	0/1614	0.56	0/2193
1	B	0.41	0/1620	0.55	0/2201
1	C	0.36	0/1538	0.55	0/2090
1	D	0.45	0/1620	0.60	0/2201
All	All	0.41	0/6392	0.56	0/8685

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	1573	0	1493	67	0
1	B	1576	0	1498	56	0
1	C	1499	0	1425	115	0
1	D	1576	0	1498	51	0
2	A	3	0	0	0	0
2	B	5	0	0	1	0
2	C	1	0	0	0	0
2	D	15	0	0	2	0
All	All	6248	0	5914	282	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 23.

All (282) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:349:ASN:HB2	1:D:399:MET:HE3	1.51	0.92
1:C:351:ASN:HB3	1:C:358:PRO:HA	1.52	0.90
1:B:407:VAL:HG11	1:A:451:ILE:HD13	1.55	0.89
1:C:347:SER:O	1:C:351:ASN:HB2	1.78	0.83
1:B:333:VAL:CG1	1:B:373:PHE:HB3	2.09	0.83
1:C:286:VAL:HG22	1:C:299:CYS:HB2	1.61	0.82
1:C:383:SER:HA	1:C:386:VAL:HG23	1.64	0.80
1:C:361:VAL:HG21	1:C:410:TRP:O	1.82	0.79
1:B:412:ALA:O	1:B:413:GLU:HB2	1.85	0.76
1:A:412:ALA:O	1:A:413:GLU:HB2	1.84	0.76
1:C:269:LEU:HD12	1:C:313:ILE:HD11	1.67	0.75
1:B:257:GLU:HB2	1:B:258:PRO:HD3	1.66	0.75
1:A:380:GLN:HB3	1:A:384:GLN:HE21	1.52	0.75
1:D:394:TYR:O	1:D:397:THR:HB	1.87	0.74
1:D:281:ASN:HB3	1:D:297:ASP:OD2	1.87	0.74
1:C:327:TYR:O	1:C:333:VAL:HA	1.89	0.73
1:D:331:GLY:O	1:D:375:ASN:HB2	1.88	0.73
1:B:333:VAL:HG13	1:B:373:PHE:HB3	1.70	0.72
1:B:313:ILE:HG12	1:B:423:PRO:HB3	1.72	0.72
1:A:267:TYR:CE1	1:A:272:ARG:HG2	2.25	0.71
1:C:285:ILE:HD11	1:C:338:LEU:HD22	1.73	0.70
1:D:412:ALA:O	1:D:413:GLU:HB2	1.91	0.70
1:C:285:ILE:HD13	1:C:324:VAL:O	1.91	0.70
1:A:333:VAL:HG13	1:A:373:PHE:HB3	1.73	0.70
1:B:270:ASN:HB3	1:B:420:THR:HB	1.74	0.70
1:C:363:LYS:HG2	1:C:365:PRO:HD3	1.74	0.70
1:B:329:VAL:HG12	1:B:332:GLU:HB2	1.74	0.70
1:B:365:PRO:O	1:B:368:CYS:HB2	1.93	0.68
1:C:344:PHE:HD2	1:C:361:VAL:HG11	1.58	0.68
1:D:349:ASN:HB2	1:D:399:MET:CE	2.23	0.67
1:C:353:GLN:HE21	1:C:377:GLU:HG2	1.59	0.67
1:B:289:PHE:O	1:B:300:CYS:HB3	1.94	0.66
1:D:295:ASN:O	1:D:297:ASP:N	2.29	0.66
1:D:322:LYS:HE3	2:D:12:HOH:O	1.96	0.65
1:B:331:GLY:HA3	1:B:375:ASN:HB2	1.78	0.65
1:C:350:CYS:C	1:C:352:TYR:H	2.00	0.65
1:D:267:TYR:CE1	1:D:272:ARG:HG2	2.31	0.65
1:A:352:TYR:CZ	1:A:381:LEU:HD21	2.32	0.65
1:B:454:VAL:HG22	1:C:414:TYR:HD1	1.61	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:333:VAL:HG13	1:C:373:PHE:HB3	1.80	0.64
1:C:333:VAL:HG22	1:C:372:ILE:HG13	1.78	0.64
1:D:349:ASN:HD22	1:D:399:MET:HE1	1.62	0.64
1:C:333:VAL:CG1	1:C:373:PHE:HB3	2.27	0.64
1:C:408:LYS:HB3	1:C:416:ARG:HH12	1.63	0.63
1:C:413:GLU:HB3	1:C:414:TYR:CD2	2.33	0.63
1:C:344:PHE:HB2	1:C:405:SER:HB3	1.79	0.63
1:C:334:TYR:CD1	1:C:371:LYS:HB2	2.34	0.62
1:A:300:CYS:O	1:A:303:GLN:NE2	2.31	0.62
1:C:289:PHE:O	1:C:300:CYS:HB3	1.99	0.62
1:C:307:VAL:C	1:C:309:ARG:H	2.02	0.62
1:D:333:VAL:HG13	1:D:373:PHE:HB3	1.81	0.61
1:D:272:ARG:NH1	1:D:274:GLY:O	2.34	0.60
1:C:268:GLU:O	1:C:269:LEU:HB2	2.02	0.60
1:C:351:ASN:CB	1:C:358:PRO:HA	2.28	0.60
1:C:443:GLN:O	1:C:444:MET:HG2	2.02	0.60
1:C:412:ALA:O	1:C:413:GLU:HB2	2.00	0.60
1:A:272:ARG:NH1	1:A:274:GLY:O	2.35	0.59
1:C:287:ASP:HB2	1:C:321:GLY:O	2.03	0.59
1:C:329:VAL:HG12	1:C:332:GLU:HB2	1.84	0.58
1:C:365:PRO:O	1:C:368:CYS:HB3	2.03	0.58
1:B:391:GLU:HG2	1:B:395:GLU:HG2	1.85	0.58
1:A:277:PHE:CD2	1:A:299:CYS:HB3	2.37	0.58
1:A:296:SER:O	1:A:297:ASP:HB2	2.02	0.58
1:C:334:TYR:HA	1:C:371:LYS:HA	1.84	0.58
1:A:296:SER:O	1:A:297:ASP:CB	2.52	0.58
1:C:349:ASN:HB2	1:C:373:PHE:CD1	2.39	0.58
1:C:364:ILE:HG12	1:C:370:LEU:HD22	1.86	0.57
1:A:267:TYR:HE1	1:A:272:ARG:HG2	1.70	0.57
1:B:274:GLY:HA3	1:B:304:LEU:HD13	1.87	0.57
1:C:383:SER:HA	1:C:386:VAL:CG2	2.34	0.57
1:C:289:PHE:HB2	1:C:298:ARG:NH2	2.20	0.57
1:A:307:VAL:C	1:A:309:ARG:H	2.08	0.57
1:A:271:CYS:O	1:A:273:VAL:HG23	2.05	0.57
1:C:349:ASN:HA	1:C:399:MET:SD	2.45	0.57
1:C:366:PRO:O	1:C:368:CYS:N	2.38	0.56
1:C:272:ARG:NH1	1:C:274:GLY:O	2.38	0.56
1:C:411:GLY:N	1:C:416:ARG:O	2.35	0.56
1:C:335:ALA:HB2	1:C:372:ILE:HD13	1.87	0.56
1:D:322:LYS:HB3	1:D:338:LEU:HB3	1.88	0.56
1:D:393:VAL:HG22	1:D:441:LEU:HD21	1.86	0.56
1:A:393:VAL:HG21	1:A:440:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:377:GLU:O	1:C:381:LEU:HD23	2.05	0.56
1:A:393:VAL:HG22	1:A:441:LEU:HD21	1.87	0.56
1:D:443:GLN:O	1:D:444:MET:HG3	2.06	0.56
1:D:377:GLU:O	1:D:381:LEU:HD23	2.06	0.56
1:D:348:ARG:NH1	1:D:398:LYS:HD3	2.21	0.55
1:A:348:ARG:NH2	1:A:398:LYS:HD3	2.21	0.55
1:A:289:PHE:O	1:A:300:CYS:HB3	2.06	0.55
1:C:403:ARG:O	1:C:404:MET:HB3	2.06	0.55
1:A:268:GLU:O	1:A:269:LEU:HB2	2.07	0.55
1:A:386:VAL:HG13	1:A:444:MET:CE	2.38	0.54
1:D:274:GLY:HA3	1:D:304:LEU:HD13	1.90	0.54
1:C:416:ARG:HD3	1:C:421:SER:HB3	1.90	0.54
1:A:382:LEU:HD13	1:A:437:LEU:HD12	1.89	0.54
1:A:439:LYS:N	1:A:439:LYS:HD3	2.23	0.53
1:C:439:LYS:N	1:C:439:LYS:HD2	2.22	0.53
1:C:341:SER:HB3	1:C:407:VAL:HG22	1.89	0.53
1:C:341:SER:CB	1:C:407:VAL:HG22	2.38	0.53
1:D:413:GLU:OE2	1:D:413:GLU:HA	2.07	0.53
1:A:348:ARG:CZ	1:A:398:LYS:HD3	2.39	0.53
1:C:268:GLU:OE2	1:C:317:ARG:HD2	2.09	0.53
1:A:286:VAL:HB	1:A:324:VAL:HG12	1.91	0.52
1:D:268:GLU:O	1:D:269:LEU:HB2	2.08	0.52
1:A:403:ARG:HD3	1:A:427:GLU:HG3	1.91	0.52
1:D:413:GLU:HG3	1:A:370:LEU:HA	1.92	0.52
1:A:380:GLN:HB3	1:A:384:GLN:NE2	2.24	0.51
1:C:349:ASN:HB2	1:C:373:PHE:CE1	2.46	0.51
1:C:350:CYS:C	1:C:352:TYR:N	2.63	0.51
1:A:452:SER:HB3	1:A:455:SER:OG	2.10	0.51
1:C:361:VAL:HG22	1:C:410:TRP:CE2	2.45	0.51
1:B:418:ASP:O	1:B:421:SER:HB2	2.11	0.51
1:C:364:ILE:O	1:C:364:ILE:HG22	2.11	0.51
1:B:434:LEU:HD22	1:C:303:GLN:HB3	1.93	0.51
1:C:267:TYR:CE1	1:C:272:ARG:HG2	2.46	0.51
1:B:350:CYS:C	1:B:352:TYR:H	2.15	0.50
1:B:396:LEU:O	1:B:399:MET:HB2	2.12	0.50
1:A:386:VAL:HG13	1:A:444:MET:HE1	1.93	0.50
1:C:349:ASN:HD22	1:C:399:MET:CE	2.24	0.50
1:C:345:VAL:HG12	1:C:346:GLN:N	2.26	0.50
1:C:334:TYR:CE1	1:C:371:LYS:HD3	2.47	0.50
1:C:376:GLN:C	1:C:378:PHE:H	2.16	0.50
1:C:366:PRO:C	1:C:368:CYS:H	2.15	0.49
1:A:352:TYR:CE1	1:A:381:LEU:HD21	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:375:ASN:OD1	1:A:436:TRP:HZ3	1.95	0.49
1:A:284:VAL:HG23	1:A:326:LEU:HB2	1.94	0.49
1:B:423:PRO:HD2	2:B:4:HOH:O	2.12	0.49
1:C:350:CYS:HA	1:C:353:GLN:HB3	1.94	0.49
1:C:370:LEU:O	1:C:371:LYS:C	2.50	0.49
1:C:307:VAL:C	1:C:309:ARG:N	2.66	0.49
1:D:393:VAL:HG22	1:D:441:LEU:CD2	2.43	0.49
1:D:347:SER:HB3	1:D:350:CYS:HB3	1.94	0.49
1:B:257:GLU:CB	1:B:258:PRO:HD3	2.37	0.49
1:A:419:VAL:HA	1:A:422:THR:HG23	1.94	0.49
1:A:339:SER:HB3	1:A:341:SER:O	2.13	0.49
1:C:410:TRP:HB3	1:C:422:THR:HG22	1.95	0.48
1:B:306:ASN:OD1	1:B:308:ASN:HB2	2.12	0.48
1:C:257:GLU:N	1:C:258:PRO:CD	2.76	0.48
1:B:380:GLN:O	1:B:384:GLN:HG3	2.13	0.48
1:C:337:CYS:SG	1:C:343:ILE:HG23	2.54	0.48
1:B:258:PRO:HB3	1:B:435:GLN:NE2	2.29	0.48
1:D:310:ASN:OD1	1:D:310:ASN:C	2.52	0.48
1:B:260:PHE:CD2	1:B:278:HIS:HB3	2.48	0.48
1:D:378:PHE:HD2	1:D:399:MET:HE2	1.78	0.48
1:C:344:PHE:O	1:C:410:TRP:CZ3	2.67	0.48
1:B:386:VAL:HG12	1:B:387:ASN:N	2.28	0.48
1:C:344:PHE:CE2	1:C:409:GLY:CA	2.97	0.48
1:D:296:SER:O	1:D:297:ASP:HB2	2.14	0.47
1:B:329:VAL:O	1:B:330:THR:C	2.52	0.47
1:C:289:PHE:HB2	1:C:298:ARG:HH22	1.78	0.47
1:A:309:ARG:HD3	1:A:314:GLU:HG3	1.95	0.47
1:B:439:LYS:HD2	1:B:439:LYS:N	2.28	0.47
1:A:365:PRO:O	1:A:368:CYS:HB2	2.13	0.47
1:B:443:GLN:HE21	1:B:443:GLN:HB2	1.49	0.47
1:D:341:SER:HB2	1:D:407:VAL:HG22	1.96	0.47
1:C:353:GLN:HE21	1:C:377:GLU:CG	2.26	0.47
1:B:380:GLN:HB3	1:B:384:GLN:HE21	1.78	0.47
1:D:330:THR:OG1	1:D:331:GLY:N	2.47	0.47
1:C:376:GLN:C	1:C:378:PHE:N	2.66	0.47
1:B:441:LEU:HB3	1:C:289:PHE:CD1	2.49	0.47
1:B:441:LEU:HB3	1:C:289:PHE:HD1	1.78	0.47
1:C:344:PHE:CD2	1:C:361:VAL:HG11	2.44	0.47
1:C:338:LEU:HD12	1:C:338:LEU:N	2.29	0.47
1:B:261:TRP:NE1	1:B:281:ASN:O	2.48	0.47
1:B:386:VAL:C	1:B:388:ASN:H	2.18	0.46
1:C:316:THR:HG23	1:C:407:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:GLU:HB2	1:A:258:PRO:HD3	1.96	0.46
1:B:390:PHE:CD1	1:B:447:PRO:HG3	2.50	0.46
1:C:333:VAL:HG13	1:C:373:PHE:O	2.15	0.46
1:A:347:SER:HB3	1:A:350:CYS:HB3	1.97	0.46
1:B:257:GLU:HB2	1:B:258:PRO:CD	2.40	0.46
1:A:300:CYS:HB2	1:A:303:GLN:HE21	1.81	0.46
1:A:281:ASN:HB3	1:A:297:ASP:CG	2.35	0.46
1:C:349:ASN:HD22	1:C:399:MET:HE1	1.79	0.46
1:A:274:GLY:HA3	1:A:304:LEU:HD22	1.97	0.46
1:D:315:ASN:O	1:D:319:HIS:HD2	1.98	0.46
1:C:320:ILE:O	1:C:339:SER:HB2	2.15	0.46
1:C:351:ASN:ND2	1:C:360:THR:O	2.46	0.46
1:A:306:ASN:HB3	1:A:309:ARG:HB2	1.96	0.46
1:D:448:HIS:CG	1:D:449:ASN:N	2.83	0.46
1:B:279:CYS:HB3	1:B:284:VAL:HG11	1.98	0.46
1:A:303:GLN:H	1:A:303:GLN:HG3	1.41	0.46
1:A:309:ARG:HG3	1:A:313:ILE:CG2	2.46	0.46
1:B:453:SER:O	1:B:454:VAL:HG23	2.16	0.45
1:C:413:GLU:HB3	1:C:414:TYR:CE2	2.50	0.45
1:D:340:ASP:HB2	2:D:17:HOH:O	2.15	0.45
1:A:282:ASN:HB3	1:A:328:TYR:O	2.16	0.45
1:D:344:PHE:HE1	1:D:407:VAL:O	1.99	0.45
1:D:378:PHE:CD2	1:D:399:MET:HE2	2.51	0.45
1:D:374:ASN:HB3	1:D:377:GLU:HB3	1.98	0.45
1:B:390:PHE:O	1:B:393:VAL:HG12	2.15	0.45
1:B:377:GLU:O	1:B:381:LEU:HD23	2.17	0.45
1:C:348:ARG:HG2	1:C:358:PRO:HB3	1.98	0.45
1:C:344:PHE:CE2	1:C:409:GLY:HA2	2.51	0.45
1:A:277:PHE:CE2	1:A:299:CYS:HB3	2.52	0.45
1:B:304:LEU:N	1:B:304:LEU:HD23	2.32	0.45
1:C:281:ASN:OD1	1:C:282:ASN:N	2.50	0.45
1:C:269:LEU:CD1	1:C:313:ILE:HD11	2.43	0.45
1:C:410:TRP:HA	1:C:416:ARG:O	2.16	0.45
1:C:333:VAL:HG11	1:C:373:PHE:HB3	1.98	0.45
1:C:326:LEU:HA	1:C:334:TYR:O	2.17	0.45
1:B:295:ASN:OD1	1:B:295:ASN:N	2.47	0.45
1:D:286:VAL:O	1:D:323:GLY:HA3	2.17	0.45
1:B:438:ASP:O	1:B:442:THR:OG1	2.35	0.44
1:C:268:GLU:HB3	1:C:313:ILE:HD13	1.99	0.44
1:C:279:CYS:HB3	1:C:284:VAL:HG11	1.98	0.44
1:B:374:ASN:HD21	1:B:376:GLN:HG3	1.83	0.44
1:C:414:TYR:CD2	1:C:414:TYR:N	2.85	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:309:ARG:HG3	1:C:313:ILE:CG2	2.47	0.44
1:D:257:GLU:HB2	1:D:258:PRO:HD3	1.98	0.44
1:A:344:PHE:O	1:A:404:MET:HA	2.18	0.44
1:A:290:THR:HA	1:A:303:GLN:HG2	1.99	0.44
1:C:285:ILE:HD12	1:C:322:LYS:O	2.18	0.44
1:B:341:SER:HB2	1:B:407:VAL:HG22	1.99	0.43
1:C:344:PHE:CE2	1:C:409:GLY:HA3	2.53	0.43
1:C:410:TRP:CE2	1:C:419:VAL:HB	2.53	0.43
1:D:286:VAL:HB	1:D:324:VAL:HG12	2.00	0.43
1:A:287:ASP:C	1:A:287:ASP:OD1	2.57	0.43
1:D:269:LEU:HA	1:D:269:LEU:HD23	1.88	0.43
1:C:257:GLU:N	1:C:258:PRO:HD3	2.34	0.43
1:A:354:HIS:HB3	1:A:356:PHE:CE1	2.53	0.43
1:D:268:GLU:HA	1:D:423:PRO:O	2.19	0.43
1:A:337:CYS:SG	1:A:366:PRO:HA	2.59	0.43
1:C:322:LYS:HB2	1:C:322:LYS:HE3	1.81	0.43
1:A:332:GLU:HG3	1:A:334:TYR:CE2	2.54	0.43
1:C:351:ASN:ND2	1:C:358:PRO:O	2.52	0.43
1:D:382:LEU:O	1:D:386:VAL:HG23	2.18	0.43
1:D:380:GLN:O	1:D:383:SER:N	2.52	0.43
1:A:412:ALA:O	1:A:413:GLU:CB	2.60	0.43
1:B:363:LYS:HB3	1:B:363:LYS:HE2	1.60	0.43
1:B:339:SER:HB3	1:B:341:SER:O	2.19	0.43
1:A:292:PRO:O	1:A:293:SER:C	2.57	0.43
1:C:356:PHE:HE2	1:C:360:THR:HG21	1.84	0.42
1:C:413:GLU:C	1:C:414:TYR:CD2	2.92	0.42
1:D:332:GLU:OE2	1:D:371:LYS:HD2	2.19	0.42
1:C:260:PHE:HB3	1:C:279:CYS:O	2.19	0.42
1:B:370:LEU:HD12	1:B:371:LYS:H	1.83	0.42
1:C:329:VAL:C	1:C:330:THR:HG1	2.22	0.42
1:C:270:ASN:HB3	1:C:420:THR:HB	2.02	0.42
1:D:411:GLY:N	1:D:416:ARG:O	2.43	0.42
1:A:381:LEU:HD13	1:A:381:LEU:HA	1.89	0.42
1:D:344:PHE:O	1:D:404:MET:HA	2.20	0.42
1:D:341:SER:CB	1:D:407:VAL:HG22	2.50	0.42
1:C:344:PHE:O	1:C:410:TRP:CH2	2.73	0.42
1:B:322:LYS:HE3	1:B:338:LEU:O	2.19	0.42
1:A:416:ARG:HB3	1:A:421:SER:HB2	2.02	0.41
1:D:304:LEU:N	1:D:304:LEU:HD23	2.34	0.41
1:A:332:GLU:HG3	1:A:334:TYR:OH	2.19	0.41
1:A:396:LEU:O	1:A:399:MET:HB2	2.20	0.41
1:C:411:GLY:O	1:C:412:ALA:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:262:ALA:HA	1:D:429:HIS:O	2.20	0.41
1:A:451:ILE:HG12	1:A:452:SER:N	2.36	0.41
1:C:411:GLY:O	1:C:413:GLU:N	2.53	0.41
1:C:303:GLN:H	1:C:303:GLN:HG3	1.59	0.41
1:C:304:LEU:HD23	1:C:304:LEU:HA	1.71	0.41
1:B:403:ARG:HD2	1:B:427:GLU:HG3	2.02	0.41
1:B:343:ILE:HG12	1:B:364:ILE:HB	2.02	0.41
1:A:311:SER:O	1:A:315:ASN:CG	2.59	0.41
1:D:306:ASN:O	1:D:309:ARG:HB2	2.20	0.41
1:B:268:GLU:HB3	1:B:313:ILE:HD13	2.02	0.41
1:A:307:VAL:C	1:A:309:ARG:N	2.73	0.41
1:D:352:TYR:CE1	1:D:381:LEU:HD21	2.56	0.41
1:A:386:VAL:HG13	1:A:444:MET:HE3	2.03	0.41
1:B:448:HIS:O	1:B:449:ASN:C	2.60	0.41
1:B:346:GLN:HG3	1:B:360:THR:O	2.21	0.41
1:C:354:HIS:O	1:C:356:PHE:N	2.44	0.40
1:A:380:GLN:O	1:A:384:GLN:HG3	2.21	0.40
1:B:291:ASN:HB3	1:B:300:CYS:SG	2.61	0.40
1:C:281:ASN:HB3	1:C:297:ASP:OD2	2.21	0.40
1:A:335:ALA:HB2	1:A:372:ILE:HD13	2.03	0.40
1:A:430:LEU:HB3	1:A:433:PRO:HD2	2.02	0.40
1:C:306:ASN:OD1	1:C:307:VAL:N	2.55	0.40
1:A:364:ILE:HD11	1:A:370:LEU:HB3	2.04	0.40
1:D:399:MET:HE2	1:D:399:MET:HB3	1.71	0.40
1:C:351:ASN:O	1:C:356:PHE:O	2.40	0.40
1:B:452:SER:O	1:C:408:LYS:HG2	2.22	0.40
1:C:333:VAL:CG2	1:C:372:ILE:HG13	2.49	0.40
1:A:443:GLN:O	1:A:444:MET:HG3	2.21	0.40
1:C:344:PHE:HB3	1:C:410:TRP:CZ3	2.57	0.40
1:C:309:ARG:HG3	1:C:313:ILE:HG21	2.03	0.40
1:C:365:PRO:O	1:C:366:PRO:O	2.40	0.40
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.88	0.40
1:B:408:LYS:HB3	1:B:416:ARG:NH1	2.37	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	197/245 (80%)	168 (85%)	21 (11%)	8 (4%)	4	14
1	B	198/245 (81%)	172 (87%)	18 (9%)	8 (4%)	5	14
1	C	186/245 (76%)	144 (77%)	31 (17%)	11 (6%)	2	6
1	D	198/245 (81%)	171 (86%)	18 (9%)	9 (4%)	4	12
All	All	779/980 (80%)	655 (84%)	88 (11%)	36 (5%)	4	11

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	ASN
1	D	296	SER
1	D	448	HIS
1	B	330	THR
1	B	386	VAL
1	A	297	ASP
1	A	413	GLU
1	C	363	LYS
1	C	413	GLU
1	D	449	ASN
1	D	450	ALA
1	B	296	SER
1	B	351	ASN
1	B	449	ASN
1	B	454	VAL
1	C	269	LEU
1	C	308	ASN
1	C	367	GLY
1	C	370	LEU
1	C	371	LYS
1	C	407	VAL
1	C	412	ALA
1	D	297	ASP
1	D	381	LEU
1	B	447	PRO
1	A	292	PRO
1	A	293	SER
1	D	269	LEU
1	B	387	ASN
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	308	ASN
1	A	412	ALA
1	C	366	PRO
1	D	407	VAL
1	C	355	GLY
1	A	444	MET

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	177/213 (83%)	163 (92%)	14 (8%)	18	44
1	B	178/213 (84%)	156 (88%)	22 (12%)	7	20
1	C	168/213 (79%)	143 (85%)	25 (15%)	4	12
1	D	178/213 (84%)	160 (90%)	18 (10%)	11	30
All	All	701/852 (82%)	622 (89%)	79 (11%)	9	24

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	272	ARG
1	D	297	ASP
1	D	301	LEU
1	D	305	SER
1	D	307	VAL
1	D	311	SER
1	D	312	THR
1	D	333	VAL
1	D	338	LEU
1	D	353	GLN
1	D	374	ASN
1	D	387	ASN
1	D	393	VAL
1	D	397	THR
1	D	404	MET
1	D	413	GLU

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Mol	Chain	Res	Type
1	D	430	LEU
1	D	439	LYS
1	B	258	PRO
1	B	267	TYR
1	B	272	ARG
1	B	284	VAL
1	B	295	ASN
1	B	301	LEU
1	B	303	GLN
1	B	312	THR
1	B	329	VAL
1	B	332	GLU
1	B	333	VAL
1	B	338	LEU
1	B	354	HIS
1	B	387	ASN
1	B	397	THR
1	B	403	ARG
1	B	413	GLU
1	B	430	LEU
1	B	436	TRP
1	B	439	LYS
1	B	442	THR
1	B	449	ASN
1	A	270	ASN
1	A	272	ARG
1	A	295	ASN
1	A	301	LEU
1	A	303	GLN
1	A	332	GLU
1	A	333	VAL
1	A	338	LEU
1	A	375	ASN
1	A	380	GLN
1	A	413	GLU
1	A	422	THR
1	A	430	LEU
1	A	439	LYS
1	C	271	CYS
1	C	272	ARG
1	C	279	CYS
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	281	ASN
1	C	285	ILE
1	C	301	LEU
1	C	303	GLN
1	C	307	VAL
1	C	312	THR
1	C	329	VAL
1	C	333	VAL
1	C	352	TYR
1	C	356	PHE
1	C	369	SER
1	C	374	ASN
1	C	387	ASN
1	C	390	PHE
1	C	395	GLU
1	C	410	TRP
1	C	413	GLU
1	C	422	THR
1	C	430	LEU
1	C	436	TRP
1	C	439	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	319	HIS
1	D	349	ASN
1	D	353	GLN
1	D	374	ASN
1	D	443	GLN
1	D	448	HIS
1	B	281	ASN
1	B	353	GLN
1	B	375	ASN
1	B	384	GLN
1	B	443	GLN
1	B	449	ASN
1	A	295	ASN
1	A	357	HIS
1	A	384	GLN
1	C	280	ASN
1	C	349	ASN

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Mol	Chain	Res	Type
1	C	353	GLN
1	C	357	HIS
1	C	387	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 ⓘ

There are no ligands in this entry.

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, 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	199/245 (81%)	0.53	8 (4%) 36 37	51, 73, 111, 127	0
1	B	199/245 (81%)	0.47	6 (3%) 48 49	47, 69, 110, 122	0
1	C	188/245 (76%)	0.88	19 (10%) 7 6	52, 95, 131, 141	0
1	D	199/245 (81%)	0.38	2 (1%) 79 79	39, 55, 94, 120	0
All	All	785/980 (80%)	0.56	35 (4%) 32 33	39, 73, 119, 141	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	372	ILE	6.1
1	C	356	PHE	3.3
1	C	327	TYR	3.1
1	B	451	ILE	2.9
1	D	436	TRP	2.9
1	C	329	VAL	2.9
1	B	327	TYR	2.9
1	C	335	ALA	2.9
1	C	375	ASN	2.8
1	C	370	LEU	2.8
1	A	436	TRP	2.7
1	B	436	TRP	2.7
1	C	396	LEU	2.6
1	C	444	MET	2.6
1	B	453	SER	2.6
1	C	380	GLN	2.6
1	C	334	TYR	2.5
1	B	331	GLY	2.5
1	A	412	ALA	2.4
1	C	363	LYS	2.4
1	B	448	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	379	ALA	2.3
1	C	436	TRP	2.3
1	C	384	GLN	2.2
1	C	390	PHE	2.2
1	C	330	THR	2.2
1	C	376	GLN	2.2
1	C	412	ALA	2.1
1	A	375	ASN	2.1
1	A	391	GLU	2.1
1	A	385	SER	2.1
1	A	376	GLN	2.1
1	D	391	GLU	2.0
1	A	387	ASN	2.0
1	A	448	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.