



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:42 AM UTC

PDB ID : 3JXA / pdb_00003jxa
Title : Immunoglobulin domains 1-4 of mouse CNTN4
Authors : Bouyain, S.
Deposited on : 2009-09-18
Resolution : 2.40 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

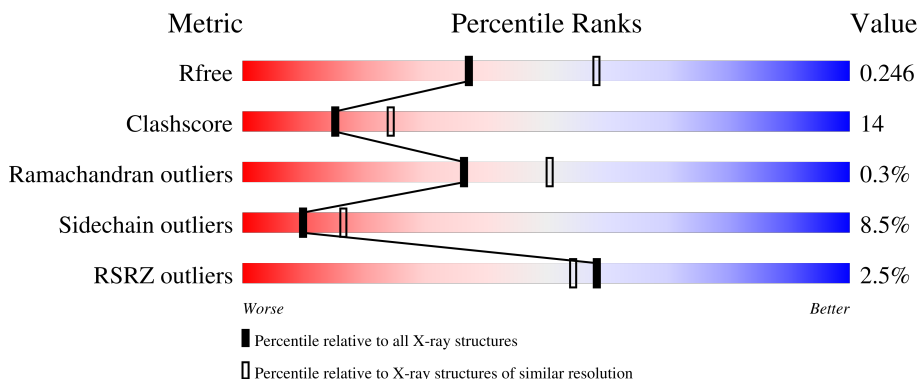
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

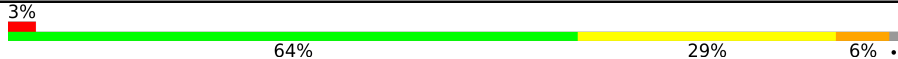
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	383	
1	B	383	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2	X	-	-	-
2	NAG	A	4	X	-	-	-
2	NAG	B	5	X	-	-	-
2	NAG	B	8	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6283 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.

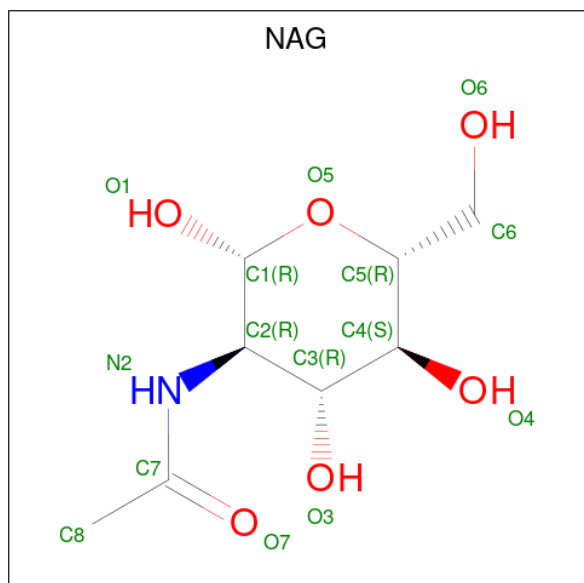
- Molecule 1 is a protein called Contactin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2971	1878	523	556	14			
1	B	383	Total	C	N	O	S	0	0	0
			3013	1902	529	568	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PRO	-	expression tag	UNP Q14BL8
A	23	GLY	-	expression tag	UNP Q14BL8
A	24	SER	-	expression tag	UNP Q14BL8
B	22	PRO	-	expression tag	UNP Q14BL8
B	23	GLY	-	expression tag	UNP Q14BL8
B	24	SER	-	expression tag	UNP Q14BL8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

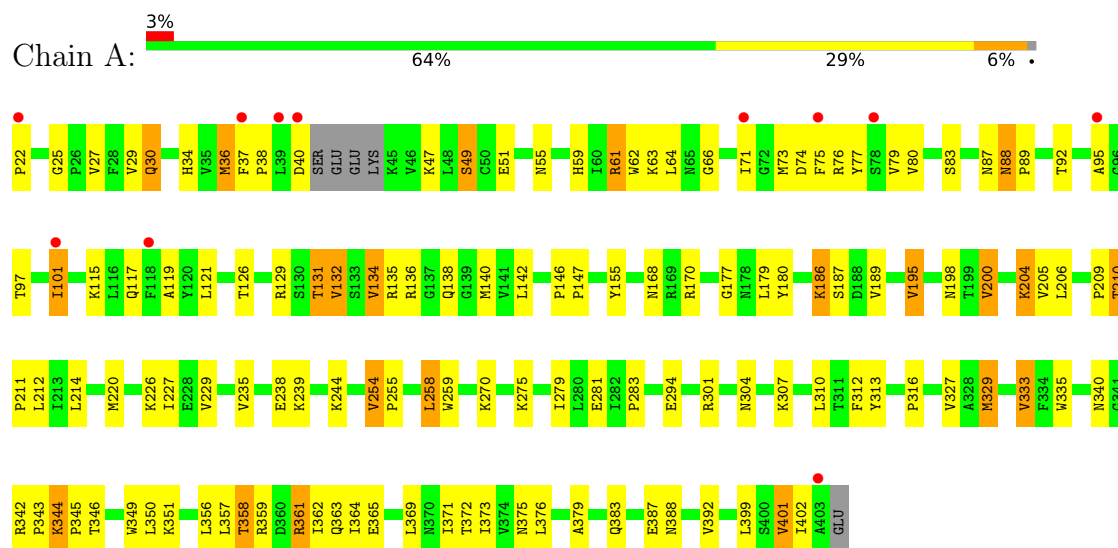
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	35	Total	O	0	0
			35	35		

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: Contactin 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	281.73Å 40.43Å 95.08Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	37.17 – 2.40 37.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.4 (37.17-2.40) 91.4 (37.17-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.252 0.194 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6283	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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

5.1 Standard geometry

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

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	0.39	0/3040	0.81	7/4127 (0.2%)
1	B	0.32	0/3083	0.77	4/4185 (0.1%)
All	All	0.36	0/6123	0.79	11/8312 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	LYS	CA-C-N	6.07	126.01	119.76
1	B	344	LYS	C-N-CA	6.07	126.01	119.76
1	A	344	LYS	CA-C-N	5.73	126.05	119.92
1	A	344	LYS	C-N-CA	5.73	126.05	119.92
1	A	88	ASN	CA-C-N	5.70	126.18	120.14
1	A	88	ASN	C-N-CA	5.70	126.18	120.14
1	B	145	GLY	CA-C-N	5.18	123.44	119.66
1	B	145	GLY	C-N-CA	5.18	123.44	119.66
1	A	25	GLY	CA-C-N	5.14	124.90	119.76
1	A	25	GLY	C-N-CA	5.14	124.90	119.76
1	A	329	MET	N-CA-C	5.02	117.14	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2971	0	2931	93	0
1	B	3013	0	2968	72	2
2	A	56	0	52	1	0
2	B	56	0	52	2	0
3	A	152	0	0	3	0
3	B	35	0	0	0	0
All	All	6283	0	6003	164	2

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 14.

All (164) 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:A:73:MET:SD	1:A:74:ASP:HB2	1.84	1.17
1:A:361:ARG:HE	1:A:361:ARG:H	0.93	0.92
1:B:190:GLY:HA2	2:B:7:NAG:H82	1.56	0.87
1:B:73:MET:HA	1:B:74:ASP:HB2	1.56	0.86
1:A:361:ARG:HE	1:A:361:ARG:N	1.77	0.82
1:A:327:VAL:HG11	1:A:333:VAL:HG12	1.62	0.82
1:A:361:ARG:H	1:A:361:ARG:NE	1.77	0.80
1:B:225:PRO:HG2	1:B:298:GLU:HA	1.64	0.80
1:A:351:LYS:HB2	1:A:356:LEU:HD12	1.64	0.80
1:B:38:PRO:HB2	1:B:41:SER:HB2	1.64	0.79
1:A:71:ILE:HD13	1:A:79:VAL:HG21	1.65	0.78
1:A:115:LYS:HE3	1:A:117:GLN:HG2	1.65	0.77
1:A:134:VAL:CG2	1:A:212:LEU:HD11	2.14	0.77
1:A:30:GLN:HB2	1:A:51:GLU:HG2	1.68	0.76
1:A:357:LEU:HA	1:A:364:ILE:HD11	1.68	0.75
1:A:138:GLN:NE2	1:A:220:MET:HE3	2.03	0.73
1:A:29:VAL:HB	1:A:51:GLU:HG3	1.72	0.72
1:A:134:VAL:HG21	1:A:212:LEU:HD11	1.71	0.71
1:B:244:LYS:HG2	1:B:281:GLU:HG2	1.73	0.71
1:B:370:ASN:HB2	2:B:8:NAG:O6	1.91	0.70
1:A:209:PRO:HG3	3:A:498:HOH:O	1.93	0.69
1:A:75:PHE:HD1	1:A:77:TYR:CE2	2.11	0.69
1:A:186:LYS:HD3	1:A:187:SER:N	2.10	0.66
1:A:227:ILE:H	1:A:304:ASN:HD22	1.45	0.65
1:A:270:LYS:HE3	1:A:283:PRO:O	1.97	0.64
1:A:49:SER:HA	1:A:83:SER:OG	1.98	0.63
1:A:71:ILE:HG21	1:A:79:VAL:HG23	1.80	0.63
1:B:336:GLU:HG3	1:B:368:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:O	1:B:89:PRO:HD3	1.98	0.63
1:A:75:PHE:CD1	1:A:77:TYR:CE2	2.87	0.62
1:A:275:LYS:HD2	1:A:279:ILE:HD12	1.81	0.62
1:B:138:GLN:HG2	1:B:139:GLY:N	2.16	0.61
1:B:212:LEU:C	1:B:212:LEU:HD12	2.25	0.60
1:A:402:ILE:HG12	3:A:528:HOH:O	2.01	0.60
1:B:44:LYS:H	1:B:44:LYS:HD3	1.67	0.60
1:B:165:TYR:HB3	1:B:170:ARG:NH2	2.16	0.60
1:B:138:GLN:HG2	1:B:139:GLY:H	1.67	0.59
1:B:183:LYS:HD2	1:B:252:ASN:OD1	2.03	0.59
1:A:76:ARG:HD3	1:A:87:ASN:HD22	1.66	0.59
1:A:131:THR:HB	1:A:211:PRO:HB2	1.82	0.59
1:B:73:MET:SD	1:B:74:ASP:HB2	2.42	0.59
1:B:267:ILE:HG23	1:B:269:ARG:H	1.67	0.59
1:A:270:LYS:HG3	1:A:283:PRO:HD2	1.84	0.59
1:A:74:ASP:O	1:A:75:PHE:CG	2.56	0.58
1:A:34:HIS:CD2	1:A:115:LYS:H	2.21	0.58
1:A:372:THR:HG22	1:A:373:ILE:HG13	1.86	0.58
1:B:101:ILE:HD12	1:B:110:VAL:HG22	1.86	0.57
1:A:34:HIS:HD2	1:A:115:LYS:H	1.53	0.57
1:B:132:VAL:HG12	1:B:133:SER:N	2.20	0.57
1:B:55:ASN:HD22	1:B:56:PRO:HA	1.70	0.57
1:A:134:VAL:HG23	1:A:212:LEU:HD11	1.87	0.56
1:A:198:ASN:OD1	1:A:200:VAL:HG13	2.05	0.56
1:A:74:ASP:O	1:A:75:PHE:CD1	2.59	0.56
1:A:186:LYS:HD3	1:A:186:LYS:C	2.31	0.56
1:A:342:ARG:HA	1:A:343:PRO:C	2.31	0.55
1:B:222:GLU:HA	1:B:252:ASN:HB3	1.88	0.55
1:A:22:PRO:HA	1:A:55:ASN:HD22	1.72	0.54
1:A:349:TRP:O	1:A:350:LEU:HD12	2.07	0.54
1:A:71:ILE:HD13	1:A:79:VAL:CG2	2.38	0.54
1:A:329:MET:HE1	1:A:376:LEU:HG	1.90	0.54
1:A:358:THR:HB	1:A:364:ILE:H	1.71	0.54
1:B:284:ASN:ND2	1:B:286:GLN:HE21	2.05	0.54
1:B:47:LYS:HG3	1:B:85:LEU:CD2	2.38	0.54
1:A:359:ARG:NH2	1:A:362:ILE:HD12	2.23	0.53
1:B:387:GLU:HB3	1:B:392:VAL:HG22	1.90	0.53
1:A:64:LEU:C	1:A:66:GLY:H	2.17	0.53
1:A:364:ILE:O	1:A:364:ILE:HG13	2.08	0.53
1:B:224:GLU:HG2	1:B:302:GLY:HA3	1.91	0.53
1:B:369:LEU:C	1:B:369:LEU:HD23	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD12	1:A:259:TRP:N	2.24	0.53
1:B:252:ASN:C	1:B:252:ASN:HD22	2.16	0.53
1:A:195:VAL:HB	1:A:206:LEU:CD2	2.39	0.52
1:A:294:GLU:HG2	1:A:307:LYS:HB3	1.90	0.52
1:A:376:LEU:HA	1:A:401:VAL:HG21	1.91	0.52
1:A:227:ILE:H	1:A:304:ASN:ND2	2.08	0.51
1:B:223:TYR:CZ	1:B:251:GLY:HA2	2.46	0.51
1:B:180:TYR:CE2	1:B:229:VAL:HG22	2.46	0.50
1:A:361:ARG:HH12	1:A:375:ASN:ND2	2.09	0.50
1:B:168:ASN:HD22	1:B:168:ASN:N	2.09	0.50
1:A:180:TYR:CZ	1:A:229:VAL:HG22	2.46	0.49
1:A:239:LYS:HE3	1:A:312:PHE:HZ	1.78	0.49
1:A:239:LYS:HB2	1:A:312:PHE:CZ	2.48	0.49
1:B:166:GLN:HE22	1:B:275:LYS:NZ	2.10	0.49
1:A:129:ARG:HD2	1:A:210:THR:HB	1.94	0.49
1:B:165:TYR:HD1	1:B:166:GLN:N	2.11	0.49
1:B:103:THR:OG1	1:B:108:THR:HB	2.13	0.48
1:A:142:LEU:HD12	1:A:179:LEU:HD23	1.95	0.48
1:A:226:LYS:NZ	1:B:403:ALA:HB3	2.28	0.48
1:A:47:LYS:NZ	1:A:49:SER:HB3	2.28	0.48
1:A:356:LEU:C	1:A:356:LEU:HD23	2.38	0.48
1:B:318:TRP:CE2	1:B:393:ILE:HD12	2.48	0.48
1:A:95:ALA:O	2:A:1:NAG:H3	2.14	0.48
1:A:195:VAL:HB	1:A:206:LEU:HD23	1.97	0.47
1:B:342:ARG:HA	1:B:343:PRO:C	2.39	0.47
1:B:222:GLU:HG2	1:B:252:ASN:ND2	2.29	0.47
1:B:360:ASP:O	1:B:361:ARG:HB2	2.14	0.47
1:B:121:LEU:HD21	1:B:196:VAL:HG22	1.97	0.47
1:B:157:TRP:CZ2	1:B:194:CYS:HB2	2.49	0.47
1:B:76:ARG:HD3	1:B:76:ARG:HA	1.45	0.47
1:A:132:VAL:HG21	1:A:140:MET:HE1	1.97	0.47
1:A:186:LYS:HA	1:A:214:LEU:HD11	1.96	0.47
1:B:101:ILE:CD1	1:B:110:VAL:HG22	2.45	0.47
1:B:227:ILE:H	1:B:304:ASN:HD22	1.63	0.47
1:A:73:MET:HA	1:A:74:ASP:HA	1.45	0.46
1:B:73:MET:SD	1:B:74:ASP:CB	3.04	0.46
1:B:99:GLN:NE2	1:B:110:VAL:HG13	2.31	0.46
1:A:189:VAL:CG2	1:A:214:LEU:HG	2.45	0.46
1:A:37:PHE:CD2	1:A:38:PRO:O	2.68	0.46
1:B:37:PHE:HA	1:B:38:PRO:HD3	1.80	0.45
1:B:203:HIS:CD2	1:B:204:LYS:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ILE:HG12	1:B:371:ILE:HG12	2.00	0.44
1:A:61:ARG:HG2	1:A:62:TRP:N	2.32	0.44
1:B:261:ARG:C	1:B:263:ASP:H	2.26	0.44
1:B:208:PRO:HA	1:B:209:PRO:HD3	1.87	0.44
1:B:295:CYS:O	1:B:305:VAL:HA	2.18	0.44
1:A:63:LYS:HE2	1:A:101:ILE:HD13	1.99	0.44
1:A:254:VAL:HA	1:A:255:PRO:HD3	1.74	0.44
1:B:75:PHE:CD1	1:B:77:TYR:CE1	3.06	0.44
1:B:124:PHE:CD1	1:B:207:GLY:HA2	2.53	0.44
1:B:227:ILE:HG13	1:B:304:ASN:HD22	1.83	0.44
1:A:121:LEU:HD21	1:A:205:VAL:HG22	2.00	0.44
1:A:76:ARG:CD	1:A:87:ASN:HD22	2.30	0.43
1:A:80:VAL:O	1:A:80:VAL:HG13	2.17	0.43
1:A:363:GLN:HE21	1:A:365:GLU:HG2	1.82	0.43
1:B:44:LYS:H	1:B:44:LYS:CD	2.31	0.43
1:B:156:ALA:HB3	1:B:195:VAL:HG13	2.00	0.43
1:A:146:PRO:HA	1:A:147:PRO:HD3	1.91	0.43
1:B:298:GLU:HB2	1:B:302:GLY:O	2.19	0.43
1:A:204:LYS:NZ	1:A:204:LYS:HB3	2.33	0.43
1:A:344:LYS:HA	1:A:345:PRO:HD3	1.80	0.43
1:B:240:GLY:O	1:B:284:ASN:HA	2.19	0.43
1:B:52:VAL:HG12	1:B:58:PRO:HG2	2.00	0.43
1:B:268:ALA:O	1:B:269:ARG:HB3	2.18	0.43
1:B:74:ASP:O	1:B:75:PHE:CG	2.72	0.43
1:B:284:ASN:HD21	1:B:286:GLN:HE21	1.64	0.43
1:B:309:GLN:HE21	1:B:309:GLN:HB3	1.54	0.43
1:A:343:PRO:HG2	1:A:388:ASN:HB2	2.01	0.43
1:B:238:GLU:HB2	1:B:313:TYR:CZ	2.54	0.43
1:B:359:ARG:HG2	1:B:360:ASP:N	2.33	0.42
1:A:59:HIS:HB2	3:A:532:HOH:O	2.19	0.42
1:A:138:GLN:HE22	1:A:220:MET:HE3	1.83	0.42
1:A:64:LEU:C	1:A:66:GLY:N	2.77	0.42
1:A:316:PRO:HA	1:A:340:ASN:O	2.19	0.42
1:B:55:ASN:HA	1:B:56:PRO:C	2.45	0.42
1:A:36:MET:CE	1:A:119:ALA:HB2	2.49	0.42
1:B:265:LYS:HA	1:B:266:PRO:HD3	1.95	0.42
1:A:244:LYS:HE2	1:A:281:GLU:OE2	2.20	0.42
1:A:333:VAL:HG22	1:A:371:ILE:HB	2.03	0.41
1:B:242:THR:HA	1:B:282:ILE:O	2.20	0.41
1:A:258:LEU:HD12	1:A:259:TRP:H	1.85	0.41
1:B:38:PRO:HG3	1:B:201:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HB2	1:A:383:GLN:HB2	2.03	0.41
1:A:238:GLU:HB2	1:A:313:TYR:CZ	2.56	0.41
1:B:45:LYS:HA	1:B:86:ILE:O	2.21	0.41
1:A:140:MET:HE3	1:A:140:MET:HB2	1.70	0.41
1:A:155:TYR:CD2	1:A:177:GLY:HA3	2.56	0.40
1:A:369:LEU:C	1:A:369:LEU:HD23	2.46	0.40
1:B:316:PRO:HA	1:B:340:ASN:O	2.21	0.40
1:A:387:GLU:CB	1:A:392:VAL:HG12	2.51	0.40
1:B:132:VAL:CG1	1:B:133:SER:N	2.83	0.40
1:B:183:LYS:HD2	1:B:252:ASN:CG	2.46	0.40
1:A:88:ASN:HA	1:A:89:PRO:HD3	1.74	0.40
1:A:135:ARG:NH2	1:A:220:MET:HE1	2.36	0.40
1:A:379:ALA:HA	1:A:399:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:TYR:CZ	1:B:162:TYR:OH[2_555]	1.38	0.82
1:B:162:TYR:CZ	1:B:162:TYR:CZ[2_555]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/383 (98%)	349 (93%)	24 (6%)	1 (0%)	36	50
1	B	381/383 (100%)	352 (92%)	28 (7%)	1 (0%)	36	50
All	All	755/766 (99%)	701 (93%)	52 (7%)	2 (0%)	36	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	B	403	ALA

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	328/333 (98%)	297 (90%)	31 (10%)	8	13
1	B	333/333 (100%)	308 (92%)	25 (8%)	12	21
All	All	661/666 (99%)	605 (92%)	56 (8%)	10	16

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	30	GLN
1	A	36	MET
1	A	40	ASP
1	A	49	SER
1	A	61	ARG
1	A	92	THR
1	A	97	THR
1	A	101	ILE
1	A	126	THR
1	A	131	THR
1	A	132	VAL
1	A	134	VAL
1	A	136	ARG
1	A	170	ARG
1	A	186	LYS
1	A	195	VAL
1	A	200	VAL
1	A	204	LYS
1	A	210	THR
1	A	235	VAL
1	A	254	VAL

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Mol	Chain	Res	Type
1	A	258	LEU
1	A	301	ARG
1	A	310	LEU
1	A	333	VAL
1	A	335	TRP
1	A	346	THR
1	A	358	THR
1	A	361	ARG
1	A	401	VAL
1	B	39	LEU
1	B	43	GLU
1	B	79	VAL
1	B	108	THR
1	B	110	VAL
1	B	128	THR
1	B	131	THR
1	B	134	VAL
1	B	141	VAL
1	B	143	LEU
1	B	168	ASN
1	B	175	GLU
1	B	189	VAL
1	B	193	THR
1	B	196	VAL
1	B	212	LEU
1	B	229	VAL
1	B	242	THR
1	B	252	ASN
1	B	267	ILE
1	B	309	GLN
1	B	359	ARG
1	B	365	GLU
1	B	399	LEU
1	B	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	55	ASN
1	A	87	ASN
1	A	203	HIS

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Mol	Chain	Res	Type
1	A	274	HIS
1	A	284	ASN
1	A	304	ASN
1	A	326	HIS
1	A	363	GLN
1	B	30	GLN
1	B	55	ASN
1	B	99	GLN
1	B	166	GLN
1	B	168	ASN
1	B	203	HIS
1	B	252	ASN
1	B	277	ASN
1	B	284	ASN
1	B	304	ASN
1	B	309	GLN
1	B	317	ASN
1	B	363	GLN

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](#)

8 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	NAG	B	7	1	14,14,15	0.56	0	17,19,21	0.71	0
2	NAG	A	3	1	14,14,15	0.64	0	17,19,21	1.20	2 (11%)
2	NAG	B	8	1	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
2	NAG	B	5	1	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
2	NAG	A	2	1	14,14,15	0.43	0	17,19,21	1.19	1 (5%)
2	NAG	A	1	1	14,14,15	0.45	0	17,19,21	1.14	1 (5%)
2	NAG	B	6	1	14,14,15	0.43	0	17,19,21	1.03	1 (5%)
2	NAG	A	4	1	14,14,15	0.49	0	17,19,21	0.73	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
2	NAG	B	7	1	-	3/6/23/26	0/1/1/1
2	NAG	A	3	1	-	0/6/23/26	0/1/1/1
2	NAG	B	8	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	5	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	2	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	1	1	-	2/6/23/26	0/1/1/1
2	NAG	B	6	1	-	0/6/23/26	0/1/1/1
2	NAG	A	4	1	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-O5-C5	3.50	116.88	112.19
2	A	2	NAG	C1-O5-C5	3.38	116.71	112.19
2	B	5	NAG	C1-O5-C5	3.15	116.40	112.19
2	B	6	NAG	C1-O5-C5	2.98	116.18	112.19
2	A	3	NAG	C4-C3-C2	2.64	114.89	111.02
2	B	8	NAG	O5-C1-C2	-2.27	107.78	111.29
2	A	3	NAG	C1-O5-C5	2.12	115.03	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	NAG	C1
2	A	4	NAG	C1
2	B	5	NAG	C1
2	B	8	NAG	C1

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	B	8	NAG	C8-C7-N2-C2
2	B	8	NAG	O7-C7-N2-C2
2	A	4	NAG	C8-C7-N2-C2
2	B	5	NAG	C8-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6
2	A	4	NAG	O7-C7-N2-C2
2	B	7	NAG	C8-C7-N2-C2
2	B	5	NAG	O7-C7-N2-C2
2	B	7	NAG	O7-C7-N2-C2
2	B	7	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7	NAG	1	0
2	B	8	NAG	1	0
2	A	1	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	378/383 (98%)	0.05	11 (2%) 53 50	23, 65, 144, 206	0
1	B	383/383 (100%)	0.35	8 (2%) 63 59	31, 93, 136, 175	0
All	All	761/766 (99%)	0.20	19 (2%) 58 54	23, 83, 138, 206	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	ALA	3.0
1	A	403	ALA	2.8
1	A	40	ASP	2.8
1	B	75	PHE	2.7
1	A	71	ILE	2.7
1	B	162	TYR	2.6
1	B	123	ASN	2.6
1	B	220	MET	2.5
1	A	75	PHE	2.4
1	A	78	SER	2.3
1	A	37	PHE	2.2
1	A	22	PRO	2.2
1	B	293	TYR	2.2
1	A	101	ILE	2.2
1	A	95	ALA	2.1
1	B	404	GLU	2.1
1	A	118	PHE	2.1
1	A	39	LEU	2.1
1	B	281	GLU	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
2	NAG	A	2	14/15	0.56	0.14	122,135,149,150	0
2	NAG	B	6	14/15	0.56	0.16	127,133,135,136	0
2	NAG	A	4	14/15	0.64	0.14	86,99,103,104	0
2	NAG	A	1	14/15	0.69	0.10	96,106,111,113	0
2	NAG	B	8	14/15	0.76	0.19	109,119,125,126	0
2	NAG	B	5	14/15	0.78	0.10	95,103,114,117	0
2	NAG	B	7	14/15	0.86	0.09	76,92,104,107	0
2	NAG	A	3	14/15	0.86	0.11	43,67,76,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.