



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1T34
Title : ROTATION MECHANISM FOR TRANSMEMBRANE SIGNALING BY
THE ATRIAL NATRIURETIC PEPTIDE RECEPTOR
Authors : Ogawa, H.; Qiu, Y.; Ogata, C.M.; Misono, K.S.
Deposited on : 2004-04-23
Resolution : 2.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

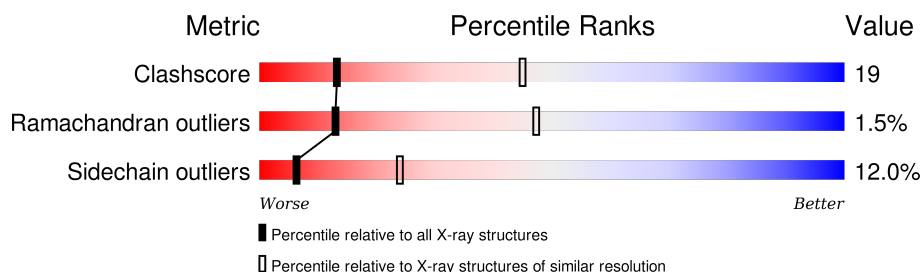
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	435	
1	B	435	
2	H	21	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7086 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 Atrial natriuretic peptide receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3349	2145	583	610	11			
1	B	421	Total	C	N	O	S	0	0	0
			3315	2123	578	603	11			

- Molecule 2 is a protein called Atrial natriuretic peptide factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	21	Total	C	N	O	S	0	21	0
			308	184	64	56	4			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

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

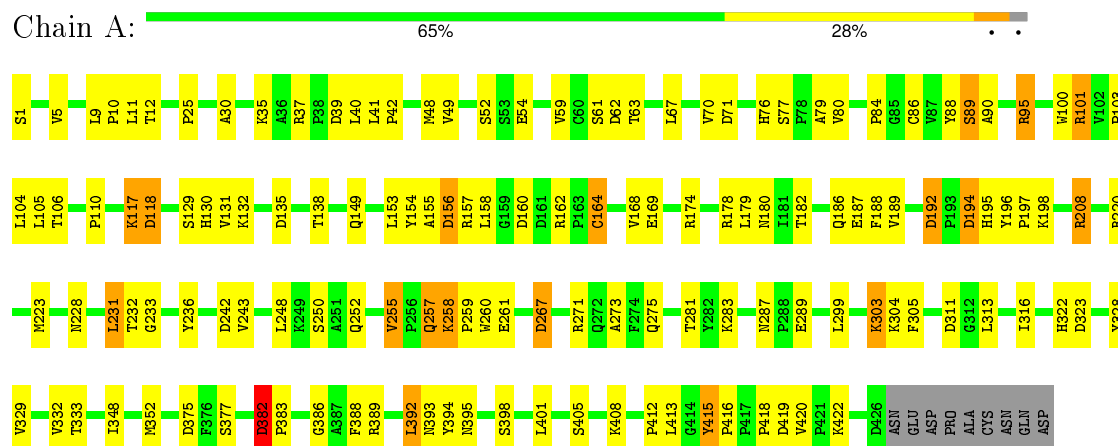
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

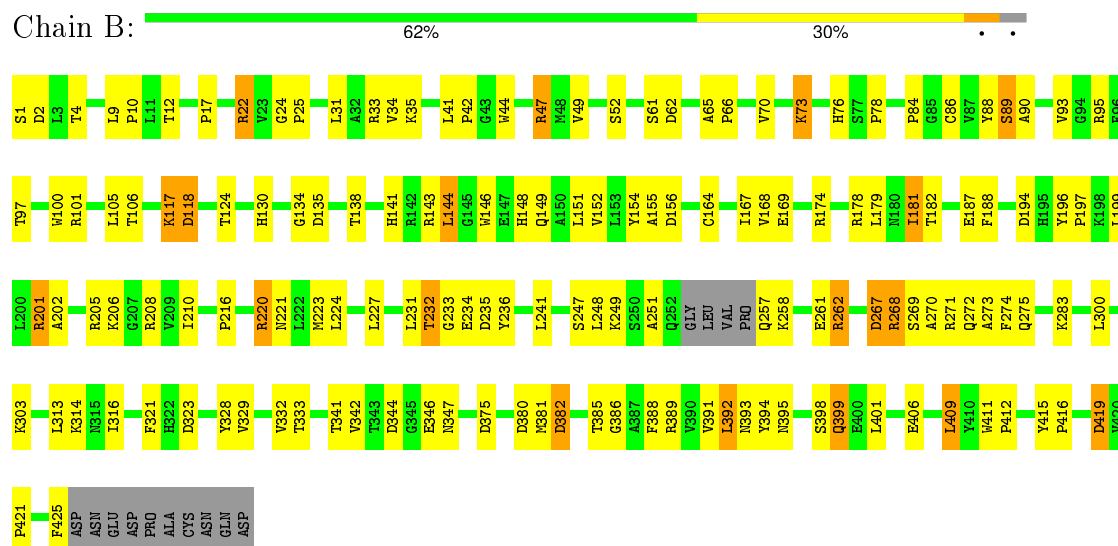
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: Atrial natriuretic peptide receptor A



• Molecule 1: Atrial natriuretic peptide receptor A



• Molecule 2: Atrial natriuretic peptide factor



C7	F8	G9	G10	R11	I12	D13	R14	I15	G16	A17	Q18	S19	G20	L21	G22	C23	N24	S25	F26	R27
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	100.13Å 100.13Å 259.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.71 – 2.95	Depositor
% Data completeness (in resolution range)	89.1 (87.71-2.95)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.237 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: NAG, 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	0.49	0/3439	0.80	11/4685 (0.2%)
1	B	0.51	0/3403	0.79	7/4633 (0.2%)
2	H	0.61	0/310	1.13	2/404 (0.5%)
All	All	0.50	0/7152	0.81	20/9722 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	11[A]	ARG	NE-CZ-NH2	7.25	123.93	120.30
2	H	11[B]	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	62	ASP	CB-CG-OD2	7.18	124.76	118.30
1	B	156	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	382	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	267	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	419	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	419	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	323	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	2	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	194	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	242	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	344	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	375	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	382	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	39	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	323	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	192	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	71	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	118	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3349	0	3299	99	0
1	B	3315	0	3264	103	0
2	H	308	0	290	79	0
3	A	56	0	50	0	0
3	B	56	0	50	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
All	All	7086	0	6953	265	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 19.

All (265) 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)
2:H:20[B]:GLY:O	2:H:21[B]:LEU:HG	1.34	1.27
2:H:10[B]:GLY:O	2:H:12[B]:ILE:HG23	1.38	1.20
2:H:8[A]:PHE:C	2:H:10[A]:GLY:H	1.47	1.12
1:A:283:LYS:HD2	1:A:393:ASN:ND2	1.62	1.12
2:H:15[B]:ILE:HD13	2:H:15[B]:ILE:O	1.51	1.09
1:A:260:TRP:CZ3	1:A:261:GLU:HA	1.97	1.00
2:H:8[B]:PHE:C	2:H:10[B]:GLY:H	1.65	0.97
1:B:409:LEU:HD12	1:B:409:LEU:H	1.29	0.96
2:H:8[A]:PHE:O	2:H:10[A]:GLY:N	1.99	0.95
2:H:10[A]:GLY:O	2:H:12[A]:ILE:HG23	1.66	0.95
2:H:8[A]:PHE:C	2:H:10[A]:GLY:N	2.20	0.94
2:H:10[B]:GLY:O	2:H:12[B]:ILE:N	2.01	0.92
2:H:21[B]:LEU:O	2:H:23[B]:CYS:SG	2.28	0.91
1:A:117:LYS:HD3	1:A:118:ASP:N	1.86	0.90
1:B:95:ARG:NH2	2:H:15[A]:ILE:HD11	1.88	0.89
1:B:95:ARG:HH22	2:H:15[A]:ILE:CG1	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10[B]:GLY:O	2:H:12[B]:ILE:CG2	2.23	0.84
2:H:14[B]:ARG:O	2:H:15[B]:ILE:C	2.16	0.84
1:A:283:LYS:HD2	1:A:393:ASN:HD21	1.37	0.83
2:H:10[B]:GLY:C	2:H:12[B]:ILE:H	1.82	0.83
1:A:258:LYS:HB2	1:A:261:GLU:HB2	1.62	0.82
1:A:260:TRP:CE3	1:A:260:TRP:C	2.53	0.82
2:H:15[A]:ILE:O	2:H:15[A]:ILE:HD13	1.79	0.82
2:H:20[B]:GLY:O	2:H:21[B]:LEU:CG	2.24	0.82
2:H:15[B]:ILE:O	2:H:15[B]:ILE:CD1	2.28	0.81
1:A:260:TRP:CE3	1:A:261:GLU:HA	2.16	0.80
2:H:10[A]:GLY:O	2:H:12[A]:ILE:N	2.15	0.78
2:H:16[A]:GLY:O	2:H:18[A]:GLN:N	2.16	0.78
2:H:16[B]:GLY:O	2:H:18[B]:GLN:N	2.16	0.77
1:B:258:LYS:HB3	1:B:261:GLU:HB3	1.65	0.77
2:H:14[B]:ARG:HH11	2:H:14[B]:ARG:HB3	1.50	0.76
2:H:14[A]:ARG:O	2:H:15[A]:ILE:C	2.25	0.75
1:B:95:ARG:HH22	2:H:15[A]:ILE:CD1	2.01	0.73
2:H:16[A]:GLY:O	2:H:17[A]:ALA:C	2.26	0.73
1:A:392:LEU:HD13	1:A:401:LEU:HD22	1.71	0.73
2:H:26[A]:PHE:O	2:H:27[A]:ARG:O	2.07	0.73
1:A:95:ARG:HH22	2:H:15[B]:ILE:CG1	2.02	0.72
1:A:252:GLN:HB3	1:A:255:VAL:HB	1.70	0.72
1:A:41:LEU:HD11	1:A:329:VAL:HG22	1.71	0.72
1:B:49:VAL:HG11	1:B:76:HIS:CD2	2.25	0.72
1:A:186:GLN:HE22	2:H:25[B]:SER:HA	1.55	0.72
1:B:148:HIS:O	1:B:181:ILE:HB	1.89	0.71
1:B:95:ARG:HH22	2:H:15[A]:ILE:HD11	1.53	0.71
1:B:392:LEU:HD23	1:B:393:ASN:H	1.54	0.71
1:A:49:VAL:HG11	1:A:76:HIS:CD2	2.25	0.70
1:B:272:GLN:O	1:B:275:GLN:HB2	1.91	0.70
1:A:260:TRP:HE3	1:A:260:TRP:O	1.74	0.70
2:H:16[B]:GLY:O	2:H:17[B]:ALA:C	2.31	0.70
1:A:192:ASP:OD2	1:A:194:ASP:HB2	1.92	0.69
1:A:258:LYS:HD3	1:A:261:GLU:HG3	1.75	0.69
1:B:380:ASP:HB3	1:B:391:VAL:HG11	1.74	0.68
1:B:233:GLY:HA3	1:B:412:PRO:HG2	1.74	0.68
1:B:381:MET:HG3	1:B:386:GLY:O	1.96	0.66
2:H:19[A]:SER:OG	2:H:20[A]:GLY:N	2.24	0.66
1:A:228:ASN:HD22	1:A:228:ASN:H	1.43	0.66
2:H:8[B]:PHE:C	2:H:10[B]:GLY:N	2.37	0.66
1:A:194:ASP:O	1:A:197:PRO:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HB3	1:B:10:PRO:CD	2.26	0.66
2:H:8[B]:PHE:O	2:H:10[B]:GLY:N	2.29	0.66
2:H:14[B]:ARG:O	2:H:16[B]:GLY:N	2.28	0.65
1:A:260:TRP:CE3	1:A:260:TRP:O	2.49	0.65
1:B:268:ARG:HA	1:B:268:ARG:HE	1.63	0.64
1:A:231:LEU:HB3	1:A:236:TYR:CD1	2.32	0.64
2:H:9[B]:GLY:O	2:H:10[B]:GLY:O	2.16	0.63
1:A:260:TRP:CE3	1:A:261:GLU:CA	2.81	0.62
1:A:283:LYS:CD	1:A:393:ASN:ND2	2.53	0.62
1:B:227:LEU:HD11	1:B:272:GLN:NE2	2.15	0.62
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.65	0.62
1:A:283:LYS:CD	1:A:393:ASN:HD21	2.11	0.62
2:H:12[B]:ILE:O	2:H:12[B]:ILE:HG13	1.99	0.61
1:A:260:TRP:CD2	1:A:260:TRP:C	2.72	0.61
2:H:25[B]:SER:O	2:H:26[B]:PHE:CD1	2.53	0.61
1:B:221:ASN:HA	1:B:224:LEU:HD12	1.82	0.61
1:B:382:ASP:HB3	1:B:386:GLY:H	1.64	0.61
1:B:138:THR:HG23	1:B:179:LEU:HG	1.83	0.61
1:A:233:GLY:HA3	1:A:412:PRO:HG2	1.83	0.60
1:A:260:TRP:CE3	1:A:261:GLU:N	2.69	0.60
1:A:117:LYS:HD3	1:A:117:LYS:C	2.22	0.60
1:A:88:TYR:CE2	2:H:14[B]:ARG:HB2	2.37	0.60
1:A:25:PRO:HG3	1:A:305:PHE:CD1	2.36	0.59
2:H:19[B]:SER:OG	2:H:20[B]:GLY:N	2.34	0.59
2:H:16[A]:GLY:C	2:H:18[A]:GLN:N	2.53	0.59
1:B:220:ARG:HD2	1:B:262:ARG:HD3	1.85	0.59
2:H:17[B]:ALA:O	2:H:19[B]:SER:N	2.35	0.59
1:B:42:PRO:HD3	1:B:333:THR:HG23	1.85	0.59
2:H:14[B]:ARG:NH1	2:H:14[B]:ARG:HB3	2.16	0.59
1:A:313:LEU:O	1:A:316:ILE:HG12	2.03	0.59
1:B:152:VAL:HG11	1:B:168:VAL:HG13	1.84	0.59
2:H:17[A]:ALA:O	2:H:19[A]:SER:N	2.36	0.58
1:A:9:LEU:HB3	1:A:10:PRO:CD	2.32	0.58
1:B:95:ARG:HH22	2:H:15[A]:ILE:HG13	1.67	0.58
1:B:392:LEU:HD21	1:B:401:LEU:HB3	1.85	0.58
1:A:49:VAL:HG11	1:A:76:HIS:CG	2.37	0.58
1:A:418:PRO:HG2	1:A:420:VAL:O	2.02	0.58
1:B:248:LEU:O	1:B:249:LYS:HG3	2.04	0.58
2:H:13[A]:ASP:O	2:H:14[A]:ARG:C	2.41	0.58
1:A:174:ARG:O	1:A:178:ARG:HG3	2.03	0.58
1:B:267:ASP:OD1	1:B:267:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9[A]:GLY:O	2:H:10[A]:GLY:O	2.21	0.58
1:B:154:TYR:HB3	1:B:168:VAL:HG21	1.86	0.58
2:H:15[A]:ILE:O	2:H:15[A]:ILE:CD1	2.49	0.57
1:A:95:ARG:HH22	2:H:15[B]:ILE:HG13	1.69	0.57
1:A:9:LEU:HB3	1:A:10:PRO:HD2	1.85	0.57
1:A:418:PRO:C	1:A:420:VAL:H	2.08	0.57
2:H:15[B]:ILE:C	2:H:15[B]:ILE:HD13	2.24	0.57
2:H:13[A]:ASP:O	2:H:16[A]:GLY:N	2.36	0.57
1:B:178:ARG:HH22	1:B:399:GLN:HE22	1.52	0.57
2:H:12[B]:ILE:C	2:H:14[B]:ARG:N	2.56	0.57
1:B:381:MET:HG2	1:B:386:GLY:HA2	1.86	0.57
1:A:95:ARG:HH22	2:H:15[B]:ILE:HG12	1.70	0.56
1:B:328:TYR:O	1:B:332:VAL:HG23	2.04	0.56
1:B:22:ARG:HH11	1:B:22:ARG:HB2	1.71	0.56
2:H:26[B]:PHE:O	2:H:27[B]:ARG:HB2	2.06	0.56
1:B:201:ARG:HD2	1:B:205:ARG:CZ	2.36	0.56
1:B:169:GLU:OE2	2:H:10[B]:GLY:HA2	2.06	0.55
1:B:143:ARG:NH1	1:B:401:LEU:HB2	2.20	0.55
1:B:380:ASP:HB3	1:B:391:VAL:CG1	2.35	0.55
2:H:13[B]:ASP:O	2:H:14[B]:ARG:C	2.45	0.55
1:A:186:GLN:NE2	2:H:25[B]:SER:HA	2.21	0.55
1:A:117:LYS:CD	1:A:118:ASP:N	2.64	0.55
1:B:273:ALA:C	1:B:275:GLN:H	2.08	0.55
1:B:117:LYS:HG3	1:B:118:ASP:H	1.72	0.55
1:A:259:PRO:HG2	1:A:388:PHE:CD1	2.42	0.55
2:H:10[A]:GLY:C	2:H:12[A]:ILE:N	2.61	0.54
2:H:12[B]:ILE:O	2:H:14[B]:ARG:N	2.41	0.54
2:H:25[B]:SER:O	2:H:26[B]:PHE:HD1	1.90	0.54
2:H:10[A]:GLY:C	2:H:12[A]:ILE:H	2.11	0.54
1:B:17:PRO:HG3	1:B:314:LYS:HD3	1.90	0.53
1:B:24:GLY:N	1:B:25:PRO:HD2	2.22	0.53
2:H:26[A]:PHE:C	2:H:27[A]:ARG:O	2.45	0.53
1:B:194:ASP:O	1:B:197:PRO:HD2	2.09	0.53
1:A:138:THR:HG23	1:A:179:LEU:HD21	1.91	0.53
1:A:63:THR:O	1:A:67:LEU:HB2	2.08	0.53
1:B:101:ARG:NH1	1:B:346:GLU:OE2	2.41	0.52
1:A:395:ASN:HB3	1:A:398:SER:OG	2.09	0.52
1:B:146:TRP:CD1	1:B:419:ASP:HB3	2.45	0.52
2:H:9[B]:GLY:O	2:H:10[B]:GLY:C	2.48	0.52
2:H:9[A]:GLY:O	2:H:10[A]:GLY:C	2.48	0.52
2:H:16[B]:GLY:C	2:H:18[B]:GLN:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD12	1:B:409:LEU:N	2.11	0.51
2:H:21[A]:LEU:O	2:H:22[A]:GLY:C	2.48	0.51
1:B:233:GLY:CA	1:B:412:PRO:HG2	2.41	0.51
1:B:267:ASP:HA	1:B:270:ALA:HB3	1.93	0.51
1:B:196:TYR:N	1:B:197:PRO:CD	2.74	0.51
1:B:86:CYS:HB2	1:B:89:SER:HB2	1.93	0.51
1:A:37:ARG:HB2	1:A:40:LEU:HD12	1.92	0.51
1:B:257:GLN:OE1	1:B:257:GLN:HA	2.11	0.51
1:B:273:ALA:O	1:B:275:GLN:N	2.44	0.51
1:A:154:TYR:HB3	1:A:168:VAL:HG21	1.92	0.50
1:A:228:ASN:H	1:A:228:ASN:ND2	2.08	0.50
1:B:231:LEU:CD2	1:B:236:TYR:CE1	2.94	0.50
1:A:155:ALA:HB2	1:A:188:PHE:CZ	2.47	0.50
1:B:100:TRP:O	1:B:101:ARG:HB2	2.11	0.50
1:A:79:ALA:O	1:A:103:PRO:HD2	2.11	0.50
1:A:154:TYR:CZ	1:A:187:GLU:HB2	2.47	0.50
1:B:154:TYR:CZ	1:B:187:GLU:HB2	2.46	0.49
1:A:223:MET:HA	1:A:223:MET:CE	2.41	0.49
1:A:86:CYS:HB2	1:A:89:SER:HB2	1.94	0.49
1:A:189:VAL:H	1:A:195:HIS:CE1	2.29	0.49
1:A:328:TYR:O	1:A:332:VAL:HG23	2.12	0.49
2:H:14[A]:ARG:O	2:H:16[A]:GLY:N	2.46	0.48
1:A:223:MET:HA	1:A:223:MET:HE2	1.95	0.48
1:A:105:LEU:HD11	1:A:328:TYR:HB2	1.95	0.48
2:H:12[B]:ILE:O	2:H:13[B]:ASP:C	2.52	0.48
1:A:138:THR:HA	1:A:179:LEU:HD11	1.95	0.48
1:B:65:ALA:HB3	1:B:66:PRO:CD	2.44	0.48
1:B:41:LEU:HB3	1:B:44:TRP:HB2	1.95	0.48
1:B:105:LEU:HD23	1:B:124:THR:HB	1.95	0.47
1:B:65:ALA:HB3	1:B:66:PRO:HD3	1.96	0.47
1:B:149:GLN:HA	1:B:182:THR:O	2.14	0.47
1:A:186:GLN:HG2	1:A:198:LYS:HZ1	1.80	0.47
1:B:208:ARG:HD3	1:B:236:TYR:CE2	2.50	0.47
1:B:411:TRP:CE2	1:B:416:PRO:HB3	2.49	0.47
1:B:88:TYR:CE2	2:H:14[A]:ARG:HB2	2.49	0.47
2:H:14[A]:ARG:HB3	2:H:14[A]:ARG:HH11	1.79	0.47
1:B:313:LEU:O	1:B:316:ILE:HG12	2.14	0.47
1:B:93:VAL:O	1:B:97:THR:HG23	2.15	0.47
1:B:9:LEU:HB3	1:B:10:PRO:HD2	1.95	0.47
1:B:188:PHE:CD2	1:B:199:LEU:HD21	2.50	0.47
1:A:243:VAL:HA	1:A:281:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ASP:O	1:B:388:PHE:HA	2.15	0.46
1:A:260:TRP:CD2	1:A:261:GLU:N	2.83	0.46
1:B:273:ALA:C	1:B:275:GLN:N	2.68	0.46
2:H:12[B]:ILE:C	2:H:14[B]:ARG:H	2.17	0.46
1:A:196:TYR:N	1:A:197:PRO:CD	2.78	0.46
1:B:144:LEU:HD13	1:B:411:TRP:HZ2	1.81	0.46
1:A:70:VAL:HG11	1:B:70:VAL:HG11	1.98	0.46
1:B:95:ARG:HH21	2:H:15[A]:ILE:HD11	1.76	0.46
2:H:13[A]:ASP:O	2:H:15[A]:ILE:N	2.48	0.46
1:A:208:ARG:HD2	1:A:236:TYR:CE2	2.51	0.46
1:B:231:LEU:HD22	1:B:236:TYR:CE1	2.51	0.46
1:A:84:PRO:HD2	1:A:90:ALA:HA	1.98	0.46
2:H:25[B]:SER:HB2	2:H:26[B]:PHE:H	1.53	0.45
2:H:14[A]:ARG:H	2:H:14[A]:ARG:HG2	1.58	0.45
1:B:395:ASN:O	1:B:399:GLN:N	2.47	0.45
1:A:273:ALA:C	1:A:275:GLN:H	2.19	0.45
1:B:101:ARG:HA	1:B:101:ARG:HD3	1.84	0.45
1:A:231:LEU:HD22	1:A:236:TYR:CE1	2.51	0.45
1:B:84:PRO:HB3	4:B:601:CL:CL	2.54	0.45
2:H:10[A]:GLY:O	2:H:11[A]:ARG:C	2.55	0.45
1:B:73:LYS:HD3	1:B:100:TRP:CD2	2.52	0.45
1:A:299:LEU:O	1:A:303:LYS:HB2	2.17	0.45
2:H:12[A]:ILE:C	2:H:14[A]:ARG:N	2.68	0.44
1:B:392:LEU:HD22	1:B:401:LEU:HD22	1.97	0.44
1:A:135:ASP:HB3	1:A:394:TYR:OH	2.16	0.44
1:B:421:PRO:HG2	1:B:425:PHE:HA	1.99	0.44
1:A:5:VAL:HG22	1:A:80:VAL:CG1	2.47	0.44
1:B:151:LEU:HB3	1:B:210:ILE:HG13	1.99	0.44
1:A:11:LEU:HG	1:A:52:SER:HA	2.00	0.44
1:B:411:TRP:CD1	1:B:416:PRO:HD3	2.53	0.44
1:A:153:LEU:HD23	1:A:186:GLN:HB3	1.99	0.43
1:B:101:ARG:HD2	1:B:346:GLU:OE2	2.18	0.43
1:A:52:SER:OG	1:A:54:GLU:HG2	2.18	0.43
1:A:160:ASP:CG	1:A:162:ARG:H	2.22	0.43
1:A:95:ARG:CG	1:A:95:ARG:HH11	2.31	0.43
1:A:117:LYS:HD3	1:A:118:ASP:H	1.75	0.43
1:B:4:THR:HB	1:B:78:PRO:HA	2.00	0.43
2:H:15[A]:ILE:C	2:H:15[A]:ILE:HD13	2.37	0.43
1:B:231:LEU:HD23	1:B:236:TYR:CE1	2.54	0.43
1:A:174:ARG:HD2	1:A:178:ARG:HD3	2.01	0.43
1:B:84:PRO:HD2	1:B:90:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:PRO:HB3	1:B:247:SER:HB3	2.01	0.43
1:A:348:ILE:O	1:A:352:MET:HG3	2.19	0.43
1:A:186:GLN:NE2	1:A:187:GLU:O	2.49	0.42
1:B:151:LEU:HD23	1:B:210:ILE:HG12	2.00	0.42
1:A:42:PRO:HD3	1:A:333:THR:HG23	2.01	0.42
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.73	0.42
1:A:415:TYR:HB2	1:A:416:PRO:HD2	2.02	0.42
1:B:223:MET:CE	1:B:223:MET:HA	2.49	0.42
1:B:65:ALA:N	1:B:66:PRO:HD2	2.35	0.41
1:B:411:TRP:CZ2	1:B:416:PRO:HB3	2.55	0.41
1:A:231:LEU:CD2	1:A:236:TYR:CE1	3.03	0.41
1:A:257:GLN:O	1:A:259:PRO:HD3	2.21	0.41
1:B:130:HIS:CE1	1:B:167:ILE:HG12	2.55	0.41
1:A:158:LEU:HD11	2:H:19[A]:SER:HB2	2.02	0.41
1:A:283:LYS:HG3	1:A:377:SER:OG	2.20	0.41
1:B:332:VAL:HG11	1:B:342:VAL:HG12	2.02	0.41
1:A:156:ASP:OD2	1:A:164:CYS:N	2.53	0.41
1:B:392:LEU:HD23	1:B:393:ASN:N	2.28	0.41
1:B:241:LEU:HA	1:B:241:LEU:HD23	1.89	0.41
1:B:381:MET:CG	1:B:386:GLY:HA2	2.50	0.41
1:B:232:THR:C	1:B:234:GLU:H	2.23	0.41
1:A:149:GLN:HA	1:A:182:THR:O	2.21	0.41
1:B:31:LEU:O	1:B:34:VAL:HB	2.21	0.41
1:B:134:GLY:HA3	1:B:174:ARG:HB3	2.01	0.41
1:A:100:TRP:O	1:A:101:ARG:HB2	2.21	0.41
1:B:409:LEU:H	1:B:409:LEU:CD1	2.05	0.41
1:A:30:ALA:HB2	1:A:322:HIS:CD2	2.55	0.41
1:A:382:ASP:O	1:A:386:GLY:N	2.47	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.54	0.41
2:H:25[A]:SER:HB2	2:H:26[A]:PHE:H	1.63	0.41
1:B:199:LEU:O	1:B:202:ALA:HB3	2.21	0.41
1:A:287:ASN:HD22	1:A:289:GLU:HB2	1.86	0.41
1:A:418:PRO:C	1:A:420:VAL:N	2.74	0.40
1:B:135:ASP:HB3	1:B:394:TYR:OH	2.21	0.40
1:B:411:TRP:CD2	1:B:416:PRO:HA	2.56	0.40
1:A:129:SER:HB2	1:A:132:LYS:HG2	2.03	0.40
1:A:132:LYS:O	1:A:135:ASP:HB2	2.21	0.40
1:A:5:VAL:HG22	1:A:80:VAL:HG12	2.03	0.40
1:A:117:LYS:CD	1:A:118:ASP:H	2.29	0.40
1:B:341:THR:OG1	1:B:342:VAL:N	2.54	0.40
1:A:382:ASP:HA	1:A:383:PRO:HD2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:HB2	1:A:130:HIS:CE1	2.56	0.40
1:B:196:TYR:N	1:B:197:PRO:HD3	2.36	0.40
1:B:155:ALA:HB2	1:B:188:PHE:CE1	2.57	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	424/435 (98%)	399 (94%)	24 (6%)	1 (0%)	52	86
1	B	417/435 (96%)	390 (94%)	25 (6%)	2 (0%)	34	74
2	H	38/21 (181%)	10 (26%)	8 (21%)	20 (53%)	0	0
All	All	879/891 (99%)	799 (91%)	57 (6%)	23 (3%)	13	30

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	11[A]	ARG
2	H	11[B]	ARG
2	H	17[A]	ALA
2	H	17[B]	ALA
2	H	18[A]	GLN
2	H	18[B]	GLN
2	H	19[A]	SER
2	H	19[B]	SER
2	H	21[A]	LEU
2	H	21[B]	LEU
1	B	251	ALA
1	B	274	PHE
2	H	10[A]	GLY
2	H	10[B]	GLY

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Mol	Chain	Res	Type
2	H	15[A]	ILE
2	H	15[B]	ILE
2	H	22[A]	GLY
2	H	22[B]	GLY
1	A	157	ARG
2	H	25[A]	SER
2	H	25[B]	SER
2	H	14[A]	ARG
2	H	14[B]	ARG

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	353/361 (98%)	313 (89%)	40 (11%)	7	26
1	B	349/361 (97%)	307 (88%)	42 (12%)	6	24
2	H	30/15 (200%)	22 (73%)	8 (27%)	0	2
All	All	732/737 (99%)	642 (88%)	90 (12%)	6	23

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	12	THR
1	A	35	LYS
1	A	48	MET
1	A	59	VAL
1	A	61	SER
1	A	77	SER
1	A	89	SER
1	A	95	ARG
1	A	101	ARG
1	A	104	LEU
1	A	106	THR
1	A	117	LYS

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Mol	Chain	Res	Type
1	A	118	ASP
1	A	131	VAL
1	A	156	ASP
1	A	164	CYS
1	A	169	GLU
1	A	180	ASN
1	A	208	ARG
1	A	220	ARG
1	A	231	LEU
1	A	232	THR
1	A	248	LEU
1	A	250	SER
1	A	255	VAL
1	A	257	GLN
1	A	258	LYS
1	A	271	ARG
1	A	303	LYS
1	A	304	LYS
1	A	311	ASP
1	A	382	ASP
1	A	389	ARG
1	A	392	LEU
1	A	405	SER
1	A	408	LYS
1	A	413	LEU
1	A	415	TYR
1	A	422	LYS
1	B	1	SER
1	B	12	THR
1	B	22	ARG
1	B	33	ARG
1	B	35	LYS
1	B	47	ARG
1	B	52	SER
1	B	61	SER
1	B	62	ASP
1	B	73	LYS
1	B	89	SER
1	B	106	THR
1	B	117	LYS
1	B	141	HIS
1	B	144	LEU

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Mol	Chain	Res	Type
1	B	164	CYS
1	B	181	ILE
1	B	201	ARG
1	B	206	LYS
1	B	220	ARG
1	B	232	THR
1	B	235	ASP
1	B	262	ARG
1	B	267	ASP
1	B	268	ARG
1	B	269	SER
1	B	271	ARG
1	B	283	LYS
1	B	300	LEU
1	B	303	LYS
1	B	321	PHE
1	B	329	VAL
1	B	347	ASN
1	B	375	ASP
1	B	385	THR
1	B	389	ARG
1	B	392	LEU
1	B	398	SER
1	B	399	GLN
1	B	406	GLU
1	B	409	LEU
1	B	415	TYR
2	H	14[A]	ARG
2	H	14[B]	ARG
2	H	15[A]	ILE
2	H	15[B]	ILE
2	H	25[A]	SER
2	H	25[B]	SER
2	H	26[A]	PHE
2	H	26[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	228	ASN
1	A	306	ASN

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Mol	Chain	Res	Type
1	A	322	HIS
1	A	347	ASN
1	A	393	ASN
1	A	399	GLN
1	B	186	GLN
1	B	272	GLN
1	B	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 carbohydrates 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	$\# Z > 2$
3	NAG	A	451	1,3	14,14,15	0.76	1 (7%)	15,19,21	1.29	1 (6%)
3	NAG	A	452	3	14,14,15	0.50	0	15,19,21	0.80	0
3	NAG	A	461	1,3	14,14,15	0.46	0	15,19,21	1.15	1 (6%)
3	NAG	A	462	3	14,14,15	0.50	0	15,19,21	1.07	0
3	NAG	B	451	1,3	14,14,15	0.73	0	15,19,21	1.04	1 (6%)
3	NAG	B	452	3	14,14,15	0.49	0	15,19,21	0.96	0
3	NAG	B	461	1,3	14,14,15	0.53	0	15,19,21	1.16	2 (13%)
3	NAG	B	462	3	14,14,15	0.46	0	15,19,21	0.92	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
3	NAG	A	451	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	452	3	-	0/6/23/26	0/1/1/1
3	NAG	A	461	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	462	3	-	0/6/23/26	0/1/1/1
3	NAG	B	451	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	452	3	-	0/6/23/26	0/1/1/1
3	NAG	B	461	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	462	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	451	NAG	O5-C1	-2.03	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	461	NAG	C4-C3-C2	-2.50	107.34	111.23
3	B	451	NAG	C1-O5-C5	2.94	115.98	112.25
3	B	461	NAG	C1-O5-C5	3.01	116.07	112.25
3	A	451	NAG	C1-O5-C5	3.64	116.87	112.25
3	A	461	NAG	C1-O5-C5	3.67	116.91	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.