



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:44 AM UTC

PDB ID : 6N4X / pdb_00006n4x
Title : Metabotropic Glutamate Receptor 5 Apo Form Ligand Binding Domain
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Weis, W.I.; Skiniotis, G.S.; Mathiesen, J.M.; Kobilka, B.K.
Deposited on : 2018-11-20
Resolution : 4.00 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

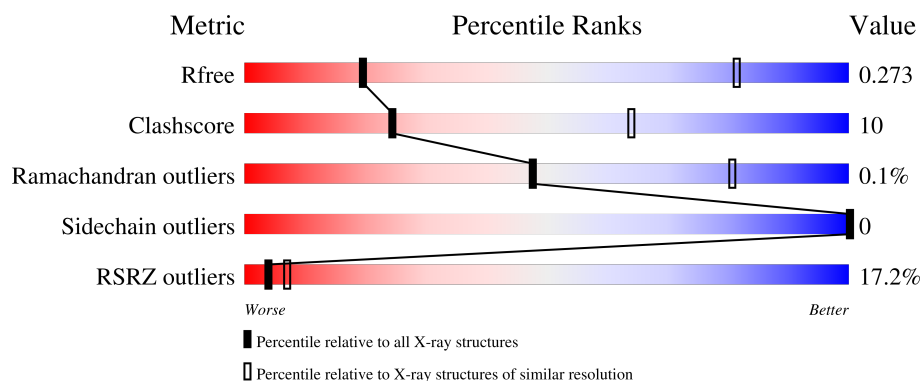
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 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	877	10% 44% 13% 42%
1	B	877	10% 43% 13% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7736 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3897	2456	666	739	36			
1	B	487	Total	C	N	O	S	0	0	0
			3754	2362	646	712	34			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	THR	-	expression tag	UNP P41594
A	-2	ILE	-	expression tag	UNP P41594
A	-1	ILE	-	expression tag	UNP P41594
A	0	ALA	-	expression tag	UNP P41594
A	1	LEU	-	expression tag	UNP P41594
A	2	SER	-	expression tag	UNP P41594
A	3	TYR	-	expression tag	UNP P41594
A	4	ILE	-	expression tag	UNP P41594
A	5	PHE	-	expression tag	UNP P41594
A	6	CYS	-	expression tag	UNP P41594
A	7	LEU	-	expression tag	UNP P41594
A	8	VAL	-	expression tag	UNP P41594
A	9	PHE	-	expression tag	UNP P41594
A	10	ALA	-	expression tag	UNP P41594
A	11	ASP	-	expression tag	UNP P41594
A	12	TYR	-	expression tag	UNP P41594
A	13	LYS	-	expression tag	UNP P41594
A	14	ASP	-	expression tag	UNP P41594
A	15	ASP	-	expression tag	UNP P41594
A	16	ASP	-	expression tag	UNP P41594
A	17	ASP	-	expression tag	UNP P41594
A	18	ALA	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	866	HIS	-	expression tag	UNP P41594
A	867	HIS	-	expression tag	UNP P41594
A	868	HIS	-	expression tag	UNP P41594
A	869	HIS	-	expression tag	UNP P41594
A	870	HIS	-	expression tag	UNP P41594
A	871	HIS	-	expression tag	UNP P41594
B	-5	MET	-	initiating methionine	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	THR	-	expression tag	UNP P41594
B	-2	ILE	-	expression tag	UNP P41594
B	-1	ILE	-	expression tag	UNP P41594
B	0	ALA	-	expression tag	UNP P41594
B	1	LEU	-	expression tag	UNP P41594
B	2	SER	-	expression tag	UNP P41594
B	3	TYR	-	expression tag	UNP P41594
B	4	ILE	-	expression tag	UNP P41594
B	5	PHE	-	expression tag	UNP P41594
B	6	CYS	-	expression tag	UNP P41594
B	7	LEU	-	expression tag	UNP P41594
B	8	VAL	-	expression tag	UNP P41594
B	9	PHE	-	expression tag	UNP P41594
B	10	ALA	-	expression tag	UNP P41594
B	11	ASP	-	expression tag	UNP P41594
B	12	TYR	-	expression tag	UNP P41594
B	13	LYS	-	expression tag	UNP P41594
B	14	ASP	-	expression tag	UNP P41594
B	15	ASP	-	expression tag	UNP P41594
B	16	ASP	-	expression tag	UNP P41594
B	17	ASP	-	expression tag	UNP P41594
B	18	ALA	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	866	HIS	-	expression tag	UNP P41594
B	867	HIS	-	expression tag	UNP P41594
B	868	HIS	-	expression tag	UNP P41594
B	869	HIS	-	expression tag	UNP P41594
B	870	HIS	-	expression tag	UNP P41594
B	871	HIS	-	expression tag	UNP P41594

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

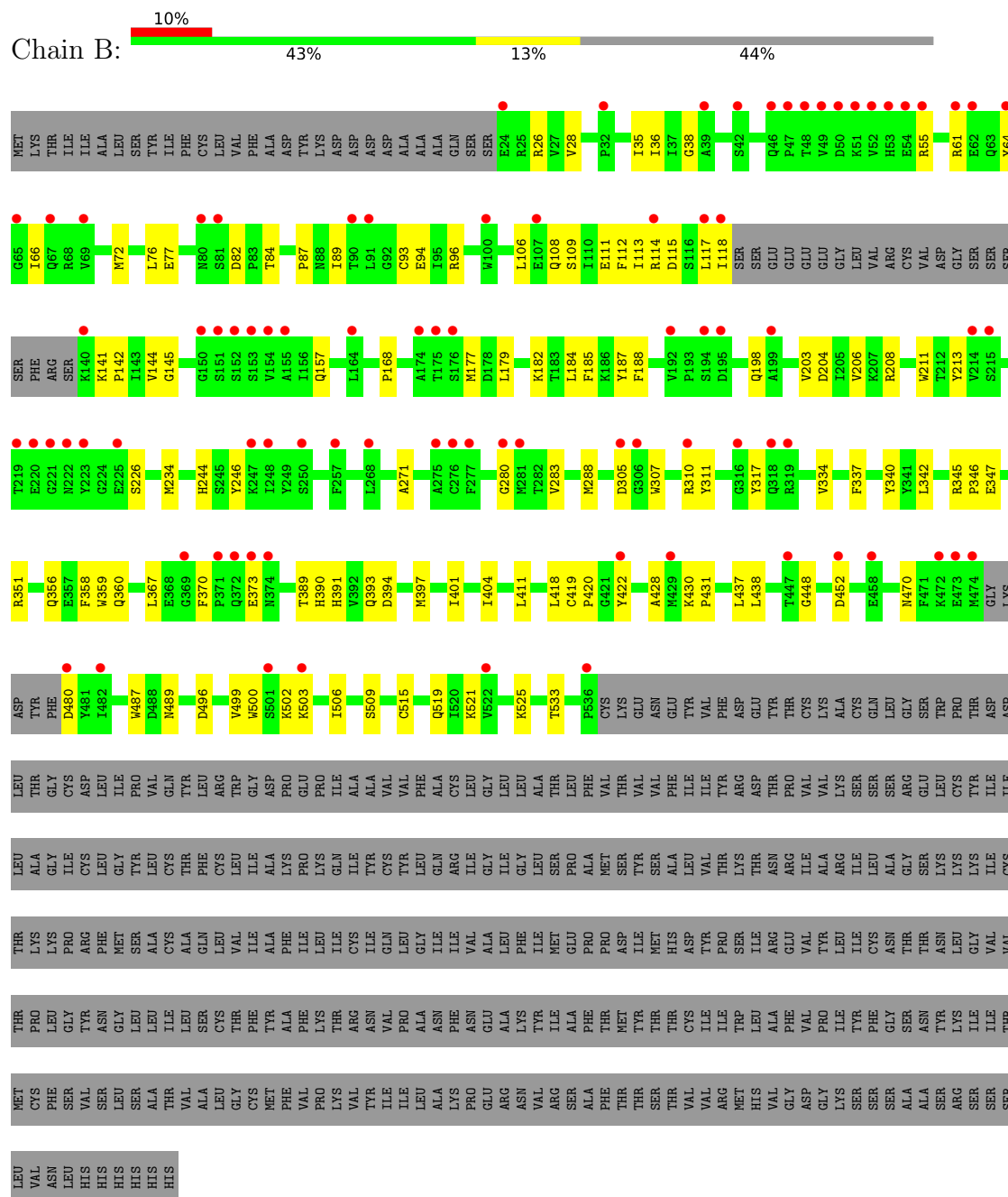


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 1: Metabotropic glutamate receptor 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.08Å 174.10Å 180.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 4.00 49.57 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.57-4.00) 93.1 (49.57-4.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.270 , 0.282 (Not available) , 0.273	Depositor DCC
R_{free} test set	1541 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	172.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 163.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h,l,k	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å ²)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, MG

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	0.13	0/3985	0.39	0/5407
1	B	0.12	0/3836	0.38	0/5200
All	All	0.13	0/7821	0.39	0/10607

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3897	0	3649	76	0
1	B	3754	0	3546	74	0
2	A	56	0	52	0	0
2	B	28	0	26	0	0
3	B	1	0	0	0	0
All	All	7736	0	7273	149	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 10.

All (149) 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:520:ILE:HD13	1:A:546:GLU:C	1.90	0.94
1:A:77:GLU:OE2	1:A:351:ARG:NH1	2.18	0.76
1:B:77:GLU:OE2	1:B:351:ARG:NH1	2.19	0.74
1:B:360:GLN:HE22	1:B:373:GLU:HA	1.52	0.74
1:A:360:GLN:HE22	1:A:373:GLU:HA	1.53	0.73
1:A:522:VAL:HG22	1:A:547:TYR:HA	1.72	0.70
1:B:419:CYS:HB3	1:B:422:TYR:HB2	1.74	0.69
1:B:198:GLN:HE22	1:B:305:ASP:H	1.40	0.69
1:A:182:LYS:NZ	1:A:188:PHE:O	2.27	0.67
1:A:198:GLN:HE22	1:A:305:ASP:H	1.42	0.66
1:B:182:LYS:NZ	1:B:188:PHE:O	2.29	0.65
1:A:82:ASP:OD2	1:A:84:THR:OG1	2.11	0.64
1:A:94:GLU:OE2	1:A:96:ARG:NH2	2.32	0.63
1:A:447:THR:HG21	1:B:428:ALA:HB2	1.80	0.63
1:B:213:TYR:O	1:B:509:SER:OG	2.16	0.63
1:B:106:LEU:HD21	1:B:157:GLN:HB3	1.81	0.61
1:A:198:GLN:NE2	1:A:305:ASP:H	1.97	0.61
1:B:525:LYS:HG2	1:B:533:THR:HG23	1.82	0.61
1:A:345:ARG:HD3	1:A:346:PRO:HD2	1.83	0.60
1:A:106:LEU:HD21	1:A:157:GLN:HB3	1.83	0.60
1:B:311:TYR:OH	1:B:480:ASP:OD1	2.16	0.60
1:B:109:SER:HA	1:B:112:PHE:HD2	1.65	0.60
1:A:520:ILE:HD13	1:A:546:GLU:O	2.02	0.60
1:B:345:ARG:HD3	1:B:346:PRO:HD2	1.84	0.59
1:A:35:ILE:HG23	1:A:144:VAL:HG21	1.83	0.59
1:A:310:ARG:HG2	1:A:312:ASP:OD1	2.03	0.59
1:B:208:ARG:NH1	1:B:496:ASP:OD1	2.31	0.58
1:B:342:LEU:HD21	1:B:391:HIS:CG	2.39	0.57
1:B:35:ILE:HG23	1:B:144:VAL:HG21	1.86	0.57
1:A:487:TRP:HD1	1:A:492:LEU:HD13	1.71	0.56
1:A:213:TYR:O	1:A:509:SER:OG	2.22	0.56
1:A:342:LEU:HD21	1:A:391:HIS:CG	2.41	0.55
1:A:525:LYS:HG3	1:A:527:GLU:H	1.71	0.55
1:A:26:ARG:HD2	1:A:108:GLN:NE2	2.21	0.55
1:A:168:PRO:HG2	1:A:437:LEU:HD23	1.88	0.55
1:A:203:VAL:HG21	1:A:234:MET:HB2	1.89	0.54
1:A:208:ARG:NH1	1:A:496:ASP:OD1	2.27	0.54
1:A:28:VAL:HG11	1:A:94:GLU:HG3	1.88	0.54
1:A:340:TYR:OH	1:A:351:ARG:NH2	2.33	0.54
1:A:519:GLN:HB3	1:A:536:PRO:HA	1.89	0.54
1:B:198:GLN:NE2	1:B:305:ASP:H	2.04	0.54
1:B:206:VAL:HG13	1:B:211:TRP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:CD1	1:A:546:GLU:C	2.75	0.53
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.41	0.53
1:A:520:ILE:HG13	1:A:521:LYS:H	1.74	0.53
1:B:203:VAL:HG21	1:B:234:MET:HB2	1.90	0.53
1:B:82:ASP:OD2	1:B:84:THR:OG1	2.13	0.53
1:A:345:ARG:HG3	1:A:347:GLU:H	1.74	0.53
1:B:109:SER:O	1:B:113:ILE:HG12	2.09	0.53
1:B:394:ASP:HB3	1:B:397:MET:HE2	1.91	0.52
1:B:288:MET:HG2	1:B:317:TYR:CZ	2.45	0.52
1:B:345:ARG:HG3	1:B:347:GLU:H	1.74	0.52
1:B:72:MET:HE3	1:B:76:LEU:HD11	1.91	0.51
1:B:489:ASN:C	1:B:489:ASN:HD22	2.18	0.51
1:A:44:HIS:ND1	1:A:97:ASP:OD2	2.42	0.51
1:A:72:MET:HE3	1:A:76:LEU:HD11	1.91	0.51
1:A:500:TRP:CD1	1:A:506:ILE:HG12	2.46	0.51
1:A:489:ASN:C	1:A:489:ASN:HD22	2.19	0.51
1:A:273:VAL:HG22	1:A:300:LEU:HD23	1.93	0.51
1:A:519:GLN:HB3	1:A:537:CYS:H	1.76	0.51
1:A:177:MET:HE2	1:A:226:SER:HB3	1.92	0.50
1:A:334:VAL:HG21	1:A:401:ILE:HD12	1.94	0.50
1:B:179:LEU:HD13	1:B:188:PHE:CZ	2.47	0.50
1:B:418:LEU:O	1:B:420:PRO:HD3	2.11	0.50
1:A:394:ASP:HB3	1:A:397:MET:HE2	1.93	0.49
1:B:26:ARG:HD2	1:B:108:GLN:NE2	2.27	0.49
1:B:499:VAL:HG13	1:B:500:TRP:CD1	2.47	0.49
1:B:61:ARG:HG2	1:B:64:TYR:HB2	1.93	0.49
1:A:499:VAL:HG13	1:A:500:TRP:CD1	2.47	0.49
1:B:36:ILE:HD12	1:B:141:LYS:HB3	1.94	0.49
1:A:448:GLY:N	1:A:452:ASP:O	2.31	0.49
1:B:28:VAL:HG11	1:B:94:GLU:HG3	1.93	0.49
1:B:76:LEU:CD1	1:B:93:CYS:HB3	2.43	0.48
1:B:334:VAL:HG21	1:B:401:ILE:HD12	1.94	0.48
1:A:515:CYS:SG	1:A:532:TRP:NE1	2.85	0.48
1:A:248:ILE:HB	1:A:260:LEU:HD13	1.94	0.48
1:A:474:MET:O	1:A:478:TYR:HB3	2.12	0.48
1:A:418:LEU:O	1:A:420:PRO:HD3	2.13	0.48
1:A:179:LEU:HD13	1:A:188:PHE:CZ	2.49	0.47
1:A:288:MET:HG2	1:A:317:TYR:CZ	2.49	0.47
1:A:445:ASN:HB2	1:A:455:LEU:HD12	1.95	0.47
1:A:206:VAL:HG13	1:A:211:TRP:HB2	1.96	0.47
1:A:144:VAL:HG11	1:A:411:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD11	1:B:93:CYS:HB3	1.96	0.47
1:B:168:PRO:HG2	1:B:437:LEU:HD23	1.97	0.47
1:A:76:LEU:CD1	1:A:93:CYS:HB3	2.45	0.47
1:B:28:VAL:HG22	1:B:96:ARG:HG2	1.97	0.47
1:B:470:ASN:ND2	1:B:499:VAL:HG23	2.30	0.47
1:B:187:TYR:CD1	1:B:438:LEU:HD22	2.50	0.46
1:B:87:PRO:O	1:B:89:ILE:HD12	2.16	0.45
1:B:117:LEU:HD13	1:B:117:LEU:O	2.15	0.45
1:A:521:LYS:HD3	1:A:537:CYS:HA	1.99	0.45
1:A:187:TYR:CD1	1:A:438:LEU:HD22	2.51	0.45
1:B:502:LYS:HG2	1:B:503:LYS:N	2.32	0.45
1:A:28:VAL:HG22	1:A:96:ARG:HG2	1.97	0.45
1:A:96:ARG:HD3	1:A:108:GLN:HB3	1.98	0.45
1:A:470:ASN:ND2	1:A:499:VAL:HG23	2.31	0.45
1:B:283:VAL:HG11	1:B:307:TRP:CE3	2.52	0.45
1:B:367:LEU:HB3	1:B:370:PHE:CD2	2.51	0.44
1:B:244:HIS:CE1	1:B:246:TYR:CZ	3.05	0.44
1:B:448:GLY:N	1:B:452:ASP:O	2.37	0.44
1:A:389:THR:HG22	1:A:390:HIS:ND1	2.33	0.44
1:B:114:ARG:O	1:B:117:LEU:HB2	2.18	0.44
1:B:184:LEU:HD22	1:B:185:PHE:CZ	2.53	0.44
1:B:356:GLN:O	1:B:360:GLN:HG3	2.18	0.44
1:A:251:ASN:OD1	1:A:252:ALA:N	2.51	0.44
1:B:389:THR:HG22	1:B:390:HIS:ND1	2.32	0.44
1:A:87:PRO:O	1:A:89:ILE:HD12	2.16	0.44
1:B:394:ASP:HB3	1:B:397:MET:HB2	2.00	0.44
1:B:500:TRP:CD1	1:B:506:ILE:HG12	2.52	0.44
1:A:315:ASP:HA	1:A:318:GLN:HE21	1.82	0.44
1:B:144:VAL:HG11	1:B:411:LEU:HD21	2.00	0.44
1:A:94:GLU:HG2	1:A:112:PHE:HE1	1.83	0.44
1:A:356:GLN:O	1:A:360:GLN:HG3	2.18	0.43
1:B:204:ASP:OD2	1:B:487:TRP:HH2	2.01	0.43
1:B:346:PRO:HD3	1:B:359:TRP:CE3	2.53	0.43
1:A:213:TYR:CD2	1:A:271:ALA:HB2	2.54	0.43
1:A:63:GLN:HG2	1:A:394:ASP:HA	2.00	0.43
1:B:430:LYS:HA	1:B:431:PRO:HA	1.86	0.43
1:B:26:ARG:NH2	1:B:55:ARG:O	2.52	0.43
1:A:182:LYS:HZ3	1:A:188:PHE:HB3	1.84	0.42
1:B:337:PHE:HD2	1:B:393:GLN:HE21	1.66	0.42
1:B:38:GLY:N	1:B:145:GLY:O	2.52	0.42
1:B:213:TYR:CD2	1:B:271:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG12	1:A:337:PHE:H	1.84	0.42
1:A:346:PRO:HD3	1:A:359:TRP:CE3	2.54	0.42
1:B:66:ILE:HG13	1:B:358:PHE:CG	2.54	0.42
1:B:334:VAL:HG12	1:B:337:PHE:H	1.85	0.42
1:A:66:ILE:HG13	1:A:358:PHE:CG	2.55	0.42
1:A:184:LEU:HD22	1:A:185:PHE:CZ	2.55	0.42
1:A:283:VAL:HG11	1:A:307:TRP:CE3	2.55	0.41
1:A:308:ALA:HB1	1:A:328:LYS:HA	2.01	0.41
1:B:182:LYS:HZ3	1:B:188:PHE:HB3	1.85	0.41
1:B:280:GLY:HA3	1:B:310:ARG:NH1	2.34	0.41
1:B:515:CYS:HB3	1:B:519:GLN:O	2.20	0.41
1:B:346:PRO:HG3	1:B:359:TRP:CG	2.55	0.41
1:A:214:VAL:HG12	1:A:273:VAL:HB	2.02	0.41
1:B:359:TRP:CD1	1:B:367:LEU:HD21	2.56	0.41
1:B:168:PRO:HA	1:B:187:TYR:HB3	2.03	0.41
1:B:118:ILE:HD12	1:B:142:PRO:HD3	2.03	0.41
1:A:113:ILE:HG22	1:A:167:ILE:HD12	2.03	0.41
1:A:217:VAL:HG22	1:A:246:TYR:HB2	2.02	0.41
1:B:72:MET:HA	1:B:404:ILE:HD13	2.03	0.41
1:B:340:TYR:OH	1:B:351:ARG:NH2	2.36	0.41
1:A:153:SER:O	1:A:157:GLN:NE2	2.54	0.41
1:A:359:TRP:CD1	1:A:367:LEU:HD21	2.55	0.41
1:B:177:MET:HE2	1:B:226:SER:HB3	2.03	0.41
1:A:430:LYS:HA	1:A:431:PRO:HA	1.84	0.40
1:B:111:GLU:O	1:B:115:ASP:HB2	2.22	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	502/877 (57%)	471 (94%)	31 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	481/877 (55%)	453 (94%)	27 (6%)	1 (0%)	43	75
All	All	983/1754 (56%)	924 (94%)	58 (6%)	1 (0%)	48	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	LYS

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	412/763 (54%)	412 (100%)	0	100	100
1	B	399/763 (52%)	399 (100%)	0	100	100
All	All	811/1526 (53%)	811 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	157	GLN
1	A	166	ASN
1	A	198	GLN
1	A	218	HIS
1	A	318	GLN
1	B	74	HIS
1	B	157	GLN
1	B	166	ASN
1	B	198	GLN
1	B	218	HIS
1	B	244	HIS
1	B	318	GLN

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Mol	Chain	Res	Type
1	B	361	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	902	1	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
2	NAG	A	901	1	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	A	903	1	14,14,15	0.38	0	17,19,21	0.50	0
2	NAG	A	904	1	14,14,15	0.47	0	17,19,21	0.68	1 (5%)
2	NAG	B	903	1	14,14,15	0.47	0	17,19,21	0.57	0
2	NAG	A	902	1	14,14,15	0.28	0	17,19,21	0.61	1 (5%)

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	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	2/6/23/26	0/1/1/1
2	NAG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	902	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NAG	C1-O5-C5	2.25	115.20	112.19
2	A	904	NAG	C1-O5-C5	2.21	115.15	112.19
2	A	902	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	506/877 (57%)	0.89	84 (16%) 4 8	127, 180, 254, 270	0
1	B	487/877 (55%)	0.95	87 (17%) 3 6	114, 183, 252, 292	0
All	All	993/1754 (56%)	0.92	171 (17%) 4 7	114, 181, 254, 292	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	14.9
1	A	51	LYS	10.6
1	B	222	ASN	8.6
1	A	62	GLU	8.0
1	B	151	SER	7.8
1	A	52	VAL	7.3
1	A	53	HIS	7.0
1	A	390	HIS	6.8
1	A	222	ASN	6.6
1	A	298	GLU	6.4
1	A	56	LYS	6.3
1	A	296	ALA	6.3
1	A	30	HIS	6.0
1	A	50	ASP	6.0
1	B	371	PRO	5.8
1	A	55	ARG	5.8
1	B	458	GLU	5.2
1	B	474	MET	5.1
1	A	42	SER	4.9
1	B	221	GLY	4.7
1	B	81	SER	4.7
1	B	52	VAL	4.4
1	A	316	GLY	4.3
1	B	175	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	54	GLU	4.2
1	B	473	GLU	4.2
1	A	297	GLY	4.1
1	B	536	PRO	3.9
1	B	195	ASP	3.9
1	B	305	ASP	3.9
1	A	350	HIS	3.8
1	A	47	PRO	3.8
1	B	223	TYR	3.8
1	B	310	ARG	3.7
1	B	51	LYS	3.7
1	B	372	GLN	3.7
1	A	351	ARG	3.6
1	A	329	LEU	3.6
1	A	337	PHE	3.5
1	B	46	GLN	3.5
1	B	53	HIS	3.5
1	A	74	HIS	3.4
1	A	533	THR	3.4
1	B	42	SER	3.4
1	A	48	THR	3.4
1	B	306	GLY	3.4
1	B	32	PRO	3.4
1	A	65	GLY	3.4
1	B	118	ILE	3.3
1	A	372	GLN	3.3
1	A	326	THR	3.3
1	A	203	VAL	3.3
1	B	50	ASP	3.3
1	A	207	LYS	3.3
1	B	174	ALA	3.3
1	A	49	VAL	3.3
1	B	80	ASN	3.3
1	B	522	VAL	3.3
1	B	91	LEU	3.3
1	A	458	GLU	3.2
1	B	277	PHE	3.2
1	B	316	GLY	3.2
1	A	294	GLY	3.2
1	B	281	MET	3.2
1	B	154	VAL	3.2
1	A	46	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	215	SER	3.1
1	A	525	LYS	3.1
1	A	523	ILE	3.1
1	A	348	THR	3.1
1	B	275	ALA	3.0
1	B	49	VAL	3.0
1	B	150	GLY	3.0
1	A	308	ALA	2.9
1	A	319	ARG	2.9
1	A	349	ASN	2.9
1	B	24	GLU	2.9
1	B	318	GLN	2.9
1	B	503	LYS	2.8
1	B	100	TRP	2.8
1	B	55	ARG	2.8
1	A	25	ARG	2.8
1	B	117	LEU	2.8
1	B	176	SER	2.8
1	B	501	SER	2.8
1	A	24	GLU	2.8
1	A	325	ILE	2.7
1	A	61	ARG	2.7
1	B	319	ARG	2.7
1	A	540	ASN	2.7
1	B	220	GLU	2.7
1	B	276	CYS	2.7
1	B	153	SER	2.7
1	A	41	PHE	2.7
1	B	194	SER	2.6
1	B	268	LEU	2.6
1	B	452	ASP	2.6
1	A	64	TYR	2.6
1	A	548	THR	2.6
1	B	250	SER	2.5
1	B	447	THR	2.5
1	B	64	TYR	2.5
1	B	247	LYS	2.5
1	A	63	GLN	2.5
1	B	219	THR	2.5
1	A	250	SER	2.5
1	B	482	ILE	2.5
1	A	140	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	464	GLY	2.5
1	A	380	THR	2.4
1	A	353	PRO	2.4
1	A	339	ASP	2.4
1	A	517	LYS	2.4
1	A	252	ALA	2.4
1	B	248	ILE	2.4
1	B	214	VAL	2.4
1	B	65	GLY	2.4
1	A	118	ILE	2.4
1	A	251	ASN	2.4
1	B	67	GLN	2.4
1	A	200	ARG	2.4
1	B	369	GLY	2.3
1	A	328	LYS	2.3
1	B	422	TYR	2.3
1	A	487	TRP	2.3
1	A	421	GLY	2.3
1	A	443	LYS	2.3
1	B	155	ALA	2.3
1	B	47	PRO	2.3
1	B	280	GLY	2.3
1	B	39	ALA	2.3
1	B	199	ALA	2.3
1	A	27	VAL	2.3
1	A	268	LEU	2.3
1	A	405	TYR	2.3
1	A	197	GLN	2.3
1	A	513	GLU	2.3
1	B	374	ASN	2.2
1	B	257	PHE	2.2
1	B	61	ARG	2.2
1	B	373	GLU	2.2
1	B	480	ASP	2.2
1	B	107	GLU	2.2
1	B	140	LYS	2.2
1	A	43	VAL	2.2
1	B	69	VAL	2.2
1	B	114	ARG	2.2
1	A	32	PRO	2.2
1	A	444	THR	2.2
1	A	331	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	461	ASP	2.2
1	A	379	LYS	2.2
1	B	164	LEU	2.2
1	B	192	VAL	2.1
1	A	199	ALA	2.1
1	A	507	ILE	2.1
1	A	295	LEU	2.1
1	A	60	VAL	2.1
1	B	429	MET	2.1
1	A	238	GLU	2.1
1	B	152	SER	2.1
1	A	101	HIS	2.1
1	A	272	ARG	2.1
1	A	204	ASP	2.1
1	B	472	LYS	2.1
1	B	90	THR	2.1
1	A	549	CYS	2.0
1	B	62	GLU	2.0
1	B	225	GLU	2.0
1	A	466	TYR	2.0
1	B	48	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	903	14/15	0.53	0.16	222,240,245,248	0
2	NAG	A	903	14/15	0.61	0.20	214,233,238,244	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	902	14/15	0.63	0.17	184,210,226,226	0
2	NAG	A	901	14/15	0.67	0.16	200,209,217,221	0
2	NAG	A	902	14/15	0.70	0.16	200,219,226,230	0
2	NAG	A	904	14/15	0.79	0.17	193,206,212,217	0
3	MG	B	901	1/1	0.98	0.08	165,165,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.