



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:22 AM UTC

PDB ID : 6N50 / pdb_00006n50
Title : Metabotropic Glutamate Receptor 5 Extracellular Domain in Complex with Nb43 and L-quisqualic acid
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Chu, M.; Weis, W.I.; Skiniotis, G.; Mathiesen, J.M.; Kobilka, B.K.
Deposited on : 2018-11-20
Resolution : 3.75 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

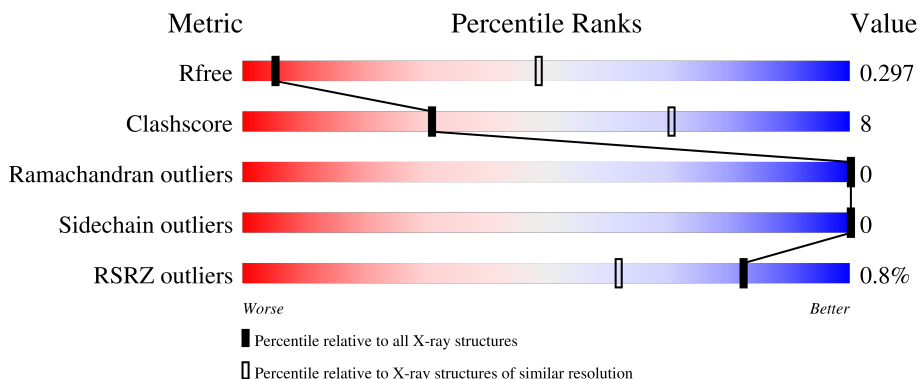
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	596	% 68% 19% 13%
1	B	596	60% 14% 26%
1	C	596	% 69% 17% 14%
2	E	123	% 80% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12146 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	518	Total	C	N	O	S	0	0	0
			3977	2511	673	755	38			
1	B	444	Total	C	N	O	S	0	0	0
			3262	2063	559	611	29			
1	C	511	Total	C	N	O	S	0	0	0
			3873	2448	652	736	37			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP P41594
A	-15	LEU	-	expression tag	UNP P41594
A	-14	LEU	-	expression tag	UNP P41594
A	-13	VAL	-	expression tag	UNP P41594
A	-12	ASN	-	expression tag	UNP P41594
A	-11	GLN	-	expression tag	UNP P41594
A	-10	SER	-	expression tag	UNP P41594
A	-9	HIS	-	expression tag	UNP P41594
A	-8	GLN	-	expression tag	UNP P41594
A	-7	GLY	-	expression tag	UNP P41594
A	-6	PHE	-	expression tag	UNP P41594
A	-5	ASN	-	expression tag	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	GLU	-	expression tag	UNP P41594
A	-2	HIS	-	expression tag	UNP P41594
A	-1	THR	-	expression tag	UNP P41594
A	0	SER	-	expression tag	UNP P41594
A	1	LYS	-	expression tag	UNP P41594
A	2	MET	-	expression tag	UNP P41594
A	3	VAL	-	expression tag	UNP P41594
A	4	SER	-	expression tag	UNP P41594
A	5	ALA	-	expression tag	UNP P41594
A	6	ILE	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	VAL	-	expression tag	UNP P41594
A	8	LEU	-	expression tag	UNP P41594
A	9	TYR	-	expression tag	UNP P41594
A	10	VAL	-	expression tag	UNP P41594
A	11	LEU	-	expression tag	UNP P41594
A	12	LEU	-	expression tag	UNP P41594
A	13	ALA	-	expression tag	UNP P41594
A	14	ALA	-	expression tag	UNP P41594
A	15	ALA	-	expression tag	UNP P41594
A	16	ALA	-	expression tag	UNP P41594
A	17	HIS	-	expression tag	UNP P41594
A	18	SER	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594
A	20	PHE	-	expression tag	UNP P41594
A	572	HIS	-	expression tag	UNP P41594
A	573	HIS	-	expression tag	UNP P41594
A	574	HIS	-	expression tag	UNP P41594
A	575	HIS	-	expression tag	UNP P41594
A	576	HIS	-	expression tag	UNP P41594
A	577	HIS	-	expression tag	UNP P41594
A	578	HIS	-	expression tag	UNP P41594
A	579	HIS	-	expression tag	UNP P41594
B	-16	MET	-	initiating methionine	UNP P41594
B	-15	LEU	-	expression tag	UNP P41594
B	-14	LEU	-	expression tag	UNP P41594
B	-13	VAL	-	expression tag	UNP P41594
B	-12	ASN	-	expression tag	UNP P41594
B	-11	GLN	-	expression tag	UNP P41594
B	-10	SER	-	expression tag	UNP P41594
B	-9	HIS	-	expression tag	UNP P41594
B	-8	GLN	-	expression tag	UNP P41594
B	-7	GLY	-	expression tag	UNP P41594
B	-6	PHE	-	expression tag	UNP P41594
B	-5	ASN	-	expression tag	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	GLU	-	expression tag	UNP P41594
B	-2	HIS	-	expression tag	UNP P41594
B	-1	THR	-	expression tag	UNP P41594
B	0	SER	-	expression tag	UNP P41594
B	1	LYS	-	expression tag	UNP P41594
B	2	MET	-	expression tag	UNP P41594
B	3	VAL	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	expression tag	UNP P41594
B	5	ALA	-	expression tag	UNP P41594
B	6	ILE	-	expression tag	UNP P41594
B	7	VAL	-	expression tag	UNP P41594
B	8	LEU	-	expression tag	UNP P41594
B	9	TYR	-	expression tag	UNP P41594
B	10	VAL	-	expression tag	UNP P41594
B	11	LEU	-	expression tag	UNP P41594
B	12	LEU	-	expression tag	UNP P41594
B	13	ALA	-	expression tag	UNP P41594
B	14	ALA	-	expression tag	UNP P41594
B	15	ALA	-	expression tag	UNP P41594
B	16	ALA	-	expression tag	UNP P41594
B	17	HIS	-	expression tag	UNP P41594
B	18	SER	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	20	PHE	-	expression tag	UNP P41594
B	572	HIS	-	expression tag	UNP P41594
B	573	HIS	-	expression tag	UNP P41594
B	574	HIS	-	expression tag	UNP P41594
B	575	HIS	-	expression tag	UNP P41594
B	576	HIS	-	expression tag	UNP P41594
B	577	HIS	-	expression tag	UNP P41594
B	578	HIS	-	expression tag	UNP P41594
B	579	HIS	-	expression tag	UNP P41594
C	-16	MET	-	initiating methionine	UNP P41594
C	-15	LEU	-	expression tag	UNP P41594
C	-14	LEU	-	expression tag	UNP P41594
C	-13	VAL	-	expression tag	UNP P41594
C	-12	ASN	-	expression tag	UNP P41594
C	-11	GLN	-	expression tag	UNP P41594
C	-10	SER	-	expression tag	UNP P41594
C	-9	HIS	-	expression tag	UNP P41594
C	-8	GLN	-	expression tag	UNP P41594
C	-7	GLY	-	expression tag	UNP P41594
C	-6	PHE	-	expression tag	UNP P41594
C	-5	ASN	-	expression tag	UNP P41594
C	-4	LYS	-	expression tag	UNP P41594
C	-3	GLU	-	expression tag	UNP P41594
C	-2	HIS	-	expression tag	UNP P41594
C	-1	THR	-	expression tag	UNP P41594
C	0	SER	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LYS	-	expression tag	UNP P41594
C	2	MET	-	expression tag	UNP P41594
C	3	VAL	-	expression tag	UNP P41594
C	4	SER	-	expression tag	UNP P41594
C	5	ALA	-	expression tag	UNP P41594
C	6	ILE	-	expression tag	UNP P41594
C	7	VAL	-	expression tag	UNP P41594
C	8	LEU	-	expression tag	UNP P41594
C	9	TYR	-	expression tag	UNP P41594
C	10	VAL	-	expression tag	UNP P41594
C	11	LEU	-	expression tag	UNP P41594
C	12	LEU	-	expression tag	UNP P41594
C	13	ALA	-	expression tag	UNP P41594
C	14	ALA	-	expression tag	UNP P41594
C	15	ALA	-	expression tag	UNP P41594
C	16	ALA	-	expression tag	UNP P41594
C	17	HIS	-	expression tag	UNP P41594
C	18	SER	-	expression tag	UNP P41594
C	19	ALA	-	expression tag	UNP P41594
C	20	PHE	-	expression tag	UNP P41594
C	572	HIS	-	expression tag	UNP P41594
C	573	HIS	-	expression tag	UNP P41594
C	574	HIS	-	expression tag	UNP P41594
C	575	HIS	-	expression tag	UNP P41594
C	576	HIS	-	expression tag	UNP P41594
C	577	HIS	-	expression tag	UNP P41594
C	578	HIS	-	expression tag	UNP P41594
C	579	HIS	-	expression tag	UNP P41594

- Molecule 2 is a protein called Nanobody 43.

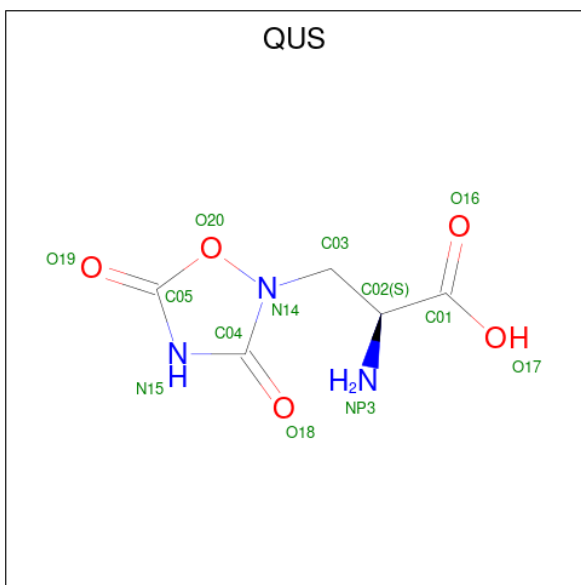
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	123	Total	C	N	O	S	0	0	0
			925	575	159	186	5			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (CCD ID: QUS) (formula: C₅H₇N₃O₅).

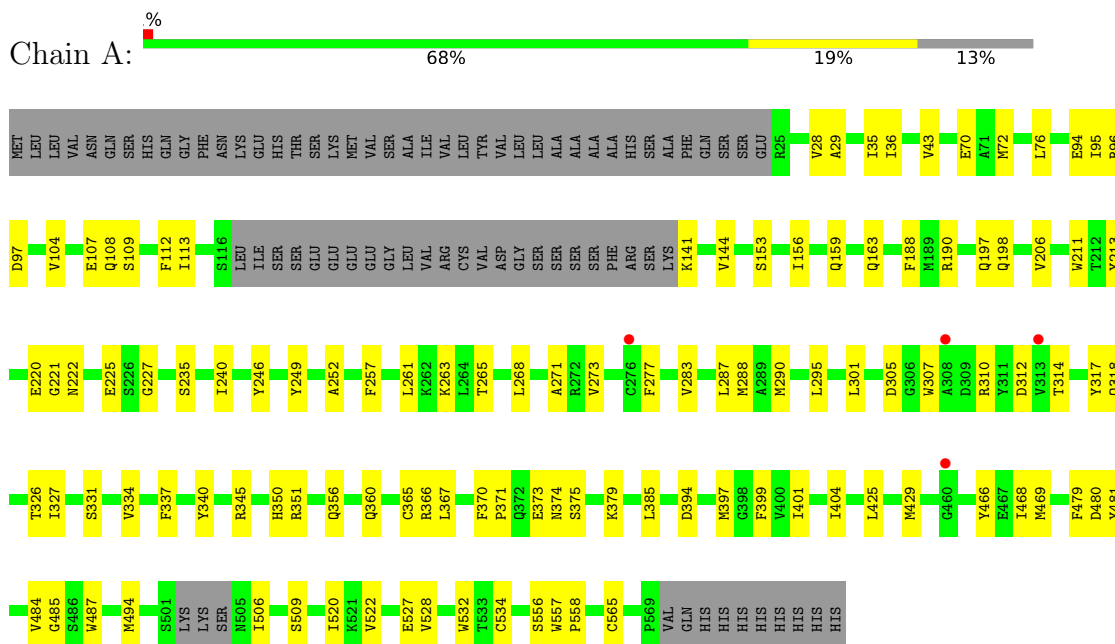


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	5	3	5		
4	B	1	Total	C	N	O	0	0
			13	5	3	5		
4	C	1	Total	C	N	O	0	0
			13	5	3	5		

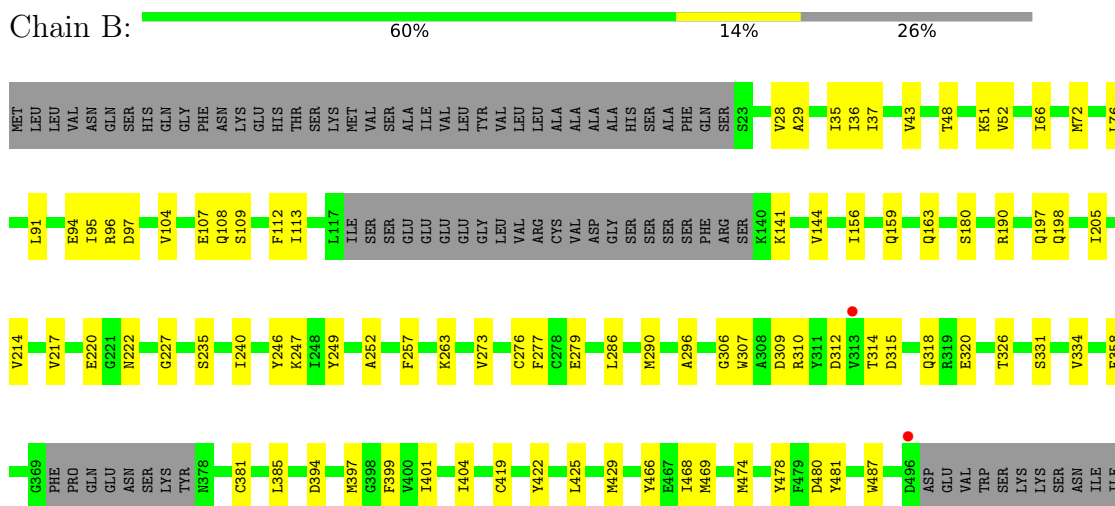
3 Residue-property plots [i](#)

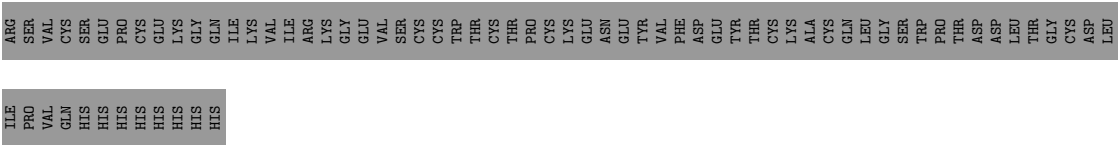
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Metabotropic glutamate receptor 5

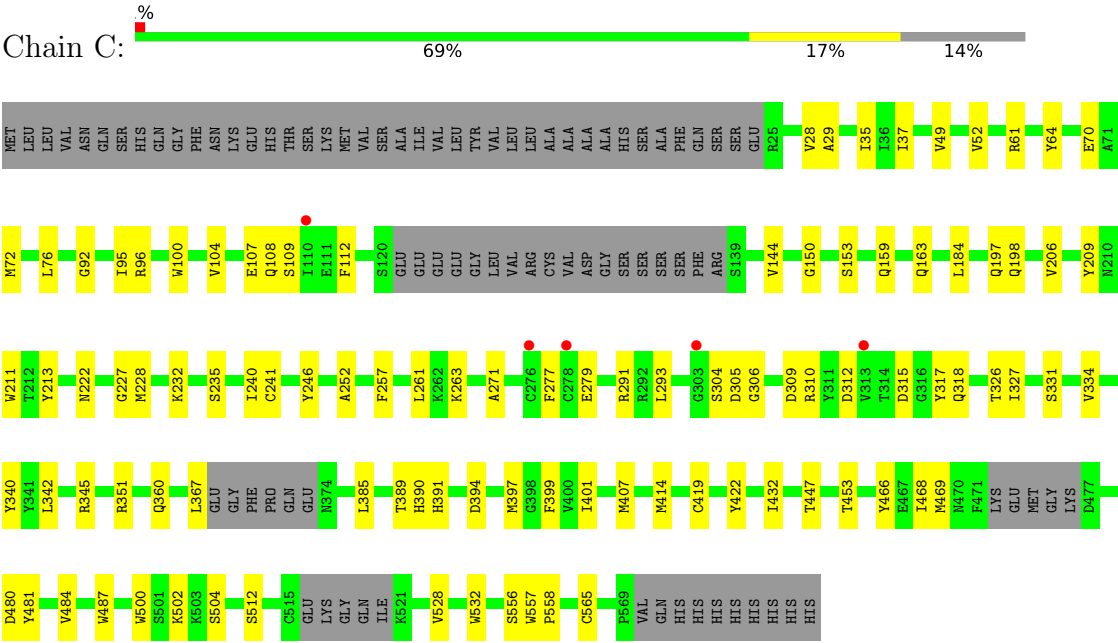


• Molecule 1: Metabotropic glutamate receptor 5

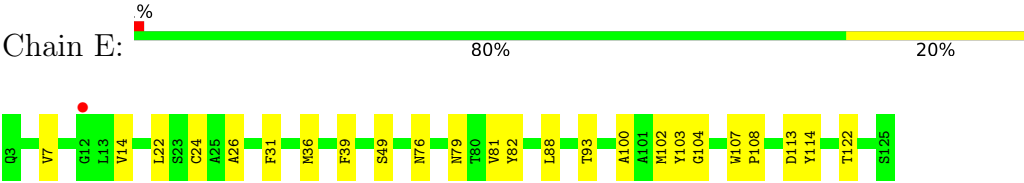




● Molecule 1: Metabotropic glutamate receptor 5



● Molecule 2: Nanobody 43



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	150.43Å 157.16Å 208.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 3.75 39.29 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.29-3.75) 98.3 (39.29-3.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.14 _3211	Depositor
R, R_{free}	0.266 , 0.300 0.264 , 0.297	Depositor DCC
R_{free} test set	2003 reflections (7.95%)	wwPDB-VP
Wilson B-factor (Å ²)	122.2	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 124.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12146	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/4069	0.46	0/5526
1	B	0.13	0/3334	0.37	0/4537
1	C	0.16	0/3961	0.46	0/5385
2	E	0.20	0/947	0.56	0/1284
All	All	0.16	0/12311	0.45	0/16732

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 [i](#)

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	3977	0	3704	72	0
1	B	3262	0	2975	48	0
1	C	3873	0	3578	58	0
2	E	925	0	852	17	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	26	0	0
4	A	13	0	6	0	0
4	B	13	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	13	0	6	0	0
All	All	12146	0	11192	192	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 8.

All (192) 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:C:29:ALA:HB3	1:C:95:ILE:HB	1.55	0.88
1:A:527:GLU:HG2	1:A:528:VAL:HG23	1.63	0.81
1:A:29:ALA:HB3	1:A:95:ILE:HB	1.62	0.80
1:A:72:MET:HE3	1:A:76:LEU:HD11	1.67	0.75
1:A:360:GLN:HE22	1:A:373:GLU:HA	1.50	0.75
1:C:198:GLN:NE2	1:C:304:SER:OG	2.20	0.75
1:C:340:TYR:OH	1:C:351:ARG:NH2	2.20	0.75
1:B:29:ALA:HB3	1:B:95:ILE:HB	1.67	0.75
1:B:72:MET:HE3	1:B:76:LEU:HD11	1.67	0.74
1:C:72:MET:HE3	1:C:76:LEU:HD11	1.69	0.73
1:A:340:TYR:OH	1:A:351:ARG:NH2	2.23	0.72
1:A:290:MET:HE1	1:A:301:LEU:HD11	1.74	0.70
1:A:350:HIS:HB3	2:E:103:TYR:HB3	1.75	0.69
1:B:37:ILE:HD11	1:B:91:LEU:HD22	1.77	0.67
1:A:109:SER:HA	1:A:112:PHE:HD2	1.60	0.67
1:A:220:GLU:HG2	1:A:249:TYR:CE1	2.30	0.66
1:C:252:ALA:HB3	1:C:257:PHE:HE1	1.60	0.66
1:B:381:CYS:HB2	1:B:385:LEU:HD21	1.76	0.66
2:E:93:THR:HG23	2:E:122:THR:HA	1.78	0.66
1:A:252:ALA:HB3	1:A:257:PHE:HE1	1.61	0.66
1:B:252:ALA:HB3	1:B:257:PHE:HE1	1.62	0.65
1:B:220:GLU:HG2	1:B:249:TYR:CE1	2.32	0.65
1:C:228:MET:HG3	1:C:232:LYS:HE3	1.79	0.64
1:C:109:SER:HA	1:C:112:PHE:HD2	1.64	0.63
1:C:326:THR:HG23	1:C:469:MET:HB2	1.81	0.62
1:C:419:CYS:HB3	1:C:422:TYR:HB2	1.81	0.62
1:B:109:SER:HA	1:B:112:PHE:HD2	1.64	0.62
2:E:26:ALA:O	2:E:79:ASN:ND2	2.35	0.60
1:B:36:ILE:HD13	1:B:141:LYS:HE3	1.83	0.60
1:B:326:THR:HG23	1:B:469:MET:HB2	1.82	0.60
1:B:35:ILE:HG23	1:B:144:VAL:HG21	1.83	0.59
1:A:556:SER:HB3	1:A:565:CYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:O	1:B:290:MET:HG3	2.03	0.59
1:A:326:THR:HG23	1:A:469:MET:HB2	1.84	0.58
1:C:556:SER:HB3	1:C:565:CYS:HB3	1.85	0.58
1:B:227:GLY:HA3	1:B:277:PHE:CE2	2.38	0.58
1:A:425:LEU:HD23	1:A:429:MET:HE2	1.86	0.58
1:A:28:VAL:HG11	1:A:94:GLU:HG3	1.85	0.57
1:A:227:GLY:HA3	1:A:277:PHE:CE2	2.40	0.57
1:A:35:ILE:HG23	1:A:144:VAL:HG21	1.86	0.56
1:A:334:VAL:HG13	1:A:337:PHE:HB3	1.87	0.56
1:B:419:CYS:HB3	1:B:422:TYR:HB3	1.87	0.55
2:E:102:MET:HE3	2:E:103:TYR:CE1	2.42	0.55
1:A:356:GLN:HE22	1:A:370:PHE:HD2	1.56	0.54
1:C:291:ARG:HD2	1:C:317:TYR:CE2	2.42	0.54
1:B:480:ASP:OD1	1:B:481:TYR:N	2.41	0.54
1:B:246:TYR:HE1	1:B:263:LYS:HE2	1.73	0.54
2:E:107:TRP:CD1	2:E:108:PRO:HA	2.43	0.53
1:A:520:ILE:HG21	1:A:534:CYS:HB3	1.90	0.53
1:C:197:GLN:HB3	1:C:487:TRP:CZ3	2.44	0.53
1:B:28:VAL:HG11	1:B:94:GLU:HG3	1.91	0.53
1:B:197:GLN:HB3	1:B:487:TRP:CZ3	2.45	0.52
1:C:163:GLN:NE2	1:C:184:LEU:O	2.42	0.52
1:C:159:GLN:OE1	1:C:163:GLN:HG2	2.08	0.52
1:C:241:CYS:HB3	1:C:528:VAL:HG11	1.92	0.52
1:B:159:GLN:OE1	1:B:163:GLN:HB3	2.10	0.52
2:E:22:LEU:O	2:E:82:TYR:HA	2.10	0.52
1:C:252:ALA:HB3	1:C:257:PHE:CE1	2.44	0.52
1:B:425:LEU:HD23	1:B:429:MET:HE2	1.92	0.51
1:A:506:ILE:H	1:A:506:ILE:HD12	1.75	0.51
1:A:246:TYR:HE1	1:A:263:LYS:HE2	1.76	0.51
1:A:265:THR:HG21	1:A:295:LEU:HD13	1.92	0.51
1:A:527:GLU:N	1:A:527:GLU:OE1	2.44	0.51
1:C:246:TYR:HE1	1:C:263:LYS:HE2	1.76	0.51
1:B:246:TYR:CE1	1:B:263:LYS:HE2	2.46	0.51
1:B:217:VAL:O	1:B:276:CYS:HA	2.10	0.50
1:C:502:LYS:HD3	1:C:504:SER:H	1.77	0.50
1:C:35:ILE:HG23	1:C:144:VAL:HG21	1.92	0.50
1:C:227:GLY:HA3	1:C:277:PHE:CE2	2.47	0.50
1:A:198:GLN:HB2	1:A:466:TYR:CE2	2.47	0.50
1:A:360:GLN:HE21	1:A:367:LEU:H	1.59	0.50
1:A:261:LEU:HD23	1:A:295:LEU:HD12	1.94	0.50
1:A:197:GLN:HB3	1:A:487:TRP:CZ3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:HG22	1:A:268:LEU:HD12	1.93	0.49
1:C:104:VAL:O	1:C:107:GLU:HG2	2.12	0.49
1:C:198:GLN:HB2	1:C:466:TYR:CE2	2.47	0.49
1:C:480:ASP:OD1	1:C:481:TYR:N	2.43	0.49
1:A:252:ALA:HB3	1:A:257:PHE:CE1	2.45	0.49
1:A:480:ASP:OD1	1:A:481:TYR:N	2.44	0.49
1:A:522:VAL:HG13	1:A:532:TRP:CG	2.47	0.49
1:B:331:SER:HB2	1:B:399:PHE:CE2	2.48	0.49
1:C:246:TYR:CE1	1:C:263:LYS:HE2	2.47	0.49
1:C:331:SER:HB2	1:C:399:PHE:CE2	2.48	0.49
1:A:310:ARG:HB3	1:A:312:ASP:OD1	2.13	0.49
1:A:371:PRO:HG2	2:E:104:GLY:H	1.78	0.49
1:A:246:TYR:CE1	1:A:263:LYS:HE2	2.48	0.49
1:A:283:VAL:O	1:A:287:LEU:HG	2.13	0.49
1:C:345:ARG:NH2	1:C:385:LEU:O	2.43	0.49
1:A:331:SER:HB2	1:A:399:PHE:CE2	2.48	0.48
1:A:557:TRP:CG	1:A:558:PRO:HD2	2.48	0.48
1:A:235:SER:HB2	1:A:240:ILE:HB	1.94	0.48
1:C:70:GLU:HB3	1:C:340:TYR:HE2	1.78	0.48
1:A:371:PRO:HG2	2:E:104:GLY:N	2.29	0.48
1:B:310:ARG:HB3	1:B:312:ASP:OD1	2.14	0.48
1:C:557:TRP:CG	1:C:558:PRO:HD2	2.48	0.47
1:C:235:SER:HB2	1:C:240:ILE:HB	1.97	0.47
1:C:261:LEU:HD23	1:C:293:LEU:HD22	1.95	0.47
1:A:520:ILE:CG2	1:A:534:CYS:HB3	2.44	0.47
1:B:198:GLN:HB2	1:B:466:TYR:CE2	2.49	0.47
1:C:310:ARG:HB3	1:C:312:ASP:OD1	2.14	0.47
1:A:305:ASP:HA	1:A:327:ILE:O	2.15	0.47
1:C:315:ASP:HA	1:C:318:GLN:NE2	2.30	0.47
2:E:102:MET:HG2	2:E:103:TYR:CD1	2.50	0.47
1:B:474:MET:HB2	1:B:478:TYR:CD2	2.50	0.46
1:A:527:GLU:HG2	1:A:528:VAL:N	2.29	0.46
1:B:235:SER:HB2	1:B:240:ILE:HB	1.97	0.46
1:B:279:GLU:HA	1:B:306:GLY:HA3	1.97	0.46
1:B:309:ASP:N	1:B:309:ASP:OD1	2.48	0.46
1:C:512:SER:HB3	1:C:532:TRP:CH2	2.50	0.46
1:C:159:GLN:O	1:C:163:GLN:HG3	2.16	0.46
1:A:104:VAL:O	1:A:107:GLU:HG2	2.15	0.46
1:B:104:VAL:O	1:B:107:GLU:HG2	2.15	0.46
1:A:43:VAL:HB	1:A:97:ASP:OD1	2.16	0.46
1:A:109:SER:HA	1:A:112:PHE:CD2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ASP:HB3	1:C:397:MET:HE2	1.96	0.46
1:A:213:TYR:CD2	1:A:271:ALA:HB2	2.51	0.46
1:C:153:SER:OG	1:C:222:ASN:N	2.38	0.46
1:B:180:SER:OG	1:B:190:ARG:NH2	2.49	0.46
1:A:394:ASP:HB3	1:A:397:MET:HE2	1.97	0.46
2:E:36:MET:HG3	2:E:81:VAL:HG11	1.96	0.46
1:A:345:ARG:NH2	1:A:385:LEU:O	2.46	0.45
1:B:394:ASP:HB3	1:B:397:MET:HE2	1.97	0.45
1:A:394:ASP:HB3	1:A:397:MET:HB2	1.98	0.45
1:C:228:MET:O	1:C:232:LYS:HG3	2.16	0.45
1:A:159:GLN:OE1	1:A:163:GLN:HB3	2.17	0.45
1:A:188:PHE:HE2	1:A:190:ARG:HD2	1.81	0.45
1:C:96:ARG:HD3	1:C:108:GLN:HB3	1.98	0.45
1:C:206:VAL:HG13	1:C:211:TRP:HB2	1.98	0.45
1:C:309:ASP:N	1:C:309:ASP:OD1	2.49	0.45
1:C:334:VAL:HG21	1:C:401:ILE:HD12	1.98	0.45
1:A:318:GLN:HB3	1:A:479:PHE:CD2	2.51	0.45
1:B:48:THR:O	1:B:52:VAL:HG13	2.17	0.45
1:B:334:VAL:HG21	1:B:401:ILE:HD12	1.99	0.45
1:C:305:ASP:HA	1:C:327:ILE:O	2.16	0.45
1:A:288:MET:HG2	1:A:317:TYR:CZ	2.53	0.44
1:C:279:GLU:HA	1:C:306:GLY:HA3	1.99	0.44
1:B:220:GLU:OE1	1:B:247:LYS:HD2	2.17	0.44
1:B:48:THR:HG23	1:B:51:LYS:H	1.82	0.44
1:B:43:VAL:HB	1:B:97:ASP:OD1	2.17	0.44
1:A:366:ARG:HG2	1:A:379:LYS:O	2.17	0.44
1:B:66:ILE:HG13	1:B:358:PHE:CG	2.53	0.44
1:B:307:TRP:HE1	1:B:314:THR:HG23	1.82	0.44
2:E:14:VAL:HG11	2:E:88:LEU:HD13	1.99	0.44
1:C:414:MET:HE1	1:C:432:ILE:HG23	2.00	0.43
1:A:206:VAL:HG13	1:A:211:TRP:HB2	2.00	0.43
2:E:102:MET:HE3	2:E:103:TYR:HE1	1.82	0.43
1:A:485:GLY:HA3	1:A:494:MET:SD	2.58	0.43
1:C:468:ILE:HG22	1:C:484:VAL:HG23	2.00	0.43
1:C:61:ARG:HE	1:C:64:TYR:HB2	1.82	0.43
1:C:342:LEU:HD21	1:C:391:HIS:CG	2.53	0.43
1:B:252:ALA:HB3	1:B:257:PHE:CE1	2.47	0.43
1:A:36:ILE:HD12	1:A:141:LYS:HB2	2.00	0.43
1:B:109:SER:O	1:B:113:ILE:HG12	2.19	0.43
1:B:290:MET:HE2	1:B:296:ALA:HA	2.01	0.43
1:A:374:ASN:HD22	1:A:375:SER:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HG22	1:C:92:GLY:O	2.18	0.43
1:C:360:GLN:HE21	1:C:367:LEU:H	1.67	0.42
1:C:28:VAL:HG12	1:C:96:ARG:HG2	2.01	0.42
2:E:7:VAL:O	2:E:24:CYS:HA	2.20	0.42
1:C:37:ILE:HD12	1:C:407:MET:HG2	2.00	0.42
1:A:468:ILE:HG22	1:A:484:VAL:HG23	2.01	0.42
1:A:70:GLU:HB3	1:A:340:TYR:HE2	1.84	0.42
1:A:221:GLY:O	1:A:225:GLU:HB2	2.19	0.42
1:B:156:ILE:HD11	1:B:222:ASN:OD1	2.19	0.42
1:A:307:TRP:HE1	1:A:314:THR:HG23	1.85	0.41
1:C:213:TYR:CD2	1:C:271:ALA:HB2	2.56	0.41
1:A:273:VAL:HG12	1:A:509:SER:OG	2.20	0.41
1:A:334:VAL:HG11	1:A:401:ILE:HD12	2.03	0.41
1:A:96:ARG:HD3	1:A:108:GLN:HB3	2.03	0.41
1:B:205:ILE:HD11	1:B:468:ILE:HG12	2.03	0.41
1:C:512:SER:HB3	1:C:532:TRP:CZ2	2.56	0.41
1:B:290:MET:HB2	1:B:320:GLU:HG2	2.03	0.41
1:C:100:TRP:CZ3	1:C:150:GLY:HA3	2.56	0.41
1:C:389:THR:HG22	1:C:390:HIS:ND1	2.36	0.41
2:E:113:ASP:OD1	2:E:113:ASP:N	2.52	0.41
1:A:370:PHE:N	1:A:370:PHE:CD1	2.89	0.41
2:E:31:PHE:HE2	2:E:76:ASN:HA	1.85	0.41
2:E:100:ALA:HB3	2:E:114:TYR:HB2	2.03	0.41
1:C:209:TYR:HE2	1:C:500:TRP:HE1	1.69	0.40
1:A:156:ILE:HD11	1:A:222:ASN:OD1	2.20	0.40
1:A:360:GLN:HG2	1:A:365:CYS:O	2.21	0.40
1:B:72:MET:HA	1:B:404:ILE:HD13	2.03	0.40
1:A:109:SER:O	1:A:113:ILE:HG12	2.22	0.40
1:A:153:SER:HG	1:A:222:ASN:H	1.67	0.40
1:A:265:THR:CG2	1:A:295:LEU:HD13	2.51	0.40
1:B:315:ASP:HA	1:B:318:GLN:NE2	2.37	0.40
1:B:96:ARG:HD3	1:B:108:GLN:HB3	2.03	0.40
1:C:447:THR:HA	1:C:453:THR:HA	2.04	0.40
1:A:72:MET:HA	1:A:404:ILE:HD13	2.04	0.40
1:B:214:VAL:HG12	1:B:273:VAL:HG23	2.03	0.40
1:C:49:VAL:HA	1:C:52:VAL:HG23	2.03	0.40
2:E:39:PHE:HB3	2:E:49:SER:HA	2.03	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	512/596 (86%)	478 (93%)	34 (7%)	0	100	100
1	B	438/596 (74%)	424 (97%)	14 (3%)	0	100	100
1	C	501/596 (84%)	472 (94%)	29 (6%)	0	100	100
2	E	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
All	All	1572/1911 (82%)	1488 (95%)	84 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	418/520 (80%)	418 (100%)	0	100	100
1	B	321/520 (62%)	321 (100%)	0	100	100
1	C	404/520 (78%)	404 (100%)	0	100	100
2	E	94/97 (97%)	94 (100%)	0	100	100
All	All	1237/1657 (75%)	1237 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	360	GLN
1	A	374	ASN
1	A	415	GLN
1	B	361	HIS
1	B	489	ASN
1	C	198	GLN
1	C	361	HIS
1	C	470	ASN
1	C	489	ASN

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	$\# Z > 2$
4	QUS	B	602	-	9,13,13	1.94	3 (33%)	10,18,18	2.84	6 (60%)
3	NAG	A	602	1	14,14,15	0.35	0	17,19,21	0.56	0
3	NAG	C	601	1	14,14,15	0.34	0	17,19,21	0.56	0
4	QUS	C	603	-	9,13,13	1.96	3 (33%)	10,18,18	2.91	5 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	C	602	1	14,14,15	0.29	0	17,19,21	0.32	0
4	QUS	A	603	-	9,13,13	1.96	3 (33%)	10,18,18	2.92	6 (60%)

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
4	QUS	B	602	-	-	1/6/8/8	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
4	QUS	C	603	-	-	2/6/8/8	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	602	1	-	2/6/23/26	0/1/1/1
4	QUS	A	603	-	-	2/6/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	QUS	C04-N14	-3.74	1.32	1.39
4	B	602	QUS	C04-N14	-3.71	1.32	1.39
4	A	603	QUS	C04-N14	-3.70	1.32	1.39
4	A	603	QUS	O18-C04	-2.37	1.18	1.23
4	B	602	QUS	O18-C04	-2.33	1.18	1.23
4	C	603	QUS	O18-C04	-2.32	1.19	1.23
4	A	603	QUS	C04-N15	-2.26	1.34	1.38
4	C	603	QUS	C04-N15	-2.25	1.34	1.38
4	B	602	QUS	C04-N15	-2.24	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	QUS	O20-N14-C03	6.44	126.64	113.83
4	A	603	QUS	O20-N14-C03	6.44	126.63	113.83
4	B	602	QUS	O20-N14-C03	6.31	126.37	113.83
4	A	603	QUS	O20-C05-O19	4.00	126.43	122.95
4	C	603	QUS	O20-C05-O19	4.00	126.43	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	QUS	O20-C05-O19	3.79	126.25	122.95
4	A	603	QUS	C04-N15-C05	-2.68	108.08	112.62
4	C	603	QUS	C04-N15-C05	-2.66	108.11	112.62
4	B	602	QUS	C04-N15-C05	-2.64	108.14	112.62
4	A	603	QUS	O19-C05-N15	-2.49	125.61	129.68
4	C	603	QUS	O19-C05-N15	-2.44	125.69	129.68
4	B	602	QUS	O19-C05-N15	-2.38	125.78	129.68
4	A	603	QUS	N15-C04-N14	2.18	108.19	106.10
4	C	603	QUS	N15-C04-N14	2.14	108.15	106.10
4	B	602	QUS	O20-C05-N15	2.04	107.97	106.14
4	A	603	QUS	O20-C05-N15	2.02	107.96	106.14
4	B	602	QUS	N15-C04-N14	2.01	108.03	106.10

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
4	A	603	QUS	C01-C02-C03-N14
4	B	602	QUS	C01-C02-C03-N14
4	C	603	QUS	C01-C02-C03-N14
4	A	603	QUS	NP3-C02-C03-N14
4	C	603	QUS	NP3-C02-C03-N14
3	C	602	NAG	C4-C5-C6-O6

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 [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	518/596 (86%)	-0.12	4 (0%)	82 62	90, 123, 169, 193	0
1	B	444/596 (74%)	-0.16	2 (0%)	87 70	122, 160, 197, 221	0
1	C	511/596 (85%)	0.00	5 (0%)	79 57	122, 167, 204, 239	0
2	E	123/123 (100%)	-0.26	1 (0%)	82 62	114, 138, 164, 180	0
All	All	1596/1911 (83%)	-0.10	12 (0%)	82 62	90, 152, 194, 239	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	303	GLY	2.7
1	C	276	CYS	2.6
1	B	496	ASP	2.5
1	C	278	CYS	2.3
1	C	313	VAL	2.3
1	B	313	VAL	2.3
1	A	313	VAL	2.1
1	A	308	ALA	2.1
1	C	110	ILE	2.1
2	E	12	GLY	2.1
1	A	460	GLY	2.1
1	A	276	CYS	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
3	NAG	C	602	14/15	0.34	0.10	209,214,219,220	0
3	NAG	C	601	14/15	0.39	0.09	235,237,238,238	0
3	NAG	B	601	14/15	0.79	0.08	186,187,188,189	0
3	NAG	A	601	14/15	0.81	0.09	160,161,164,165	0
4	QUS	C	603	13/13	0.81	0.10	149,156,161,162	0
4	QUS	B	602	13/13	0.84	0.08	145,152,157,158	0
3	NAG	A	602	14/15	0.85	0.09	177,179,180,180	0
4	QUS	A	603	13/13	0.88	0.09	100,106,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.