Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:03 PM EDT

PDB ID	:	6N50
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 (i) 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 (i)) were used in the production of this report:

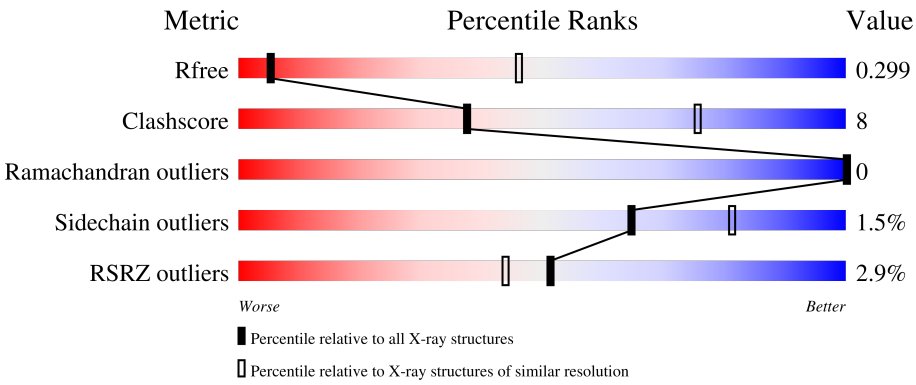
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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 <=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% 18% • 13%
1	B	596	2% 61% 13% 26%
1	C	596	3% 69% 16% 14%
2	E	123	7% 80% 20%

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
4	QUS	C	603	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	518	3977	2511	673	755	38	0	0	0
1	B	444	3262	2063	559	611	29	0	0	0
1	C	511	3873	2448	652	736	37	0	0	0

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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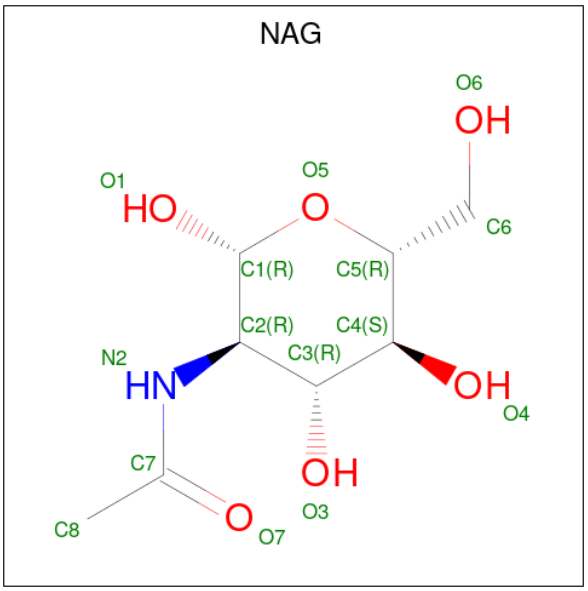
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LYS	-	expression tag	UNP P41594
C	2	MET	-	expression tag	UNP P41594
C	3	VAL	-	expression tag	UNP P41594
C	4	SER	-	expression tag	UNP P41594
C	5	ALA	-	expression tag	UNP P41594
C	6	ILE	-	expression tag	UNP P41594
C	7	VAL	-	expression tag	UNP P41594
C	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.

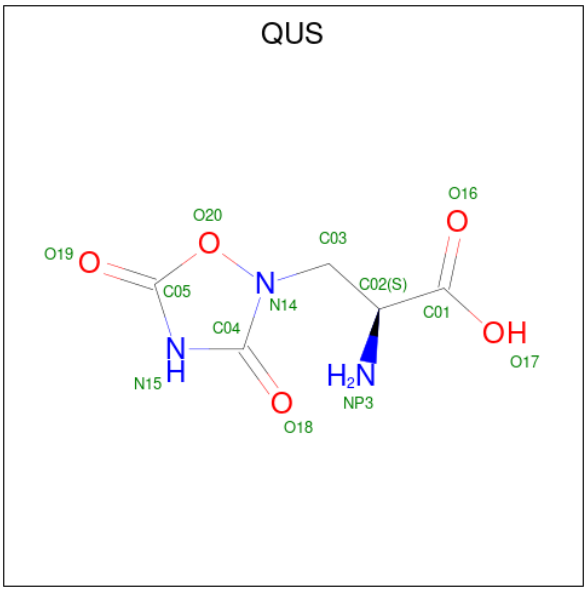
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	123	925	575	159	186	5	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: $C_5H_7N_3O_5$).



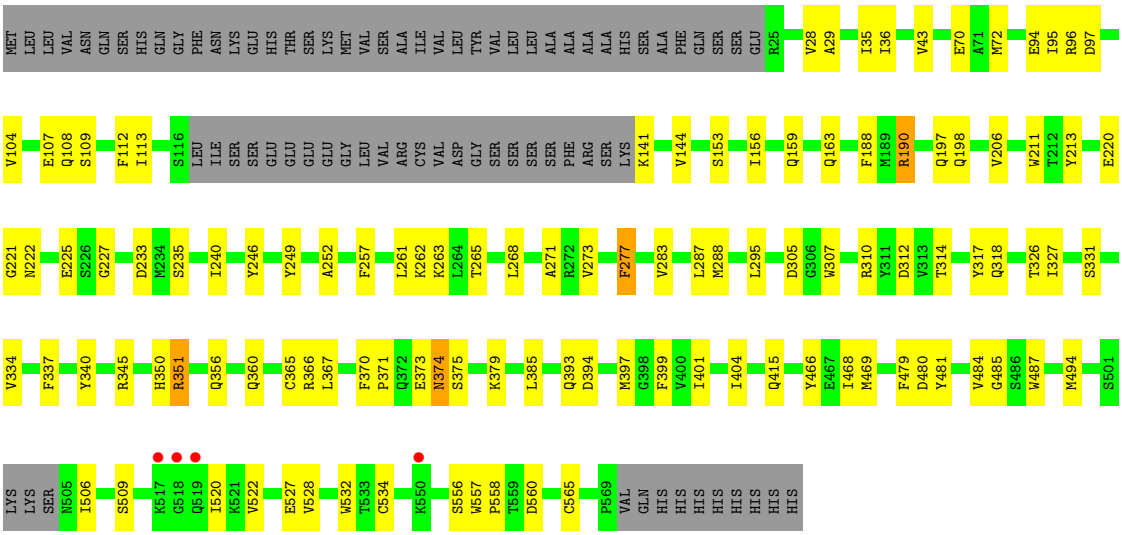
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	13	5	3	5	0	0
			Total	C	N	O		
4	B	1	13	5	3	5	0	0
			Total	C	N	O		
4	C	1	13	5	3	5	0	0

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.

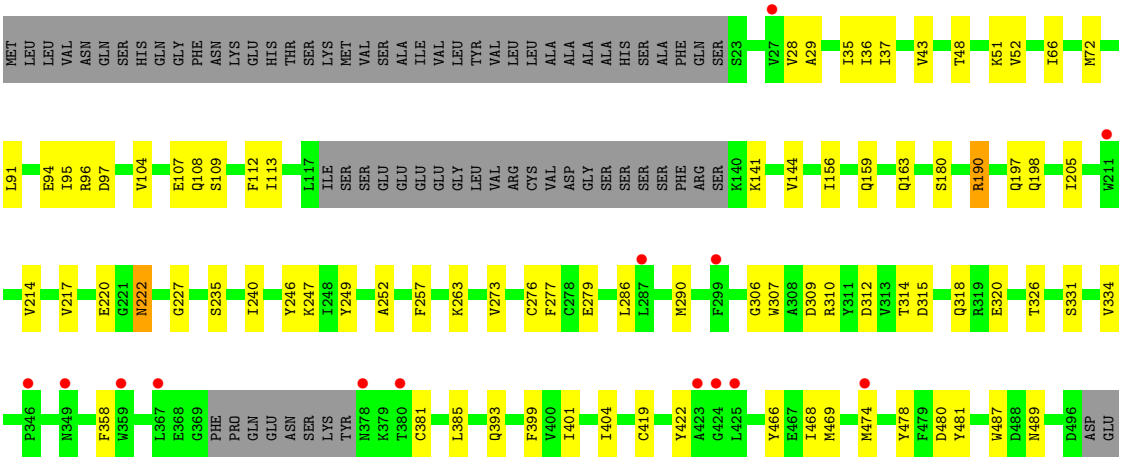
• Molecule 1: Metabotropic glutamate receptor 5

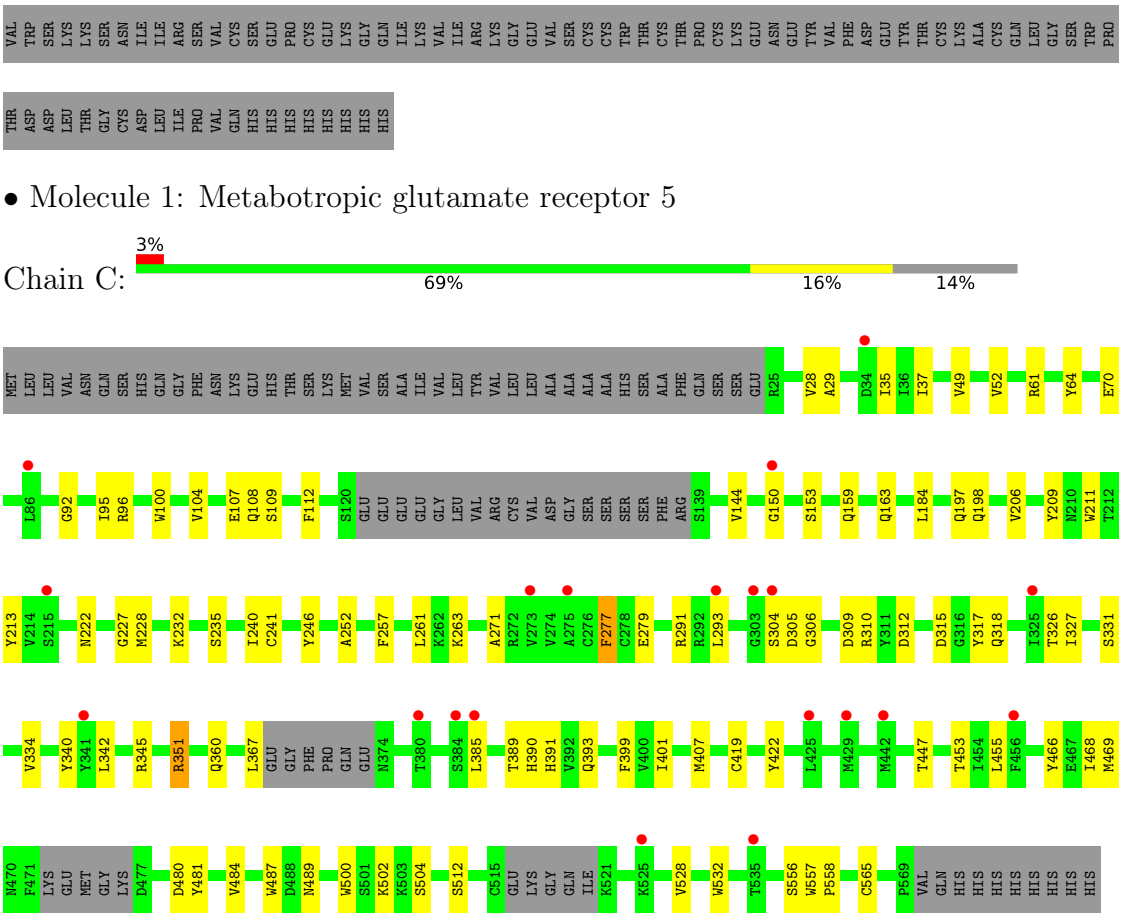
Chain A:



• Molecule 1: Metabotropic glutamate receptor 5

Chain B:




VAL TRP SER LYS LYS SER ASN ILE ILE ARG SER VAL CYS SER GLU PRO CYS GLU LYS GLY GLN ILE LYS VAL ILE ARG LYS GLY GLU VAL SER CYS CYS TRP THR CYS THR PRO CYS LYS GLU ASN GLU TYR VAL PHE ASP GLU TYR THR CYS LYS ALA CYS GLN LEU GLY SER TRP PRO
THR ASP ASP LEU THR GLY CYS ASP LEU ILE PRO VAL GLN HIS HIS HIS HIS HIS HIS HIS HIS
• Molecule 1: Metabotropic glutamate receptor 5
Chain C:
3%
69%
16%
14%
MET LEU LEU VAL ASN GLN SER HIS GLN GLY PHE ASN LYS GLU HIS THR SER LYS MET VAL SER ALA ILE VAL LEU TYR VAL LEU LEU ALA ALA ALA ALA HIS SER ALA PHE GLN SER SER GLU R25 V28 A29 D34 I35 I36 I37 V49 V52 R61 Y64 E70
L86 G92 I95 R96 W100 V104 E107 Q108 S109 F112 S120 GLU GLU GLU GLY LEU VAL ARG CYS VAL ASP GLY SER SER SER SER PHE ARG S139 V144 G150 S153 Q159 Q163 L184 Q197 Q198 V206 Y209 N210 W211 T212
Y213 V214 S215 N222 G227 M228 K232 S235 I240 C241 Y246 A252 F257 L261 K262 K263 A271 R272 V273 V274 A275 C276 F277 C278 E279 R291 R292 L293 G303 S304 D305 G306 D309 R310 Y311 D312 D315 G316 Y317 Q318 I325 T326 I327 S331
V334 Y340 Y341 L342 R345 R351 Q360 L367 GLU GLY PHE PRO GLN GLU N374 T380 S384 L385 T389 H390 H391 V392 Q393 F399 V400 I401 M407 C419 Y422 L425 M429 M442 T447 T453 I454 L455 F456 Y466 E467 I468 M469
N470 F471 LYS GLU MET GLY LYS D477 D480 Y481 V484 W487 D488 N489 W500 S501 K502 K503 S504 S512 C515 GLU LYS GLY GLN ILE K521 K525 V528 W532 T535 S556 W557 P558 C565 P569 VAL GLN HIS HIS HIS HIS HIS HIS HIS HIS
• Molecule 2: Nanobody 43
Chain E:
7%
80%
20%
Q3 V7 G11 G12 L13 V14 Q15 L22 S23 C24 A25 A26 F31 M36 F39 S49 I72 N76 N79 T80 V81 Y82 M85 L88 E91 D92 T93 A100 A101 M102 Y103 G104 W107 P108 D113 Y114 T119 T122 V123 S124 S125

4 Data and refinement statistics (i)

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) 98.5 (39.29-3.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.266 , 0.300 0.265 , 0.299	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)	0.30 , 111.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: QUS, 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	0.26	0/4069	0.49	0/5526
1	B	0.25	0/3334	0.45	0/4537
1	C	0.26	0/3961	0.48	0/5385
2	E	0.27	0/947	0.58	0/1284
All	All	0.26	0/12311	0.49	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	68	0
1	B	3262	0	2975	44	0
1	C	3873	0	3578	55	0
2	E	925	0	852	15	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	179	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 (179) 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: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:A:340:TYR:OH	1:A:351:ARG:NH2	2.23	0.72
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:206:VAL:HG13	1:A:211:TRP:HB2	2.00	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:A:374:ASN:HD22	1:A:375:SER:N	2.17	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	512/596 (86%)	478 (93%)	34 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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%)	409 (98%)	9 (2%)	52	73
1	B	321/520 (62%)	317 (99%)	4 (1%)	71	84
1	C	404/520 (78%)	399 (99%)	5 (1%)	71	84
2	E	94/97 (97%)	94 (100%)	0	100	100
All	All	1237/1657 (75%)	1219 (98%)	18 (2%)	65	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	233	ASP
1	A	262	LYS
1	A	277	PHE
1	A	351	ARG
1	A	374	ASN
1	A	393	GLN
1	A	415	GLN
1	A	560	ASP
1	B	190	ARG
1	B	222	ASN
1	B	393	GLN
1	B	489	ASN

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Mol	Chain	Res	Type
1	C	277	PHE
1	C	351	ARG
1	C	393	GLN
1	C	455	LEU
1	C	489	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	HIS
1	A	360	GLN
1	A	374	ASN
1	A	415	GLN
1	B	489	ASN
1	C	44	HIS
1	C	198	GLN
1	C	489	ASN
2	E	79	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 monosaccharides 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	$\#\|Z\| > 2$
3	NAG	A	602	1	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	A	601	1	14,14,15	0.27	0	17,19,21	0.54	0
4	QUS	B	602	-	6,13,13	0.92	0	4,18,18	1.36	0
4	QUS	C	603	-	6,13,13	0.93	0	4,18,18	1.30	0
3	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	C	602	1	14,14,15	0.28	0	17,19,21	0.31	0
4	QUS	A	603	-	6,13,13	0.94	0	4,18,18	1.33	0
3	NAG	C	601	1	14,14,15	0.32	0	17,19,21	0.55	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	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	QUS	B	602	-	-	1/6/8/8	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	C	602	1	-	2/6/23/26	0/1/1/1
4	QUS	A	603	-	-	2/6/8/8	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Atoms
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 (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	518/596 (86%)	0.01	4 (0%)	86	84	90, 123, 169, 193	0
1	B	444/596 (74%)	0.09	14 (3%)	47	40	122, 160, 197, 221	0
1	C	511/596 (85%)	0.26	20 (3%)	39	34	122, 167, 204, 239	0
2	E	123/123 (100%)	0.44	8 (6%)	18	15	114, 138, 164, 180	0
All	All	1596/1911 (83%)	0.15	46 (2%)	51	44	90, 152, 194, 239	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	12	GLY	6.3
1	C	303	GLY	5.0
2	E	11	GLY	4.5
1	A	518	GLY	3.9
1	B	380	THR	3.5
1	C	150	GLY	3.4
2	E	85	MET	3.3
1	C	425	LEU	3.0
1	A	519	GLN	3.0
1	C	442	MET	3.0
1	C	325	ILE	2.8
1	C	304	SER	2.6
1	B	349	ASN	2.5
1	B	424	GLY	2.5
1	B	346	PRO	2.5
1	B	367	LEU	2.4
1	B	211	TRP	2.4
1	B	425	LEU	2.4
1	B	474	MET	2.4
1	C	525	LYS	2.4
1	C	535	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	517	LYS	2.3
2	E	124	SER	2.3
1	C	34	ASP	2.3
1	B	423	ALA	2.2
1	C	273	VAL	2.2
1	B	27	VAL	2.2
1	C	275	ALA	2.2
2	E	119	THR	2.2
2	E	91	GLU	2.2
2	E	72	ILE	2.2
1	C	215	SER	2.2
1	A	550	LYS	2.2
1	C	429	MET	2.2
1	C	293	LEU	2.1
1	C	385	LEU	2.1
1	C	384	SER	2.1
1	B	359	TRP	2.1
1	B	299	PHE	2.1
1	B	378	ASN	2.1
1	C	456	PHE	2.1
1	C	341	TYR	2.1
1	B	287	LEU	2.1
2	E	15	GLN	2.1
1	C	86	LEU	2.0
1	C	380	THR	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 monosaccharides 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	601	14/15	0.67	0.31	235,237,238,238	0
3	NAG	A	602	14/15	0.72	0.18	177,179,180,180	0
3	NAG	C	602	14/15	0.75	0.34	209,214,219,220	0
3	NAG	B	601	14/15	0.78	0.28	186,187,188,189	0
4	QUS	C	603	13/13	0.79	0.43	149,156,161,162	0
3	NAG	A	601	14/15	0.80	0.33	160,161,164,165	0
4	QUS	B	602	13/13	0.84	0.27	145,152,157,158	0
4	QUS	A	603	13/13	0.91	0.29	100,106,111,112	0

6.5 Other polymers (i)

There are no such residues in this entry.