



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2023 – 04:14 PM EST

PDB ID : 5CNK
Title : mglur3 with glutamate
Authors : Monn, J.A.; Clawson, D.K.
Deposited on : 2015-07-17
Resolution : 3.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.1
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) : 2.32.1

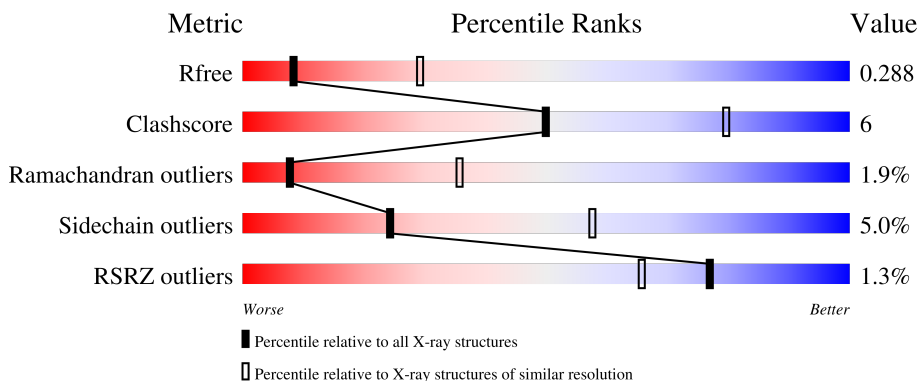
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	517	 74% 10% • 14%
1	B	517	 68% 14% • 15%
1	C	517	 69% 16% • 13%

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
3	IOD	A	604	-	-	X	-
3	IOD	B	602	-	-	X	-
3	IOD	C	603	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10563 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3518	2237	608	659	14	0	0	0
1	B	438	3478	2210	600	654	14	0	0	0
1	C	448	3525	2234	607	670	14	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

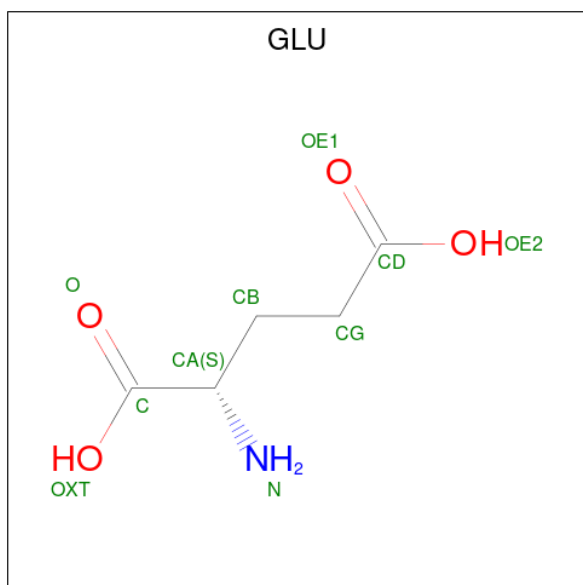
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q14832
A	0	ALA	-	expression tag	UNP Q14832
A	1	LEU	-	expression tag	UNP Q14832
A	240	SER	CYS	conflict	UNP Q14832
A	508	GLU	-	expression tag	UNP Q14832
A	509	GLY	-	expression tag	UNP Q14832
A	510	HIS	-	expression tag	UNP Q14832
A	511	HIS	-	expression tag	UNP Q14832
A	512	HIS	-	expression tag	UNP Q14832
A	513	HIS	-	expression tag	UNP Q14832
A	514	HIS	-	expression tag	UNP Q14832
A	515	HIS	-	expression tag	UNP Q14832
B	-1	MET	-	initiating methionine	UNP Q14832
B	0	ALA	-	expression tag	UNP Q14832
B	1	LEU	-	expression tag	UNP Q14832
B	240	SER	CYS	conflict	UNP Q14832
B	508	GLU	-	expression tag	UNP Q14832
B	509	GLY	-	expression tag	UNP Q14832
B	510	HIS	-	expression tag	UNP Q14832
B	511	HIS	-	expression tag	UNP Q14832
B	512	HIS	-	expression tag	UNP Q14832
B	513	HIS	-	expression tag	UNP Q14832
B	514	HIS	-	expression tag	UNP Q14832

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Chain	Residue	Modelled	Actual	Comment	Reference
B	515	HIS	-	expression tag	UNP Q14832
C	-1	MET	-	initiating methionine	UNP Q14832
C	0	ALA	-	expression tag	UNP Q14832
C	1	LEU	-	expression tag	UNP Q14832
C	240	SER	CYS	conflict	UNP Q14832
C	508	GLU	-	expression tag	UNP Q14832
C	509	GLY	-	expression tag	UNP Q14832
C	510	HIS	-	expression tag	UNP Q14832
C	511	HIS	-	expression tag	UNP Q14832
C	512	HIS	-	expression tag	UNP Q14832
C	513	HIS	-	expression tag	UNP Q14832
C	514	HIS	-	expression tag	UNP Q14832
C	515	HIS	-	expression tag	UNP Q14832

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	5	1	4	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total 4 I	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total I 3 3	0	0
3	C	3	Total I 3 3	0	0

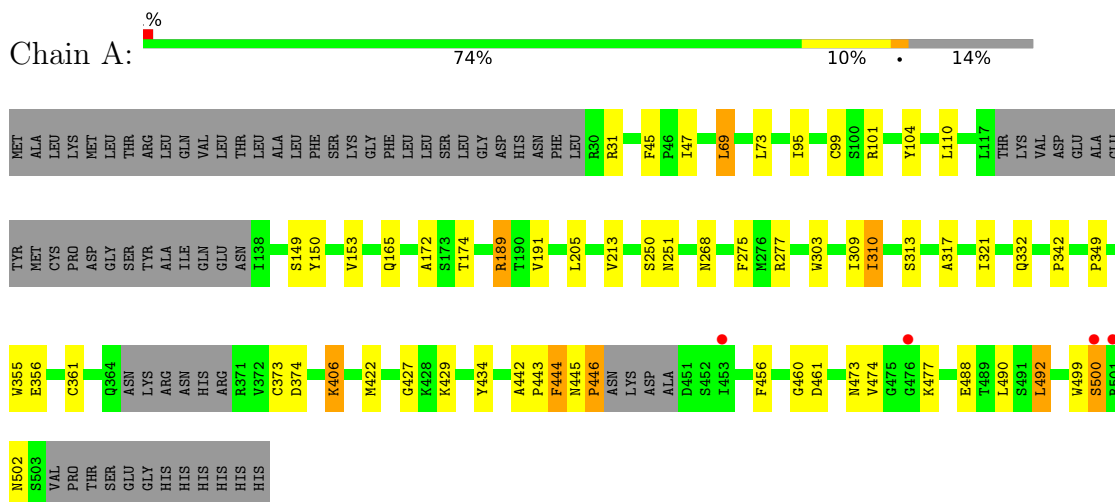
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0

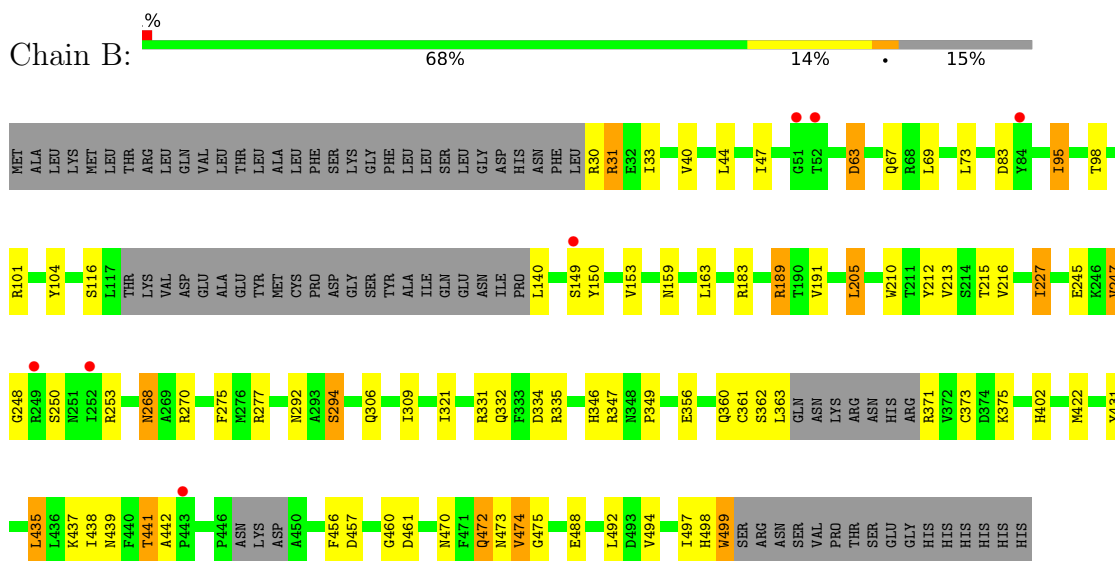
3 Residue-property plots [i](#)

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 3

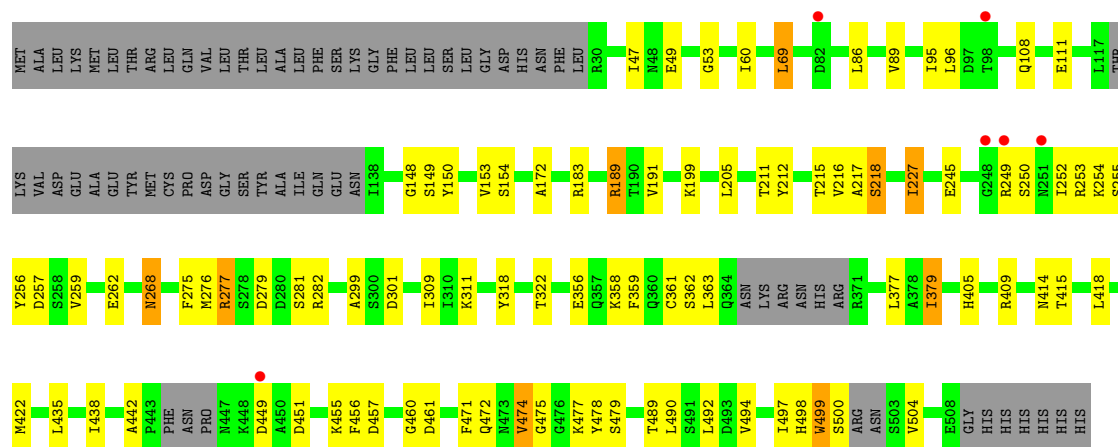


- Molecule 1: Metabotropic glutamate receptor 3



- Molecule 1: Metabotropic glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.34Å 80.00Å 206.86Å 90.00° 130.73° 90.00°	Depositor
Resolution (Å)	78.38 – 3.15 78.38 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (78.38-3.15) 97.8 (78.38-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.13Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.221 , 0.258 0.243 , 0.288	Depositor DCC
R_{free} test set	873 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.055 for $-1/2^*h+3/2^*k, 1/2^*h+1/2^*k, -1/2^*h-3/2^*k-l$ 0.059 for $-1/2^*h-3/2^*k, -1/2^*h+1/2^*k, -1/2^*h+3/2^*k-l$ 0.105 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -3/2^*h-3/2^*k-l$ 0.078 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -3/2^*h+3/2^*k-l$ 0.064 for $-h, -k, 2^*h+1$	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10563	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: IOD

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	0.55	1/3592 (0.0%)	0.72	0/4856
1	B	0.51	0/3551	0.76	1/4800 (0.0%)
1	C	0.51	0/3596	0.76	2/4866 (0.0%)
All	All	0.53	1/10739 (0.0%)	0.75	3/14522 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	PRO	N-CD	14.88	1.68	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ARG	C-N-CA	5.97	136.64	121.70
1	C	249	ARG	C-N-CA	5.47	135.38	121.70
1	C	255	SER	N-CA-C	-5.27	96.76	111.00

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	3518	0	3425	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3478	0	3378	50	0
1	C	3525	0	3402	40	0
2	A	10	0	5	2	0
3	A	4	0	0	3	0
3	B	3	0	0	2	0
3	C	3	0	0	2	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	1	0
All	All	10563	0	10210	121	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 6.

All (121) 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:446:PRO:N	1:A:446:PRO:CD	1.68	1.43
1:B:216:VAL:HG22	1:B:245:GLU:HB2	1.38	1.03
1:C:216:VAL:HG22	1:C:245:GLU:HB2	1.42	0.98
1:C:438:ILE:HG22	1:C:455:LYS:HB3	1.50	0.92
1:B:247:VAL:HG23	1:B:248:GLY:H	1.38	0.89
1:A:321:ILE:HD11	1:A:499:TRP:HZ3	1.42	0.81
1:A:442:ALA:O	1:A:444:PHE:N	2.13	0.81
1:B:83:ASP:O	1:B:83:ASP:OD1	2.02	0.78
1:B:474:VAL:HG23	1:B:475:GLY:H	1.51	0.74
1:A:321:ILE:HD11	1:A:499:TRP:CZ3	2.25	0.70
1:A:101:ARG:HE	1:A:104:TYR:HB2	1.58	0.68
1:B:494:VAL:HA	1:B:497:ILE:HD12	1.76	0.68
1:C:149:SER:HB3	3:C:603:IOD:I	2.65	0.67
1:C:494:VAL:HA	1:C:497:ILE:HD12	1.76	0.65
1:C:414:ASN:ND2	4:C:701:HOH:O	2.24	0.65
1:A:174:THR:HG1	2:A:601:GLU:N	1.95	0.65
1:B:470:ASN:ND2	1:B:497:ILE:HG23	2.14	0.63
1:B:149:SER:HB3	3:B:602:IOD:I	2.69	0.63
1:C:217:ALA:HB2	1:C:227:ILE:HG13	1.81	0.61
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.82	0.61
1:C:356:GLU:HA	1:C:361:CYS:HB2	1.83	0.61
1:C:299:ALA:HB3	1:C:322:THR:HG22	1.84	0.60
1:B:402:HIS:HB3	1:B:437:LYS:CE	2.32	0.59
1:B:360:GLN:HB2	1:B:371:ARG:HH22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HG23	1:B:438:ILE:O	2.04	0.57
1:C:475:GLY:C	1:C:477:LYS:H	2.08	0.57
1:A:303:TRP:HA	1:A:309:ILE:CD1	2.36	0.56
1:A:189:ARG:HG3	1:A:191:VAL:O	2.04	0.56
1:B:189:ARG:HG3	1:B:191:VAL:O	2.07	0.55
1:C:471:PHE:CZ	1:C:478:TYR:HB3	2.42	0.55
1:B:153:VAL:HG21	3:B:602:IOD:I	2.77	0.55
1:B:474:VAL:HG23	1:B:475:GLY:N	2.22	0.54
1:C:47:ILE:HD12	1:C:69:LEU:HD12	1.88	0.54
1:A:374:ASP:OD1	1:C:199:LYS:HE2	2.07	0.54
1:B:470:ASN:HD22	1:B:497:ILE:HG23	1.71	0.54
1:C:189:ARG:HG3	1:C:191:VAL:O	2.07	0.54
1:A:251:ASN:HA	1:B:375:LYS:HG3	1.89	0.54
1:B:63:ASP:O	1:B:67:GLN:HB2	2.08	0.54
1:B:306:GLN:HB2	1:B:309:ILE:HD12	1.91	0.53
1:B:402:HIS:HB3	1:B:437:LYS:HE2	1.91	0.52
1:C:256:TYR:HA	1:C:259:VAL:HG22	1.92	0.52
1:A:205:LEU:HD13	1:A:213:VAL:HG11	1.91	0.52
1:B:44:LEU:HD22	1:B:98:THR:HG22	1.91	0.52
1:A:47:ILE:HD12	1:A:69:LEU:HD12	1.91	0.52
1:A:473:ASN:O	1:A:477:LYS:O	2.27	0.52
1:A:189:ARG:HD3	1:A:461:ASP:OD1	2.10	0.51
1:B:402:HIS:HB3	1:B:437:LYS:CD	2.41	0.51
1:C:218:SER:HB2	1:C:276:MET:HA	1.92	0.51
1:C:359:PHE:CD1	1:C:377:LEU:HD22	2.46	0.50
1:A:149:SER:HB2	3:A:604:IOD:I	2.82	0.50
1:A:172:ALA:HB1	2:A:601:GLU:HG3	1.93	0.50
1:C:472:GLN:HG2	1:C:498:HIS:HB2	1.93	0.50
1:B:205:LEU:HD23	1:B:210:TRP:HE3	1.77	0.50
1:B:247:VAL:HG23	1:B:248:GLY:N	2.17	0.50
1:C:414:ASN:OD1	1:C:415:THR:HG23	2.13	0.49
1:B:189:ARG:HD3	1:B:461:ASP:OD1	2.12	0.49
1:C:489:THR:HG22	1:C:490:LEU:N	2.28	0.49
1:C:189:ARG:HD3	1:C:461:ASP:OD1	2.13	0.49
1:B:457:ASP:HB2	1:B:461:ASP:H	1.78	0.48
1:B:402:HIS:HB3	1:B:437:LYS:HD3	1.95	0.48
1:C:457:ASP:HB2	1:C:461:ASP:H	1.79	0.48
1:B:472:GLN:HG3	1:B:498:HIS:HB2	1.96	0.48
1:A:150:TYR:HB2	1:A:153:VAL:HG13	1.96	0.48
1:B:431:TYR:HA	1:B:435:LEU:HB2	1.94	0.48
3:A:605:IOD:I	1:B:346:HIS:NE2	3.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:CG2	1:B:245:GLU:HB2	2.27	0.47
1:C:277:ARG:HD3	1:C:279:ASP:OD1	2.14	0.47
1:C:358:LYS:HE2	1:C:379:ILE:HG23	1.96	0.47
1:B:101:ARG:HE	1:B:104:TYR:HB2	1.79	0.47
1:C:282:ARG:HD3	1:C:309:ILE:HA	1.97	0.46
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.98	0.46
1:B:31:ARG:HD2	1:B:349:PRO:HB2	1.98	0.46
1:A:310:ILE:HD11	1:A:317:ALA:HB1	1.98	0.45
1:B:159:ASN:O	1:B:163:LEU:HD13	2.16	0.45
1:A:499:TRP:O	1:A:500:SER:C	2.53	0.45
1:C:215:THR:HB	1:C:227:ILE:HD11	1.98	0.45
1:B:101:ARG:HH21	1:B:104:TYR:HB2	1.81	0.45
1:B:362:SER:O	1:B:363:LEU:HD22	2.16	0.45
1:A:99:CYS:SG	1:A:104:TYR:CE2	3.10	0.45
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.99	0.45
1:C:499:TRP:CZ2	1:C:504:VAL:HG22	2.51	0.45
1:C:456:PHE:HB3	1:C:460:GLY:HA2	1.99	0.45
1:C:149:SER:HA	1:C:172:ALA:HB3	2.00	0.44
1:C:362:SER:O	1:C:363:LEU:HD22	2.17	0.44
1:A:406:LYS:HD3	1:A:434:TYR:HD1	1.83	0.44
1:C:318:TYR:CE2	1:C:500:SER:HB3	2.53	0.44
1:B:73:LEU:HD23	1:B:347:ARG:HD2	2.00	0.44
1:C:212:TYR:HE2	1:C:268:ASN:HD22	1.65	0.43
1:B:456:PHE:HB3	1:B:460:GLY:HA2	2.00	0.43
1:A:73:LEU:HD11	1:A:95:ILE:HD12	2.01	0.43
1:A:165:GLN:O	1:A:427:GLY:HA3	2.19	0.43
1:C:150:TYR:HB2	1:C:153:VAL:HG13	2.01	0.43
1:C:254:LYS:HA	1:C:257:ASP:H	1.84	0.43
1:C:276:MET:HE3	1:C:281:SER:HA	2.00	0.43
1:B:331:ARG:HA	1:B:334:ASP:OD2	2.19	0.42
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.42
1:C:405:HIS:CE1	1:C:409:ARG:HD2	2.54	0.42
1:A:73:LEU:CD1	1:A:95:ILE:HD12	2.50	0.42
1:B:33:ILE:HB	1:B:95:ILE:HB	2.02	0.42
1:B:205:LEU:HD22	1:B:213:VAL:HG11	2.02	0.42
1:A:456:PHE:HB3	1:A:460:GLY:HA2	2.02	0.42
1:B:47:ILE:CD1	1:B:69:LEU:HD12	2.50	0.42
1:B:356:GLU:HG2	1:B:361:CYS:HB2	2.02	0.42
1:C:474:VAL:HG21	1:C:479:SER:OG	2.20	0.42
1:B:321:ILE:HD11	1:B:499:TRP:CZ3	2.55	0.41
1:B:150:TYR:HB2	1:B:153:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASN:O	1:B:474:VAL:HG22	2.20	0.41
1:B:270:ARG:HH21	1:B:294:SER:N	2.18	0.41
1:A:153:VAL:HG21	3:A:604:IOD:I	2.90	0.41
1:C:86:LEU:HD22	1:C:89:VAL:HB	2.02	0.41
1:A:45:PHE:HB2	1:A:47:ILE:HD11	2.03	0.41
1:B:215:THR:HB	1:B:227:ILE:HD11	2.01	0.41
1:A:490:LEU:HG	1:A:492:LEU:HD22	2.02	0.41
1:A:342:PRO:HD3	1:A:355:TRP:CD2	2.55	0.41
1:B:212:TYR:CE2	1:B:268:ASN:HB2	2.56	0.40
1:C:96:LEU:HD13	1:C:108:GLN:HB3	2.03	0.40
1:A:69:LEU:C	1:A:69:LEU:HD23	2.41	0.40
1:C:153:VAL:HG21	3:C:603:IOD:I	2.92	0.40
1:C:148:GLY:HA3	1:C:154:SER:OG	2.21	0.40
1:A:149:SER:HA	1:A:172:ALA:HB3	2.03	0.40
1:B:332:GLN:OE1	1:B:335:ARG:NH2	2.54	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	436/517 (84%)	413 (95%)	17 (4%)	6 (1%)	11	43
1	B	430/517 (83%)	390 (91%)	30 (7%)	10 (2%)	6	31
1	C	438/517 (85%)	394 (90%)	35 (8%)	9 (2%)	7	33
All	All	1304/1551 (84%)	1197 (92%)	82 (6%)	25 (2%)	8	36

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	A	443	PRO

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Mol	Chain	Res	Type
1	A	500	SER
1	B	253	ARG
1	B	441	THR
1	C	250	SER
1	C	253	ARG
1	B	247	VAL
1	C	53	GLY
1	C	252	ILE
1	C	435	LEU
1	B	250	SER
1	B	292	ASN
1	B	474	VAL
1	C	449	ASP
1	C	451	ASP
1	A	502	ASN
1	B	31	ARG
1	B	488	GLU
1	C	474	VAL
1	A	474	VAL
1	A	488	GLU
1	B	294	SER
1	B	442	ALA
1	C	442	ALA

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	373/445 (84%)	357 (96%)	16 (4%)	29	62
1	B	368/445 (83%)	350 (95%)	18 (5%)	25	59
1	C	372/445 (84%)	350 (94%)	22 (6%)	19	51
All	All	1113/1335 (83%)	1057 (95%)	56 (5%)	24	57

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

Mol	Chain	Res	Type
1	A	69	LEU
1	A	110	LEU
1	A	189	ARG
1	A	268	ASN
1	A	275	PHE
1	A	277	ARG
1	A	310	ILE
1	A	313	SER
1	A	332	GLN
1	A	373	CYS
1	A	406	LYS
1	A	422	MET
1	A	429	LYS
1	A	444	PHE
1	A	445	ASN
1	A	492	LEU
1	B	63	ASP
1	B	95	ILE
1	B	116	SER
1	B	183	ARG
1	B	189	ARG
1	B	205	LEU
1	B	227	ILE
1	B	268	ASN
1	B	275	PHE
1	B	277	ARG
1	B	373	CYS
1	B	422	MET
1	B	435	LEU
1	B	439	ASN
1	B	441	THR
1	B	472	GLN
1	B	492	LEU
1	B	499	TRP
1	C	49	GLU
1	C	60	ILE
1	C	69	LEU
1	C	95	ILE
1	C	111	GLU
1	C	183	ARG
1	C	189	ARG
1	C	205	LEU
1	C	211	THR

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Mol	Chain	Res	Type
1	C	218	SER
1	C	227	ILE
1	C	262	GLU
1	C	268	ASN
1	C	275	PHE
1	C	277	ARG
1	C	301	ASP
1	C	311	LYS
1	C	379	ILE
1	C	418	LEU
1	C	422	MET
1	C	492	LEU
1	C	499	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	GLN
1	C	268	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](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 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	GLU	A	601	-	8,9,9	2.02	2 (25%)	10,11,11	1.98	4 (40%)

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	GLU	A	601	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GLU	O-C	4.88	1.37	1.22
2	A	601	GLU	OXT-C	-2.40	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GLU	OXT-C-CA	3.59	125.61	113.38
2	A	601	GLU	O-C-CA	-2.73	112.52	122.14
2	A	601	GLU	CG-CB-CA	-2.37	108.31	113.84
2	A	601	GLU	OE2-CD-OE1	-2.22	117.77	123.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLU	CA-CB-CG-CD
2	A	601	GLU	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLU	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/517 (85%)	0.04	4 (0%) 84 75	25, 55, 87, 119	0
1	B	438/517 (84%)	-0.03	7 (1%) 72 59	17, 52, 80, 103	0
1	C	448/517 (86%)	0.01	6 (1%) 77 66	22, 53, 85, 101	0
All	All	1330/1551 (85%)	0.01	17 (1%) 77 66	17, 54, 85, 119	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	PRO	3.2
1	C	249	ARG	2.7
1	C	251	ASN	2.7
1	C	82	ASP	2.7
1	C	248	GLY	2.6
1	B	249	ARG	2.4
1	B	84	TYR	2.3
1	A	476	GLY	2.3
1	C	98	THR	2.1
1	A	501	ARG	2.1
1	B	149	SER	2.1
1	B	51	GLY	2.1
1	C	449	ASP	2.1
1	A	500	SER	2.1
1	B	252	ILE	2.1
1	A	453	ILE	2.1
1	B	52	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
2	GLU	A	601	10/10	0.95	0.23	33,39,40,41	0
3	IOD	C	603	1/1	0.98	0.06	78,78,78,78	0
3	IOD	A	604	1/1	0.99	0.10	69,69,69,69	0
3	IOD	A	605	1/1	0.99	0.07	92,92,92,92	0
3	IOD	B	601	1/1	0.99	0.12	57,57,57,57	0
3	IOD	B	603	1/1	0.99	0.15	51,51,51,51	0
3	IOD	C	601	1/1	0.99	0.12	62,62,62,62	0
3	IOD	A	602	1/1	0.99	0.13	53,53,53,53	0
3	IOD	B	602	1/1	1.00	0.08	84,84,84,84	0
3	IOD	C	602	1/1	1.00	0.14	42,42,42,42	0
3	IOD	A	603	1/1	1.00	0.12	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.