



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 03:11 am GMT

PDB ID : 4L17  
Title : GluA2-L483Y-A665C ligand-binding domain in complex with the antagonist DNQX  
Authors : Lau, A.Y.; Blachowicz, L.; Roux, B.  
Deposited on : 2013-06-02  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

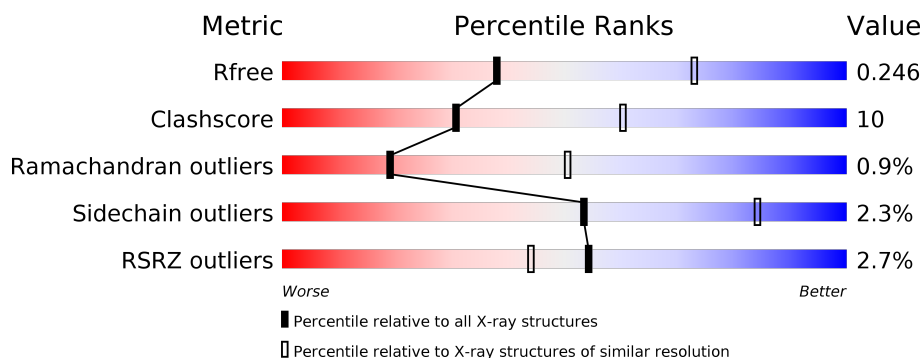
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 80%, yellow 18%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>10%</span> <span>80%</span> <span>18%</span> <span>..</span> </div> </div>
1	C	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 16%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>81%</span> <span>16%</span> <span>..</span> </div> </div>
1	E	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 77%, yellow 21%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>77%</span> <span>21%</span> <span>..</span> </div> </div>
1	G	263	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, green 62%, yellow 35%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>10%</span> <span>62%</span> <span>35%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8128 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2008	1281	330	382	15			
1	C	258	Total	C	N	O	S	0	0	0
			2001	1276	331	379	15			
1	E	259	Total	C	N	O	S	0	0	0
			1984	1268	326	375	15			
1	G	258	Total	C	N	O	S	0	0	0
			1911	1220	312	364	15			

There are 24 discrepancies between the modelled and reference sequences:

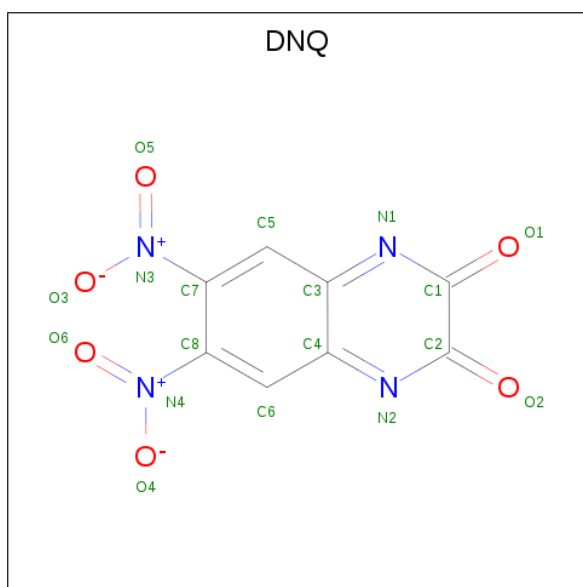
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P19491
A	2	ALA	-	EXPRESSION TAG	UNP P19491
A	94	TYR	LEU	ENGINEERED MUTATION	UNP P19491
A	118	GLY	-	LINKER	UNP P19491
A	119	THR	-	LINKER	UNP P19491
A	153	CYS	ALA	ENGINEERED MUTATION	UNP P19491
C	1	GLY	-	EXPRESSION TAG	UNP P19491
C	2	ALA	-	EXPRESSION TAG	UNP P19491
C	94	TYR	LEU	ENGINEERED MUTATION	UNP P19491
C	118	GLY	-	LINKER	UNP P19491
C	119	THR	-	LINKER	UNP P19491
C	153	CYS	ALA	ENGINEERED MUTATION	UNP P19491
E	1	GLY	-	EXPRESSION TAG	UNP P19491
E	2	ALA	-	EXPRESSION TAG	UNP P19491
E	94	TYR	LEU	ENGINEERED MUTATION	UNP P19491
E	118	GLY	-	LINKER	UNP P19491
E	119	THR	-	LINKER	UNP P19491
E	153	CYS	ALA	ENGINEERED MUTATION	UNP P19491
G	1	GLY	-	EXPRESSION TAG	UNP P19491
G	2	ALA	-	EXPRESSION TAG	UNP P19491
G	94	TYR	LEU	ENGINEERED MUTATION	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
G	118	GLY	-	LINKER	UNP P19491
G	119	THR	-	LINKER	UNP P19491
G	153	CYS	ALA	ENGINEERED MUTATION	UNP P19491

- Molecule 2 is 6,7-DINITROQUINOXALINE-2,3-DIONE (three-letter code: DNQ) (formula:  $C_8H_2N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	8	4	6		
2	C	1	Total	C	N	O	0	0
			18	8	4	6		
2	E	1	Total	C	N	O	0	0
			18	8	4	6		
2	G	1	Total	C	N	O	0	0
			18	8	4	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

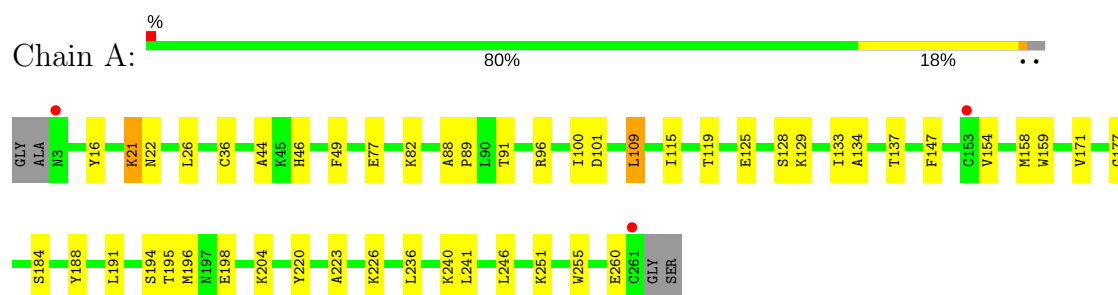
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	C	50	Total	O	0	0
			50	50		
4	E	24	Total	O	0	0
			24	24		
4	G	2	Total	O	0	0
			2	2		

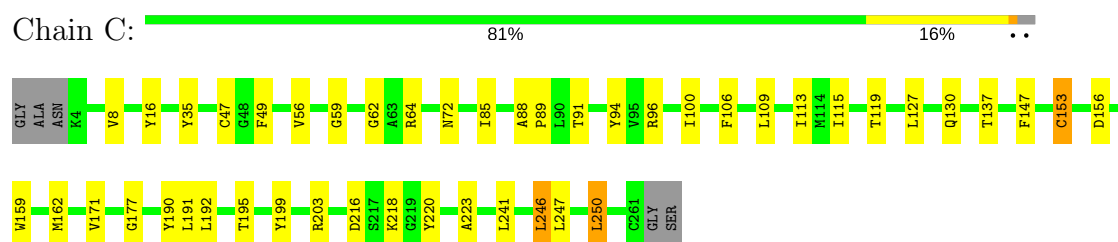
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

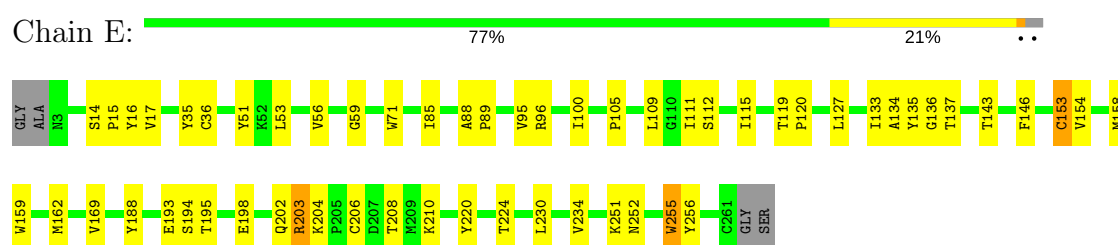
#### • Molecule 1: Glutamate receptor 2



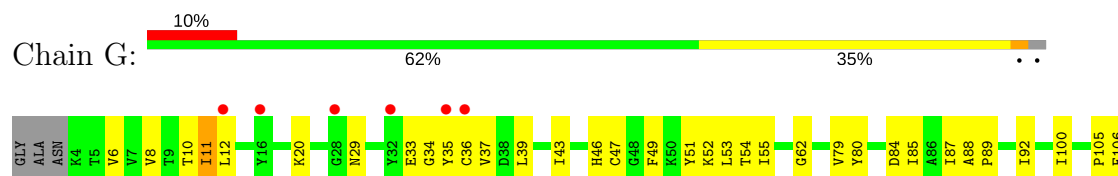
#### • Molecule 1: Glutamate receptor 2

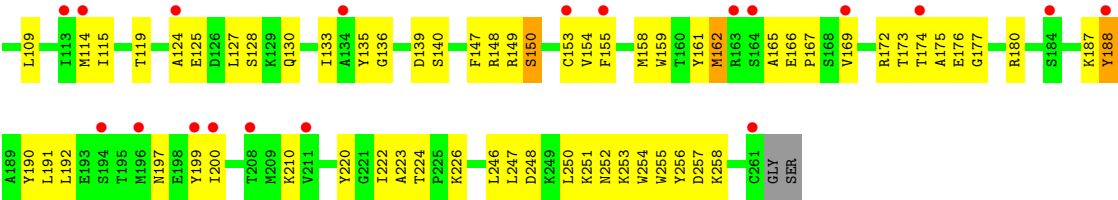


#### • Molecule 1: Glutamate receptor 2



#### • Molecule 1: Glutamate receptor 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.85Å 96.79Å 252.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.92 – 2.80 52.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (52.92-2.80) 95.4 (52.92-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.195 , 0.244 0.198 , 0.246	Depositor DCC
$R_{free}$ test set	1476 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DNQ, SO4

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	0.20	0/2045	0.35	0/2754
1	C	0.21	0/2038	0.35	0/2745
1	E	0.21	0/2021	0.35	0/2726
1	G	0.21	0/1948	0.35	0/2641
All	All	0.21	0/8052	0.35	0/10866

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	2008	0	2013	35	0
1	C	2001	0	2007	27	0
1	E	1984	0	1974	32	1
1	G	1911	0	1818	62	1
2	A	18	0	2	1	0
2	C	18	0	2	0	0
2	E	18	0	2	1	0
2	G	18	0	2	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	A	61	0	0	2	0
4	C	50	0	0	0	0
4	E	24	0	0	2	0
4	G	2	0	0	0	0
All	All	8128	0	7820	156	1

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 (156) 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:G:85:ILE:HD11	1:G:222:ILE:HG22	1.50	0.91
1:C:137:THR:HG22	1:C:191:LEU:HB2	1.55	0.88
1:A:21:LYS:H	1:A:21:LYS:HD3	1.36	0.87
1:E:115:ILE:HD12	1:E:119:THR:HB	1.58	0.84
1:G:85:ILE:HD13	1:G:224:THR:HG22	1.66	0.77
1:G:147:PHE:HB3	1:G:159:TRP:HB2	1.66	0.77
1:G:115:ILE:HD12	1:G:119:THR:HB	1.67	0.77
1:A:137:THR:HG22	1:A:191:LEU:HB2	1.68	0.75
1:E:252:ASN:HA	1:E:256:TYR:HD2	1.62	0.65
1:C:241:LEU:HD22	1:C:246:LEU:HD22	1.79	0.65
1:G:150:SER:OG	1:G:155:PHE:HB2	1.99	0.63
1:E:119:THR:HG23	1:E:133:ILE:HD13	1.82	0.62
1:G:33:GLU:HA	1:G:37:VAL:HG11	1.81	0.62
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.82	0.61
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.83	0.61
1:A:46:HIS:CD2	1:A:240:LYS:HZ3	2.20	0.60
1:G:35:TYR:HA	1:G:250:LEU:HD21	1.85	0.59
1:A:21:LYS:HG2	1:A:22:ASN:H	1.68	0.58
1:C:35:TYR:CE1	1:C:250:LEU:HB3	2.39	0.58
1:A:115:ILE:HD12	1:A:119:THR:HB	1.87	0.56
1:G:35:TYR:CD1	1:G:250:LEU:HD22	2.40	0.56
1:C:115:ILE:HD12	1:C:119:THR:HB	1.87	0.55
1:G:92:ILE:HD12	1:G:105:PRO:HG3	1.88	0.55
1:G:29:ASN:HD21	1:G:52:LYS:HA	1.72	0.55
1:E:194:SER:O	1:E:198:GLU:HG2	2.07	0.55
1:E:204:LYS:HA	1:E:206:CYS:N	2.21	0.55
1:A:251:LYS:O	1:A:255:TRP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:LEU:HD21	1:G:135:TYR:CG	2.42	0.55
1:G:187:LYS:O	1:G:188:TYR:HB2	2.07	0.55
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.89	0.54
1:G:11:ILE:H	1:G:11:ILE:HD12	1.72	0.54
1:E:127:LEU:HD11	1:E:135:TYR:HB3	1.88	0.54
1:C:137:THR:HG23	1:C:162:MET:HE1	1.89	0.53
1:G:149:ARG:O	1:G:150:SER:C	2.46	0.53
1:A:125:GLU:HG2	1:A:129:LYS:HZ2	1.73	0.52
1:G:199:TYR:HB2	1:G:255:TRP:NE1	2.25	0.52
1:C:127:LEU:HA	1:C:130:GLN:HE21	1.75	0.52
1:G:36:CYS:HB3	1:G:87:ILE:HG22	1.90	0.52
1:G:147:PHE:HD1	1:G:155:PHE:O	1.92	0.52
1:A:154:VAL:O	1:A:158:MET:HG3	2.09	0.52
1:C:100:ILE:HD12	1:C:223:ALA:HB1	1.91	0.51
1:E:51:TYR:HE2	1:E:53:LEU:HD11	1.75	0.51
1:G:197:ASN:HA	1:G:200:ILE:HG22	1.92	0.51
1:G:85:ILE:HD12	1:G:223:ALA:O	2.11	0.51
1:G:161:TYR:O	1:G:165:ALA:HB2	2.11	0.51
1:G:100:ILE:HA	1:G:226:LYS:HB2	1.93	0.51
1:A:171:VAL:HG11	1:A:177:GLY:HA2	1.93	0.51
1:G:124:ALA:O	1:G:154:VAL:HG11	2.10	0.51
1:A:21:LYS:H	1:A:21:LYS:CD	2.17	0.51
1:A:16:TYR:HB3	1:A:36:CYS:SG	2.51	0.51
1:G:250:LEU:HD23	1:G:254:TRP:CD1	2.47	0.50
1:G:34:GLY:O	1:G:37:VAL:HG12	2.11	0.50
1:A:100:ILE:HD12	1:A:223:ALA:HB1	1.93	0.50
1:G:154:VAL:O	1:G:158:MET:HG2	2.12	0.50
1:G:35:TYR:HD1	1:G:255:TRP:HZ3	1.58	0.50
1:G:177:GLY:HA3	1:G:190:TYR:CE2	2.47	0.50
1:E:111:ILE:HD13	1:E:143:THR:HG23	1.95	0.49
1:E:56:VAL:HG13	1:E:59:GLY:HA2	1.95	0.49
1:E:109:LEU:HB3	1:E:195:THR:HG23	1.94	0.49
1:A:241:LEU:HD22	1:A:246:LEU:HD13	1.95	0.49
1:G:130:GLN:OE1	1:G:133:ILE:HG12	2.13	0.48
1:A:21:LYS:HG2	1:A:22:ASN:N	2.27	0.48
1:G:253:LYS:HA	1:G:257:ASP:HB2	1.95	0.48
1:G:88:ALA:HB1	1:G:89:PRO:HD2	1.94	0.48
1:G:128:SER:HB2	1:G:158:MET:CE	2.43	0.48
1:E:251:LYS:O	1:E:255:TRP:HB2	2.14	0.48
1:A:134:ALA:O	1:A:188:TYR:HA	2.14	0.48
1:E:159:TRP:HA	1:E:162:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:TYR:HB3	1:E:36:CYS:SG	2.54	0.48
1:A:204:LYS:HG2	1:A:260:GLU:OE1	2.12	0.47
1:C:96:ARG:O	1:C:100:ILE:HG12	2.13	0.47
1:E:134:ALA:O	1:E:188:TYR:HA	2.13	0.47
1:G:51:TYR:HE2	1:G:53:LEU:HD11	1.79	0.47
1:A:128:SER:CB	1:A:154:VAL:HG13	2.45	0.47
1:E:16:TYR:HA	1:E:35:TYR:HB3	1.96	0.47
1:G:136:GLY:HA2	1:G:162:MET:SD	2.54	0.47
1:G:6:VAL:HG13	1:G:84:ASP:HB2	1.96	0.46
1:G:85:ILE:HG13	1:G:87:ILE:HD12	1.97	0.46
1:E:119:THR:HA	1:E:120:PRO:HD3	1.81	0.46
1:C:199:TYR:O	1:C:203:ARG:HG2	2.15	0.46
1:E:85:ILE:HG13	1:E:224:THR:HG22	1.97	0.46
1:A:204:LYS:HE2	1:A:260:GLU:HB3	1.98	0.45
1:G:35:TYR:HD1	1:G:255:TRP:CZ3	2.35	0.45
1:C:113:ILE:HG12	1:C:191:LEU:CD2	2.46	0.45
1:E:143:THR:HG22	4:E:424:HOH:O	2.17	0.45
1:E:203:ARG:HE	1:E:203:ARG:HA	1.80	0.45
1:A:91:THR:HG22	1:A:220:TYR:HE1	1.81	0.45
1:G:197:ASN:ND2	1:G:210:LYS:HB3	2.31	0.45
1:C:109:LEU:HB3	1:C:195:THR:HG23	1.99	0.45
1:G:85:ILE:HD11	1:G:222:ILE:CG2	2.36	0.45
1:A:128:SER:OG	1:A:154:VAL:HG13	2.17	0.45
1:C:113:ILE:HG12	1:C:191:LEU:HD23	1.98	0.45
1:E:154:VAL:O	1:E:158:MET:HG3	2.17	0.44
1:E:204:LYS:HA	1:E:206:CYS:H	1.81	0.44
1:A:194:SER:O	1:A:198:GLU:HG2	2.17	0.44
1:C:153:CYS:HA	1:C:156:ASP:HB3	1.99	0.44
1:G:246:LEU:O	1:G:250:LEU:HB2	2.17	0.44
1:C:190:TYR:CE2	1:C:192:LEU:HB3	2.52	0.44
1:C:216:ASP:OD2	1:C:218:LYS:HE3	2.18	0.44
1:A:101:ASP:OD2	1:A:226:LYS:HA	2.18	0.44
2:E:301:DNQ:O5	2:E:301:DNQ:O4	2.36	0.44
1:G:187:LYS:O	1:G:187:LYS:HG2	2.18	0.44
1:G:54:THR:C	1:G:55:ILE:HD12	2.38	0.44
1:C:16:TYR:HA	1:C:35:TYR:HB3	2.00	0.43
1:A:22:ASN:O	1:A:26:LEU:HG	2.18	0.43
1:C:147:PHE:HB3	1:C:159:TRP:HB2	2.00	0.43
1:E:143:THR:O	1:E:146:PHE:HB3	2.18	0.43
1:C:91:THR:HG22	1:C:220:TYR:HE1	1.84	0.43
1:G:174:THR:HG23	1:G:175:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:VAL:HA	1:G:180:ARG:HH12	1.84	0.43
1:A:196:MET:HB2	2:A:301:DNQ:O6	2.19	0.43
1:A:96:ARG:O	1:A:100:ILE:HG12	2.19	0.43
1:G:253:LYS:O	1:G:258:LYS:HG2	2.19	0.43
1:C:106:PHE:O	1:C:247:LEU:HD13	2.19	0.42
1:G:114:MET:HE2	1:G:190:TYR:HB3	2.00	0.42
1:G:166:GLU:HA	1:G:167:PRO:C	2.39	0.42
1:G:136:GLY:HA3	1:G:169:VAL:O	2.19	0.42
1:A:125:GLU:HG2	1:A:129:LYS:NZ	2.34	0.42
1:G:100:ILE:HD12	1:G:223:ALA:HB1	2.01	0.42
1:G:252:ASN:HA	1:G:256:TYR:HD2	1.85	0.42
1:C:91:THR:HG22	1:C:220:TYR:CE1	2.54	0.42
1:E:14:SER:HA	1:E:15:PRO:HA	1.85	0.42
1:G:174:THR:HG23	1:G:175:ALA:N	2.35	0.42
1:G:190:TYR:CD1	1:G:191:LEU:N	2.85	0.42
1:E:137:THR:HG21	4:E:424:HOH:O	2.20	0.41
1:E:71:TRP:CH2	1:E:95:VAL:HG12	2.55	0.41
1:G:109:LEU:HD13	1:G:220:TYR:OH	2.20	0.41
1:G:106:PHE:O	1:G:247:LEU:HD23	2.20	0.41
1:A:184:SER:HB2	4:A:442:HOH:O	2.19	0.41
1:E:105:PRO:HA	1:E:220:TYR:O	2.19	0.41
1:C:62:GLY:HA2	1:C:72:ASN:O	2.21	0.41
1:C:8:VAL:HG22	1:C:85:ILE:CG2	2.51	0.41
1:E:230:LEU:O	1:E:234:VAL:HG23	2.20	0.41
1:A:236:LEU:HB3	1:C:94:TYR:CE1	2.54	0.41
1:E:71:TRP:HH2	1:E:95:VAL:HG12	1.85	0.41
1:G:10:THR:HG22	1:G:54:THR:O	2.21	0.41
1:C:171:VAL:HG11	1:C:177:GLY:HA2	2.01	0.41
1:E:112:SER:CB	1:E:210:LYS:HE2	2.50	0.41
1:G:173:THR:OG1	1:G:176:GLU:HB2	2.21	0.41
1:A:109:LEU:HB3	1:A:195:THR:HG23	2.01	0.41
1:A:119:THR:HG23	1:A:133:ILE:HD13	2.03	0.41
1:C:47:CYS:HB2	1:C:49:PHE:CE2	2.56	0.41
1:E:96:ARG:O	1:E:100:ILE:HG12	2.20	0.41
1:G:199:TYR:HB2	1:G:255:TRP:CD1	2.56	0.41
1:G:39:LEU:O	1:G:43:ILE:HG13	2.21	0.41
1:A:147:PHE:HB3	1:A:159:TRP:HB2	2.02	0.41
1:C:56:VAL:HG13	1:C:59:GLY:HA2	2.03	0.41
1:G:36:CYS:SG	1:G:88:ALA:HA	2.61	0.41
1:G:47:CYS:HB2	1:G:49:PHE:CE2	2.55	0.40
1:A:91:THR:HG21	4:A:461:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:VAL:HG23	1:G:80:TYR:CD1	2.56	0.40
1:G:8:VAL:HG22	1:G:85:ILE:CG2	2.51	0.40
1:E:136:GLY:HA3	1:E:169:VAL:O	2.21	0.40
1:A:44:ALA:HA	1:A:49:PHE:CE2	2.56	0.40
1:A:77:GLU:HA	1:A:82:LYS:NZ	2.36	0.40
1:G:251:LYS:O	1:G:255:TRP:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:CYS:SG	1:G:153:CYS:CB[2_565]	2.18	0.02

## 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	257/263 (98%)	246 (96%)	11 (4%)	0	100	100
1	C	256/263 (97%)	246 (96%)	10 (4%)	0	100	100
1	E	257/263 (98%)	239 (93%)	18 (7%)	0	100	100
1	G	256/263 (97%)	227 (89%)	20 (8%)	9 (4%)	4	13
All	All	1026/1052 (98%)	958 (93%)	59 (6%)	9 (1%)	19	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	20	LYS
1	G	148	ARG
1	G	150	SER
1	G	139	ASP

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Mol	Chain	Res	Type
1	G	125	GLU
1	G	140	SER
1	G	172	ARG
1	G	188	TYR
1	G	62	GLY

### 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	214/220 (97%)	212 (99%)	2 (1%)	81	95
1	C	213/220 (97%)	209 (98%)	4 (2%)	60	87
1	E	208/220 (94%)	201 (97%)	7 (3%)	40	74
1	G	189/220 (86%)	183 (97%)	6 (3%)	42	76
All	All	824/880 (94%)	805 (98%)	19 (2%)	53	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	109	LEU
1	C	64	ARG
1	C	153	CYS
1	C	246	LEU
1	C	250	LEU
1	E	17	VAL
1	E	153	CYS
1	E	193	GLU
1	E	202	GLN
1	E	203	ARG
1	E	208	THR
1	E	255	TRP
1	G	11	ILE
1	G	12	LEU
1	G	46	HIS

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Mol	Chain	Res	Type
1	G	162	MET
1	G	192	LEU
1	G	248	ASP

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

Mol	Chain	Res	Type
1	G	197	ASN
1	G	214	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
2	DNQ	A	301	-	15,19,19	4.85	9 (60%)	12,28,28	1.27	2 (16%)
3	SO4	A	302	-	4,4,4	0.17	0	6,6,6	0.07	0
2	DNQ	C	301	-	15,19,19	4.83	9 (60%)	12,28,28	1.20	1 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	302	-	4,4,4	0.17	0	6,6,6	0.08	0
2	DNQ	E	301	-	15,19,19	4.84	9 (60%)	12,28,28	1.19	1 (8%)
3	SO4	E	302	-	4,4,4	0.15	0	6,6,6	0.07	0
2	DNQ	G	301	-	15,19,19	4.83	9 (60%)	12,28,28	1.22	1 (8%)

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	DNQ	A	301	-	-	0/4/20/20	0/2/2/2
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	DNQ	C	301	-	-	0/4/20/20	0/2/2/2
3	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	DNQ	E	301	-	-	0/4/20/20	0/2/2/2
3	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	DNQ	G	301	-	-	0/4/20/20	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	DNQ	C2-C1	-5.84	1.40	1.52
2	A	301	DNQ	C2-C1	-5.83	1.40	1.52
2	E	301	DNQ	C2-C1	-5.83	1.40	1.52
2	C	301	DNQ	C2-C1	-5.83	1.40	1.52
2	G	301	DNQ	C5-C3	2.74	1.43	1.40
2	E	301	DNQ	C5-C3	2.74	1.43	1.40
2	C	301	DNQ	C5-C3	2.78	1.43	1.40
2	A	301	DNQ	C5-C3	2.85	1.43	1.40
2	C	301	DNQ	C1-N1	3.26	1.44	1.38
2	E	301	DNQ	C1-N1	3.32	1.44	1.38
2	G	301	DNQ	C1-N1	3.34	1.44	1.38
2	A	301	DNQ	C1-N1	3.35	1.44	1.38
2	A	301	DNQ	C6-C4	4.21	1.45	1.40
2	C	301	DNQ	C6-C4	4.28	1.45	1.40
2	G	301	DNQ	C6-C4	4.30	1.45	1.40
2	E	301	DNQ	C6-C4	4.33	1.45	1.40
2	G	301	DNQ	O5-N3	4.82	1.31	1.22
2	A	301	DNQ	O5-N3	4.88	1.31	1.22
2	E	301	DNQ	O5-N3	4.88	1.31	1.22
2	C	301	DNQ	O5-N3	4.90	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	DNQ	O6-N4	5.20	1.32	1.22
2	C	301	DNQ	O6-N4	5.22	1.32	1.22
2	A	301	DNQ	O6-N4	5.24	1.32	1.22
2	G	301	DNQ	O6-N4	5.26	1.32	1.22
2	A	301	DNQ	C4-N2	7.77	1.44	1.33
2	E	301	DNQ	C4-N2	7.79	1.44	1.33
2	C	301	DNQ	C4-N2	7.81	1.44	1.33
2	G	301	DNQ	C4-N2	7.83	1.44	1.33
2	C	301	DNQ	O1-C1	8.86	1.38	1.24
2	G	301	DNQ	O2-C2	8.89	1.38	1.24
2	E	301	DNQ	O1-C1	8.90	1.38	1.24
2	G	301	DNQ	O1-C1	8.93	1.38	1.24
2	A	301	DNQ	O1-C1	8.99	1.38	1.24
2	E	301	DNQ	O2-C2	8.99	1.38	1.24
2	C	301	DNQ	O2-C2	9.00	1.38	1.24
2	A	301	DNQ	O2-C2	9.04	1.38	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DNQ	C4-N2-C2	2.05	120.06	116.90
2	E	301	DNQ	C6-C8-N4	2.30	119.14	116.05
2	C	301	DNQ	C6-C8-N4	2.33	119.17	116.05
2	G	301	DNQ	C6-C8-N4	2.49	119.39	116.05
2	A	301	DNQ	C6-C8-N4	2.49	119.39	116.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	DNQ	1	0
2	E	301	DNQ	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	259/263 (98%)	-0.30	3 (1%) 79 72	9, 28, 70, 124	0
1	C	258/263 (98%)	-0.34	0 100 100	11, 30, 68, 128	0
1	E	259/263 (98%)	-0.14	0 100 100	20, 47, 90, 115	0
1	G	258/263 (98%)	0.66	25 (9%) 8 4	54, 97, 139, 163	0
All	All	1034/1052 (98%)	-0.03	28 (2%) 54 44	9, 44, 122, 163	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	164	SER	5.1
1	G	184	SER	4.9
1	G	153	CYS	4.0
1	G	208	THR	3.8
1	G	114	MET	3.6
1	G	113	ILE	3.1
1	G	199	TYR	3.1
1	G	32	TYR	2.9
1	G	261	CYS	2.9
1	G	163	ARG	2.8
1	G	174	THR	2.8
1	A	3	ASN	2.8
1	A	261	CYS	2.7
1	G	211	VAL	2.6
1	G	188	TYR	2.6
1	G	35	TYR	2.5
1	G	194	SER	2.5
1	G	36	CYS	2.4
1	G	124	ALA	2.4
1	G	169	VAL	2.3
1	A	153	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	155	PHE	2.3
1	G	196	MET	2.3
1	G	134	ALA	2.3
1	G	12	LEU	2.1
1	G	28	GLY	2.1
1	G	16	TYR	2.1
1	G	200	ILE	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	A	302	5/5	0.89	0.25	105,109,112,114	0
3	SO4	C	302	5/5	0.90	0.19	75,86,89,94	0
3	SO4	E	302	5/5	0.90	0.20	100,104,107,109	0
2	DNQ	G	301	18/18	0.92	0.34	59,92,127,127	0
2	DNQ	E	301	18/18	0.94	0.25	20,40,78,82	0
2	DNQ	A	301	18/18	0.94	0.21	34,48,78,93	0
2	DNQ	C	301	18/18	0.95	0.22	27,40,90,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.