



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U94  
Title : Crystal structure of the GluK3 ligand binding domain complex with glutamate and zinc: P21212 form  
Authors : Kumar, J.; Mayer, M.L.  
Deposited on : 2011-10-17  
Resolution : 1.96 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

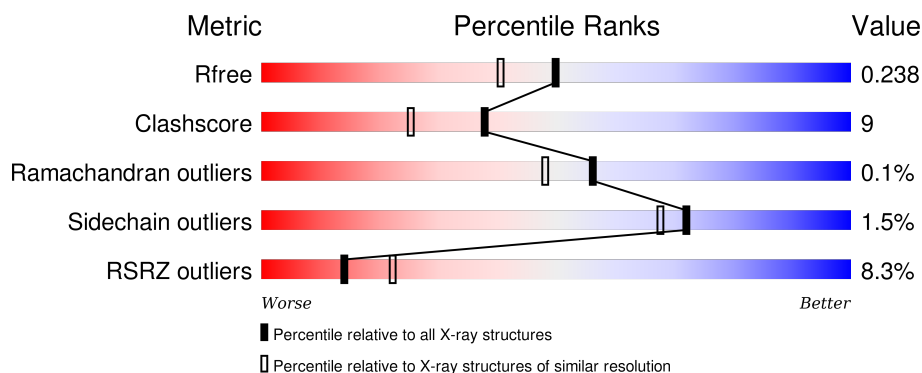
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	257	<div> <div>10%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	B	257	<div> <div>9%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	257	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	257	<div> <div>7%</div> <div>81%</div> <div>18%</div> <div>..</div> </div>

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	SO4	C	263	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16935 atoms, of which 8128 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, ionotropic kainate 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	H	N	O	S	0	0	0
			4048	1288	2030	337	381	12			
1	B	253	Total	C	H	N	O	S	0	0	0
			4034	1284	2024	335	379	12			
1	C	253	Total	C	H	N	O	S	1	0	0
			4034	1283	2023	336	380	12			
1	D	254	Total	C	H	N	O	S	0	0	0
			4045	1286	2028	337	382	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P42264
A	2	SER	-	EXPRESSION TAG	UNP P42264
A	117	GLY	-	LINKER	UNP P42264
A	118	THR	-	LINKER	UNP P42264
B	1	GLY	-	EXPRESSION TAG	UNP P42264
B	2	SER	-	EXPRESSION TAG	UNP P42264
B	117	GLY	-	LINKER	UNP P42264
B	118	THR	-	LINKER	UNP P42264
C	1	GLY	-	EXPRESSION TAG	UNP P42264
C	2	SER	-	EXPRESSION TAG	UNP P42264
C	117	GLY	-	LINKER	UNP P42264
C	118	THR	-	LINKER	UNP P42264
D	1	GLY	-	EXPRESSION TAG	UNP P42264
D	2	SER	-	EXPRESSION TAG	UNP P42264
D	117	GLY	-	LINKER	UNP P42264
D	118	THR	-	LINKER	UNP P42264

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			18	5	8	1	4		
2	B	1	Total	C	H	N	O	0	0
			15	5	5	1	4		
2	C	1	Total	C	H	N	O	0	0
			15	5	5	1	4		
2	D	1	Total	C	H	N	O	0	0
			15	5	5	1	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	3	Total	Zn	0	0
			3	3		
3	D	4	Total	Zn	0	0
			4	4		
3	C	4	Total	Zn	0	0
			4	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

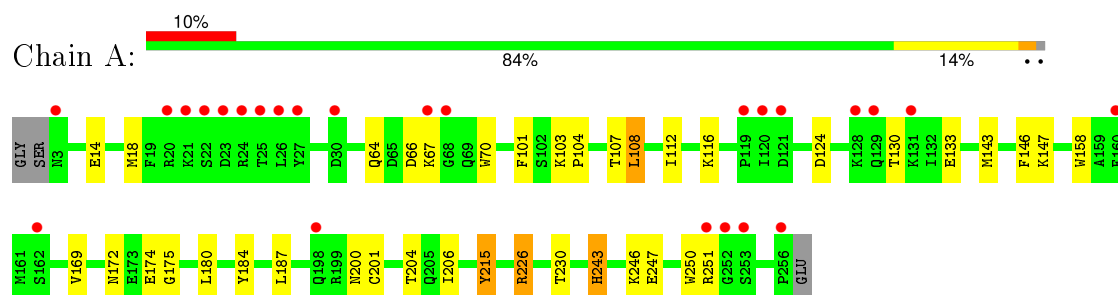
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total	O	0	0
			191	191		
6	B	130	Total	O	0	0
			130	130		
6	C	204	Total	O	0	0
			204	204		
6	D	162	Total	O	0	0
			162	162		

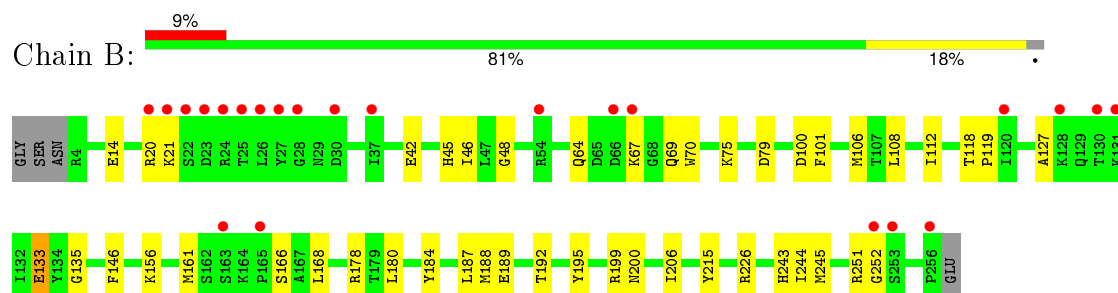
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

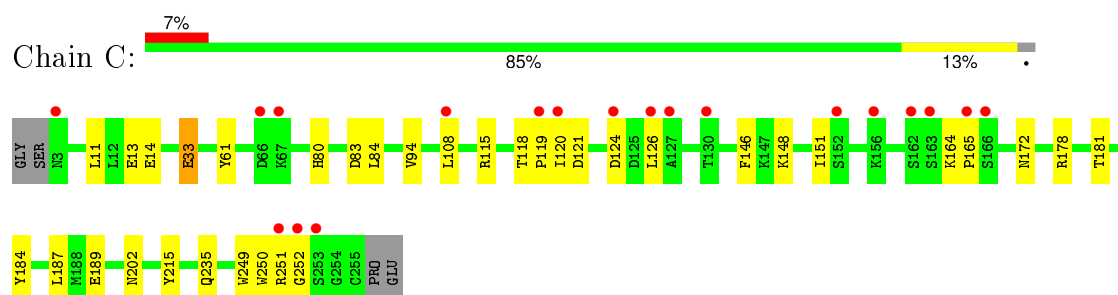
- Molecule 1: Glutamate receptor, ionotropic kainate 3



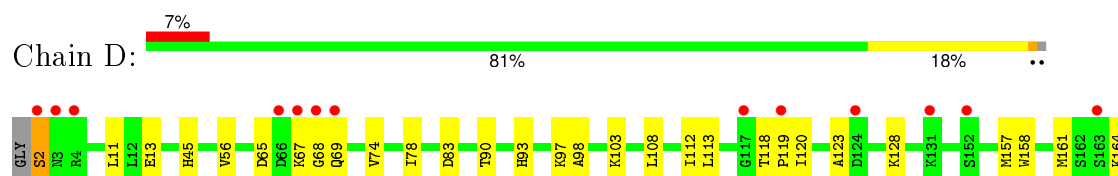
- Molecule 1: Glutamate receptor, ionotropic kainate 3

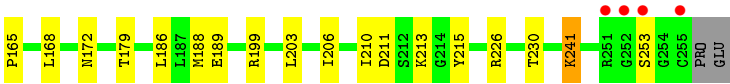


- Molecule 1: Glutamate receptor, ionotropic kainate 3



- Molecule 1: Glutamate receptor, ionotropic kainate 3







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.16 Å   111.37 Å   129.85 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	38.94 – 1.96 39.43 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.94-1.96) 97.5 (39.43-1.96)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 1.97 Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.193   ,   0.247 0.184   ,   0.238	Depositor DCC
$R_{free}$ test set	4529 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtrriage
Anisotropy	0.544	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40   ,   50.4	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	1 of 90933 reflections (0.001%)	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.05 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1227e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, SO4, CL

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	0.62	2/2057 (0.1%)	0.70	1/2770 (0.0%)
1	B	0.54	0/2049	0.68	0/2759
1	C	0.64	0/2049	0.70	0/2758
1	D	0.55	0/2055	0.68	0/2766
All	All	0.59	2/8210 (0.0%)	0.69	1/11053 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ARG	CG-CD	-5.68	1.37	1.51
1	A	215	TYR	CD1-CE1	5.48	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	CA-CB-CG	-5.35	101.64	113.40

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	2018	2030	2034	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2010	2024	2028	51	0
1	C	2011	2023	2027	27	2
1	D	2017	2028	2032	43	0
2	A	10	8	5	0	0
2	B	10	5	5	0	0
2	C	10	5	5	0	0
2	D	10	5	5	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
5	D	1	0	0	0	0
6	A	191	0	0	3	0
6	B	130	0	0	3	0
6	C	204	0	0	7	0
6	D	162	0	0	4	0
All	All	8807	8128	8141	150	2

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 9.

All (150) 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:143:MET:SD	6:A:349:HOH:O	2.11	1.09
1:B:108:LEU:HD22	1:B:215:TYR:CZ	2.01	0.95
1:B:251:ARG:HB3	1:B:252:GLY:CA	1.99	0.93
1:C:172:ASN:OD1	6:C:655:HOH:O	1.92	0.86
1:B:251:ARG:HB3	1:B:252:GLY:HA2	1.57	0.85
1:B:188:MET:HE2	1:B:192:THR:HB	1.58	0.85
1:B:251:ARG:CB	1:B:252:GLY:CA	2.56	0.82
1:D:128:LYS:O	6:D:561:HOH:O	2.00	0.79
1:D:123:ALA:O	1:D:157:MET:HE3	1.83	0.78
1:B:251:ARG:CB	1:B:252:GLY:HA3	2.14	0.77
1:D:172:ASN:OD1	6:D:654:HOH:O	2.02	0.77
1:B:108:LEU:CD2	1:B:215:TYR:CZ	2.68	0.76
1:B:14:GLU:OE1	6:B:481:HOH:O	2.08	0.72
1:A:64:GLN:OE1	6:A:641:HOH:O	2.07	0.70
1:B:45:HIS:ND1	6:B:387:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HB2	1:D:188:MET:HE3	1.75	0.67
1:C:235:GLN:OE1	6:C:482:HOH:O	2.12	0.67
1:B:188:MET:CE	1:B:192:THR:HG22	2.25	0.67
1:B:188:MET:HE2	1:B:192:THR:CB	2.24	0.67
1:D:108:LEU:HD22	1:D:215:TYR:CZ	2.30	0.66
1:B:45:HIS:NE2	4:B:261:SO4:O2	2.28	0.66
1:B:108:LEU:CD2	1:B:215:TYR:CE1	2.79	0.66
1:B:251:ARG:HB2	1:B:252:GLY:HA3	1.76	0.66
1:B:106:MET:HE1	1:B:215:TYR:CE2	2.31	0.65
1:A:147:LYS:HD3	1:A:158:TRP:CZ2	2.31	0.65
1:A:108:LEU:HD22	1:A:215:TYR:CZ	2.32	0.64
1:B:188:MET:CE	1:B:192:THR:CG2	2.76	0.63
1:D:113:LEU:HD22	1:D:188:MET:HE1	1.80	0.63
1:D:78:ILE:HD11	1:D:98:ALA:HB1	1.81	0.62
1:B:166:SER:O	1:B:178:ARG:NH2	2.32	0.62
1:B:106:MET:HE1	1:B:215:TYR:CD2	2.36	0.61
1:D:241:LYS:NZ	6:D:499:HOH:O	2.33	0.61
1:A:169:VAL:HG11	1:A:175:GLY:N	2.17	0.60
1:C:33:GLU:HG3	1:C:249:TRP:CH2	2.37	0.60
1:C:108:LEU:HD22	1:C:215:TYR:CZ	2.37	0.60
1:B:101:PHE:O	1:B:226:ARG:HD2	2.02	0.60
1:D:113:LEU:CD2	1:D:188:MET:HE1	2.32	0.59
1:C:120:ILE:HD12	1:C:126:LEU:HD11	1.84	0.59
1:A:169:VAL:HG13	1:A:174:GLU:HB3	1.85	0.58
1:A:243:HIS:O	1:A:247:GLU:HG2	2.03	0.58
1:D:78:ILE:CD1	1:D:98:ALA:HB1	2.34	0.58
1:A:130:THR:HG22	1:A:130:THR:O	2.04	0.58
1:D:118:THR:CG2	1:D:119:PRO:HD2	2.34	0.57
1:B:195:TYR:O	1:B:199:ARG:HG2	2.04	0.57
1:B:106:MET:CE	1:B:215:TYR:CE2	2.87	0.57
1:A:108:LEU:HD22	1:A:215:TYR:CE1	2.40	0.56
1:B:161:MET:CE	1:B:168:LEU:HD21	2.34	0.56
1:C:251:ARG:HG2	1:C:252:GLY:HA3	1.88	0.56
1:B:135:GLY:HA2	1:B:161:MET:HG2	1.88	0.56
1:A:14:GLU:HG3	1:A:18:MET:SD	2.46	0.55
1:D:2:SER:HA	1:D:83:ASP:OD1	2.06	0.55
1:C:120:ILE:O	6:C:327:HOH:O	2.18	0.55
1:D:158:TRP:CE3	1:D:161:MET:HE2	2.41	0.55
1:C:115:ARG:HG2	6:C:673:HOH:O	2.06	0.55
1:A:107:THR:HG22	1:A:108:LEU:N	2.22	0.55
1:D:226:ARG:O	1:D:226:ARG:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HD11	1:C:61:TYR:CZ	2.42	0.54
1:C:94:VAL:HG11	1:C:148:LYS:NZ	2.22	0.54
1:C:164:LYS:HD2	1:C:165:PRO:HD2	1.89	0.54
1:A:101:PHE:O	1:A:226:ARG:HD2	2.07	0.54
1:D:186:LEU:HD23	1:D:188:MET:HE2	1.88	0.54
6:C:362:HOH:O	1:D:45:HIS:HD2	1.91	0.54
1:A:103:LYS:HD2	1:A:230:THR:HG23	1.89	0.53
1:D:67:LYS:HD3	1:D:69:GLN:N	2.23	0.53
1:D:112:ILE:HB	1:D:206:ILE:HB	1.90	0.53
1:D:74:VAL:O	1:D:78:ILE:HG12	2.09	0.53
1:D:118:THR:HG22	1:D:119:PRO:HD2	1.90	0.53
1:A:130:THR:O	1:A:130:THR:CG2	2.57	0.53
1:B:108:LEU:HD21	1:B:215:TYR:CE1	2.43	0.53
1:D:241:LYS:HE3	6:D:579:HOH:O	2.08	0.53
1:A:172:ASN:OD1	6:A:334:HOH:O	2.19	0.52
1:A:247:GLU:O	1:A:251:ARG:HB2	2.09	0.52
1:B:42:GLU:OE1	1:B:42:GLU:HA	2.09	0.52
1:B:106:MET:CE	1:B:215:TYR:HE2	2.23	0.51
1:D:93:HIS:CD2	1:D:97:LYS:HE2	2.45	0.51
1:A:246:LYS:HD2	1:A:250:TRP:CE3	2.45	0.51
1:D:120:ILE:HG22	1:D:206:ILE:HG21	1.92	0.51
1:D:90:THR:CG2	1:D:213:LYS:HD3	2.41	0.51
1:B:188:MET:HE3	1:B:192:THR:CG2	2.40	0.51
1:A:116:LYS:HG2	1:A:204:THR:HB	1.93	0.51
1:A:112:ILE:HB	1:A:206:ILE:HB	1.93	0.51
1:C:108:LEU:HD13	1:C:189:GLU:HB3	1.92	0.51
1:B:195:TYR:CE1	1:B:199:ARG:NH2	2.79	0.51
1:B:112:ILE:HB	1:B:206:ILE:HB	1.93	0.51
1:D:103:LYS:HG3	1:D:230:THR:HG23	1.93	0.50
1:D:211:ASP:OD2	1:D:213:LYS:HE3	2.12	0.50
1:C:118:THR:HB	1:C:119:PRO:CD	2.42	0.50
1:C:13:GLU:OE2	1:C:172:ASN:HB2	2.12	0.49
1:A:146:PHE:CE2	1:A:187:LEU:HD13	2.48	0.49
1:D:93:HIS:NE2	1:D:97:LYS:CE	2.76	0.48
1:D:186:LEU:HD23	1:D:188:MET:CE	2.44	0.48
1:D:93:HIS:CD2	1:D:97:LYS:CE	2.96	0.48
1:C:151:ILE:HD12	1:C:151:ILE:N	2.27	0.48
1:C:14:GLU:OE2	6:C:379:HOH:O	2.20	0.47
1:B:42:GLU:O	1:B:46:ILE:HG12	2.14	0.47
1:B:67:LYS:HE2	1:B:69:GLN:HG2	1.96	0.47
1:B:161:MET:HE2	1:B:168:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ALA:O	1:B:156:LYS:HD3	2.14	0.47
1:C:83:ASP:O	1:C:84:LEU:HD23	2.15	0.46
1:B:75:LYS:HE3	1:B:79:ASP:OD2	2.16	0.46
1:A:64:GLN:HG3	1:A:70:TRP:CE2	2.51	0.46
1:D:123:ALA:O	1:D:157:MET:CE	2.59	0.45
1:B:188:MET:HE2	1:B:192:THR:CG2	2.46	0.45
1:C:94:VAL:HG11	1:C:148:LYS:HZ1	1.82	0.44
1:D:67:LYS:HD3	1:D:68:GLY:N	2.32	0.44
1:D:113:LEU:CB	1:D:188:MET:HE3	2.46	0.44
1:D:108:LEU:HD13	1:D:189:GLU:HB3	1.99	0.44
1:B:244:ILE:HG22	1:B:245:MET:N	2.32	0.44
1:B:133:GLU:OE2	1:B:178:ARG:NH1	2.51	0.44
1:B:118:THR:HB	1:B:119:PRO:HD2	2.00	0.44
1:C:124:ASP:CB	6:C:302:HOH:O	2.65	0.44
1:B:178:ARG:NH2	6:B:425:HOH:O	2.51	0.43
1:C:33:GLU:HG3	1:C:249:TRP:HH2	1.79	0.43
1:A:169:VAL:CG1	1:A:174:GLU:HB3	2.47	0.43
1:B:100:ASP:HB3	1:B:226:ARG:HD3	1.99	0.43
1:B:161:MET:HE3	1:B:168:LEU:CD2	2.48	0.43
1:B:133:GLU:HG2	1:B:184:TYR:HD2	1.83	0.43
1:C:118:THR:HB	1:C:119:PRO:HD2	2.00	0.43
1:C:164:LYS:HA	1:C:165:PRO:HD2	1.86	0.43
1:C:178:ARG:HG2	1:C:184:TYR:CD1	2.54	0.43
1:B:146:PHE:CE2	1:B:187:LEU:HD13	2.54	0.43
1:D:164:LYS:HA	1:D:165:PRO:HD3	1.90	0.43
1:A:133:GLU:O	1:A:184:TYR:HA	2.19	0.43
1:A:180:LEU:HD21	1:A:200:ASN:HD21	1.84	0.43
1:B:161:MET:HE3	1:B:168:LEU:HD21	2.00	0.43
1:A:66:ASP:OD1	1:A:67:LYS:N	2.52	0.43
1:C:250:TRP:O	1:C:251:ARG:HB2	2.19	0.42
1:B:20:ARG:HG2	1:B:21:LYS:N	2.34	0.42
1:D:11:LEU:HB3	1:D:56:VAL:HG12	2.01	0.42
1:D:179:THR:HG21	1:D:203:LEU:HD22	2.00	0.42
1:B:108:LEU:HD13	1:B:189:GLU:HB3	2.00	0.42
1:B:180:LEU:HD21	1:B:200:ASN:ND2	2.34	0.42
1:B:106:MET:CE	1:B:215:TYR:CD2	3.03	0.42
1:A:180:LEU:HD21	1:A:200:ASN:ND2	2.34	0.42
1:A:226:ARG:HG2	1:A:226:ARG:O	2.13	0.42
1:D:13:GLU:OE2	1:D:172:ASN:HB2	2.20	0.42
1:D:161:MET:HE3	1:D:168:LEU:HD21	2.01	0.42
1:B:64:GLN:HG3	1:B:70:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HE2	1:A:201:CYS:O	2.20	0.41
1:A:104:PRO:HA	1:A:215:TYR:O	2.19	0.41
1:C:146:PHE:CE2	1:C:187:LEU:HD13	2.56	0.41
1:D:103:LYS:HG3	1:D:230:THR:CG2	2.50	0.41
1:B:251:ARG:HB3	1:B:252:GLY:HA3	1.80	0.41
1:C:251:ARG:HA	1:C:252:GLY:HA3	1.93	0.41
1:B:133:GLU:CG	1:B:184:TYR:HD2	2.33	0.41
1:D:90:THR:HG23	1:D:213:LYS:HD3	2.03	0.41
1:C:178:ARG:HG2	1:C:184:TYR:CG	2.55	0.41
1:D:210:ILE:O	1:D:210:ILE:CG2	2.68	0.40
1:D:210:ILE:O	1:D:210:ILE:HG22	2.21	0.40
1:D:65:ASP:O	1:D:67:LYS:O	2.38	0.40

All (2) 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:C:80:HIS:CE1	1:C:80:HIS:HE1[2_555]	1.06	0.54
1:C:80:HIS:CE1	1:C:80:HIS:CE1[2_555]	2.11	0.09

## 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	252/257 (98%)	249 (99%)	3 (1%)	0	100	100
1	B	251/257 (98%)	241 (96%)	9 (4%)	1 (0%)	39	27
1	C	251/257 (98%)	244 (97%)	7 (3%)	0	100	100
1	D	252/257 (98%)	240 (95%)	12 (5%)	0	100	100
All	All	1006/1028 (98%)	974 (97%)	31 (3%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	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	219/221 (99%)	216 (99%)	3 (1%)	74	70
1	B	218/221 (99%)	216 (99%)	2 (1%)	84	83
1	C	218/221 (99%)	214 (98%)	4 (2%)	66	60
1	D	219/221 (99%)	215 (98%)	4 (2%)	66	60
All	All	874/884 (99%)	861 (98%)	13 (2%)	72	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	124	ASP
1	A	243	HIS
1	B	133	GLU
1	B	243	HIS
1	C	33	GLU
1	C	121	ASP
1	C	181	THR
1	C	202	ASN
1	D	2	SER
1	D	199	ARG
1	D	241	LYS
1	D	253	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	45	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLU	A	258	-	3,9,9	0.35	0	2,11,11	0.19	0
2	GLU	B	258	-	3,9,9	0.32	0	2,11,11	0.35	0
4	SO4	B	261	-	4,4,4	0.14	0	6,6,6	0.24	0
2	GLU	C	258	-	3,9,9	0.27	0	2,11,11	0.11	0
4	SO4	C	263	-	4,4,4	0.19	0	6,6,6	0.07	0
2	GLU	D	258	-	3,9,9	0.32	0	2,11,11	0.18	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
2	GLU	A	258	-	-	0/3/9/9	0/0/0/0
2	GLU	B	258	-	-	0/3/9/9	0/0/0/0
4	SO4	B	261	-	-	0/0/0/0	0/0/0/0
2	GLU	C	258	-	-	0/3/9/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	263	-	-	0/0/0/0	0/0/0/0
2	GLU	D	258	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	261	SO4	1	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

### 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	254/257 (98%)	0.46	25 (9%) 10 15	16, 34, 67, 87	0
1	B	253/257 (98%)	0.66	23 (9%) 11 18	22, 39, 74, 112	0
1	C	253/257 (98%)	0.59	19 (7%) 17 26	15, 28, 59, 121	0
1	D	254/257 (98%)	0.49	17 (6%) 21 31	19, 35, 76, 109	0
All	All	1014/1028 (98%)	0.55	84 (8%) 14 22	15, 34, 72, 121	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	GLY	16.4
1	B	27	TYR	9.3
1	B	26	LEU	9.2
1	B	25	THR	7.8
1	C	3	ASN	6.6
1	D	3	ASN	6.4
1	A	25	THR	6.4
1	C	253	SER	6.4
1	A	27	TYR	6.3
1	B	24	ARG	6.2
1	D	253	SER	5.7
1	A	24	ARG	5.7
1	A	26	LEU	5.5
1	C	120	ILE	5.2
1	A	129	GLN	5.0
1	B	21	LYS	4.9
1	D	66	ASP	4.8
1	C	119	PRO	4.7
1	B	22	SER	4.6
1	A	21	LYS	4.5
1	B	67	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	256	PRO	4.1
1	B	23	ASP	4.0
1	A	20	ARG	3.9
1	C	251	ARG	3.8
1	D	252	GLY	3.8
1	B	28	GLY	3.8
1	D	117	GLY	3.7
1	A	251	ARG	3.6
1	D	2	SER	3.6
1	B	253	SER	3.5
1	C	67	LYS	3.5
1	B	163	SER	3.5
1	C	152	SER	3.4
1	A	23	ASP	3.4
1	B	130	THR	3.3
1	A	253	SER	3.2
1	B	252	GLY	3.2
1	A	3	ASN	3.2
1	C	130	THR	3.1
1	C	66	ASP	3.0
1	C	165	PRO	2.9
1	B	30	ASP	2.9
1	D	152	SER	2.9
1	B	20	ARG	2.8
1	A	252	GLY	2.8
1	D	68	GLY	2.8
1	D	255	CYS	2.7
1	C	163	SER	2.7
1	B	54	ARG	2.6
1	A	160	PHE	2.6
1	C	124	ASP	2.6
1	D	119	PRO	2.6
1	A	131	LYS	2.5
1	D	4	ARG	2.5
1	D	124	ASP	2.5
1	B	165	PRO	2.5
1	D	67	LYS	2.5
1	A	68	GLY	2.5
1	C	108	LEU	2.4
1	B	128	LYS	2.4
1	A	256	PRO	2.4
1	C	162	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	131	LYS	2.4
1	C	156	LYS	2.4
1	D	131	LYS	2.4
1	B	66	ASP	2.4
1	A	67	LYS	2.3
1	A	30	ASP	2.3
1	A	128	LYS	2.3
1	A	120	ILE	2.3
1	A	22	SER	2.2
1	A	198	GLN	2.2
1	A	162	SER	2.2
1	D	69	GLN	2.2
1	A	119	PRO	2.2
1	C	127	ALA	2.1
1	D	163	SER	2.1
1	C	126	LEU	2.1
1	B	37	ILE	2.1
1	B	120	ILE	2.1
1	C	166	SER	2.1
1	D	251	ARG	2.0
1	A	121	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	263	5/5	0.91	0.24	2.22	102,108,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLU	D	258	10/10	0.97	0.17	1.79	22,32,41,44	0
3	ZN	C	261	1/1	0.87	0.15	1.54	33,33,33,33	1
2	GLU	B	258	10/10	0.96	0.12	0.73	21,27,34,34	0
2	GLU	C	258	10/10	0.98	0.15	0.42	17,20,23,26	0
3	ZN	D	261	1/1	0.95	0.11	-0.15	31,31,31,31	1
2	GLU	A	258	10/10	0.96	0.11	-0.32	18,22,26,27	0
3	ZN	B	260	1/1	0.98	0.10	-0.78	50,50,50,50	1
3	ZN	A	259	1/1	0.98	0.09	-1.84	33,33,33,33	0
3	ZN	B	259	1/1	0.95	0.10	-3.24	35,35,35,35	0
3	ZN	D	260	1/1	0.87	0.13	-	36,36,36,36	1
3	ZN	D	262	1/1	0.99	0.07	-	47,47,47,47	1
3	ZN	C	260	1/1	0.91	0.12	-	37,37,37,37	1
3	ZN	A	261	1/1	0.94	0.10	-	52,52,52,52	1
3	ZN	C	259	1/1	0.99	0.15	-	18,18,18,18	1
3	ZN	D	259	1/1	0.99	0.13	-	20,20,20,20	0
3	ZN	C	262	1/1	0.98	0.07	-	32,32,32,32	1
5	CL	D	263	1/1	0.94	0.09	-	69,69,69,69	0
3	ZN	A	260	1/1	0.94	0.11	-	58,58,58,58	0
4	SO4	B	261	5/5	0.90	0.14	-	80,90,91,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.