



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:48 AM GMT

PDB ID : 2I3V  
Title : Measurement of conformational changes accompanying desensitization in an ionotropic glutamate receptor: Structure of G725C mutant  
Authors : Armstrong, N.; Jasti, J.; Beich-Frandsen, M.; Gouaux, E.  
Deposited on : 2006-08-21  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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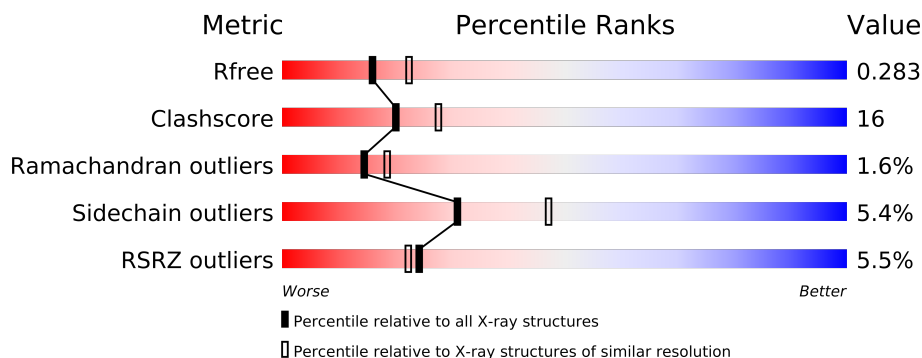
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	C	259	
1	D	259	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8367 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			2029	1291	338	385	15			
1	B	259	Total	C	N	O	S	0	0	0
			2029	1291	338	385	15			
1	C	258	Total	C	N	O	S	0	0	0
			2021	1287	336	383	15			
1	D	258	Total	C	N	O	S	0	0	0
			2021	1287	336	383	15			

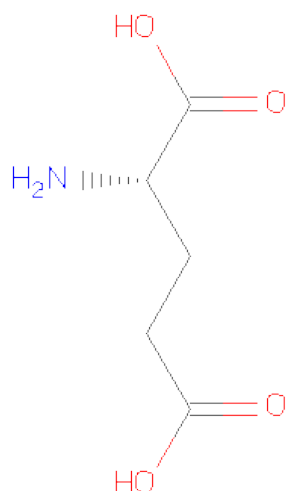
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	PRO	-	LINKER	UNP P19491
A	121	ILE	-	LINKER	UNP P19491
B	120	PRO	-	LINKER	UNP P19491
B	121	ILE	-	LINKER	UNP P19491
C	120	PRO	-	LINKER	UNP P19491
C	121	ILE	-	LINKER	UNP P19491
D	120	PRO	-	LINKER	UNP P19491
D	121	ILE	-	LINKER	UNP P19491

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	2	Total	Zn	0	0
			2	2		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).

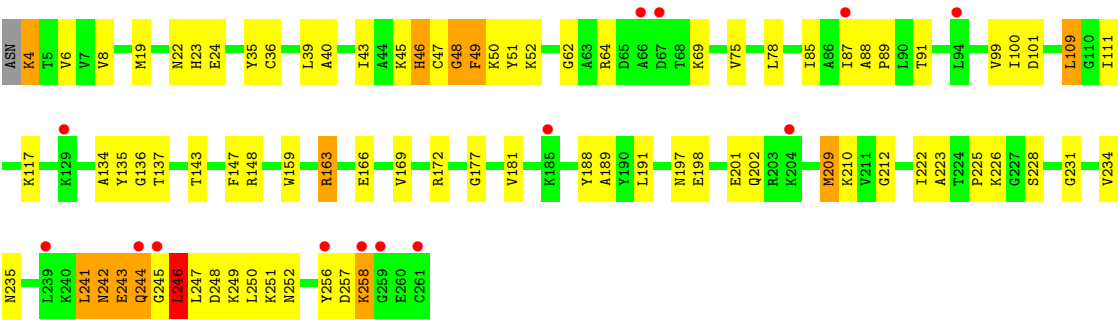


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total	O	0	0
			86	86		
4	B	52	Total	O	0	0
			52	52		
4	C	38	Total	O	0	0
			38	38		
4	D	44	Total	O	0	0
			44	44		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.19Å 106.29Å 192.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 28.89 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.3 (28.89-2.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.281 0.236 , 0.283	Depositor DCC
$R_{free}$ test set	2337 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49915 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/2065	0.64	0/2776
1	B	0.37	0/2065	0.61	0/2776
1	C	0.32	0/2057	0.57	0/2765
1	D	0.36	0/2057	0.77	4/2765 (0.1%)
All	All	0.36	0/8244	0.65	4/11082 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	LEU	N-CA-C	15.15	151.91	111.00
1	D	242	ASN	N-CA-CB	-13.86	85.65	110.60
1	D	241	LEU	CB-CA-C	-9.88	91.43	110.20
1	D	258	LYS	N-CA-C	-5.72	95.55	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2029	0	2057	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2029	0	2057	66	0
1	C	2021	0	2051	84	0
1	D	2021	0	2051	71	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	3	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
4	A	86	0	0	5	0
4	B	52	0	0	2	0
4	C	38	0	0	1	0
4	D	44	0	0	2	0
All	All	8367	0	8236	260	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (260) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:172:ARG:HG3	1:B:173:THR:HG23	1.42	1.00
1:D:242:ASN:HA	1:D:247:LEU:H	1.27	0.99
1:D:43:ILE:O	1:D:47:CYS:HB3	1.66	0.94
1:A:241:LEU:HD22	1:A:246:LEU:HD23	1.47	0.94
1:C:43:ILE:O	1:C:47:CYS:HB3	1.70	0.90
1:C:249:LYS:HA	1:C:252:ASN:HD22	1.33	0.89
1:D:244:GLN:HE21	1:D:244:GLN:H	1.33	0.76
1:A:202:GLN:HG2	1:A:257:ASP:CG	2.07	0.75
1:D:242:ASN:HB3	1:D:243:GLU:OE2	1.86	0.75
1:D:241:LEU:O	1:D:245:GLY:HA3	1.87	0.75
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.69	0.74
1:B:121:ILE:HD13	1:B:127:LEU:CD2	2.17	0.74
1:C:253:LYS:NZ	1:C:258:LYS:HE2	2.03	0.73
1:C:36:CYS:SG	1:C:88:ALA:HA	2.28	0.72
1:C:240:LYS:HG3	1:C:244:GLN:HE21	1.55	0.72
1:C:40:ALA:O	1:C:43:ILE:HG22	1.90	0.71
1:D:242:ASN:HA	1:D:247:LEU:N	2.05	0.71
1:D:244:GLN:N	1:D:244:GLN:HE21	1.89	0.70
1:D:88:ALA:HB1	1:D:89:PRO:HD2	1.72	0.69
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.73	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:130:GLN:HE22	1:C:133:ILE:H	1.39	0.69
1:A:128:SER:O	1:A:157:LYS:HE3	1.92	0.69
1:D:198:GLU:O	1:D:202:GLN:HG2	1.94	0.68
1:D:212:GLY:HA3	4:D:442:HOH:O	1.93	0.68
1:D:225:PRO:HG2	1:D:228:SER:HB2	1.75	0.68
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.75	0.67
1:C:10:THR:HG23	1:C:11:ILE:N	2.09	0.67
1:D:23:HIS:CE1	1:D:24:GLU:HG2	2.30	0.66
1:B:115:ILE:HD12	1:B:119:THR:HB	1.76	0.66
1:B:256:TYR:O	1:B:257:ASP:HB3	1.96	0.66
1:D:137:THR:HG22	1:D:191:LEU:HB2	1.78	0.65
1:B:68:THR:HG22	1:B:70:ILE:H	1.61	0.64
1:A:172:ARG:HH21	1:A:172:ARG:HG3	1.62	0.64
1:C:179:ALA:O	1:C:183:LYS:HD3	1.97	0.64
1:C:10:THR:OG1	1:C:88:ALA:HB2	1.98	0.63
1:D:258:LYS:C	1:D:258:LYS:HD3	2.19	0.63
1:C:50:LYS:HD3	1:C:50:LYS:N	2.14	0.62
1:C:21:LYS:HG3	1:C:22:ASN:OD1	1.99	0.62
1:C:234:VAL:O	1:C:238:VAL:HG23	1.98	0.62
1:D:243:GLU:CD	1:D:243:GLU:H	2.03	0.62
1:B:121:ILE:HD13	1:B:127:LEU:HD23	1.80	0.62
1:B:4:LYS:HE3	1:B:4:LYS:HA	1.81	0.61
1:A:244:GLN:HE21	1:A:244:GLN:HA	1.66	0.61
1:C:196:MET:HE1	4:C:404:HOH:O	1.99	0.61
1:C:130:GLN:HE22	1:C:133:ILE:HB	1.66	0.61
1:D:242:ASN:CG	1:D:247:LEU:HB2	2.21	0.60
1:C:25:MET:HG2	1:C:25:MET:O	2.01	0.60
1:A:139:ASP:O	1:A:144:LYS:HD2	2.02	0.60
1:B:88:ALA:HB1	1:B:89:PRO:HD2	1.83	0.60
1:C:130:GLN:NE2	1:C:133:ILE:H	1.98	0.60
1:C:246:LEU:HA	1:C:249:LYS:HD2	1.82	0.60
1:B:64:ARG:NH2	1:B:69:LYS:HE2	2.17	0.60
1:B:101:ASP:OD2	1:B:226:LYS:HA	2.02	0.59
1:D:99:VAL:O	1:D:226:LYS:HD3	2.03	0.58
1:C:240:LYS:HG3	1:C:244:GLN:NE2	2.16	0.58
1:A:184:SER:HB2	4:A:480:HOH:O	2.03	0.58
1:B:121:ILE:HD13	1:B:127:LEU:HD21	1.85	0.57
1:A:240:LYS:O	1:A:244:GLN:HG2	2.04	0.57
1:C:109:LEU:HD22	1:C:109:LEU:C	2.24	0.57
1:B:68:THR:CG2	1:B:70:ILE:H	2.17	0.57
1:D:4:LYS:O	1:D:50:LYS:HB2	2.04	0.57
1:C:134:ALA:O	1:C:188:TYR:HA	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:137:THR:HG22	1:C:191:LEU:HB2	1.87	0.57
1:D:49:PHE:C	1:D:49:PHE:CD1	2.79	0.56
1:C:251:LYS:HG3	1:C:255:TRP:CE3	2.40	0.56
1:B:180:ARG:HA	1:B:183:LYS:HE2	1.87	0.56
1:C:249:LYS:NZ	1:C:249:LYS:HB2	2.20	0.56
1:A:149:ARG:NH2	1:B:243:GLU:O	2.39	0.56
1:C:93:THR:O	1:C:97:GLU:HG3	2.06	0.56
1:C:253:LYS:HZ1	1:C:258:LYS:HE2	1.69	0.56
1:D:39:LEU:O	1:D:43:ILE:HG13	2.06	0.56
1:D:23:HIS:ND1	1:D:24:GLU:N	2.54	0.55
1:A:95:VAL:HG13	4:A:408:HOH:O	2.05	0.55
1:D:258:LYS:O	1:D:258:LYS:HD3	2.07	0.55
1:B:180:ARG:HG2	1:B:188:TYR:CD2	2.42	0.55
1:B:149:ARG:O	1:B:149:ARG:HG3	2.07	0.55
1:D:242:ASN:HB2	1:D:247:LEU:HD12	1.89	0.55
1:C:230:LEU:O	1:C:234:VAL:HG22	2.08	0.54
1:D:109:LEU:HD22	1:D:109:LEU:C	2.27	0.54
1:D:163:ARG:HG2	1:D:163:ARG:NH1	2.22	0.54
1:D:45:LYS:HG2	1:D:46:HIS:HD2	1.73	0.53
1:C:246:LEU:O	1:C:246:LEU:HD23	2.08	0.53
1:C:147:PHE:CZ	1:C:191:LEU:HD23	2.43	0.53
1:D:242:ASN:CB	1:D:247:LEU:HB2	2.39	0.53
1:B:4:LYS:CE	1:B:5:THR:N	2.72	0.53
1:D:177:GLY:O	1:D:181:VAL:HG23	2.09	0.53
1:C:199:TYR:CZ	1:C:203:ARG:HD2	2.43	0.53
1:A:251:LYS:HD2	1:A:255:TRP:CE3	2.44	0.53
1:A:202:GLN:HG3	4:A:474:HOH:O	2.09	0.53
1:B:120:PRO:O	1:B:121:ILE:HG13	2.09	0.53
1:C:41:ALA:O	1:C:45:LYS:HG2	2.08	0.53
1:B:240:LYS:O	1:B:244:GLN:HG3	2.09	0.53
1:A:171:VAL:HG11	1:A:177:GLY:HA2	1.91	0.53
1:D:201:GLU:OE1	1:D:210:LYS:N	2.42	0.52
1:C:100:ILE:HD12	1:C:223:ALA:HB1	1.91	0.52
1:A:137:THR:HG22	1:A:191:LEU:HB2	1.91	0.52
1:B:237:ALA:O	1:B:241:LEU:HG	2.10	0.52
1:D:23:HIS:ND1	1:D:24:GLU:HG2	2.25	0.52
1:A:225:PRO:HD2	1:A:228:SER:HB2	1.92	0.52
1:C:5:THR:HG22	1:C:6:VAL:H	1.75	0.52
1:A:192:LEU:HD23	1:A:192:LEU:H	1.75	0.52
1:B:86:ALA:HB3	1:B:223:ALA:HB3	1.91	0.52
1:A:203:ARG:HD3	4:A:457:HOH:O	2.08	0.52
1:D:134:ALA:O	1:D:188:TYR:HA	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:45:LYS:C	1:D:47:CYS:H	2.13	0.51
1:A:121:ILE:HD12	1:A:127:LEU:HD23	1.92	0.51
1:D:85:ILE:HG13	1:D:223:ALA:O	2.09	0.51
1:D:163:ARG:HH11	1:D:163:ARG:HG2	1.74	0.51
1:C:139:ASP:O	1:C:144:LYS:HE3	2.11	0.51
1:C:237:ALA:O	1:C:241:LEU:HG	2.10	0.51
1:C:10:THR:HG23	1:C:11:ILE:H	1.73	0.51
1:C:215:LEU:HD12	1:C:215:LEU:N	2.26	0.51
1:B:8:VAL:HG22	1:B:85:ILE:CG2	2.41	0.51
1:D:8:VAL:HG23	1:D:51:TYR:HB2	1.93	0.50
1:A:202:GLN:HG2	1:A:257:ASP:OD2	2.11	0.50
1:B:36:CYS:SG	1:B:88:ALA:HA	2.52	0.50
1:A:109:LEU:HD22	1:A:109:LEU:C	2.32	0.50
1:B:109:LEU:C	1:B:109:LEU:HD22	2.33	0.49
1:C:258:LYS:O	1:C:260:GLU:HG3	2.12	0.49
1:D:136:GLY:HA3	1:D:169:VAL:O	2.12	0.49
1:B:121:ILE:HD12	1:B:133:ILE:HD12	1.94	0.49
1:C:5:THR:HG22	1:C:6:VAL:N	2.27	0.49
1:C:139:ASP:N	1:C:171:VAL:O	2.42	0.49
1:C:80:TYR:O	1:C:82:LYS:HG2	2.12	0.49
1:D:246:LEU:O	1:D:250:LEU:HB2	2.13	0.49
1:D:43:ILE:CD1	1:D:222:ILE:HD13	2.43	0.49
1:C:130:GLN:NE2	1:C:133:ILE:HB	2.27	0.49
1:B:4:LYS:HE2	1:B:5:THR:N	2.27	0.49
1:C:129:LYS:HD3	1:C:157:LYS:HZ3	1.78	0.49
1:A:230:LEU:O	1:A:234:VAL:HG13	2.12	0.49
1:D:49:PHE:C	1:D:49:PHE:HD1	2.16	0.49
1:B:135:TYR:HA	1:B:189:ALA:O	2.13	0.49
1:C:40:ALA:C	1:C:43:ILE:HG22	2.33	0.48
1:D:241:LEU:O	1:D:246:LEU:N	2.43	0.48
1:A:180:ARG:HG2	1:A:188:TYR:CD2	2.49	0.48
1:C:40:ALA:HA	1:C:43:ILE:HG22	1.95	0.48
1:A:196:MET:O	1:A:200:ILE:HG12	2.13	0.48
1:A:22:ASN:HB3	1:A:25:MET:CG	2.44	0.48
1:A:204:LYS:HG2	1:A:260:GLU:HG2	1.94	0.48
1:A:174:THR:O	1:A:178:VAL:HG23	2.13	0.48
1:C:130:GLN:HE22	1:C:133:ILE:N	2.09	0.48
1:A:20:LYS:HD2	1:A:30:GLU:O	2.14	0.48
1:D:100:ILE:N	1:D:226:LYS:HE2	2.29	0.48
1:B:3:ASN:N	1:B:3:ASN:HD22	2.12	0.47
1:C:91:THR:HG1	3:C:403:GLU:N	2.12	0.47
1:D:244:GLN:N	1:D:244:GLN:NE2	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:241:LEU:HB3	1:B:246:LEU:HD23	1.96	0.47
1:D:252:ASN:HD22	1:D:256:TYR:HE2	1.61	0.47
1:B:193:GLU:OE1	3:B:402:GLU:HG2	2.15	0.47
1:C:32:TYR:CE1	1:C:55:ILE:HD11	2.49	0.47
1:B:4:LYS:CE	1:B:5:THR:H	2.27	0.47
1:B:91:THR:HG1	3:B:402:GLU:N	2.12	0.47
1:C:106:PHE:CD1	1:C:106:PHE:C	2.87	0.47
1:C:71:TRP:CE3	1:C:75:VAL:HG11	2.49	0.47
1:B:149:ARG:CG	1:B:149:ARG:O	2.62	0.47
1:B:241:LEU:HD13	1:B:246:LEU:CD2	2.44	0.47
1:B:4:LYS:HD3	1:B:5:THR:O	2.15	0.47
1:D:64:ARG:NH1	1:D:69:LYS:HD2	2.28	0.47
1:A:75:VAL:O	1:A:79:VAL:HG23	2.15	0.47
1:A:201:GLU:HG3	1:A:209:MET:HA	1.97	0.47
1:B:192:LEU:HD23	1:B:192:LEU:N	2.30	0.47
1:C:105:PRO:HA	1:C:220:TYR:O	2.15	0.47
1:B:107:MET:CE	1:B:251:LYS:HD2	2.45	0.47
1:B:174:THR:O	1:B:178:VAL:HG23	2.15	0.47
1:B:256:TYR:O	1:B:257:ASP:CB	2.61	0.46
1:C:191:LEU:HD12	1:C:191:LEU:N	2.30	0.46
1:B:68:THR:CG2	1:B:70:ILE:HB	2.46	0.46
1:B:135:TYR:HB3	1:B:189:ALA:HB3	1.97	0.46
1:B:192:LEU:H	1:B:192:LEU:HD23	1.81	0.46
1:B:107:MET:HE2	4:B:407:HOH:O	2.16	0.46
1:B:258:LYS:O	1:B:260:GLU:N	2.48	0.46
1:B:21:LYS:HG3	1:B:22:ASN:N	2.30	0.46
1:B:132:GLU:H	1:B:132:GLU:HG3	1.50	0.46
1:D:243:GLU:CD	1:D:243:GLU:N	2.68	0.45
1:D:48:GLY:O	1:D:49:PHE:HB3	2.17	0.45
1:C:58:ASP:OD2	1:C:73:GLY:HA2	2.17	0.45
1:B:99:VAL:HG23	1:B:100:ILE:HG23	1.98	0.45
1:D:43:ILE:CD1	1:D:222:ILE:CD1	2.95	0.45
1:D:101:ASP:O	1:D:223:ALA:HA	2.16	0.45
1:C:151:LYS:HD3	1:C:151:LYS:HA	1.72	0.45
1:C:139:ASP:HB2	1:C:172:ARG:HA	1.98	0.45
1:A:22:ASN:HB3	1:A:25:MET:SD	2.57	0.45
1:D:40:ALA:HA	1:D:87:ILE:HD13	1.99	0.45
1:C:130:GLN:HE22	1:C:133:ILE:CB	2.28	0.45
1:D:248:ASP:O	1:D:251:LYS:HB3	2.17	0.44
1:B:50:LYS:N	1:B:50:LYS:HD2	2.32	0.44
1:C:16:TYR:CG	1:C:89:PRO:HD3	2.53	0.44
1:B:56:VAL:HG23	1:B:77:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:128:SER:HB3	1:C:158:MET:CG	2.47	0.44
1:C:128:SER:HB3	1:C:158:MET:HG2	1.98	0.44
1:A:88:ALA:HB1	1:A:89:PRO:CD	2.44	0.44
1:D:197:ASN:ND2	1:D:210:LYS:HG3	2.32	0.44
1:D:99:VAL:HG23	1:D:100:ILE:HG23	2.00	0.44
1:B:241:LEU:HD22	1:B:246:LEU:HD22	2.00	0.44
1:C:24:GLU:O	1:C:26:LEU:N	2.51	0.44
1:C:20:LYS:HD2	1:C:30:GLU:O	2.18	0.44
1:D:35:TYR:CE2	1:D:250:LEU:HB3	2.52	0.44
1:C:135:TYR:HA	1:C:189:ALA:O	2.18	0.44
1:C:236:LEU:O	1:C:240:LYS:HB2	2.18	0.43
1:B:259:GLY:O	1:B:260:GLU:C	2.57	0.43
1:C:24:GLU:C	1:C:26:LEU:H	2.22	0.43
1:A:207:ASP:OD1	1:A:208:THR:HG23	2.18	0.43
1:C:166:GLU:HA	1:C:167:PRO:C	2.39	0.43
1:C:62:GLY:HA2	1:C:72:ASN:O	2.17	0.43
1:D:148:ARG:HG3	1:D:159:TRP:CZ2	2.52	0.43
1:C:32:TYR:HE1	1:C:55:ILE:HD11	1.84	0.43
1:A:232:ASN:O	1:A:236:LEU:HD23	2.17	0.43
1:A:95:VAL:HG22	4:A:408:HOH:O	2.18	0.43
1:B:30:GLU:OE1	1:D:172:ARG:NE	2.51	0.43
1:B:3:ASN:O	1:B:4:LYS:CB	2.66	0.43
1:A:244:GLN:NE2	1:A:244:GLN:HA	2.31	0.43
1:B:134:ALA:O	1:B:188:TYR:HA	2.19	0.43
1:D:252:ASN:HA	1:D:256:TYR:CD2	2.54	0.43
1:B:121:ILE:CD1	1:B:133:ILE:HD12	2.49	0.43
1:B:256:TYR:HA	4:B:434:HOH:O	2.19	0.42
1:B:22:ASN:OD1	1:B:26:LEU:HD11	2.18	0.42
1:A:100:ILE:HD12	1:A:223:ALA:HB1	2.02	0.42
1:D:43:ILE:HD11	1:D:222:ILE:CD1	2.50	0.42
1:D:117:LYS:HE3	1:D:209:MET:HG2	2.01	0.42
1:D:36:CYS:SG	1:D:88:ALA:HA	2.59	0.42
1:B:113:ILE:HG12	1:B:191:LEU:CD2	2.49	0.42
1:C:104:LYS:HB2	1:C:239:LEU:HD21	2.00	0.42
1:C:129:LYS:HA	1:C:129:LYS:HD3	1.85	0.42
1:D:91:THR:HG1	3:D:404:GLU:N	2.17	0.42
1:C:14:SER:HA	1:C:15:PRO:HA	1.87	0.42
1:C:50:LYS:N	1:C:50:LYS:CD	2.79	0.42
1:C:99:VAL:HG23	1:C:100:ILE:HG23	2.02	0.42
1:C:147:PHE:HZ	1:C:191:LEU:HD23	1.82	0.42
1:B:142:SER:N	3:B:402:GLU:O	2.49	0.42
1:C:8:VAL:HG22	1:C:85:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:192:LEU:HD23	1:A:192:LEU:N	2.33	0.42
1:C:119:THR:HA	1:C:120:PRO:HD3	1.89	0.41
1:C:119:THR:CG2	1:C:133:ILE:HD13	2.50	0.41
1:D:135:TYR:HB3	1:D:189:ALA:HB3	2.02	0.41
1:C:86:ALA:HB3	1:C:223:ALA:HB3	2.02	0.41
1:D:45:LYS:O	1:D:47:CYS:N	2.48	0.41
1:D:49:PHE:HE1	1:D:51:TYR:HB3	1.85	0.41
1:A:166:GLU:HA	1:A:167:PRO:C	2.39	0.41
1:D:231:GLY:O	1:D:234:VAL:HG22	2.20	0.41
1:D:6:VAL:O	1:D:51:TYR:HA	2.20	0.41
1:C:148:ARG:HH11	1:C:148:ARG:HG3	1.86	0.41
1:D:135:TYR:HA	1:D:189:ALA:O	2.20	0.41
1:B:46:HIS:CE1	1:D:166:GLU:OE2	2.74	0.41
1:A:136:GLY:HA3	1:A:169:VAL:O	2.20	0.41
1:B:4:LYS:HE2	1:B:5:THR:H	1.85	0.41
1:D:117:LYS:HE2	4:D:428:HOH:O	2.20	0.41
1:C:192:LEU:HD23	1:C:192:LEU:H	1.85	0.41
1:D:111:ILE:HD13	1:D:143:THR:HG23	2.03	0.41
1:B:105:PRO:HA	1:B:220:TYR:O	2.20	0.41
1:C:249:LYS:HA	1:C:252:ASN:ND2	2.16	0.41
1:A:172:ARG:HB2	1:A:176:GLU:OE1	2.21	0.41
1:B:109:LEU:HD23	1:B:193:GLU:HG2	2.03	0.41
1:C:29:ASN:HD22	1:C:29:ASN:N	2.18	0.41
1:B:258:LYS:O	1:B:259:GLY:C	2.59	0.41
1:D:62:GLY:HA3	1:D:75:VAL:CG2	2.51	0.40
1:D:147:PHE:HB3	1:D:159:TRP:HB2	2.04	0.40
1:C:104:LYS:HB3	1:C:104:LYS:HE3	1.97	0.40
1:A:109:LEU:N	1:A:109:LEU:HD13	2.37	0.40
1:C:116:LYS:O	1:C:117:LYS:C	2.60	0.40
1:B:119:THR:CG2	1:B:120:PRO:HD2	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/259 (99%)	241 (94%)	16 (6%)	0	100	100
1	B	257/259 (99%)	235 (91%)	16 (6%)	6 (2%)	10	10
1	C	256/259 (99%)	224 (88%)	27 (10%)	5 (2%)	11	13
1	D	256/259 (99%)	229 (90%)	22 (9%)	5 (2%)	11	13
All	All	1026/1036 (99%)	929 (90%)	81 (8%)	16 (2%)	14	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	GLU
1	D	243	GLU
1	B	228	SER
1	B	257	ASP
1	B	259	GLY
1	C	25	MET
1	C	139	ASP
1	D	48	GLY
1	D	246	LEU
1	D	257	ASP
1	C	20	LYS
1	D	46	HIS
1	B	4	LYS
1	C	140	SER
1	C	46	HIS
1	B	231	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	219/219 (100%)	212 (97%)	7 (3%)	51	72
1	B	219/219 (100%)	206 (94%)	13 (6%)	28	42
1	C	218/219 (100%)	204 (94%)	14 (6%)	25	37
1	D	218/219 (100%)	205 (94%)	13 (6%)	27	41
All	All	874/876 (100%)	827 (95%)	47 (5%)	31	47



All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	78	LEU
1	A	109	LEU
1	A	163	ARG
1	A	172	ARG
1	A	234	VAL
1	A	235	ASN
1	B	3	ASN
1	B	4	LYS
1	B	19	MET
1	B	50	LYS
1	B	53	LEU
1	B	68	THR
1	B	97	GLU
1	B	109	LEU
1	B	132	GLU
1	B	172	ARG
1	B	215	LEU
1	B	226	LYS
1	B	250	LEU
1	C	21	LYS
1	C	22	ASN
1	C	23	HIS
1	C	49	PHE
1	C	50	LYS
1	C	109	LEU
1	C	129	LYS
1	C	130	GLN
1	C	140	SER
1	C	149	ARG
1	C	226	LYS
1	C	242	ASN
1	C	246	LEU
1	C	249	LYS
1	D	4	LYS
1	D	19	MET
1	D	22	ASN
1	D	49	PHE
1	D	52	LYS
1	D	78	LEU
1	D	109	LEU
1	D	163	ARG

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Mol	Chain	Res	Type
1	D	209	MET
1	D	235	ASN
1	D	244	GLN
1	D	246	LEU
1	D	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	232	ASN
1	A	244	GLN
1	B	202	GLN
1	C	29	ASN
1	C	130	GLN
1	C	242	ASN
1	C	244	GLN
1	C	252	ASN
1	D	46	HIS
1	D	202	GLN
1	D	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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$
3	GLU	A	401	-	9,9,9	0.84	0	11,11,11	0.90	0
3	GLU	B	402	-	9,9,9	0.81	0	11,11,11	0.96	1 (9%)
3	GLU	C	403	-	9,9,9	0.77	0	11,11,11	0.84	0
3	GLU	D	404	-	9,9,9	0.87	0	11,11,11	0.65	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	GLU	A	401	-	-	0/9/9/9	0/0/0/0
3	GLU	B	402	-	-	0/9/9/9	0/0/0/0
3	GLU	C	403	-	-	0/9/9/9	0/0/0/0
3	GLU	D	404	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	GLU	C-CA-N	2.15	112.92	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	259/259 (100%)	0.15	7 (2%) 52 49	28, 42, 64, 78	0
1	B	259/259 (100%)	0.29	7 (2%) 52 49	30, 51, 75, 87	0
1	C	258/259 (99%)	0.65	29 (11%) 6 5	43, 69, 99, 100	0
1	D	258/259 (99%)	0.39	14 (5%) 25 23	41, 58, 82, 96	0
All	All	1034/1036 (99%)	0.37	57 (5%) 24 22	28, 55, 88, 100	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	TYR	5.6
1	C	261	CYS	4.8
1	B	3	ASN	4.7
1	C	25	MET	4.5
1	C	246	LEU	4.4
1	C	257	ASP	4.3
1	C	26	LEU	4.3
1	C	4	LYS	4.1
1	D	245	GLY	4.1
1	C	259	GLY	4.0
1	D	66	ALA	4.0
1	C	24	GLU	3.9
1	C	21	LYS	3.9
1	C	22	ASN	3.9
1	D	67	ASP	3.9
1	D	261	CYS	3.8
1	A	25	MET	3.6
1	D	256	TYR	3.6
1	C	202	GLN	3.5
1	C	50	LYS	3.5
1	A	3	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	129	LYS	3.4
1	C	87	ILE	3.4
1	C	258	LYS	3.3
1	C	81	GLY	3.3
1	C	131	THR	3.1
1	A	24	GLU	3.0
1	C	20	LYS	3.0
1	C	31	ARG	2.9
1	B	25	MET	2.9
1	D	244	GLN	2.9
1	B	24	GLU	2.9
1	B	258	LYS	2.8
1	C	36	CYS	2.7
1	D	239	LEU	2.7
1	C	27	GLU	2.7
1	D	87	ILE	2.6
1	D	258	LYS	2.6
1	C	89	PRO	2.6
1	D	259	GLY	2.5
1	A	27	GLU	2.4
1	C	5	THR	2.4
1	A	22	ASN	2.4
1	C	129	LYS	2.4
1	C	32	TYR	2.4
1	B	259	GLY	2.3
1	C	260	GLU	2.3
1	B	90	LEU	2.2
1	D	94	LEU	2.2
1	D	185	LYS	2.2
1	A	192	LEU	2.2
1	C	49	PHE	2.1
1	C	28	GLY	2.1
1	D	204	LYS	2.1
1	A	149	ARG	2.1
1	C	23	HIS	2.1
1	B	141	GLY	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GLU	D	404	10/10	0.23	1.16	44,45,49,49	0
3	GLU	B	402	10/10	0.26	0.86	41,44,45,45	0
3	GLU	A	401	10/10	0.21	0.10	24,26,27,29	0
2	ZN	C	306	1/1	0.16	-0.44	62,62,62,62	0
3	GLU	C	403	10/10	0.15	-0.61	59,59,61,61	0
2	ZN	B	305	1/1	0.14	-0.71	80,80,80,80	0
2	ZN	A	302	1/1	0.03	-1.57	91,91,91,91	0
2	ZN	B	303	1/1	0.07	-2.27	77,77,77,77	0
2	ZN	D	307	1/1	0.13	-2.91	90,90,90,90	0
2	ZN	A	301	1/1	0.08	-4.26	69,69,69,69	0
2	ZN	B	304	1/1	0.09	-	93,93,93,93	0

### 6.5 Other polymers

There are no such residues in this entry.