



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:55 AM EST

PDB ID : 3M3K
Title : Ligand binding domain (S1S2) of GluA3 (flop)
Authors : Ahmed, A.H.; Ptak, C.P.; Oswald, R.E.
Deposited on : 2010-03-09
Resolution : 1.79 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 : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

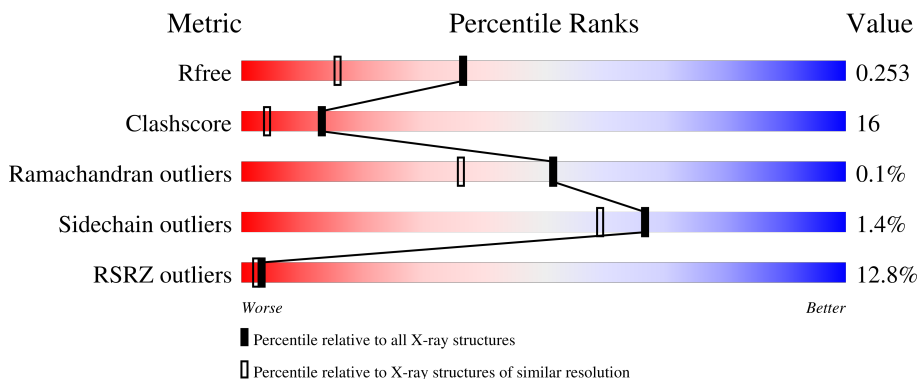
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	258	
1	C	258	
1	E	258	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6930 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.

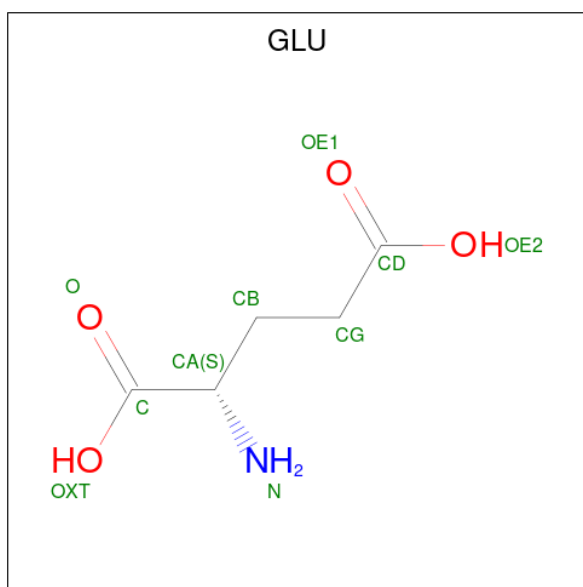
- Molecule 1 is a protein called Glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2033	1298	340	384	11	0	0	0
1	C	258	2033	1298	340	384	11	0	0	0
1	E	258	2029	1296	339	383	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	GLY	-	linker	UNP P19492
A	119	THR	-	linker	UNP P19492
C	118	GLY	-	linker	UNP P19492
C	119	THR	-	linker	UNP P19492
E	118	GLY	-	linker	UNP P19492
E	119	THR	-	linker	UNP P19492

- 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
2	C	1	10	5	1	4	0	0
2	E	1	10	5	1	4	0	0

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

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

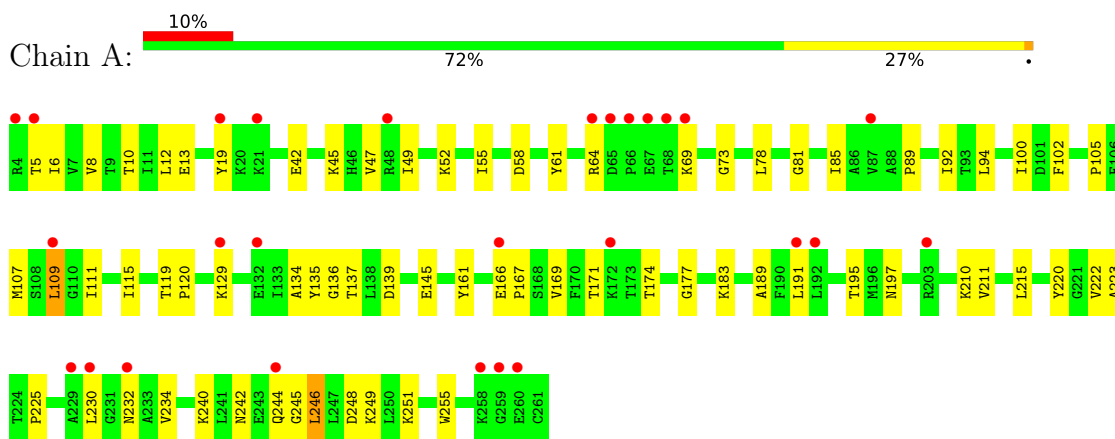
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	266	266	266	0	0
4	C	258	258	258	0	0
4	E	277	277	277	0	0

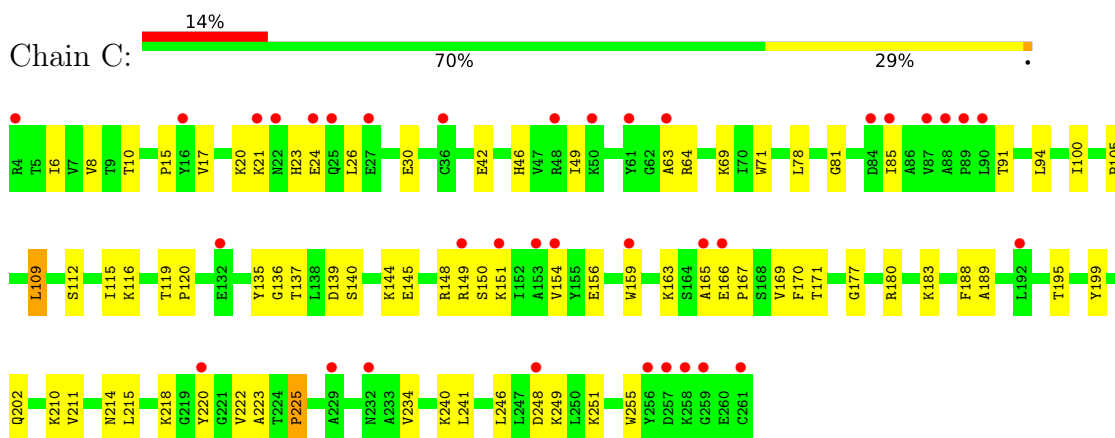
3 Residue-property plots [i](#)

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.

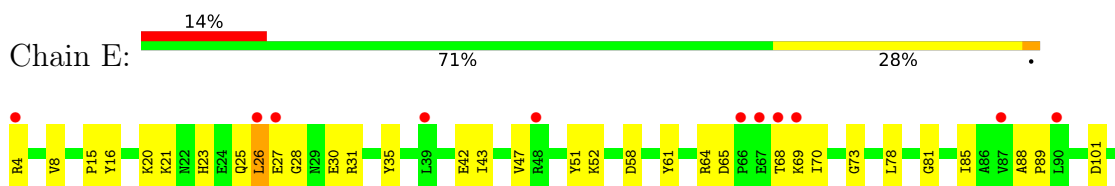
- Molecule 1: Glutamate receptor 3

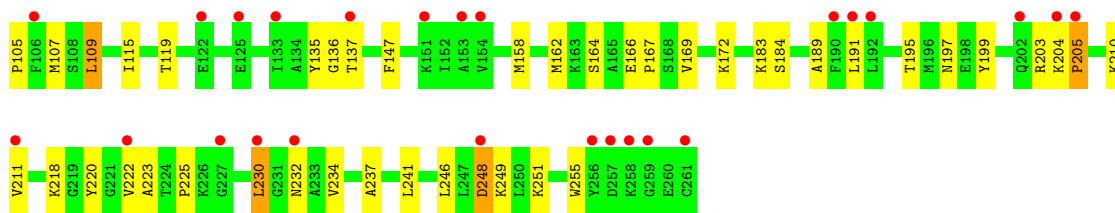


- Molecule 1: Glutamate receptor 3



- Molecule 1: Glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.03Å 110.33Å 161.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.73 – 1.79 28.73 – 1.79	Depositor EDS
% Data completeness (in resolution range)	89.0 (28.73-1.79) 89.0 (28.73-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.88 (at 1.79Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.201 , 0.240 0.223 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6930	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.08% 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

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	0.50	1/2071 (0.0%)	0.62	1/2786 (0.0%)
1	C	0.52	2/2071 (0.1%)	0.64	1/2786 (0.0%)
1	E	0.49	1/2067 (0.0%)	0.66	3/2781 (0.1%)
All	All	0.50	4/6209 (0.1%)	0.64	5/8353 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLY	C-N	-5.83	1.20	1.34
1	C	225	PRO	C-N	-5.71	1.21	1.34
1	C	225	PRO	N-CD	5.50	1.55	1.47
1	E	25	GLN	C-N	-5.27	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	GLN	O-C-N	-5.62	113.71	122.70
1	E	26	LEU	O-C-N	5.59	131.65	122.70
1	C	248	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	248	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	248	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	204	LYS	Peptide

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	2033	0	2064	63	0
1	C	2033	0	2065	72	0
1	E	2029	0	2058	74	0
2	A	10	0	5	0	0
2	C	10	0	5	0	0
2	E	10	0	5	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	266	0	0	10	0
4	C	258	0	0	10	0
4	E	277	0	0	14	0
All	All	6930	0	6202	200	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 16.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:NH2	1:C:69:LYS:HG3	1.72	1.04
1:E:42:GLU:HG3	1:E:246:LEU:HD21	1.39	1.02
1:C:64:ARG:CZ	1:C:69:LYS:HG3	1.91	1.00
1:A:137:THR:HG22	1:A:191:LEU:HB2	1.42	1.00
1:E:241:LEU:HD22	1:E:246:LEU:HD23	1.44	0.99
1:A:249:LYS:HD2	1:E:167:PRO:HD3	1.43	0.96
1:C:64:ARG:HH22	1:C:69:LYS:HE3	1.33	0.92
1:C:64:ARG:NH2	1:C:69:LYS:CG	2.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:HD22	1:C:246:LEU:HD23	1.54	0.85
1:A:64:ARG:HE	1:A:69:LYS:HG3	1.40	0.83
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.64	0.80
1:C:42:GLU:HG3	1:C:246:LEU:HD21	1.64	0.78
1:E:64:ARG:HE	1:E:69:LYS:HG3	1.48	0.77
1:C:149:ARG:HG3	4:C:501:HOH:O	1.85	0.76
1:E:85:ILE:HD11	1:E:222:VAL:HG11	1.69	0.74
1:C:202:GLN:HG3	4:C:630:HOH:O	1.89	0.73
1:E:85:ILE:HD11	1:E:222:VAL:CG1	2.20	0.72
1:C:85:ILE:HD11	1:C:222:VAL:HG11	1.71	0.71
1:E:42:GLU:CG	1:E:246:LEU:HD21	2.19	0.70
1:A:81:GLY:HA2	4:A:510:HOH:O	1.93	0.69
1:C:85:ILE:HD12	1:C:234:VAL:HG21	1.75	0.69
1:E:81:GLY:HA2	4:E:601:HOH:O	1.92	0.68
1:A:12:LEU:HD13	1:A:19:TYR:CE2	2.27	0.68
1:E:47:VAL:HG11	1:E:230:LEU:HD11	1.74	0.67
1:A:12:LEU:CD1	1:A:19:TYR:CE2	2.78	0.67
1:A:183:LYS:HG3	4:A:605:HOH:O	1.94	0.67
1:C:183:LYS:HG3	4:C:667:HOH:O	1.94	0.67
1:C:64:ARG:HH22	1:C:69:LYS:CE	2.06	0.67
1:A:12:LEU:HD13	1:A:19:TYR:HE2	1.58	0.66
1:A:64:ARG:NE	1:A:69:LYS:HG3	2.11	0.66
1:A:85:ILE:HD11	1:A:222:VAL:HG11	1.78	0.66
1:E:85:ILE:HD12	4:E:587:HOH:O	1.93	0.66
1:E:230:LEU:HD12	1:E:234:VAL:HG23	1.75	0.66
1:E:64:ARG:HH21	1:E:69:LYS:HE3	1.61	0.66
1:A:242:ASN:ND2	4:A:731:HOH:O	2.30	0.64
1:C:64:ARG:NH2	1:C:69:LYS:HE3	2.09	0.64
1:A:8:VAL:HG22	1:A:85:ILE:CG2	2.26	0.64
1:A:105:PRO:HA	1:A:220:TYR:O	1.97	0.64
1:C:145:GLU:HG2	4:C:623:HOH:O	1.96	0.64
1:E:183:LYS:HG3	4:E:555:HOH:O	1.98	0.64
1:A:78:LEU:HD22	1:A:225:PRO:HD3	1.80	0.63
1:C:136:GLY:HA3	1:C:169:VAL:O	2.01	0.61
1:E:27:GLU:HG2	4:E:713:HOH:O	2.00	0.61
1:C:105:PRO:HA	1:C:220:TYR:O	2.02	0.60
1:E:184:SER:HB2	4:E:518:HOH:O	2.01	0.60
1:C:85:ILE:HD11	1:C:222:VAL:CG1	2.33	0.59
1:A:12:LEU:HD11	1:A:19:TYR:CZ	2.37	0.59
1:E:183:LYS:HE3	4:E:555:HOH:O	2.03	0.59
1:E:28:GLY:HA2	1:E:52:LYS:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HD11	1:A:222:VAL:CG1	2.34	0.58
1:A:115:ILE:HD11	1:A:211:VAL:HG11	1.85	0.58
1:E:26:LEU:HD12	1:E:26:LEU:N	2.18	0.58
1:A:136:GLY:HA3	1:A:169:VAL:O	2.04	0.57
1:C:165:ALA:HB1	1:C:169:VAL:HG13	1.85	0.57
1:A:64:ARG:HH21	1:A:69:LYS:CE	2.17	0.57
1:C:6:ILE:HD12	1:C:85:ILE:HG22	1.87	0.57
1:E:64:ARG:NE	1:E:69:LYS:HG3	2.17	0.57
1:E:136:GLY:HA3	1:E:169:VAL:O	2.04	0.57
1:A:6:ILE:CD1	1:A:49:ILE:HD12	2.36	0.56
1:C:42:GLU:CG	1:C:246:LEU:HD21	2.34	0.56
1:E:23:HIS:HA	1:E:26:LEU:HD13	1.88	0.56
1:C:6:ILE:CD1	1:C:49:ILE:HD12	2.36	0.56
1:C:15:PRO:HG3	1:C:199:TYR:CD1	2.41	0.56
1:E:8:VAL:HG22	1:E:85:ILE:CG2	2.36	0.55
1:E:20:LYS:NZ	1:E:30:GLU:OE1	2.36	0.55
1:E:251:LYS:HD2	1:E:255:TRP:CE3	2.42	0.55
1:C:64:ARG:NH2	1:C:69:LYS:CE	2.68	0.55
1:A:115:ILE:CD1	1:A:211:VAL:HG11	2.36	0.55
1:A:197:ASN:ND2	1:A:210:LYS:HG3	2.22	0.55
1:C:249:LYS:NZ	1:C:249:LYS:HB2	2.21	0.54
1:E:21:LYS:HE2	4:E:572:HOH:O	2.05	0.54
1:C:30:GLU:HG2	4:C:705:HOH:O	2.06	0.54
1:C:116:LYS:NZ	4:C:704:HOH:O	2.39	0.54
1:E:205:PRO:HA	4:E:655:HOH:O	2.09	0.53
1:A:5:THR:HG21	1:A:52:LYS:HG2	1.91	0.53
1:A:210:LYS:HD2	4:A:623:HOH:O	2.07	0.53
1:C:112:SER:CB	1:C:210:LYS:HE2	2.39	0.53
1:C:91:THR:HG21	1:C:218:LYS:HD2	1.90	0.53
1:A:5:THR:HG21	1:A:52:LYS:CG	2.39	0.52
1:A:246:LEU:HB2	1:E:166:GLU:CG	2.39	0.52
1:C:23:HIS:HA	1:C:26:LEU:HD12	1.92	0.52
1:E:28:GLY:HA2	1:E:52:LYS:HE3	1.90	0.52
1:A:12:LEU:HD11	1:A:19:TYR:CE2	2.45	0.52
1:E:4:ARG:HG2	4:E:737:HOH:O	2.08	0.52
1:E:26:LEU:N	1:E:26:LEU:CD1	2.73	0.52
1:E:248:ASP:OD1	4:E:760:HOH:O	2.19	0.52
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.91	0.51
1:E:52:LYS:HE2	4:E:505:HOH:O	2.10	0.51
1:E:78:LEU:HD22	1:E:225:PRO:HD3	1.92	0.51
1:E:249:LYS:HB2	1:E:249:LYS:NZ	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HB2	1:E:166:GLU:HG3	1.93	0.51
1:C:154:VAL:HG12	4:C:726:HOH:O	2.11	0.51
1:A:240:LYS:HB2	1:C:94:LEU:HD22	1.93	0.50
1:C:215:LEU:HD12	1:C:215:LEU:N	2.26	0.50
1:E:20:LYS:HB2	1:E:23:HIS:CG	2.46	0.50
1:A:85:ILE:HD12	1:A:234:VAL:HG21	1.93	0.50
1:C:63:ALA:CB	1:C:140:SER:HA	2.41	0.50
1:E:232:ASN:ND2	4:E:519:HOH:O	2.39	0.50
1:A:61:TYR:HE1	1:A:89:PRO:HG2	1.77	0.50
1:A:145:GLU:HG2	4:A:614:HOH:O	2.12	0.50
1:C:8:VAL:HA	1:C:85:ILE:O	2.12	0.50
1:A:232:ASN:ND2	4:A:601:HOH:O	2.44	0.50
1:C:109:LEU:HB3	1:C:195:THR:HG23	1.94	0.50
1:E:42:GLU:HG3	1:E:246:LEU:CD2	2.29	0.50
1:C:100:ILE:HD12	1:C:223:ALA:HB1	1.93	0.49
1:A:166:GLU:HA	1:A:167:PRO:C	2.32	0.49
1:C:21:LYS:NZ	1:C:21:LYS:HB3	2.26	0.49
1:E:105:PRO:HA	1:E:220:TYR:O	2.13	0.49
1:E:61:TYR:HE1	1:E:89:PRO:HG2	1.78	0.49
1:E:15:PRO:HB3	1:E:199:TYR:CE1	2.48	0.49
1:A:5:THR:CG2	1:A:52:LYS:HG2	2.43	0.49
1:A:10:THR:HG23	1:A:55:ILE:HD13	1.93	0.49
1:C:112:SER:HB3	1:C:210:LYS:HE2	1.94	0.49
1:C:81:GLY:HA2	4:C:525:HOH:O	2.12	0.48
1:C:180:ARG:HG2	1:C:188:PHE:CD2	2.48	0.48
1:A:94:LEU:HD22	1:C:240:LYS:HB2	1.95	0.47
1:E:43:ILE:CD1	1:E:222:VAL:HG21	2.45	0.47
1:E:135:TYR:HA	1:E:189:ALA:O	2.13	0.47
1:E:115:ILE:HB	1:E:119:THR:HB	1.96	0.47
1:E:64:ARG:HH21	1:E:69:LYS:CE	2.26	0.47
1:E:26:LEU:O	1:E:31:ARG:HD3	2.14	0.47
1:E:47:VAL:HG11	1:E:230:LEU:CD1	2.43	0.47
1:A:135:TYR:HA	1:A:189:ALA:O	2.15	0.47
1:C:63:ALA:HB2	1:C:140:SER:HA	1.97	0.46
1:C:166:GLU:HA	1:C:167:PRO:C	2.34	0.46
1:C:115:ILE:HD11	1:C:211:VAL:HG11	1.96	0.46
1:C:116:LYS:HE3	4:C:536:HOH:O	2.15	0.46
1:A:12:LEU:HD11	1:A:19:TYR:OH	2.16	0.46
1:A:100:ILE:HD12	1:A:223:ALA:HB1	1.97	0.46
1:C:20:LYS:O	1:C:23:HIS:ND1	2.41	0.46
1:C:210:LYS:NZ	1:C:214:ASN:OD1	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HH21	1:A:69:LYS:HE3	1.79	0.46
1:C:148:ARG:HA	1:C:159:TRP:CE2	2.51	0.45
1:A:45:LYS:HE2	4:A:557:HOH:O	2.16	0.45
1:C:64:ARG:HB2	1:C:71:TRP:CE2	2.51	0.45
1:C:42:GLU:O	1:C:46:HIS:HD2	2.00	0.45
1:E:28:GLY:HA2	1:E:52:LYS:HE2	1.97	0.45
1:E:101:ASP:O	1:E:223:ALA:HA	2.17	0.45
1:A:109:LEU:HB3	1:A:195:THR:HG23	1.98	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HG3	2.32	0.44
1:A:166:GLU:HG3	1:A:167:PRO:HA	1.99	0.44
1:E:237:ALA:O	1:E:241:LEU:HG	2.16	0.44
1:A:171:THR:HG21	1:A:177:GLY:HA2	1.99	0.44
1:A:64:ARG:HH21	1:A:69:LYS:HE2	1.83	0.44
1:A:107:MET:SD	1:A:195:THR:HG21	2.57	0.44
1:E:109:LEU:HB3	1:E:195:THR:HG23	1.99	0.44
1:E:35:TYR:CZ	1:E:107:MET:HE3	2.52	0.44
1:E:16:TYR:OH	1:E:195:THR:HB	2.17	0.44
1:C:151:LYS:HA	1:C:156:GLU:OE2	2.18	0.44
1:A:13:GLU:OE2	1:A:174:THR:HB	2.18	0.43
1:E:68:THR:HB	1:E:70:ILE:HG12	2.01	0.43
1:A:183:LYS:HE3	4:A:605:HOH:O	2.19	0.43
1:C:115:ILE:CD1	1:C:211:VAL:HG11	2.48	0.43
1:C:150:SER:O	1:C:156:GLU:HG2	2.19	0.43
1:C:151:LYS:HG3	1:E:164:SER:HB3	2.01	0.43
1:E:65:ASP:OD1	1:E:65:ASP:C	2.56	0.43
1:A:240:LYS:HG2	1:A:244:GLN:OE1	2.18	0.43
1:A:251:LYS:O	1:A:255:TRP:HB2	2.19	0.43
1:E:4:ARG:HB2	4:E:758:HOH:O	2.19	0.43
1:C:15:PRO:HB3	1:C:199:TYR:CE1	2.54	0.43
1:C:251:LYS:HD2	1:C:255:TRP:CE3	2.54	0.43
1:A:111:ILE:HB	1:A:215:LEU:HB2	2.01	0.43
1:C:249:LYS:HG3	4:C:626:HOH:O	2.18	0.43
1:A:6:ILE:HD11	1:A:49:ILE:HD12	2.00	0.43
1:A:58:ASP:OD1	1:A:73:GLY:HA2	2.19	0.43
1:E:230:LEU:HD13	1:E:230:LEU:HA	1.83	0.43
1:E:218:LYS:HB2	4:E:511:HOH:O	2.18	0.42
1:C:119:THR:HA	1:C:120:PRO:HD3	1.86	0.42
1:E:115:ILE:CD1	1:E:211:VAL:HG11	2.50	0.42
1:C:6:ILE:O	1:C:6:ILE:HG13	2.19	0.42
1:C:171:THR:HG21	1:C:177:GLY:HA2	2.01	0.42
1:E:172:LYS:HE2	1:E:172:LYS:HB3	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:TYR:CZ	1:E:107:MET:CE	3.02	0.42
1:A:119:THR:HA	1:A:120:PRO:HD3	1.84	0.42
1:A:92:ILE:HG12	1:A:102:PHE:CG	2.55	0.42
1:A:42:GLU:OE1	1:E:166:GLU:OE2	2.37	0.42
1:A:166:GLU:HG2	4:A:508:HOH:O	2.20	0.42
1:A:47:VAL:HG12	1:A:49:ILE:HG23	2.02	0.42
1:A:134:ALA:HA	1:A:161:TYR:OH	2.20	0.42
1:A:105:PRO:HG2	1:C:105:PRO:HG2	2.01	0.41
1:A:129:LYS:HE3	4:A:650:HOH:O	2.20	0.41
1:E:147:PHE:CZ	1:E:191:LEU:HD13	2.55	0.41
1:C:148:ARG:HA	1:C:159:TRP:CD2	2.55	0.41
1:E:8:VAL:HG23	1:E:51:TYR:HB2	2.01	0.41
1:A:246:LEU:HB2	1:E:166:GLU:HG2	2.01	0.41
1:C:135:TYR:HA	1:C:189:ALA:O	2.20	0.41
1:E:158:MET:O	1:E:162:MET:HG3	2.20	0.41
1:C:78:LEU:HD22	1:C:225:PRO:HD3	2.02	0.41
1:E:199:TYR:O	1:E:203:ARG:HG2	2.21	0.41
1:C:10:THR:OG1	1:C:17:VAL:HG21	2.21	0.40
1:C:109:LEU:N	1:C:109:LEU:HD13	2.35	0.40
1:E:58:ASP:OD1	1:E:73:GLY:HA2	2.21	0.40
1:C:148:ARG:HG2	1:C:149:ARG:HD3	2.01	0.40
1:C:165:ALA:CB	1:C:169:VAL:HG13	2.49	0.40
1:C:137:THR:O	1:C:170:PHE:HA	2.21	0.40
1:C:144:LYS:HE2	1:C:148:ARG:NH2	2.37	0.40
1:C:163:LYS:HE2	1:C:163:LYS:HB3	1.84	0.40
1:C:215:LEU:N	1:C:215:LEU:CD1	2.85	0.40
1:E:23:HIS:O	1:E:31:ARG:HG2	2.20	0.40
1:E:241:LEU:HA	1:E:241:LEU:HD23	1.85	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	256/258 (99%)	254 (99%)	2 (1%)	0	100	100
1	C	256/258 (99%)	251 (98%)	5 (2%)	0	100	100
1	E	256/258 (99%)	252 (98%)	3 (1%)	1 (0%)	34	21
All	All	768/774 (99%)	757 (99%)	10 (1%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	PRO

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	218/218 (100%)	214 (98%)	4 (2%)	59	48
1	C	218/218 (100%)	215 (99%)	3 (1%)	67	59
1	E	217/218 (100%)	215 (99%)	2 (1%)	78	75
All	All	653/654 (100%)	644 (99%)	9 (1%)	67	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LEU
1	A	139	ASP
1	A	230	LEU
1	A	246	LEU
1	C	24	GLU
1	C	109	LEU
1	C	139	ASP
1	E	109	LEU
1	E	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	242	ASN
1	A	252	ASN
1	C	252	ASN
1	E	232	ASN
1	E	252	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	E	400	-	8,9,9	1.04	1 (12%)	10,11,11	0.98	0
2	GLU	C	400	-	8,9,9	1.03	1 (12%)	10,11,11	1.23	2 (20%)
2	GLU	A	400	-	8,9,9	1.14	1 (12%)	10,11,11	1.15	1 (10%)

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	E	400	-	-	0/9/9/9	-
2	GLU	C	400	-	-	2/9/9/9	-
2	GLU	A	400	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GLU	OXT-C	-2.36	1.22	1.30
2	C	400	GLU	OXT-C	-2.02	1.23	1.30
2	E	400	GLU	OXT-C	-2.02	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLU	OXT-C-O	-2.32	118.83	124.09
2	C	400	GLU	OXT-C-CA	2.23	120.97	113.38
2	C	400	GLU	OXT-C-O	-2.14	119.24	124.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	400	GLU	OE1-CD-CG-CB
2	C	400	GLU	OE2-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	258/258 (100%)	0.81	27 (10%) 6 4	16, 26, 43, 66	0
1	C	258/258 (100%)	0.95	36 (13%) 2 2	15, 25, 45, 59	0
1	E	258/258 (100%)	0.90	36 (13%) 2 2	17, 25, 45, 71	0
All	All	774/774 (100%)	0.88	99 (12%) 3 2	15, 26, 45, 71	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	67	GLU	8.3
1	E	66	PRO	7.3
1	C	63	ALA	5.7
1	A	66	PRO	5.5
1	C	21	LYS	5.2
1	C	259	GLY	5.0
1	A	4	ARG	5.0
1	C	258	LYS	4.9
1	C	229	ALA	4.8
1	A	67	GLU	4.6
1	E	68	THR	4.5
1	A	259	GLY	4.4
1	C	25	GLN	4.3
1	E	258	LYS	4.1
1	C	232	ASN	3.9
1	C	27	GLU	3.9
1	A	258	LYS	3.8
1	C	24	GLU	3.7
1	C	90	LEU	3.7
1	A	229	ALA	3.6
1	E	154	VAL	3.6
1	A	19	TYR	3.6
1	A	192	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	256	TYR	3.5
1	C	4	ARG	3.4
1	E	26	LEU	3.4
1	E	4	ARG	3.3
1	A	232	ASN	3.3
1	A	260	GLU	3.2
1	E	204	LYS	3.2
1	E	27	GLU	3.1
1	E	90	LEU	3.1
1	A	21	LYS	3.0
1	C	22	ASN	3.0
1	C	149	ARG	3.0
1	C	61	TYR	3.0
1	E	259	GLY	3.0
1	C	261	CYS	3.0
1	A	69	LYS	3.0
1	A	48	ARG	2.9
1	C	48	ARG	2.9
1	E	39	LEU	2.9
1	E	230	LEU	2.9
1	C	192	LEU	2.8
1	C	257	ASP	2.8
1	A	132	GLU	2.8
1	A	172	LYS	2.8
1	A	244	GLN	2.8
1	C	132	GLU	2.7
1	E	261	CYS	2.7
1	E	248	ASP	2.7
1	E	153	ALA	2.7
1	C	87	VAL	2.7
1	C	248	ASP	2.7
1	E	122	GLU	2.6
1	C	36	CYS	2.6
1	E	192	LEU	2.6
1	E	137	THR	2.6
1	E	69	LYS	2.6
1	C	159	TRP	2.5
1	E	190	PHE	2.5
1	E	191	LEU	2.5
1	C	220	TYR	2.5
1	A	68	THR	2.4
1	C	151	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	232	ASN	2.4
1	A	166	GLU	2.4
1	C	16	TYR	2.4
1	C	89	PRO	2.3
1	C	154	VAL	2.3
1	E	256	TYR	2.3
1	C	85	ILE	2.3
1	C	153	ALA	2.3
1	A	109	LEU	2.3
1	A	230	LEU	2.3
1	A	64	ARG	2.3
1	C	166	GLU	2.3
1	A	191	LEU	2.2
1	E	151	LYS	2.2
1	A	65	ASP	2.2
1	A	5	THR	2.2
1	E	87	VAL	2.2
1	E	257	ASP	2.2
1	C	88	ALA	2.2
1	A	87	VAL	2.2
1	E	202	GLN	2.2
1	E	106	PHE	2.1
1	E	222	VAL	2.1
1	E	133	ILE	2.1
1	E	125	GLU	2.1
1	A	203	ARG	2.1
1	C	50	LYS	2.1
1	C	84	ASP	2.1
1	E	205	PRO	2.1
1	A	129	LYS	2.1
1	E	48	ARG	2.1
1	E	211	VAL	2.1
1	C	165	ALA	2.0
1	E	227	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	402	1/1	0.66	0.18	38,38,38,38	0
3	ZN	C	401	1/1	0.78	0.17	40,40,40,40	0
3	ZN	E	401	1/1	0.86	0.28	4,4,4,4	0
2	GLU	C	400	10/10	0.91	0.18	16,19,25,26	0
3	ZN	A	401	1/1	0.92	0.35	5,5,5,5	0
2	GLU	A	400	10/10	0.95	0.17	19,22,25,26	0
2	GLU	E	400	10/10	0.97	0.16	18,21,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.