



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:06 PM UTC

PDB ID : 3M3K / pdb_00003m3k
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

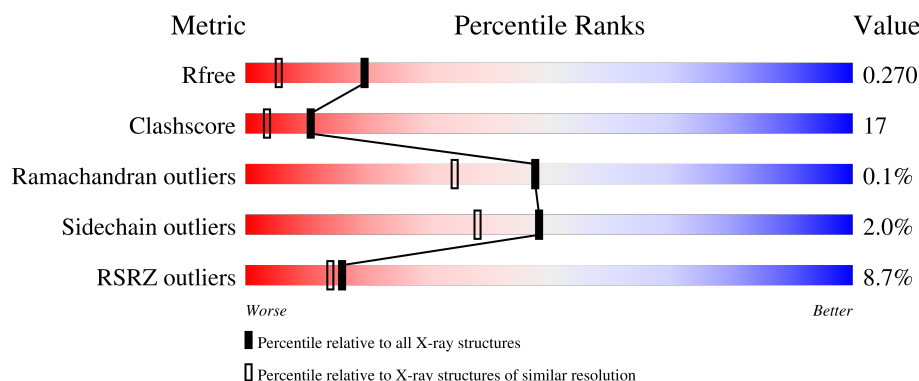
1 Overall quality at a glance

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	5% 71% 27% .
1	C	258	11% 70% 28% .
1	E	258	10% 69% 28% .

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
1	A	258	Total	C	N	O	S	0	0	0
			2033	1298	340	384	11			
1	C	258	Total	C	N	O	S	0	0	0
			2033	1298	340	384	11			
1	E	258	Total	C	N	O	S	0	0	0
			2029	1296	339	383	11			

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 (CCD ID: GLU) (formula: C₅H₉NO₄).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

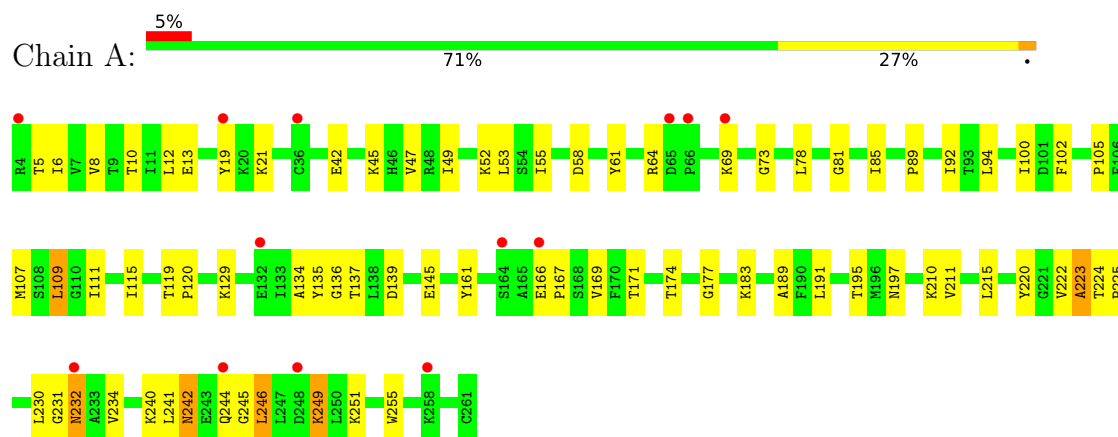
- Molecule 4 is water.

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

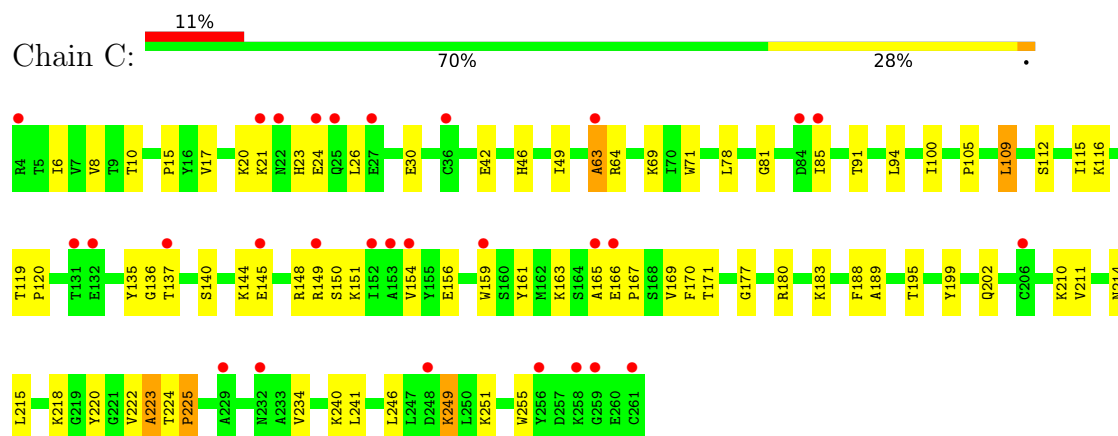
3 Residue-property plots [i](#)

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.

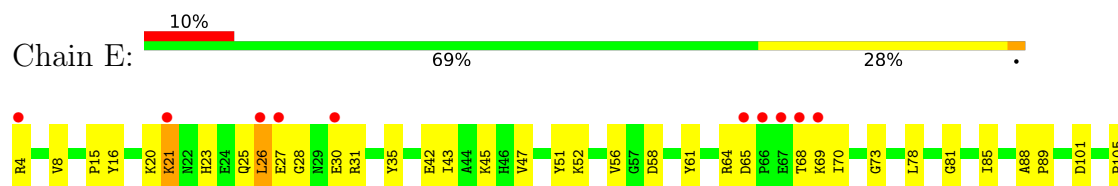
• Molecule 1: Glutamate receptor 3

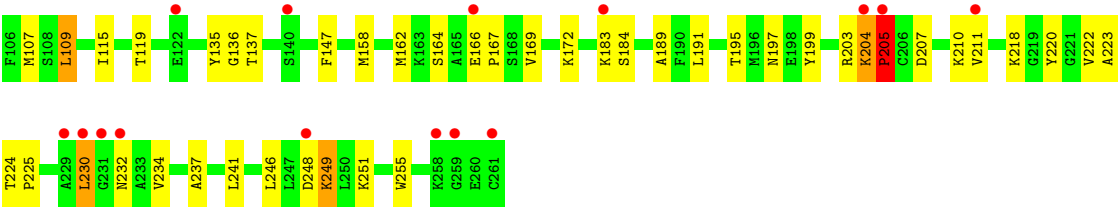


• Molecule 1: Glutamate receptor 3



• Molecule 1: Glutamate receptor 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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) 88.9 (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)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.201 , 0.240 (Not available) , 0.270	Depositor DCC
R_{free} test set	2000 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.71	6/2071 (0.3%)	0.85	2/2786 (0.1%)
1	C	0.68	4/2071 (0.2%)	0.88	4/2786 (0.1%)
1	E	0.66	2/2067 (0.1%)	0.89	7/2781 (0.3%)
All	All	0.68	12/6209 (0.2%)	0.87	13/8353 (0.2%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLY	C-N	-10.43	1.20	1.33
1	C	225	PRO	C-N	-9.29	1.21	1.33
1	E	25	GLN	C-N	-8.43	1.22	1.33
1	A	242	ASN	C-N	-7.85	1.23	1.34
1	E	45	LYS	C-N	-6.91	1.23	1.33
1	A	232	ASN	C-N	-6.87	1.25	1.33
1	A	231	GLY	C-N	-6.74	1.25	1.33
1	C	223	ALA	C-N	-6.61	1.25	1.33
1	A	241	LEU	C-N	-6.01	1.26	1.33
1	C	224	THR	C-N	-5.60	1.26	1.33
1	C	225	PRO	N-CD	5.57	1.55	1.47
1	A	223	ALA	C-N	-5.18	1.27	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	26	LEU	O-C-N	7.08	131.65	122.23
1	C	63	ALA	CA-C-N	6.84	132.34	121.66
1	C	63	ALA	C-N-CA	6.84	132.34	121.66
1	E	205	PRO	CB-CA-C	-6.37	101.05	111.56
1	A	224	THR	O-C-N	6.16	125.65	121.71
1	E	25	GLN	O-C-N	-6.13	113.71	122.41
1	E	26	LEU	CA-C-N	-5.59	113.86	122.87
1	E	26	LEU	C-N-CA	-5.59	113.86	122.87
1	E	204	LYS	CA-C-N	5.31	126.47	119.84
1	E	204	LYS	C-N-CA	5.31	126.47	119.84
1	C	224	THR	CA-C-N	5.16	125.10	119.78
1	C	224	THR	C-N-CA	5.16	125.10	119.78
1	A	53	LEU	N-CA-C	-5.14	102.67	110.28

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 ⓘ

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	2065	64	0
1	C	2033	0	2065	73	0
1	E	2029	0	2059	78	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	11	0
4	C	258	0	0	10	0
4	E	277	0	0	14	0
All	All	6930	0	6204	206	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 17.

All (206) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:52:LYS:NZ	4:A:747:HOH:O	2.30	0.61
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
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:A:166:GLU:HA	1:A:167:PRO:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:166:GLU:HA	1:C:167:PRO:C	2.34	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
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: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:E:65:ASP:OD1	1:E:65:ASP:C	2.56	0.48
1:A:94:LEU:HD22	1:C:240:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:224:THR:O	1:E:225:PRO:C	2.60	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: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:35:TYR:CZ	1:E:107:MET:HE3	2.53	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:161:TYR:CD2	1:C:161:TYR:C	2.98	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:56:VAL:HG21	1:E:73:GLY:C	2.46	0.41
1:E:199:TYR:O	1:E:203:ARG:HG2	2.21	0.41
1:E:205:PRO:HG2	1:E:207:ASP:CG	2.45	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:35:TYR:CD1	1:E:35:TYR:C	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	19
All	All	768/774 (99%)	757 (99%)	10 (1%)	1 (0%)	48	34

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%)	212 (97%)	6 (3%)	38	26
1	C	218/218 (100%)	215 (99%)	3 (1%)	59	52
1	E	217/218 (100%)	213 (98%)	4 (2%)	51	43
All	All	653/654 (100%)	640 (98%)	13 (2%)	48	38

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

Mol	Chain	Res	Type
1	A	21	LYS
1	A	109	LEU
1	A	139	ASP
1	A	230	LEU
1	A	246	LEU
1	A	249	LYS
1	C	24	GLU
1	C	109	LEU
1	C	249	LYS
1	E	21	LYS
1	E	109	LEU
1	E	230	LEU
1	E	249	LYS

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 ⓘ

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 [i](#)

There are no oligosaccharides 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	1.08	1 (12%)	8,11,11	0.92	0
2	GLU	A	400	-	8,9,9	1.18	1 (12%)	8,11,11	1.14	1 (12%)
2	GLU	C	400	-	8,9,9	1.07	1 (12%)	8,11,11	1.10	1 (12%)

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	A	400	-	-	0/9/9/9	-
2	GLU	C	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	-2.46	1.22	1.30
2	C	400	GLU	OXT-C	-2.11	1.23	1.30
2	E	400	GLU	OXT-C	-2.11	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GLU	OXT-C-O	-2.31	118.83	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	GLU	OXT-C-O	-2.13	119.24	124.08

There are no chirality outliers.

There are no torsion outliers.

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%)	0.51	13 (5%) 34 33	16, 26, 43, 66	0
1	C	258/258 (100%)	0.71	29 (11%) 10 8	15, 25, 45, 59	0
1	E	258/258 (100%)	0.63	25 (9%) 13 11	17, 25, 45, 71	0
All	All	774/774 (100%)	0.61	67 (8%) 16 14	15, 26, 45, 71	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	ALA	6.7
1	E	68	THR	5.2
1	C	24	GLU	5.0
1	E	67	GLU	4.9
1	E	66	PRO	4.5
1	C	21	LYS	4.3
1	E	205	PRO	3.8
1	C	22	ASN	3.7
1	C	261	CYS	3.7
1	C	165	ALA	3.6
1	E	248	ASP	3.4
1	C	166	GLU	3.4
1	C	232	ASN	3.4
1	A	19	TYR	3.4
1	C	25	GLN	3.4
1	C	154	VAL	3.3
1	C	259	GLY	3.3
1	A	244	GLN	3.3
1	A	166	GLU	3.2
1	C	132	GLU	3.2
1	E	258	LYS	3.1
1	C	248	ASP	3.1
1	E	211	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	4	ARG	3.0
1	E	259	GLY	3.0
1	E	30	GLU	2.9
1	E	69	LYS	2.9
1	E	65	ASP	2.9
1	C	84	ASP	2.8
1	C	229	ALA	2.8
1	E	26	LEU	2.8
1	A	164	SER	2.7
1	C	258	LYS	2.7
1	A	66	PRO	2.7
1	C	27	GLU	2.6
1	C	36	CYS	2.6
1	C	152	ILE	2.6
1	A	232	ASN	2.6
1	C	131	THR	2.6
1	A	65	ASP	2.6
1	C	4	ARG	2.6
1	C	206	CYS	2.6
1	C	159	TRP	2.6
1	E	204	LYS	2.5
1	E	27	GLU	2.5
1	E	232	ASN	2.5
1	C	149	ARG	2.5
1	C	85	ILE	2.4
1	A	69	LYS	2.4
1	E	21	LYS	2.4
1	E	230	LEU	2.4
1	E	231	GLY	2.3
1	E	261	CYS	2.3
1	C	256	TYR	2.3
1	E	140	SER	2.3
1	E	4	ARG	2.3
1	A	258	LYS	2.3
1	C	145	GLU	2.3
1	E	166	GLU	2.2
1	A	132	GLU	2.1
1	A	248	ASP	2.1
1	C	137	THR	2.1
1	E	122	GLU	2.1
1	A	36	CYS	2.0
1	C	153	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	229	ALA	2.0
1	E	183	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ZN	A	401	1/1	0.42	0.36	5,5,5,5	0
3	ZN	E	401	1/1	0.62	0.37	4,4,4,4	0
3	ZN	A	402	1/1	0.70	0.19	38,38,38,38	0
3	ZN	C	401	1/1	0.85	0.17	40,40,40,40	0
2	GLU	C	400	10/10	0.93	0.09	16,19,25,26	0
2	GLU	A	400	10/10	0.95	0.07	19,22,25,26	0
2	GLU	E	400	10/10	0.95	0.07	18,21,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.