



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 AM UTC

PDB ID : 3IL1 / pdb_00003il1
Title : Crystal structure of the AMPA subunit GluR2 bound to the allosteric modulator, IDRA-21
Authors : Ahmed, A.H.; Ptak, C.P.; Oswald, R.E.
Deposited on : 2009-08-06
Resolution : 2.00 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

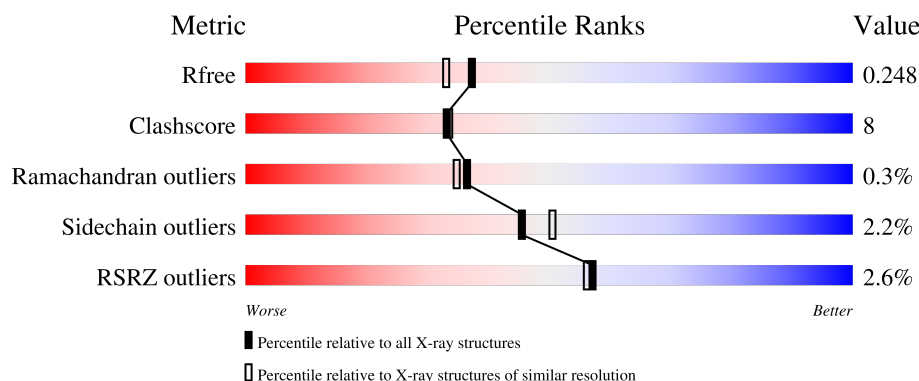
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

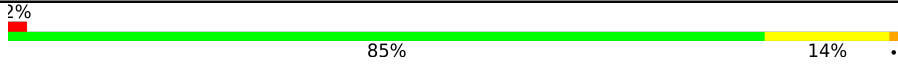
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	B	258	
1	E	258	
1	H	258	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6932 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	258	Total	C	N	O	S	0	0	0
			2012	1283	334	381	14			
1	E	258	Total	C	N	O	S	0	0	0
			2009	1282	334	379	14			
1	H	258	Total	C	N	O	S	0	0	0
			2006	1279	335	378	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
B	242	SER	ASN	engineered mutation	UNP P19491
E	118	GLY	-	linker	UNP P19491
E	119	THR	-	linker	UNP P19491
E	242	SER	ASN	engineered mutation	UNP P19491
H	118	GLY	-	linker	UNP P19491
H	119	THR	-	linker	UNP P19491
H	242	SER	ASN	engineered mutation	UNP P19491

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).

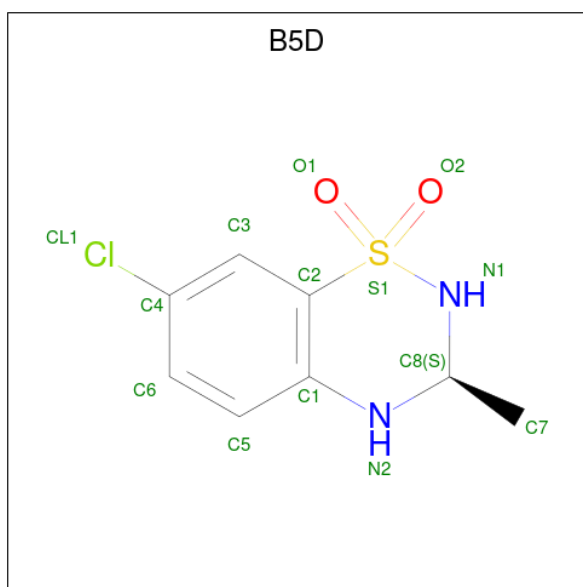


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	E	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (3S)-7-chloro-3-methyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-dioxide (CCD ID: B5D) (formula: C₈H₉ClN₂O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	S	0	0
			14	8	1	2	2	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			14	8	1	2	2	1		
4	H	1	Total	C	Cl	N	O	S	0	0
			14	8	1	2	2	1		

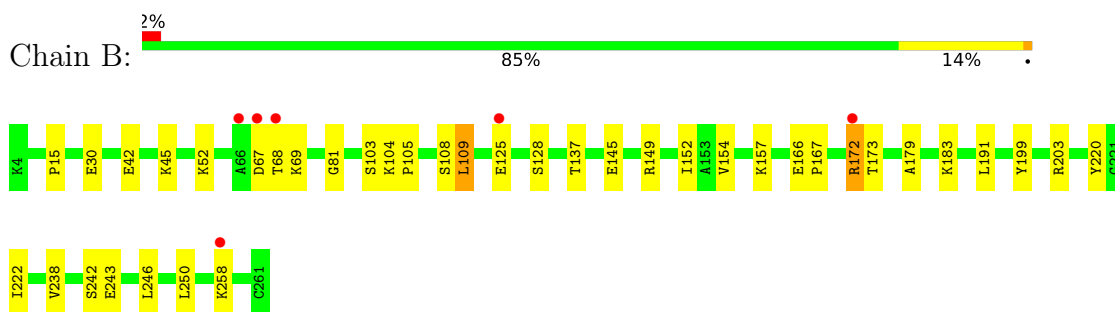
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	238	Total O 238 238	0	0
5	E	248	Total O 248 248	0	0
5	H	342	Total O 342 342	0	0

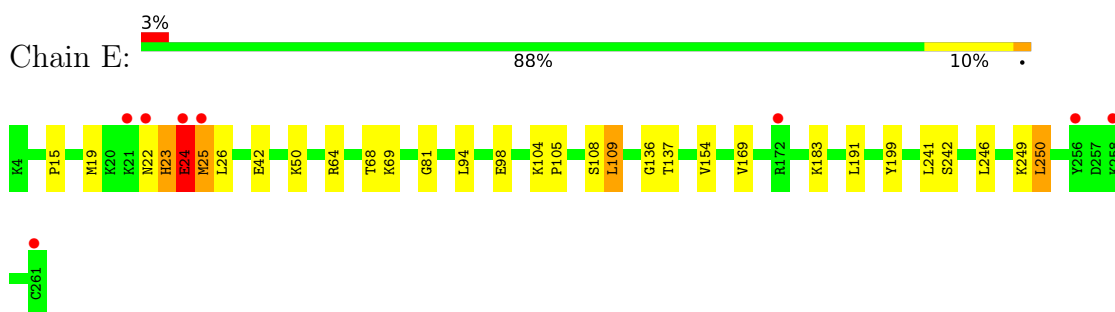
3 Residue-property plots [i](#)

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.

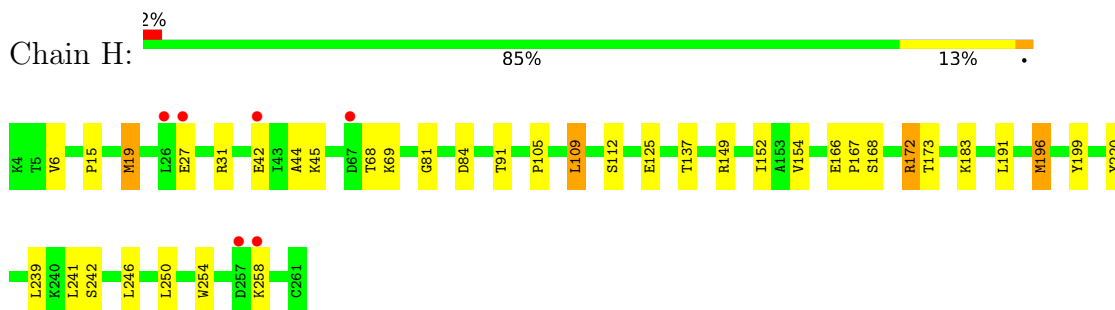
- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



- Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.33Å 114.71Å 165.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.02 – 2.00 15.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (15.02-2.00) 91.7 (15.02-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.234 0.209 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B5D, 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	B	0.41	0/2048	0.70	0/2754
1	E	0.41	0/2045	0.71	0/2750
1	H	0.49	2/2042 (0.1%)	0.72	0/2746
All	All	0.44	2/6135 (0.0%)	0.71	0/8250

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	44	ALA	C-N	-7.95	1.23	1.33
1	H	45	LYS	C-N	-5.84	1.25	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2012	0	2043	32	0
1	E	2009	0	2041	33	1
1	H	2006	0	2034	34	0
2	B	10	0	5	0	0
2	E	10	0	5	0	0
2	H	10	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	E	2	0	0	0	0
3	H	2	0	0	0	1
4	B	28	0	18	9	0
4	H	14	0	9	2	0
5	B	238	0	0	8	0
5	E	248	0	0	6	0
5	H	342	0	0	8	0
All	All	6932	0	6160	96	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (96) 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:E:23:HIS:O	1:E:25:MET:N	2.06	0.88
1:E:25:MET:HG3	1:E:25:MET:O	1.78	0.82
1:H:183:LYS:HG3	5:H:336:HOH:O	1.83	0.77
1:E:23:HIS:CD2	1:E:24:GLU:H	2.05	0.74
1:E:15:PRO:HG3	1:E:199:TYR:CD1	2.23	0.72
1:B:183:LYS:HG3	5:B:611:HOH:O	1.90	0.72
1:B:81:GLY:HA2	5:B:324:HOH:O	1.92	0.70
1:E:249:LYS:HD3	5:E:799:HOH:O	1.91	0.70
1:E:81:GLY:HA2	5:E:334:HOH:O	1.92	0.68
1:B:15:PRO:HG3	1:B:199:TYR:CD1	2.33	0.64
1:B:30:GLU:HG2	5:B:326:HOH:O	1.97	0.63
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.81	0.63
1:B:108:SER:HB3	4:B:262:B5D:CL1	2.37	0.62
1:H:15:PRO:HG3	1:H:199:TYR:CD1	2.35	0.62
1:H:42:GLU:CD	1:H:246:LEU:HD22	2.25	0.60
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.82	0.60
1:E:23:HIS:CG	1:E:24:GLU:H	2.18	0.59
1:H:27:GLU:HA	5:H:306:HOH:O	2.01	0.59
1:B:179:ALA:HB1	1:B:183:LYS:HE2	1.86	0.58
1:E:42:GLU:HG3	1:E:246:LEU:HD21	1.87	0.57
1:B:166:GLU:HA	1:B:167:PRO:C	2.30	0.57
1:E:241:LEU:HD22	1:E:246:LEU:HD22	1.84	0.57
1:H:137:THR:HG22	1:H:191:LEU:HB2	1.87	0.56
1:H:172:ARG:HD2	5:H:344:HOH:O	2.04	0.56
1:E:50:LYS:HE2	5:E:715:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ILE:HD12	1:B:152:ILE:N	2.22	0.55
1:H:241:LEU:HD22	1:H:246:LEU:CD2	2.37	0.55
1:E:183:LYS:HG3	5:E:374:HOH:O	2.06	0.54
1:B:108:SER:CB	4:B:262:B5D:CL1	2.93	0.54
1:H:112:SER:HB2	5:H:318:HOH:O	2.08	0.54
1:H:241:LEU:HD22	1:H:246:LEU:HD22	1.91	0.53
1:B:105:PRO:O	4:B:801:B5D:H7A	2.09	0.52
1:B:128:SER:O	1:B:157:LYS:HE3	2.09	0.52
1:E:154:VAL:HG23	5:E:455:HOH:O	2.09	0.52
1:H:42:GLU:HG3	1:H:246:LEU:HD21	1.92	0.52
1:H:19:MET:HE1	1:H:31:ARG:HD2	1.91	0.52
1:E:22:ASN:O	1:E:23:HIS:C	2.53	0.51
1:B:109:LEU:C	1:B:109:LEU:HD22	2.35	0.51
1:H:254:TRP:CZ3	1:H:258:LYS:HE3	2.45	0.51
1:H:242:SER:HB2	4:H:801:B5D:H7	1.93	0.50
1:B:52:LYS:HD2	5:B:322:HOH:O	2.12	0.50
1:B:258:LYS:HD3	5:B:328:HOH:O	2.12	0.50
1:B:45:LYS:HE3	1:H:168:SER:CB	2.43	0.49
1:H:183:LYS:HG2	5:H:292:HOH:O	2.12	0.49
1:B:172:ARG:CG	1:B:173:THR:HG23	2.42	0.49
1:E:23:HIS:O	1:E:26:LEU:N	2.45	0.48
1:E:94:LEU:O	1:E:98:GLU:HG3	2.13	0.48
1:H:166:GLU:HA	1:H:167:PRO:C	2.39	0.48
1:H:258:LYS:HD3	5:H:461:HOH:O	2.13	0.48
1:B:105:PRO:HA	1:B:220:TYR:O	2.14	0.47
1:E:22:ASN:OD1	1:E:26:LEU:HD11	2.14	0.47
1:B:104:LYS:HB3	4:B:801:B5D:HN1	1.78	0.47
1:E:64:ARG:CZ	1:E:69:LYS:HD2	2.44	0.47
1:H:196:MET:HG2	5:H:449:HOH:O	2.15	0.47
1:H:125:GLU:HG3	1:H:154:VAL:HG21	1.98	0.46
1:E:109:LEU:C	1:E:109:LEU:HD22	2.40	0.46
1:E:136:GLY:HA3	1:E:169:VAL:O	2.16	0.45
1:H:105:PRO:HA	1:H:220:TYR:O	2.16	0.45
1:B:172:ARG:HG3	1:B:173:THR:HG23	1.97	0.45
1:H:109:LEU:HD22	1:H:109:LEU:C	2.41	0.45
4:B:262:B5D:H7	1:E:242:SER:HB2	1.97	0.45
1:H:152:ILE:HD12	1:H:152:ILE:N	2.33	0.44
4:B:262:B5D:H7A	1:E:105:PRO:O	2.17	0.44
1:B:42:GLU:HG3	1:B:246:LEU:HD21	2.00	0.44
1:H:91:THR:HG1	2:H:400:GLU:N	2.15	0.44
1:H:42:GLU:OE1	1:H:246:LEU:HD22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:ARG:HG2	1:H:173:THR:HG23	2.00	0.43
1:E:42:GLU:HG3	1:E:246:LEU:CD2	2.48	0.43
1:E:249:LYS:HE2	1:E:249:LYS:HB2	1.71	0.43
1:E:64:ARG:NH1	1:E:69:LYS:HD2	2.33	0.43
1:H:81:GLY:HA2	5:H:329:HOH:O	2.18	0.43
1:H:42:GLU:CD	1:H:246:LEU:CD2	2.90	0.43
1:B:45:LYS:HE3	1:H:168:SER:HB2	2.01	0.43
1:E:250:LEU:HD12	1:E:250:LEU:HA	1.86	0.43
1:B:149:ARG:HA	1:B:149:ARG:HD3	1.86	0.42
1:E:68:THR:O	1:E:69:LYS:HB2	2.18	0.42
1:B:68:THR:O	1:B:69:LYS:HB2	2.20	0.42
1:E:23:HIS:CG	1:E:24:GLU:N	2.86	0.42
4:B:801:B5D:H3	1:E:105:PRO:HG3	2.01	0.42
1:H:239:LEU:HD23	4:H:801:B5D:H7B	2.02	0.42
1:E:249:LYS:HE3	5:E:714:HOH:O	2.20	0.42
4:B:801:B5D:CL1	1:E:108:SER:HB3	2.57	0.42
1:B:242:SER:HB2	4:B:801:B5D:H7	2.03	0.41
1:B:125:GLU:HG3	1:B:154:VAL:HG21	2.02	0.41
1:H:149:ARG:HA	1:H:149:ARG:HD3	1.89	0.41
1:B:103:SER:O	1:E:104:LYS:HE3	2.19	0.41
1:H:6:VAL:HG13	1:H:84:ASP:HB2	2.03	0.41
1:B:145:GLU:HG2	5:B:414:HOH:O	2.19	0.41
1:H:68:THR:O	1:H:69:LYS:HB2	2.21	0.41
1:E:109:LEU:HD13	1:E:109:LEU:N	2.36	0.41
1:H:172:ARG:CG	1:H:173:THR:HG23	2.50	0.41
1:B:243:GLU:HG3	5:B:485:HOH:O	2.19	0.40
1:B:222:ILE:HD12	1:B:238:VAL:CG2	2.51	0.40
1:B:152:ILE:N	1:B:152:ILE:CD1	2.84	0.40
1:B:203:ARG:NH1	5:B:429:HOH:O	2.48	0.40
1:H:172:ARG:HB3	1:H:172:ARG:NH1	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLU:OE1	3:H:2:ZN:ZN[3_545]	1.65	0.55

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	B	256/258 (99%)	251 (98%)	5 (2%)	0	100	100
1	E	256/258 (99%)	249 (97%)	5 (2%)	2 (1%)	16	11
1	H	256/258 (99%)	250 (98%)	6 (2%)	0	100	100
All	All	768/774 (99%)	750 (98%)	16 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	23	HIS
1	E	24	GLU

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	B	216/217 (100%)	212 (98%)	4 (2%)	50	56
1	E	215/217 (99%)	210 (98%)	5 (2%)	44	49
1	H	214/217 (99%)	209 (98%)	5 (2%)	44	49
All	All	645/651 (99%)	631 (98%)	14 (2%)	45	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	67	ASP

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Mol	Chain	Res	Type
1	B	109	LEU
1	B	172	ARG
1	B	250	LEU
1	E	19	MET
1	E	24	GLU
1	E	25	MET
1	E	109	LEU
1	E	250	LEU
1	H	19	MET
1	H	109	LEU
1	H	172	ARG
1	H	196	MET
1	H	250	LEU

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

Mol	Chain	Res	Type
1	H	22	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 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
4	B5D	B	801	-	14,15,15	1.54	2 (14%)	17,23,23	1.65	3 (17%)
2	GLU	H	400	-	8,9,9	1.11	1 (12%)	8,11,11	1.18	1 (12%)
4	B5D	B	262	-	14,15,15	1.53	2 (14%)	17,23,23	1.66	3 (17%)
2	GLU	E	400	-	8,9,9	1.20	1 (12%)	8,11,11	1.21	1 (12%)
4	B5D	H	801	-	14,15,15	1.53	2 (14%)	17,23,23	1.65	3 (17%)
2	GLU	B	400	-	8,9,9	1.10	1 (12%)	8,11,11	1.25	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
4	B5D	B	801	-	-	-	0/2/2/2
2	GLU	H	400	-	-	2/9/9/9	-
4	B5D	B	262	-	-	-	0/2/2/2
2	GLU	E	400	-	-	1/9/9/9	-
4	B5D	H	801	-	-	-	0/2/2/2
2	GLU	B	400	-	-	1/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	B5D	C2-S1	-3.75	1.72	1.75
4	B	262	B5D	C2-S1	-3.71	1.72	1.75
4	H	801	B5D	C2-S1	-3.68	1.72	1.75
4	B	262	B5D	S1-N1	-3.18	1.58	1.62
4	B	801	B5D	S1-N1	-3.18	1.58	1.62
4	H	801	B5D	S1-N1	-3.18	1.58	1.62
2	E	400	GLU	OXT-C	-2.52	1.22	1.30
2	H	400	GLU	OXT-C	-2.27	1.23	1.30
2	B	400	GLU	OXT-C	-2.12	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	B5D	O2-S1-N1	-4.20	103.83	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	262	B5D	O2-S1-N1	-4.16	103.86	108.00
4	H	801	B5D	O2-S1-N1	-4.15	103.88	108.00
4	B	262	B5D	O2-S1-O1	3.04	121.53	118.44
4	B	801	B5D	O2-S1-O1	3.03	121.52	118.44
4	H	801	B5D	O2-S1-O1	3.01	121.50	118.44
2	B	400	GLU	OXT-C-O	-2.79	117.76	124.08
2	H	400	GLU	OXT-C-O	-2.65	118.06	124.08
2	E	400	GLU	OXT-C-O	-2.42	118.58	124.08
4	H	801	B5D	C1-C2-S1	-2.27	117.29	119.00
4	B	262	B5D	C1-C2-S1	-2.26	117.31	119.00
4	B	801	B5D	C1-C2-S1	-2.24	117.32	119.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	400	GLU	OXT-C-CA-CB
2	E	400	GLU	O-C-CA-N
2	H	400	GLU	O-C-CA-CB
2	B	400	GLU	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	B5D	5	0
2	H	400	GLU	1	0
4	B	262	B5D	4	0
4	H	801	B5D	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	258/258 (100%)	-0.02	6 (2%) 61 60	15, 27, 47, 65	0
1	E	258/258 (100%)	0.08	8 (3%) 51 50	19, 29, 49, 59	0
1	H	258/258 (100%)	-0.18	6 (2%) 61 60	14, 22, 40, 53	0
All	All	774/774 (100%)	-0.04	20 (2%) 57 56	14, 26, 46, 65	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	24	GLU	5.1
1	H	27	GLU	3.5
1	B	66	ALA	3.1
1	E	25	MET	3.0
1	E	256	TYR	2.9
1	E	22	ASN	2.9
1	E	172	ARG	2.9
1	E	261	CYS	2.9
1	B	67	ASP	2.7
1	H	42	GLU	2.6
1	E	21	LYS	2.6
1	B	68	THR	2.6
1	B	258	LYS	2.5
1	H	257	ASP	2.5
1	H	258	LYS	2.4
1	H	26	LEU	2.4
1	H	67	ASP	2.2
1	E	258	LYS	2.2
1	B	172	ARG	2.1
1	B	125	GLU	2.1

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	E	1	1/1	0.74	0.29	30,30,30,30	0
4	B5D	H	801	14/14	0.85	0.33	0,0,0,0	0
4	B5D	B	262	14/14	0.86	0.31	0,0,0,0	0
4	B5D	B	801	14/14	0.86	0.33	0,0,0,0	0
3	ZN	H	3	1/1	0.91	0.06	26,26,26,26	0
3	ZN	E	262	1/1	0.93	0.28	9,9,9,9	0
3	ZN	B	263	1/1	0.94	0.14	41,41,41,41	0
3	ZN	H	2	1/1	0.94	0.06	29,29,29,29	0
2	GLU	E	400	10/10	0.95	0.06	18,20,25,29	0
2	GLU	H	400	10/10	0.95	0.06	13,17,22,24	0
2	GLU	B	400	10/10	0.96	0.05	18,21,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.