



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 1MQD / pdb_00001mqd
Title : X-ray structure of the GluR2 ligand-binding core (S1S2J) in complex with (S)-Des-Me-AMPA at 1.46 Å resolution. Crystallization in the presence of lithium sulfate.
Authors : Kasper, C.; Lunn, M.-L.; Liljefors, T.; Gouaux, E.; Egebjerg, J.; Kastrup, J.S.
Deposited on : 2002-09-16
Resolution : 1.46 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

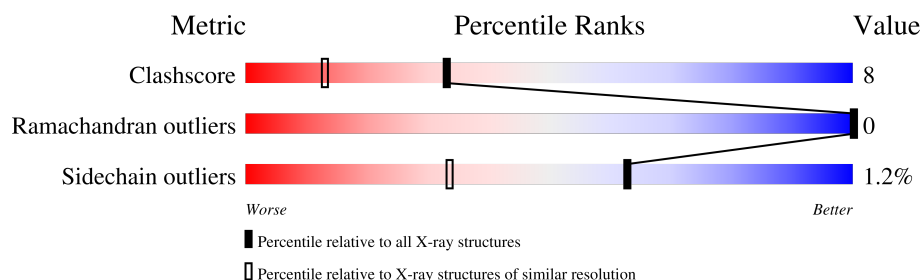
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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))
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	84% 15% .
1	B	261	84% 15% ..
1	C	261	81% 17% ..
1	D	261	83% 15% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10947 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 subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	4	0
			2053	1305	340	393	15			
1	B	258	Total	C	N	O	S	0	11	0
			2105	1336	347	407	15			
1	C	258	Total	C	N	O	S	0	5	0
			2061	1314	342	390	15			
1	D	258	Total	C	N	O	S	0	2	0
			2033	1293	338	388	14			

There are 16 discrepancies between the modelled and reference sequences:

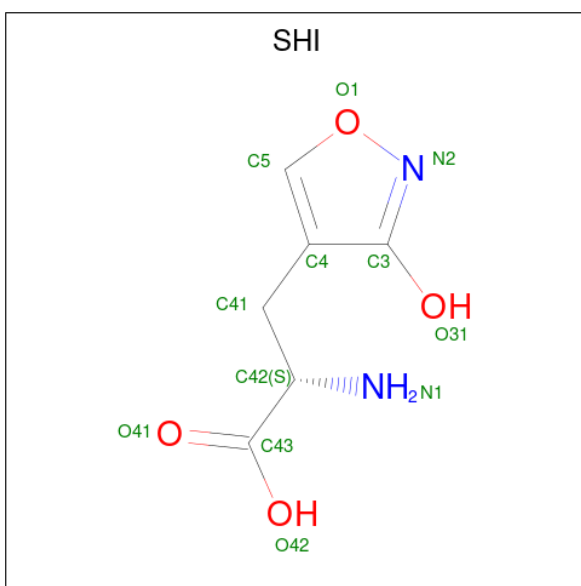
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P19491
A	-1	ALA	-	cloning artifact	UNP P19491
A	115	GLY	-	linker	UNP P19491
A	116	THR	-	linker	UNP P19491
B	-2	GLY	-	cloning artifact	UNP P19491
B	-1	ALA	-	cloning artifact	UNP P19491
B	115	GLY	-	linker	UNP P19491
B	116	THR	-	linker	UNP P19491
C	-2	GLY	-	cloning artifact	UNP P19491
C	-1	ALA	-	cloning artifact	UNP P19491
C	115	GLY	-	linker	UNP P19491
C	116	THR	-	linker	UNP P19491
D	-2	GLY	-	cloning artifact	UNP P19491
D	-1	ALA	-	cloning artifact	UNP P19491
D	115	GLY	-	linker	UNP P19491
D	116	THR	-	linker	UNP P19491

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



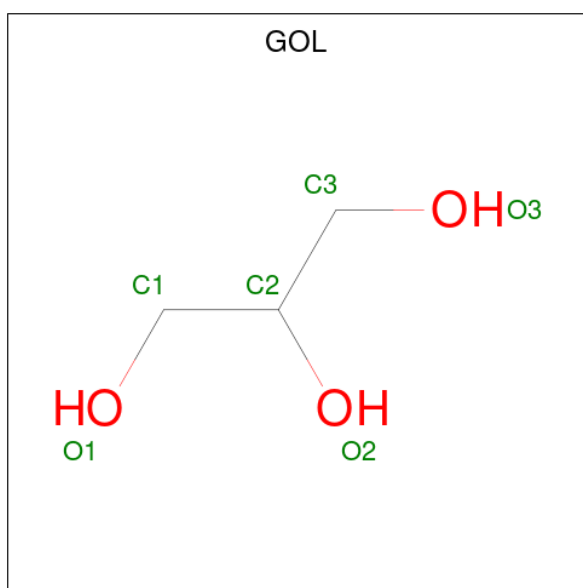
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (S)-2-AMINO-3-(3-HYDROXY-ISOXAZOL-4-YL)PROPIONIC ACID (CCD ID: SHI) (formula: C₆H₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	2	4		
3	B	1	Total	C	N	O	0	0
			12	6	2	4		
3	C	1	Total	C	N	O	0	0
			12	6	2	4		
3	D	1	Total	C	N	O	0	0
			12	6	2	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	684	Total	O	0	0
			684	684		
5	B	646	Total	O	0	0
			646	646		
5	C	639	Total	O	0	0
			639	639		
5	D	657	Total	O	0	0
			657	657		

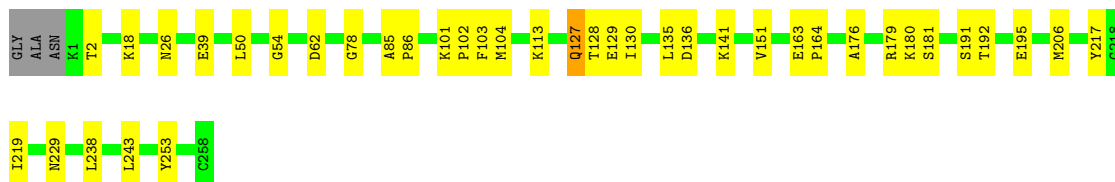
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

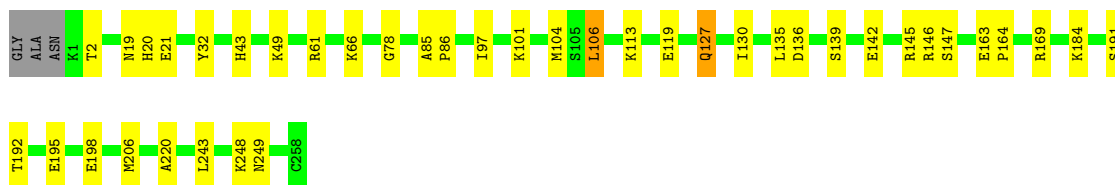
- Molecule 1: Glutamate receptor subunit 2

Chain A: 



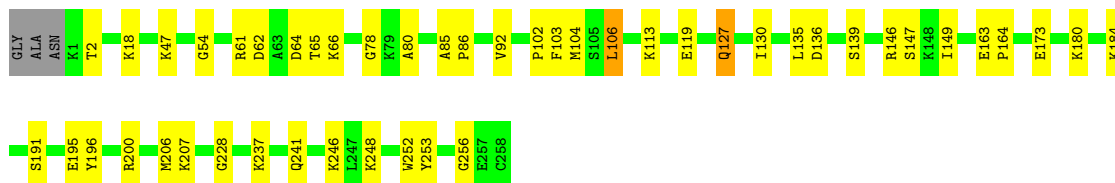
- Molecule 1: Glutamate receptor subunit 2

Chain B: 



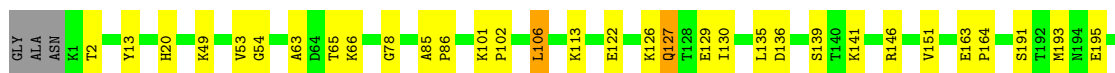
- Molecule 1: Glutamate receptor subunit 2

Chain C: 



- Molecule 1: Glutamate receptor subunit 2

Chain D: 



K206	K207	Y217	L227	G228	N229	A230	V231	L243	K246	Y253	C258
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.44Å 47.51Å 123.92Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	19.24 – 1.46	Depositor
% Data completeness (in resolution range)	98.5 (19.24-1.46)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.192	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10947	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SHI, GOL, SO4

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	0.32	0/2089	0.86	8/2807 (0.3%)
1	B	0.33	0/2141	0.88	7/2878 (0.2%)
1	C	0.33	0/2097	0.88	12/2817 (0.4%)
1	D	0.32	0/2069	0.87	7/2781 (0.3%)
All	All	0.33	0/8396	0.87	34/11283 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	N-CA-C	-7.59	99.97	110.29
1	D	135	LEU	N-CA-C	-7.03	100.78	110.35
1	B	2	THR	N-CA-C	-7.02	99.64	110.10
1	C	256	GLY	N-CA-C	-6.86	104.04	111.93
1	A	135	LEU	N-CA-C	-6.69	101.25	110.35
1	A	113	LYS	N-CA-C	-6.38	100.11	110.20
1	D	113	LYS	N-CA-C	-6.18	100.43	110.20
1	B	101	LYS	N-CA-C	-6.07	101.21	110.01
1	B	113	LYS	N-CA-C	-6.03	100.68	110.20
1	D	253	TYR	N-CA-C	6.02	121.13	113.55
1	C	135	LEU	N-CA-C	-5.94	101.61	110.23
1	A	2	THR	N-CA-C	-5.90	101.11	109.96
1	C	2	THR	N-CA-C	-5.74	101.36	109.96
1	D	2	THR	N-CA-C	-5.63	101.51	109.96
1	C	113[A]	LYS	N-CA-C	-5.61	101.34	110.20
1	C	113[B]	LYS	N-CA-C	-5.61	101.34	110.20
1	A	219	ILE	N-CA-C	-5.59	101.52	108.89
1	B	147	SER	N-CA-C	5.50	117.99	110.24
1	A	253	TYR	N-CA-C	5.46	120.43	113.55
1	A	181	SER	N-CA-C	5.33	119.42	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLY	N-CA-C	5.28	119.02	112.64
1	C	228	GLY	N-CA-C	5.26	119.01	112.64
1	C	54	GLY	N-CA-C	5.24	118.98	112.64
1	C	253	TYR	N-CA-C	5.23	120.31	113.88
1	B	139	SER	N-CA-C	5.19	117.68	111.71
1	C	139	SER	N-CA-C	5.16	117.64	111.71
1	C	102	PRO	N-CA-C	5.13	119.14	111.14
1	B	20	HIS	N-CA-C	5.12	118.30	111.75
1	C	147	SER	N-CA-C	5.12	117.46	110.24
1	D	54	GLY	N-CA-C	5.08	118.79	112.64
1	C	136	ASP	N-CA-C	5.04	119.05	113.01
1	A	101	LYS	N-CA-C	-5.02	102.97	110.20
1	D	101	LYS	N-CA-C	-5.02	102.97	110.20
1	D	139	SER	N-CA-C	5.02	117.48	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2053	0	2074	29	0
1	B	2105	0	2117	37	0
1	C	2061	0	2098	36	0
1	D	2033	0	2061	28	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
3	A	12	0	6	1	0
3	B	12	0	6	0	0
3	C	12	0	6	0	0
3	D	12	0	6	0	0
4	A	6	0	8	0	0
5	A	684	0	0	10	0
5	B	646	0	0	13	0
5	C	639	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	657	0	0	11	0
All	All	10947	0	8382	131	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 8.

All (131) 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:61:ARG:HH21	1:C:66:LYS:HD2	1.26	0.98
1:C:127:GLN:HE22	1:C:130:ILE:H	1.01	0.94
1:B:136[A]:ASP:OD2	1:B:169:ARG:HD2	1.68	0.94
1:A:127:GLN:HE22	1:A:130:ILE:H	1.15	0.93
1:B:142:GLU:HG3	5:B:4554:HOH:O	1.71	0.90
1:C:64:ASP:OD1	1:C:65:THR:HG23	1.71	0.89
1:C:61:ARG:NH2	1:C:66:LYS:HD2	1.87	0.89
1:D:127:GLN:HE22	1:D:130:ILE:H	1.21	0.83
1:A:206:MET:HE1	5:A:4173:HOH:O	1.81	0.81
1:A:238:LEU:HD22	1:A:243:LEU:HD22	1.61	0.80
1:A:176:ALA:O	1:A:180:LYS:HD3	1.81	0.80
1:C:149[B]:ILE:HD13	5:C:3484:HOH:O	1.87	0.74
1:C:127:GLN:NE2	1:C:130:ILE:H	1.83	0.71
1:C:127:GLN:HE22	1:C:130:ILE:N	1.83	0.71
1:C:206:MET:HE1	5:C:3207:HOH:O	1.94	0.68
1:D:49:LYS:HE3	5:D:4275:HOH:O	1.94	0.68
1:B:127:GLN:HE22	1:B:130:ILE:N	1.88	0.67
1:A:26:ASN:ND2	1:A:50:LEU:H	1.93	0.66
1:A:26:ASN:HD21	1:A:50:LEU:H	1.40	0.66
1:A:18:LYS:HE3	5:A:4560:HOH:O	1.96	0.66
1:D:78:GLY:HA2	5:D:4549:HOH:O	1.95	0.66
1:D:206:MET:HE1	5:D:4129:HOH:O	1.95	0.66
1:B:61:ARG:CZ	1:B:66:LYS:HE3	2.27	0.65
1:A:179:ARG:HB2	1:A:180:LYS:HZ3	1.61	0.65
1:B:146:ARG:HB3	5:B:4110:HOH:O	1.96	0.65
1:B:249:ASN:HB3	5:B:4638:HOH:O	1.97	0.65
1:C:78:GLY:HA2	5:C:3406:HOH:O	1.97	0.65
1:B:66:LYS:HB3	5:B:4478:HOH:O	1.96	0.64
1:B:78:GLY:HA2	5:B:4243:HOH:O	1.96	0.64
1:B:184:LYS:HE2	5:B:4211:HOH:O	1.96	0.64
1:A:128:THR:HG22	5:A:4637:HOH:O	1.96	0.64
1:D:207:LYS:HD3	5:D:4612:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:HH21	1:C:66:LYS:CD	2.08	0.63
1:C:85:ALA:HB1	1:C:86:PRO:HD2	1.80	0.62
1:B:85:ALA:HB1	1:B:86:PRO:HD2	1.82	0.61
1:B:66:LYS:HG2	5:B:4286:HOH:O	1.98	0.61
1:B:195[A]:GLU:HG2	5:B:4525:HOH:O	2.00	0.60
1:A:180:LYS:HD3	1:A:180:LYS:N	2.17	0.60
1:A:78:GLY:HA2	5:A:4611:HOH:O	2.01	0.59
1:D:85:ALA:HB1	1:D:86:PRO:HD2	1.84	0.59
1:A:85:ALA:HB1	1:A:86:PRO:HD2	1.85	0.58
1:C:61:ARG:NH1	5:C:3386:HOH:O	2.37	0.57
1:C:206:MET:CE	5:C:3207:HOH:O	2.52	0.56
1:D:191:SER:O	1:D:195:GLU:HG3	2.06	0.56
1:A:103:PHE:CD1	1:A:104[A]:MET:HG3	2.40	0.56
1:C:119:GLU:HB3	5:C:3576:HOH:O	2.04	0.56
1:D:227:LEU:HD23	1:D:227:LEU:O	2.06	0.56
1:A:238:LEU:HD22	1:A:243:LEU:CD2	2.35	0.55
1:A:180:LYS:N	1:A:180:LYS:CD	2.69	0.55
1:C:64:ASP:OD1	1:C:65:THR:N	2.39	0.55
1:B:61:ARG:NH1	1:B:66:LYS:HE3	2.21	0.55
1:D:227:LEU:CD2	1:D:231:VAL:HG23	2.36	0.55
1:D:246:LYS:HE2	5:D:4435:HOH:O	2.05	0.55
1:B:163[A]:GLU:HA	1:B:164:PRO:C	2.32	0.55
1:C:207:LYS:HE2	5:C:3298:HOH:O	2.05	0.55
1:A:191:SER:O	1:A:195:GLU:HG3	2.07	0.55
1:B:49:LYS:HE3	5:B:4377:HOH:O	2.06	0.54
1:A:39:GLU:HG3	1:A:243:LEU:HD21	1.89	0.54
1:D:127:GLN:HE22	1:D:130:ILE:N	2.00	0.54
1:B:106:LEU:HD22	1:B:106:LEU:C	2.33	0.53
1:A:127:GLN:HE22	1:A:130:ILE:N	1.96	0.53
1:C:80:ALA:HB2	5:C:3630:HOH:O	2.09	0.53
1:C:246:LYS:NZ	5:C:3539:HOH:O	2.42	0.52
1:A:103:PHE:HD1	1:A:104[A]:MET:HG3	1.74	0.52
1:A:151:VAL:HG23	5:A:4262:HOH:O	2.08	0.52
1:B:163[B]:GLU:HA	1:B:164:PRO:C	2.35	0.52
1:C:61:ARG:HE	1:C:66:LYS:HA	1.75	0.52
1:D:136[A]:ASP:OD1	1:D:141:LYS:NZ	2.38	0.51
1:A:127:GLN:NE2	1:A:130:ILE:H	1.96	0.51
1:D:227:LEU:HD23	1:D:231:VAL:HG23	1.91	0.51
1:C:106:LEU:HD13	1:C:106:LEU:N	2.26	0.50
1:D:20:HIS:HE1	5:D:4504:HOH:O	1.94	0.50
1:D:63:ALA:HB3	5:D:4607:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PHE:CD1	1:C:104[B]:MET:HG3	2.47	0.49
3:A:3001:SHI:H412	5:A:4686:HOH:O	2.13	0.49
1:D:227:LEU:CD2	1:D:231:VAL:CG2	2.90	0.49
1:B:192:THR:O	1:B:195[B]:GLU:HG2	2.13	0.49
1:D:243:LEU:C	1:D:243:LEU:HD13	2.38	0.48
1:B:198:GLU:OE2	1:B:206[B]:MET:SD	2.72	0.48
1:A:163:GLU:HA	1:A:164:PRO:C	2.39	0.47
1:A:136[B]:ASP:OD1	1:A:141:LYS:NZ	2.40	0.47
1:A:206:MET:HE2	5:A:4334:HOH:O	2.15	0.47
1:D:151:VAL:HG23	5:D:4137:HOH:O	2.14	0.47
1:B:61:ARG:NH2	1:B:66:LYS:HE3	2.30	0.47
1:C:103:PHE:HD1	1:C:104[B]:MET:HG3	1.80	0.47
1:C:47:LYS:HD3	5:C:3225:HOH:O	2.15	0.46
1:A:62:ASP:HB2	5:A:4534:HOH:O	2.16	0.46
1:D:106:LEU:HD13	1:D:106:LEU:N	2.30	0.45
1:B:191:SER:O	1:B:195[B]:GLU:HG2	2.16	0.45
1:A:104[B]:MET:SD	1:A:192:THR:HG21	2.57	0.45
1:B:142:GLU:CD	1:B:145:ARG:HH11	2.25	0.45
1:C:180:LYS:HE2	5:C:3372:HOH:O	2.17	0.45
1:B:66:LYS:HE2	5:B:4286:HOH:O	2.16	0.44
1:B:43:HIS:HE1	5:B:4233:HOH:O	2.00	0.44
1:B:142:GLU:CD	1:B:145:ARG:NH1	2.75	0.44
1:D:13:TYR:CE2	1:D:193:MET:HE3	2.52	0.44
1:B:195[B]:GLU:OE2	1:B:248:LYS:NZ	2.43	0.44
1:B:243:LEU:C	1:B:243:LEU:HD13	2.43	0.44
1:D:163:GLU:HA	1:D:164:PRO:C	2.42	0.44
1:C:62:ASP:HB3	1:C:65:THR:OG1	2.17	0.44
1:B:32:TYR:CZ	1:B:104:MET:HE3	2.53	0.43
1:B:119:GLU:HG2	5:B:4389:HOH:O	2.18	0.43
1:C:18:LYS:HD3	1:C:18:LYS:HA	1.65	0.43
1:C:92:VAL:HG11	1:C:146:ARG:HH22	1.84	0.43
1:D:65:THR:O	1:D:66:LYS:HB2	2.19	0.43
1:D:53:VAL:HA	5:D:4599:HOH:O	2.18	0.43
1:A:206:MET:CE	5:A:4173:HOH:O	2.54	0.42
1:C:248:LYS:O	1:C:252:TRP:HB2	2.20	0.42
1:D:206:MET:CE	5:D:4129:HOH:O	2.61	0.42
1:A:102:PRO:HA	1:A:217:TYR:O	2.19	0.42
1:C:184:LYS:HE2	5:C:3570:HOH:O	2.19	0.42
1:D:102:PRO:HA	1:D:217:TYR:O	2.19	0.42
1:B:206[A]:MET:HE1	5:B:4177:HOH:O	2.19	0.41
1:C:196:TYR:O	1:C:200:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASN:OD1	1:B:19:ASN:N	2.52	0.41
1:D:146:ARG:HA	1:D:146:ARG:HD3	1.95	0.41
1:A:229:ASN:ND2	5:A:4498:HOH:O	2.53	0.41
1:B:136[A]:ASP:OD2	1:B:169:ARG:CD	2.54	0.41
1:C:65:THR:O	1:C:66:LYS:HB2	2.20	0.41
1:D:229:ASN:ND2	5:D:4481:HOH:O	2.54	0.41
1:C:163:GLU:HA	1:C:164:PRO:C	2.45	0.41
1:C:18:LYS:NZ	5:C:3638:HOH:O	2.53	0.41
1:D:122:GLU:CG	1:D:126:LYS:HE3	2.51	0.41
1:C:191:SER:O	1:C:195:GLU:HG3	2.21	0.41
1:C:237:LYS:O	1:C:241:GLN:HG3	2.21	0.41
1:B:97:ILE:HD12	1:B:220:ALA:HB1	2.03	0.40
1:C:173[B]:GLU:HG3	5:C:3143:HOH:O	2.22	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	260/261 (100%)	256 (98%)	4 (2%)	0	100	100
1	B	267/261 (102%)	262 (98%)	5 (2%)	0	100	100
1	C	261/261 (100%)	257 (98%)	4 (2%)	0	100	100
1	D	258/261 (99%)	255 (99%)	3 (1%)	0	100	100
All	All	1046/1044 (100%)	1030 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	221/218 (101%)	219 (99%)	2 (1%)	70	46
1	B	228/218 (105%)	225 (99%)	3 (1%)	61	31
1	C	222/218 (102%)	220 (99%)	2 (1%)	70	46
1	D	219/218 (100%)	216 (99%)	3 (1%)	59	28
All	All	890/872 (102%)	880 (99%)	10 (1%)	63	38

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	129	GLU
1	B	21	GLU
1	B	106	LEU
1	B	127	GLN
1	C	106	LEU
1	C	127	GLN
1	D	106	LEU
1	D	127	GLN
1	D	129	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	127	GLN
1	A	249	ASN
1	B	43	HIS
1	B	127	GLN
1	B	199	GLN
1	B	239	ASN
1	C	127	GLN
1	C	229	ASN

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Mol	Chain	Res	Type
1	C	249	ASN
1	D	127	GLN

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 ⓘ

8 ligands are modelled in this entry.

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	SO4	B	4001	-	4,4,4	1.02	0	6,6,6	0.46	0
3	SHI	A	3001	-	11,12,12	1.58	2 (18%)	7,16,16	0.89	0
3	SHI	B	3002	-	11,12,12	1.70	2 (18%)	7,16,16	0.79	0
3	SHI	D	3004	-	11,12,12	1.68	2 (18%)	7,16,16	0.91	0
4	GOL	A	3230	-	5,5,5	0.56	0	5,5,5	1.35	1 (20%)
2	SO4	D	4003	-	4,4,4	1.03	0	6,6,6	0.43	0
3	SHI	C	3003	-	11,12,12	1.70	2 (18%)	7,16,16	0.96	0
2	SO4	A	4002	-	4,4,4	0.99	0	6,6,6	0.42	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	SHI	A	3001	-	-	0/8/8/8	0/1/1/1
3	SHI	B	3002	-	-	0/8/8/8	0/1/1/1
3	SHI	D	3004	-	-	0/8/8/8	0/1/1/1
4	GOL	A	3230	-	-	0/4/4/4	-
3	SHI	C	3003	-	-	0/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3003	SHI	C3-N2	3.93	1.34	1.31
3	B	3002	SHI	C3-N2	3.87	1.34	1.31
3	D	3004	SHI	C3-N2	3.72	1.34	1.31
3	A	3001	SHI	C3-N2	3.33	1.34	1.31
3	B	3002	SHI	O31-C3	-2.24	1.26	1.33
3	A	3001	SHI	O31-C3	-2.19	1.27	1.33
3	D	3004	SHI	O31-C3	-2.16	1.27	1.33
3	C	3003	SHI	O31-C3	-2.03	1.27	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3230	GOL	C3-C2-C1	-2.05	104.28	111.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	SHI	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.