



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:49 PM UTC

PDB ID : 4LZ5 / pdb_00004lz5
Title : Crystal structures of GLuR2 ligand-binding-domain in complex with glutamate and positive allosteric modulators
Authors : Pandit, J.
Deposited on : 2013-07-31
Resolution : 1.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

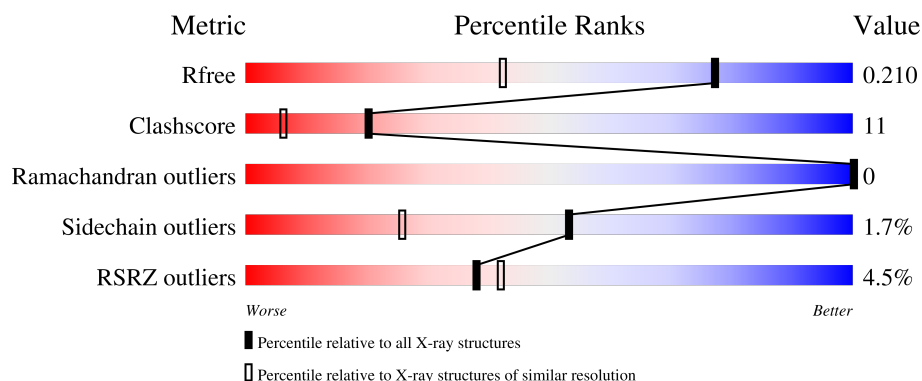
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	275	4% 68% 23% 6%
1	B	275	4% 69% 22% 7%
1	C	275	5% 71% 19% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7405 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	A	258	Total	C	N	O	S	0	0	0
			2018	1286	336	382	14			
1	B	257	Total	C	N	O	S	0	0	0
			2009	1280	334	381	14			
1	C	257	Total	C	N	O	S	0	0	0
			2008	1279	334	381	14			

There are 30 discrepancies between the modelled and reference sequences:

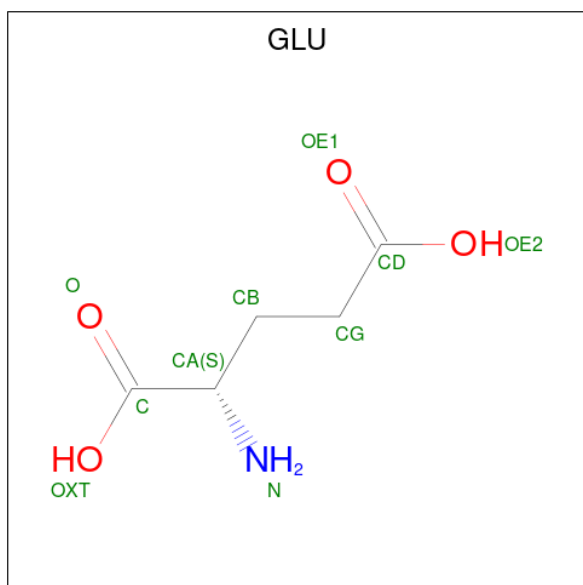
Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLY	-	expression tag	UNP P19491
A	379	SER	-	expression tag	UNP P19491
A	380	ALA	-	expression tag	UNP P19491
A	381	MET	-	expression tag	UNP P19491
A	382	GLY	-	expression tag	UNP P19491
A	389	ARG	GLY	engineered mutation	UNP P19491
A	390	GLY	LEU	engineered mutation	UNP P19491
A	391	ALA	GLU	engineered mutation	UNP P19491
A	507	GLY	-	linker	UNP P19491
A	508	THR	-	linker	UNP P19491
B	378	GLY	-	expression tag	UNP P19491
B	379	SER	-	expression tag	UNP P19491
B	380	ALA	-	expression tag	UNP P19491
B	381	MET	-	expression tag	UNP P19491
B	382	GLY	-	expression tag	UNP P19491
B	389	ARG	GLY	engineered mutation	UNP P19491
B	390	GLY	LEU	engineered mutation	UNP P19491
B	391	ALA	GLU	engineered mutation	UNP P19491
B	507	GLY	-	linker	UNP P19491
B	508	THR	-	linker	UNP P19491
C	378	GLY	-	expression tag	UNP P19491
C	379	SER	-	expression tag	UNP P19491
C	380	ALA	-	expression tag	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	381	MET	-	expression tag	UNP P19491
C	382	GLY	-	expression tag	UNP P19491
C	389	ARG	GLY	engineered mutation	UNP P19491
C	390	GLY	LEU	engineered mutation	UNP P19491
C	391	ALA	GLU	engineered mutation	UNP P19491
C	507	GLY	-	linker	UNP P19491
C	508	THR	-	linker	UNP P19491

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

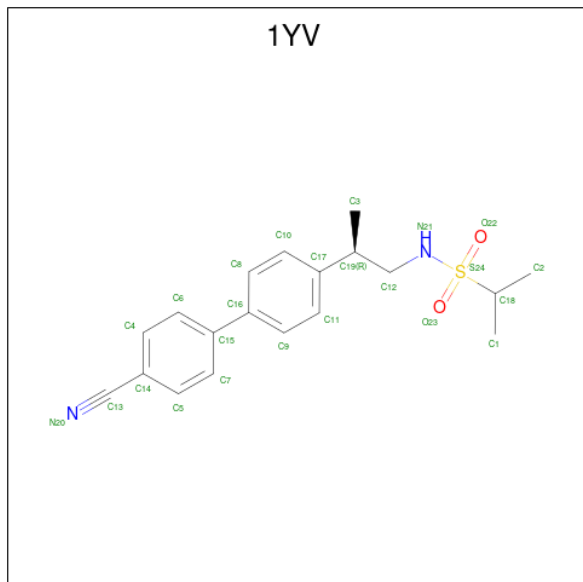


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		

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

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

- Molecule 4 is N-[(2R)-2-(4'-cyanobiphenyl-4-yl)propyl]propane-2-sulfonamide (CCD ID: 1YV) (formula: C₁₉H₂₂N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
4	C	1	Total	C	N	O	S	0	1
			48	38	4	4	2		

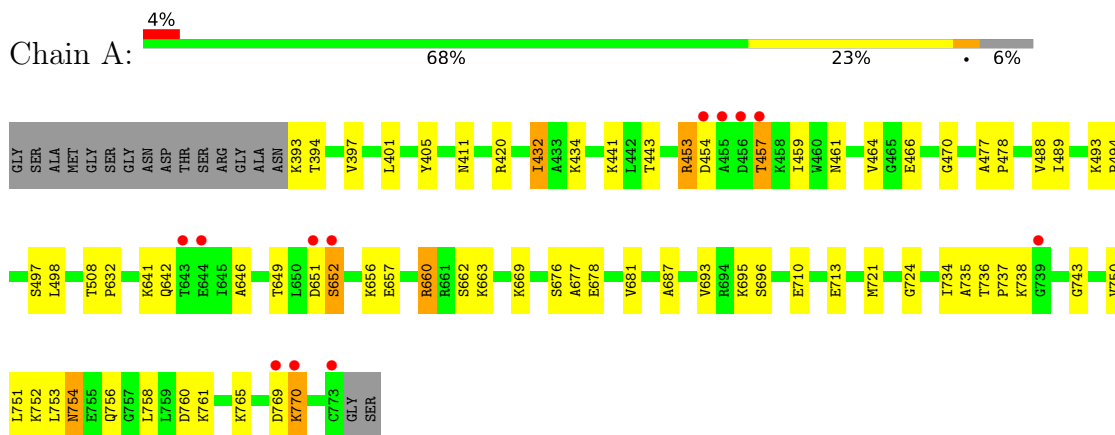
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	415	Total	O	0	0
			415	415		
5	B	475	Total	O	0	0
			475	475		
5	C	373	Total	O	0	0
			373	373		

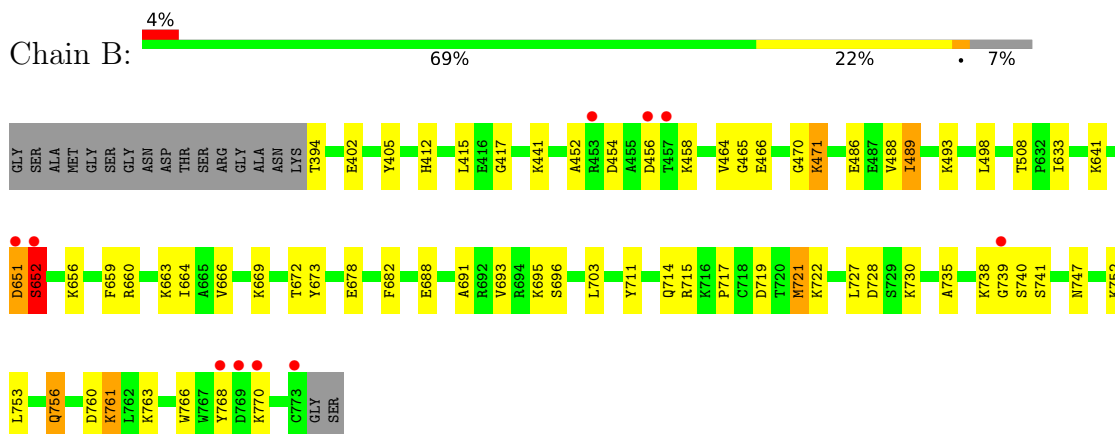
3 Residue-property plots [i](#)

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.

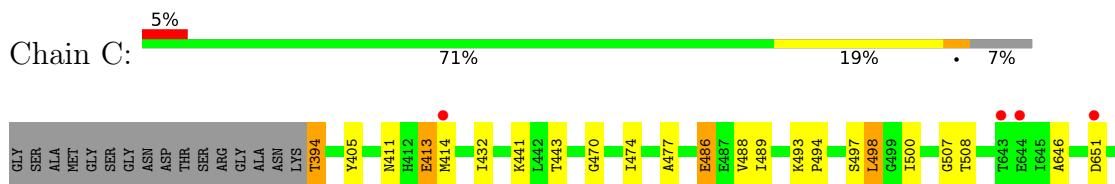
• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.75Å 164.54Å 47.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.07 – 1.50 94.07 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (94.07-1.50) 98.1 (94.07-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.203 0.177 , 0.210	Depositor DCC
R_{free} test set	7111 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7405	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.64% 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, 1YV

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	2.00	44/2054 (2.1%)	1.65	21/2762 (0.8%)
1	B	2.00	41/2045 (2.0%)	1.69	28/2751 (1.0%)
1	C	1.86	27/2044 (1.3%)	1.52	9/2749 (0.3%)
All	All	1.95	112/6143 (1.8%)	1.62	58/8262 (0.7%)

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	A	0	1

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	721	MET	SD-CE	-15.74	1.40	1.79
1	B	738	LYS	CA-C	-11.85	1.37	1.52
1	C	721	MET	SD-CE	-9.44	1.55	1.79
1	B	738	LYS	CB-CG	-8.96	1.25	1.52
1	B	652	SER	CA-C	8.85	1.67	1.52
1	C	738	LYS	CB-CG	-8.53	1.26	1.52
1	A	710	GLU	CD-OE1	8.39	1.41	1.25
1	A	662	SER	N-CA	-8.12	1.36	1.46
1	B	493	LYS	CG-CD	-7.99	1.28	1.52
1	A	652	SER	CA-C	7.98	1.64	1.53
1	B	730	LYS	CA-CB	-7.94	1.43	1.53
1	A	651	ASP	C-O	7.84	1.34	1.24
1	B	722	LYS	C-O	7.84	1.33	1.24
1	B	721	MET	CA-CB	7.78	1.67	1.53
1	B	652	SER	N-CA	7.67	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	687	ALA	N-CA	-7.66	1.37	1.46
1	A	710	GLU	CG-CD	7.61	1.71	1.52
1	C	729	SER	N-CA	-7.59	1.37	1.46
1	A	494	PRO	CA-CB	-7.49	1.43	1.53
1	B	652	SER	C-O	7.34	1.32	1.23
1	B	405	TYR	CZ-OH	7.26	1.53	1.38
1	C	709	ASN	C-O	7.15	1.32	1.24
1	C	738	LYS	CA-C	-6.92	1.43	1.52
1	A	770	LYS	CA-C	6.78	1.62	1.52
1	B	740	SER	C-O	6.64	1.31	1.23
1	A	656	LYS	N-CA	6.62	1.54	1.46
1	A	677	ALA	CA-CB	6.61	1.64	1.53
1	B	664	ILE	N-CA	-6.59	1.38	1.46
1	B	678	GLU	CD-OE1	6.55	1.37	1.25
1	C	684	ARG	C-O	6.53	1.32	1.24
1	A	432	ILE	N-CA	6.52	1.54	1.46
1	B	761	LYS	CE-NZ	6.49	1.68	1.49
1	B	696	SER	CB-OG	6.45	1.55	1.42
1	C	646	ALA	N-CA	6.42	1.54	1.45
1	B	464	VAL	CA-CB	-6.30	1.47	1.54
1	A	721	MET	CB-CG	-6.29	1.33	1.52
1	B	493	LYS	CB-CG	6.28	1.71	1.52
1	A	713	GLU	C-O	6.26	1.31	1.24
1	B	717	PRO	CG-CD	-6.25	1.34	1.51
1	A	737	PRO	C-O	6.24	1.31	1.23
1	A	405	TYR	CZ-OH	6.08	1.50	1.38
1	B	659	PHE	CA-C	6.05	1.60	1.52
1	A	641	LYS	N-CA	5.99	1.53	1.46
1	A	738	LYS	C-O	5.95	1.30	1.23
1	C	691	ALA	CA-C	-5.95	1.45	1.52
1	C	681	VAL	N-CA	5.94	1.54	1.46
1	A	660	ARG	N-CA	5.92	1.53	1.46
1	B	471	LYS	N-CA	5.88	1.53	1.46
1	A	750	VAL	N-CA	-5.87	1.39	1.46
1	B	768	TYR	C-O	5.86	1.30	1.24
1	B	673	TYR	CA-CB	-5.83	1.44	1.53
1	C	443	THR	C-O	5.83	1.30	1.24
1	C	767	TRP	C-O	5.75	1.30	1.23
1	B	719	ASP	N-CA	-5.75	1.39	1.46
1	A	394	THR	CA-CB	-5.70	1.44	1.53
1	A	721	MET	SD-CE	-5.66	1.65	1.79
1	C	474	ILE	CA-CB	-5.64	1.49	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	488	VAL	CA-CB	-5.63	1.47	1.54
1	A	488	VAL	CA-C	5.62	1.60	1.52
1	A	464	VAL	CA-CB	-5.62	1.47	1.54
1	C	762	LEU	CA-C	-5.61	1.45	1.52
1	C	669	LYS	C-O	-5.58	1.17	1.24
1	B	688	GLU	C-O	-5.57	1.17	1.24
1	B	678	GLU	CB-CG	-5.55	1.35	1.52
1	A	477	ALA	N-CA	-5.55	1.40	1.46
1	B	738	LYS	N-CA	-5.55	1.39	1.46
1	C	732	TYR	N-CA	5.54	1.52	1.46
1	B	768	TYR	N-CA	5.52	1.52	1.46
1	A	736	THR	CA-CB	5.50	1.60	1.54
1	C	493	LYS	C-N	-5.48	1.26	1.33
1	C	665	ALA	CA-CB	5.46	1.61	1.53
1	A	687	ALA	CA-CB	5.44	1.61	1.53
1	A	397	VAL	CA-C	-5.43	1.45	1.52
1	A	642	GLN	CA-C	-5.43	1.45	1.52
1	C	713	GLU	C-O	5.40	1.30	1.24
1	A	646	ALA	CA-CB	-5.38	1.44	1.53
1	B	711	TYR	CZ-OH	5.38	1.49	1.38
1	B	452	ALA	C-O	-5.36	1.17	1.23
1	C	394	THR	N-CA	5.36	1.56	1.46
1	A	441	LYS	CB-CG	-5.35	1.36	1.52
1	A	478	PRO	CA-C	5.34	1.57	1.52
1	B	672	THR	C-O	5.34	1.30	1.24
1	A	649	THR	C-O	5.33	1.30	1.23
1	B	752	LYS	CE-NZ	5.33	1.65	1.49
1	A	397	VAL	CA-CB	-5.32	1.48	1.54
1	C	500	ILE	N-CA	-5.31	1.39	1.46
1	A	508	THR	CB-OG1	-5.26	1.35	1.43
1	A	488	VAL	CA-CB	-5.26	1.48	1.54
1	A	434	LYS	CB-CG	-5.24	1.36	1.52
1	C	674	MET	C-O	-5.24	1.18	1.24
1	C	690	VAL	N-CA	5.23	1.52	1.46
1	A	632	PRO	N-CA	-5.22	1.41	1.47
1	B	682	PHE	CA-C	-5.20	1.46	1.53
1	A	738	LYS	CA-CB	5.19	1.62	1.53
1	A	743	GLY	N-CA	-5.19	1.39	1.45
1	C	670	MET	C-O	-5.15	1.18	1.24
1	B	669	LYS	N-CA	5.14	1.52	1.46
1	C	477	ALA	N-CA	-5.14	1.38	1.46
1	A	453	ARG	CA-C	5.12	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	747	ASN	N-CA	-5.12	1.40	1.46
1	B	714	GLN	C-O	5.11	1.30	1.24
1	B	756	GLN	CB-CG	-5.10	1.37	1.52
1	A	769	ASP	C-O	5.10	1.30	1.24
1	A	641	LYS	C-O	5.10	1.30	1.24
1	B	641	LYS	C-O	5.09	1.30	1.24
1	C	721	MET	CA-CB	5.08	1.64	1.54
1	A	681	VAL	N-CA	5.08	1.52	1.46
1	A	754	ASN	CG-ND2	-5.07	1.22	1.33
1	B	747	ASN	CA-C	5.05	1.59	1.52
1	B	660	ARG	N-CA	5.02	1.52	1.46
1	B	402	GLU	CA-C	-5.01	1.46	1.52
1	C	405	TYR	CZ-OH	5.01	1.48	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	THR	O-C-N	-10.21	112.22	121.30
1	A	508	THR	O-C-N	-8.93	112.35	121.28
1	B	652	SER	N-CA-C	8.65	120.83	110.44
1	C	721	MET	CG-SD-CE	-8.34	82.55	100.90
1	A	652	SER	N-CA-C	8.20	121.78	110.06
1	B	760	ASP	O-C-N	7.53	130.73	122.15
1	A	696	SER	CB-CA-C	6.85	122.14	110.56
1	B	488	VAL	N-CA-C	6.85	120.24	113.53
1	A	736	THR	O-C-N	6.84	126.88	121.55
1	B	691	ALA	CA-C-O	6.77	127.73	120.55
1	B	691	ALA	O-C-N	-6.67	115.06	122.12
1	B	652	SER	CB-CA-C	-6.59	96.74	111.77
1	B	678	GLU	CG-CD-OE1	6.59	133.56	118.40
1	C	508	THR	CA-C-O	6.59	125.94	119.75
1	B	652	SER	CA-C-O	6.58	130.38	121.89
1	B	721	MET	CG-SD-CE	-6.52	86.55	100.90
1	B	753	LEU	CA-C-O	6.25	127.17	120.55
1	B	678	GLU	OE1-CD-OE2	-6.20	108.01	122.90
1	C	508	THR	O-C-N	-6.04	115.93	121.30
1	B	766	TRP	O-C-N	6.00	130.68	122.46
1	B	656	LYS	O-C-N	5.87	128.12	122.07
1	B	738	LYS	CB-CA-C	-5.77	100.14	109.72
1	C	411	ASN	N-CA-C	5.74	119.06	112.97
1	C	443	THR	O-C-N	-5.73	116.61	123.31
1	A	752	LYS	O-C-N	-5.58	116.33	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	693	VAL	O-C-N	5.56	127.36	121.91
1	A	713	GLU	CB-CG-CD	-5.54	103.19	112.60
1	B	465	GLY	O-C-N	-5.53	116.38	122.24
1	A	736	THR	CA-C-N	-5.48	114.61	120.03
1	A	736	THR	C-N-CA	-5.48	114.61	120.03
1	C	660	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	508	THR	CA-C-N	5.40	130.16	120.88
1	A	508	THR	C-N-CA	5.40	130.16	120.88
1	C	725	GLY	N-CA-C	-5.38	104.19	112.85
1	A	646	ALA	N-CA-C	-5.36	103.31	110.55
1	B	660	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	A	693	VAL	O-C-N	5.33	127.13	121.91
1	A	669	LYS	CA-C-O	5.31	126.18	120.55
1	A	724	GLY	CA-C-O	-5.29	117.09	122.59
1	B	666	VAL	N-CA-C	-5.23	105.44	110.72
1	A	453	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	B	763	LYS	O-C-N	5.21	127.51	122.09
1	B	489	ILE	CA-C-O	-5.20	116.55	121.64
1	C	507	GLY	CA-C-O	5.19	124.75	119.10
1	B	633	ILE	CA-C-O	-5.14	114.83	120.43
1	B	659	PHE	O-C-N	5.14	128.01	122.15
1	B	728	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	761	LYS	CD-CE-NZ	5.12	128.28	111.90
1	B	703	LEU	O-C-N	-5.11	117.39	123.22
1	A	420	ARG	CA-C-O	5.08	125.62	119.38
1	B	651	ASP	CA-C-O	-5.07	113.03	119.31
1	C	750	VAL	O-C-N	5.05	126.86	121.91
1	A	676	SER	O-C-N	-5.04	116.15	122.35
1	A	411	ASN	N-CA-C	5.04	118.27	112.57
1	A	760	ASP	O-C-N	5.04	127.89	122.15
1	B	763	LYS	N-CA-C	5.02	117.14	111.11
1	A	461	ASN	OD1-CG-ND2	-5.00	117.60	122.60
1	A	678	GLU	O-C-N	5.00	126.18	121.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	THR	Mainchain

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	2018	0	2050	49	0
1	B	2009	0	2037	36	0
1	C	2008	0	2033	52	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
3	B	3	0	0	0	0
3	C	2	0	0	1	0
4	B	24	0	22	3	0
4	C	48	0	44	6	0
5	A	415	0	0	28	0
5	B	475	0	0	29	0
5	C	373	0	0	29	0
All	All	7405	0	6201	139	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 11.

All (139) 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:B:761:LYS:CE	1:B:761:LYS:NZ	1.68	1.56
4:B:805:1YV:H4	5:B:1252:HOH:O	1.12	1.25
1:A:770:LYS:HG2	5:A:1291:HOH:O	1.37	1.20
1:C:677:ALA:CA	5:C:1266:HOH:O	1.92	1.17
1:A:652:SER:N	5:A:1302:HOH:O	1.77	1.04
1:C:394:THR:N	5:C:1257:HOH:O	1.97	0.96
1:C:414:MET:CE	5:C:1244:HOH:O	2.15	0.95
1:C:432:ILE:HD13	1:C:734:ILE:HD13	1.51	0.93
1:C:432:ILE:CD1	1:C:734:ILE:CD1	2.48	0.92
1:B:695:LYS:HG2	5:B:1025:HOH:O	1.68	0.91
1:A:457:THR:HG21	5:A:1176:HOH:O	1.71	0.90
1:A:466:GLU:CD	5:A:1292:HOH:O	2.16	0.89
1:C:432:ILE:HD11	1:C:734:ILE:HD11	1.55	0.89
1:A:432:ILE:HD11	1:A:734:ILE:HD11	1.53	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:SER:CA	5:A:1302:HOH:O	2.20	0.87
1:C:413:GLU:CG	5:C:1256:HOH:O	2.23	0.87
1:B:458:LYS:HE2	5:B:1314:HOH:O	1.74	0.86
1:A:432:ILE:CD1	1:A:734:ILE:CD1	2.54	0.86
1:B:739:GLY:HA2	5:B:1363:HOH:O	1.75	0.85
1:A:432:ILE:HD13	1:A:734:ILE:HD13	1.60	0.83
1:A:756:GLN:OE1	1:C:663:LYS:NZ	2.11	0.82
1:C:413:GLU:HG2	5:C:1256:HOH:O	1.81	0.81
1:C:441:LYS:HE2	5:C:904:HOH:O	1.80	0.81
1:A:466:GLU:CG	5:A:1292:HOH:O	2.27	0.80
1:A:652:SER:O	1:A:652:SER:OG	1.96	0.80
1:C:432:ILE:HD13	1:C:734:ILE:CD1	2.10	0.79
1:C:414:MET:HE2	5:C:1244:HOH:O	1.82	0.78
1:A:695:LYS:HG3	5:A:1025:HOH:O	1.83	0.78
1:C:432:ILE:HD11	1:C:734:ILE:CD1	2.13	0.78
1:A:432:ILE:HD13	1:A:734:ILE:CD1	2.14	0.77
1:A:466:GLU:HG3	5:A:1292:HOH:O	1.83	0.76
1:B:486:GLU:OE2	5:B:1295:HOH:O	2.03	0.76
1:B:770:LYS:HG3	5:B:1318:HOH:O	1.85	0.76
1:A:432:ILE:CD1	1:A:734:ILE:HD11	2.17	0.75
1:C:432:ILE:CD1	1:C:734:ILE:HD11	2.14	0.75
1:B:739:GLY:N	5:B:1363:HOH:O	2.20	0.74
1:C:739:GLY:HA2	5:C:1229:HOH:O	1.88	0.73
1:A:770:LYS:NZ	5:A:1265:HOH:O	2.20	0.73
1:C:713:GLU:OE1	5:C:1227:HOH:O	2.07	0.73
1:B:756:GLN:OE1	5:B:1360:HOH:O	2.06	0.72
1:B:739:GLY:CA	5:B:1363:HOH:O	2.36	0.71
1:A:432:ILE:CD1	1:A:734:ILE:HD13	2.20	0.71
1:C:715:ARG:HB2	5:C:1077:HOH:O	1.91	0.69
1:B:770:LYS:HE2	5:B:1099:HOH:O	1.92	0.69
3:C:801:ZN:ZN	5:C:1241:HOH:O	1.42	0.68
1:B:651:ASP:O	5:B:1348:HOH:O	2.11	0.68
1:C:738:LYS:HE2	5:C:1025:HOH:O	1.95	0.66
1:A:432:ILE:HD11	1:A:734:ILE:CD1	2.20	0.66
1:A:493:LYS:HB2	5:A:1039:HOH:O	1.96	0.65
1:B:715:ARG:HB2	5:B:1130:HOH:O	1.97	0.64
1:B:466:GLU:OE1	5:B:1033:HOH:O	2.15	0.63
1:A:756:GLN:NE2	5:A:1294:HOH:O	2.09	0.62
1:C:432:ILE:CD1	1:C:734:ILE:HD13	2.18	0.62
1:C:713:GLU:CD	5:C:1227:HOH:O	2.43	0.61
1:A:393:LYS:N	5:A:1253:HOH:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:LYS:HE3	5:A:1031:HOH:O	2.00	0.61
1:C:738:LYS:NZ	5:C:1239:HOH:O	2.30	0.60
1:C:758:LEU:CD2	1:C:761:LYS:HE2	2.33	0.59
1:A:493:LYS:NZ	1:C:486:GLU:OE2	2.27	0.59
4:B:805:1YV:O23	5:B:1252:HOH:O	2.15	0.58
1:C:751:LEU:HD23	4:C:804[A]:1YV:H7	1.84	0.58
1:C:651:ASP:HA	5:C:1034:HOH:O	2.04	0.58
1:A:765:LYS:O	1:A:770:LYS:HE3	2.04	0.57
1:C:651:ASP:CA	5:C:1034:HOH:O	2.53	0.57
1:A:393:LYS:NZ	5:A:1182:HOH:O	2.38	0.57
1:C:675:ARG:NH1	1:C:676:SER:OG	2.38	0.57
1:B:412:HIS:HA	1:B:415:LEU:HD13	1.87	0.56
1:B:770:LYS:CG	5:B:1318:HOH:O	2.48	0.56
1:A:695:LYS:HG2	5:A:1268:HOH:O	2.04	0.56
1:C:497:SER:HB3	4:C:804[B]:1YV:H20	1.87	0.56
1:B:441:LYS:HD2	5:B:917:HOH:O	2.08	0.54
1:A:770:LYS:CE	5:A:1061:HOH:O	2.56	0.54
1:A:652:SER:CB	5:A:1302:HOH:O	2.55	0.53
1:A:695:LYS:NZ	5:A:1185:HOH:O	2.41	0.53
1:C:755:GLU:HG3	5:C:1210:HOH:O	2.08	0.53
1:A:770:LYS:HE2	5:A:1061:HOH:O	2.07	0.53
1:B:770:LYS:HD2	5:B:1335:HOH:O	2.08	0.53
1:A:457:THR:HG22	1:A:459:ILE:H	1.73	0.52
1:A:453:ARG:NH1	5:A:1183:HOH:O	2.41	0.52
1:A:756:GLN:CD	5:A:1101:HOH:O	2.51	0.52
1:C:651:ASP:CB	5:C:1034:HOH:O	2.58	0.52
1:C:498:LEU:HD23	1:C:705:GLU:HG2	1.92	0.51
1:B:470:GLY:HA2	5:B:1006:HOH:O	2.10	0.51
1:C:761:LYS:HE3	5:C:1268:HOH:O	2.09	0.51
1:C:751:LEU:HD23	4:C:804[A]:1YV:C1	2.41	0.51
1:C:738:LYS:CE	5:C:1025:HOH:O	2.54	0.51
1:A:454:ASP:HB3	1:A:457:THR:HG22	1.92	0.51
1:A:663:LYS:NZ	5:A:1279:HOH:O	2.42	0.51
1:C:668:ASP:OD1	5:C:1261:HOH:O	2.19	0.51
1:C:413:GLU:HG3	5:C:1256:HOH:O	2.00	0.50
1:A:652:SER:HB3	5:A:1302:HOH:O	2.12	0.49
1:B:770:LYS:C	5:B:1346:HOH:O	2.55	0.49
1:A:754:ASN:HD22	4:C:804[B]:1YV:H1	1.79	0.48
1:C:756:GLN:HG3	5:C:1211:HOH:O	2.12	0.48
1:B:770:LYS:CB	5:B:1346:HOH:O	2.62	0.48
4:B:805:1YV:C2	5:B:1252:HOH:O	2.00	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:LYS:HD3	5:B:1355:HOH:O	2.12	0.48
1:B:454:ASP:OD1	1:B:456:ASP:N	2.46	0.48
1:C:715:ARG:HA	1:C:772:GLU:HG2	1.95	0.48
1:B:394:THR:N	5:B:1008:HOH:O	2.47	0.48
1:A:401:LEU:HD12	5:A:1283:HOH:O	2.14	0.47
1:B:652:SER:HB3	5:B:1011:HOH:O	2.13	0.47
1:C:721:MET:HG2	1:C:723:VAL:HG13	1.96	0.47
1:C:758:LEU:HD23	1:C:761:LYS:HE2	1.96	0.47
1:A:657:GLU:OE1	1:A:660:ARG:NH1	2.44	0.47
1:C:716:LYS:H	1:C:772:GLU:HG3	1.80	0.46
1:B:695:LYS:CG	5:B:1025:HOH:O	2.44	0.46
1:C:470:GLY:HA2	5:C:945:HOH:O	2.16	0.45
1:B:741:SER:HB3	5:B:1353:HOH:O	2.16	0.45
1:C:679:PRO:HB3	5:C:1254:HOH:O	2.16	0.45
1:A:453:ARG:NH2	5:A:1264:HOH:O	2.50	0.45
1:A:457:THR:HG23	1:A:459:ILE:HG13	1.99	0.45
1:B:721:MET:HE2	1:B:721:MET:HB2	1.58	0.45
1:A:657:GLU:HG2	5:A:1004:HOH:O	2.17	0.45
1:C:716:LYS:HG3	1:C:772:GLU:HG3	1.99	0.45
1:C:721:MET:HB3	1:C:721:MET:HE3	1.62	0.44
1:A:454:ASP:OD1	1:A:457:THR:HB	2.17	0.44
1:A:497:SER:HB3	4:C:804[A]:1YV:H20	2.00	0.44
1:B:721:MET:HB3	1:B:721:MET:HE3	1.47	0.44
1:C:721:MET:HB2	1:C:721:MET:HE2	1.25	0.44
1:C:414:MET:HE3	5:C:1244:HOH:O	2.00	0.43
1:A:493:LYS:CB	5:A:1039:HOH:O	2.63	0.43
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.01	0.43
1:B:715:ARG:HD3	5:B:1346:HOH:O	2.19	0.43
1:B:454:ASP:O	1:B:458:LYS:HA	2.20	0.42
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.01	0.42
1:B:761:LYS:HE3	1:B:761:LYS:HB2	1.85	0.42
1:C:494:PRO:HA	1:C:732:TYR:O	2.19	0.42
1:B:761:LYS:NZ	5:B:1164:HOH:O	2.49	0.41
1:C:666:VAL:HG12	5:C:1127:HOH:O	2.20	0.41
1:B:695:LYS:HA	1:B:695:LYS:HD3	1.80	0.41
1:B:471:LYS:HG2	5:B:1333:HOH:O	2.19	0.41
1:C:675:ARG:NE	5:C:1240:HOH:O	2.49	0.41
1:A:489:ILE:HD12	1:A:735:ALA:HB1	2.02	0.41
1:A:753:LEU:HD22	1:A:758:LEU:HD23	2.03	0.41
1:A:751:LEU:HD23	4:C:804[B]:1YV:C1	2.51	0.40
1:B:417:GLY:HA2	1:B:441:LYS:HE2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLY:HA2	5:A:955:HOH:O	2.20	0.40
1:C:770:LYS:NZ	5:C:1141:HOH:O	2.54	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	256/275 (93%)	254 (99%)	2 (1%)	0	100	100
1	B	255/275 (93%)	251 (98%)	4 (2%)	0	100	100
1	C	255/275 (93%)	249 (98%)	6 (2%)	0	100	100
All	All	766/825 (93%)	754 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	217/227 (96%)	215 (99%)	2 (1%)	70	49
1	B	216/227 (95%)	213 (99%)	3 (1%)	59	33
1	C	216/227 (95%)	210 (97%)	6 (3%)	38	11
All	All	649/681 (95%)	638 (98%)	11 (2%)	53	26

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	457	THR
1	A	498	LEU
1	B	498	LEU
1	B	652	SER
1	B	727	LEU
1	C	413	GLU
1	C	486	GLU
1	C	498	LEU
1	C	666	VAL
1	C	675	ARG
1	C	721	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	754	ASN
1	B	411	ASN
1	B	714	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	GLU	A	801	-	8,9,9	1.25	1 (12%)	8,11,11	1.52	2 (25%)
2	GLU	B	804	-	8,9,9	1.32	1 (12%)	8,11,11	1.68	2 (25%)
2	GLU	C	803	-	8,9,9	1.85	3 (37%)	8,11,11	2.07	3 (37%)
4	1YV	B	805	-	24,25,25	2.11	5 (20%)	31,35,35	1.90	8 (25%)
4	1YV	C	804[B]	-	24,25,25	2.15	2 (8%)	31,35,35	2.20	5 (16%)
4	1YV	C	804[A]	-	24,25,25	1.88	5 (20%)	31,35,35	1.92	4 (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	A	801	-	-	3/9/9/9	-
2	GLU	B	804	-	-	1/9/9/9	-
2	GLU	C	803	-	-	2/9/9/9	-
4	1YV	B	805	-	-	2/20/22/22	0/2/2/2
4	1YV	C	804[B]	-	-	1/20/22/22	0/2/2/2
4	1YV	C	804[A]	-	-	2/20/22/22	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	1YV	C14-C13	-7.86	1.28	1.44
4	C	804[B]	1YV	C14-C13	-7.39	1.29	1.44
4	C	804[A]	1YV	C14-C13	-6.11	1.31	1.44
4	C	804[B]	1YV	O23-S24	5.89	1.50	1.43
4	C	804[A]	1YV	O23-S24	4.16	1.48	1.43
4	B	805	1YV	O23-S24	3.81	1.47	1.43
4	B	805	1YV	O22-S24	3.13	1.47	1.43
2	C	803	GLU	CG-CD	2.69	1.56	1.50
2	C	803	GLU	OE2-CD	-2.59	1.22	1.30
2	C	803	GLU	OE1-CD	2.59	1.30	1.22
4	B	805	1YV	C11-C17	2.42	1.42	1.39
4	C	804[A]	1YV	C6-C15	2.39	1.44	1.39
2	A	801	GLU	OE1-CD	2.36	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	804[A]	1YV	C12-N21	2.34	1.50	1.47
4	C	804[A]	1YV	S24-N21	-2.28	1.55	1.61
2	B	804	GLU	OE1-CD	2.12	1.29	1.22
4	B	805	1YV	C2-C18	2.07	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804[B]	1YV	O22-S24-O23	-8.09	107.07	118.88
4	C	804[A]	1YV	O22-S24-O23	-6.59	109.26	118.88
4	C	804[B]	1YV	O22-S24-N21	5.03	113.51	107.65
4	B	805	1YV	C11-C17-C10	-4.90	112.23	118.30
4	C	804[A]	1YV	O22-S24-C18	4.63	114.58	107.99
4	C	804[B]	1YV	O22-S24-C18	4.36	114.19	107.99
2	C	803	GLU	OXT-C-O	4.20	133.61	124.08
4	C	804[B]	1YV	O23-S24-N21	-3.90	103.09	107.65
4	B	805	1YV	C9-C11-C17	3.88	125.05	121.18
4	C	804[A]	1YV	C1-C18-C2	-3.59	106.67	112.79
4	B	805	1YV	O22-S24-N21	3.51	111.74	107.65
2	B	804	GLU	OE2-CD-CG	3.37	124.63	114.00
2	C	803	GLU	OE2-CD-CG	2.81	122.88	114.00
2	A	801	GLU	OE1-CD-CG	-2.74	114.39	123.09
4	B	805	1YV	O23-S24-N21	-2.67	104.53	107.65
2	A	801	GLU	OE2-CD-CG	2.64	122.35	114.00
4	B	805	1YV	C8-C16-C15	2.64	125.81	121.25
2	B	804	GLU	OE1-CD-CG	-2.41	115.45	123.09
4	C	804[B]	1YV	C11-C17-C10	-2.31	115.45	118.30
4	B	805	1YV	C10-C8-C16	2.23	123.98	121.12
4	B	805	1YV	C3-C19-C12	-2.19	101.99	112.74
2	C	803	GLU	OE1-CD-CG	-2.15	116.27	123.09
4	C	804[A]	1YV	C14-C13-N20	-2.08	172.74	177.87
4	B	805	1YV	C8-C16-C9	-2.02	114.07	117.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	805	1YV	C10-C17-C19-C12
4	C	804[B]	1YV	C11-C17-C19-C12
4	B	805	1YV	C11-C17-C19-C12
2	A	801	GLU	O-C-CA-N
2	B	804	GLU	O-C-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	803	GLU	O-C-CA-N
4	C	804[A]	1YV	C11-C17-C19-C12
2	A	801	GLU	OXT-C-CA-CB
2	C	803	GLU	OXT-C-CA-CB
2	A	801	GLU	O-C-CA-CB
4	C	804[A]	1YV	N20-C13-C14-C5

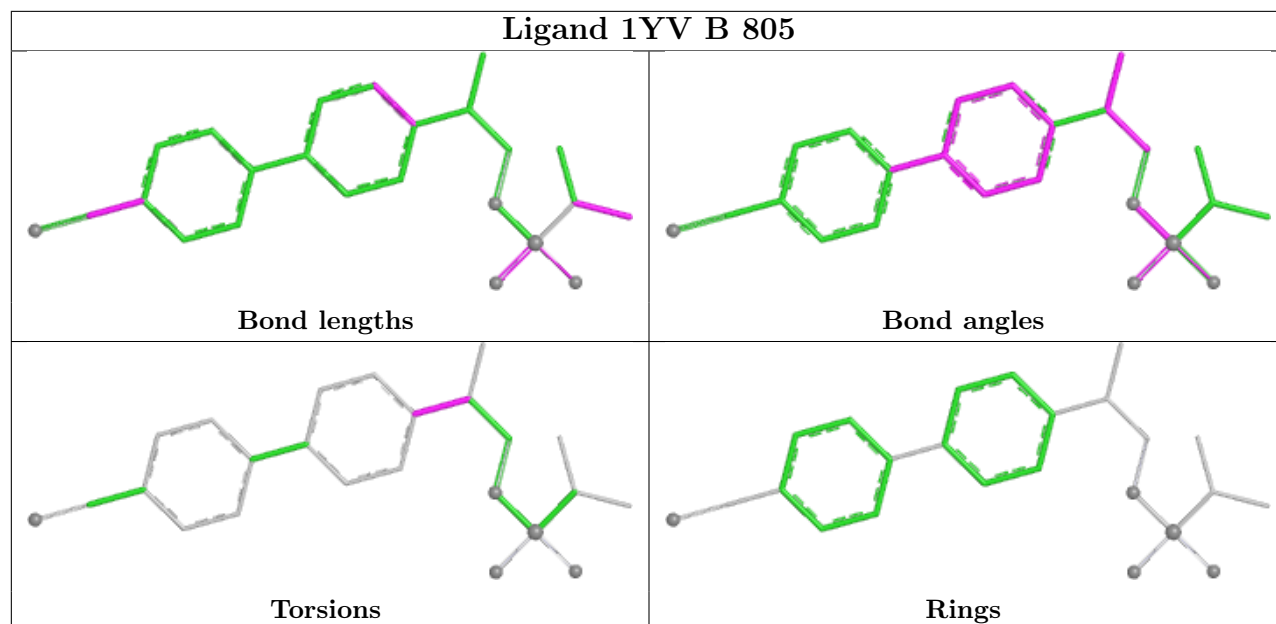
There are no ring outliers.

3 monomers are involved in 9 short contacts:

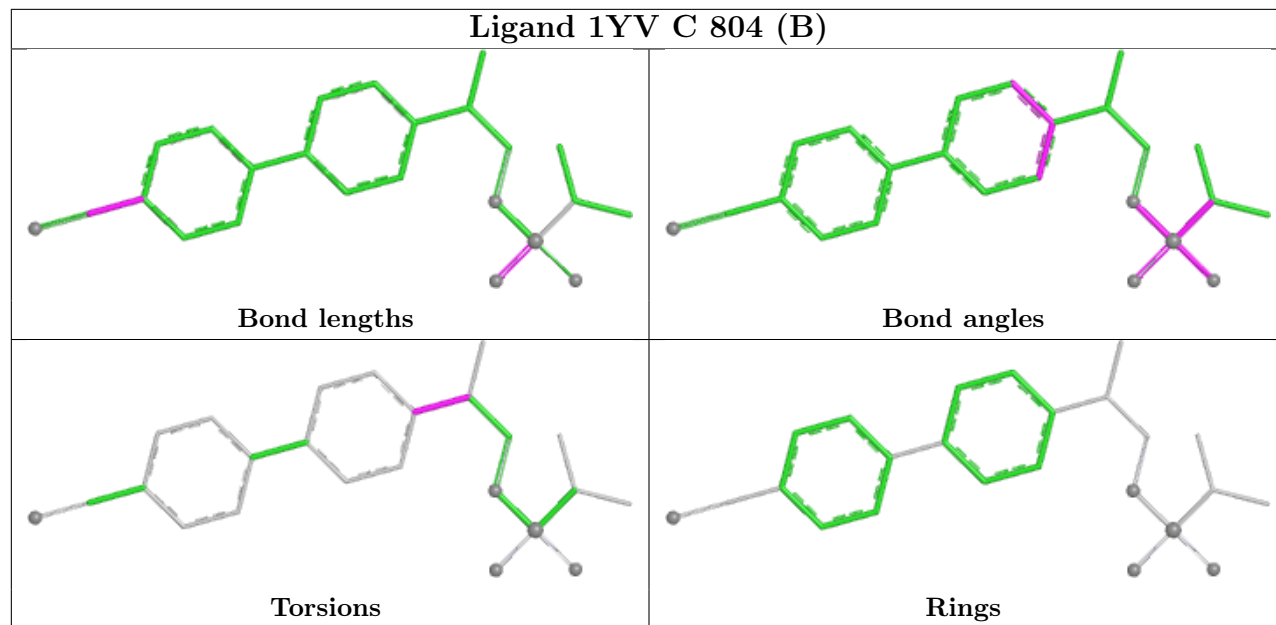
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	805	1YV	3	0
4	C	804[B]	1YV	3	0
4	C	804[A]	1YV	3	0

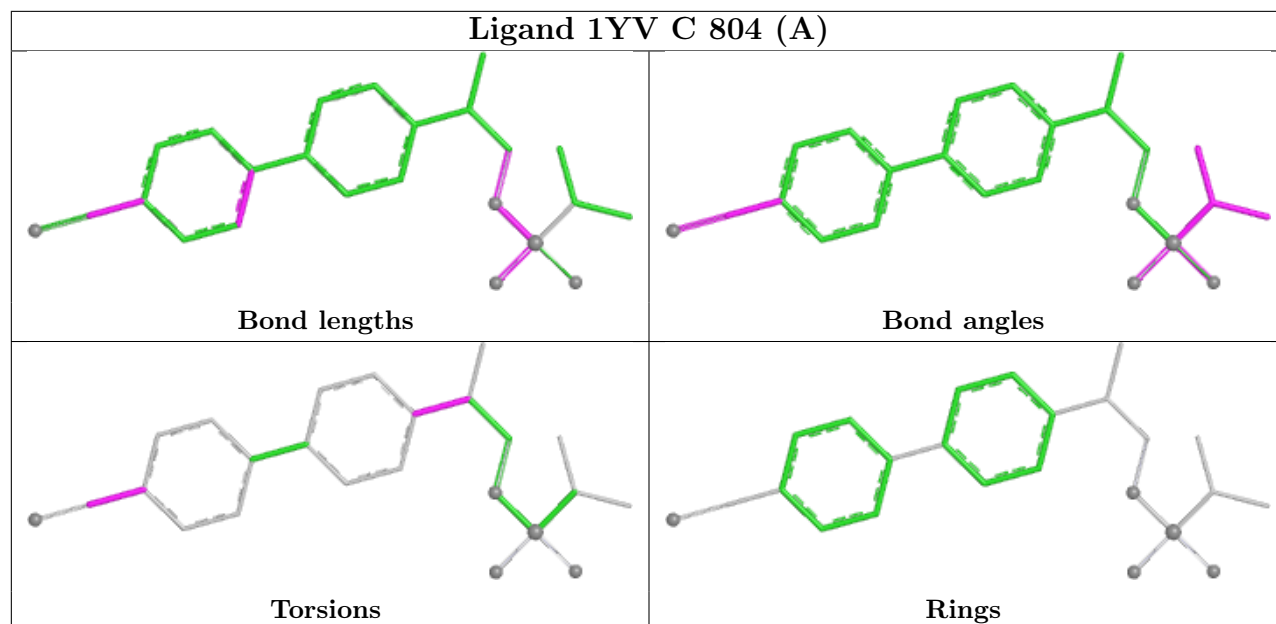
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 1YV B 805



Ligand 1YV C 804 (B)





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	258/275 (93%)	0.16	12 (4%) 36 40	8, 15, 29, 49	0
1	B	257/275 (93%)	-0.01	10 (3%) 43 47	7, 13, 27, 46	0
1	C	257/275 (93%)	0.33	13 (5%) 33 36	9, 17, 33, 45	0
All	All	772/825 (93%)	0.16	35 (4%) 38 42	7, 15, 31, 49	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	739	GLY	4.4
1	C	770	LYS	4.3
1	A	457	THR	3.7
1	B	768	TYR	3.7
1	C	773	CYS	3.4
1	C	651	ASP	3.3
1	B	770	LYS	3.2
1	A	456	ASP	3.2
1	B	456	ASP	3.2
1	B	651	ASP	3.2
1	C	771	GLY	3.2
1	B	652	SER	3.1
1	C	768	TYR	3.0
1	A	651	ASP	3.0
1	C	769	ASP	2.9
1	C	643	THR	2.9
1	A	770	LYS	2.8
1	B	769	ASP	2.7
1	A	773	CYS	2.7
1	A	643	THR	2.7
1	B	773	CYS	2.7
1	A	644	GLU	2.6
1	A	652	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	457	THR	2.5
1	C	665	ALA	2.5
1	C	664	ILE	2.5
1	B	453	ARG	2.4
1	A	455	ALA	2.4
1	A	739	GLY	2.4
1	C	644	GLU	2.3
1	B	739	GLY	2.1
1	C	414	MET	2.1
1	A	454	ASP	2.1
1	A	769	ASP	2.1
1	C	672	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

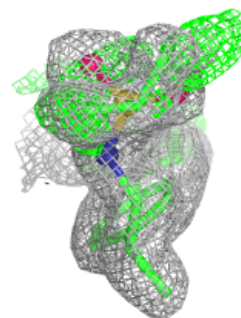
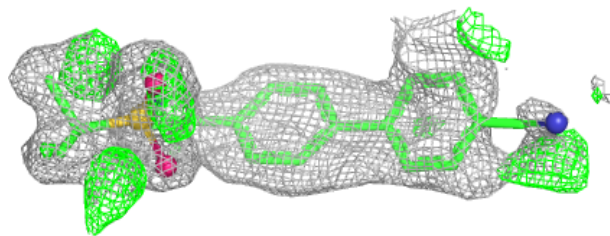
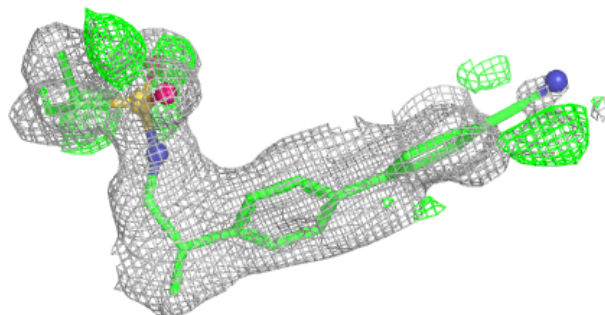
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1YV	C	804[A]	24/24	0.93	0.11	9,14,19,25	24
4	1YV	C	804[B]	24/24	0.93	0.11	8,15,23,27	24
4	1YV	B	805	24/24	0.94	0.09	9,13,23,25	24
3	ZN	C	802	1/1	0.97	0.14	34,34,34,34	0
3	ZN	C	801	1/1	0.97	0.06	19,19,19,19	0
2	GLU	B	804	10/10	0.98	0.04	7,8,10,10	0
2	GLU	C	803	10/10	0.98	0.05	8,12,14,15	0
3	ZN	B	802	1/1	0.98	0.04	18,18,18,18	0
2	GLU	A	801	10/10	0.98	0.04	8,10,13,14	0
3	ZN	B	803	1/1	0.99	0.03	14,14,14,14	0
3	ZN	B	801	1/1	0.99	0.03	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

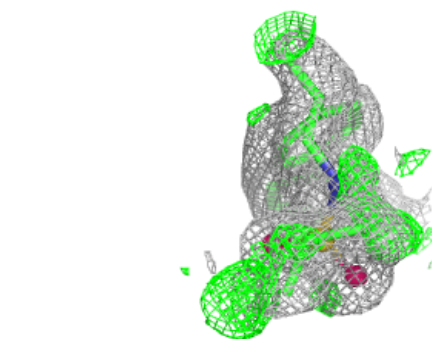
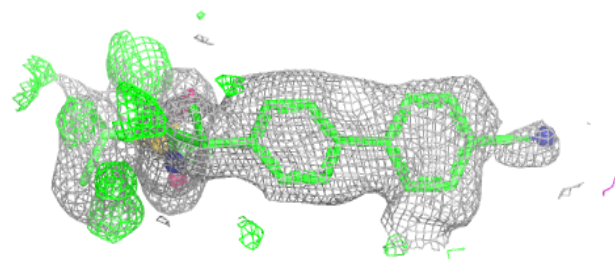
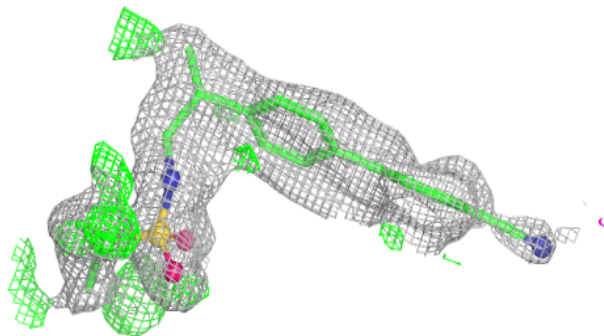
Electron density around 1YV C 804 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

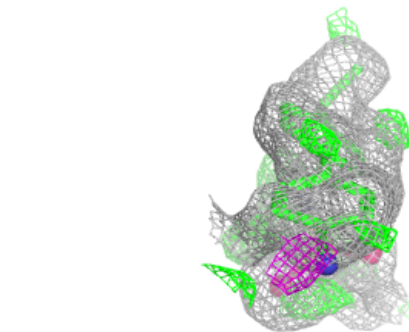
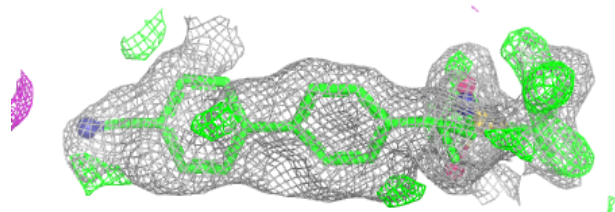
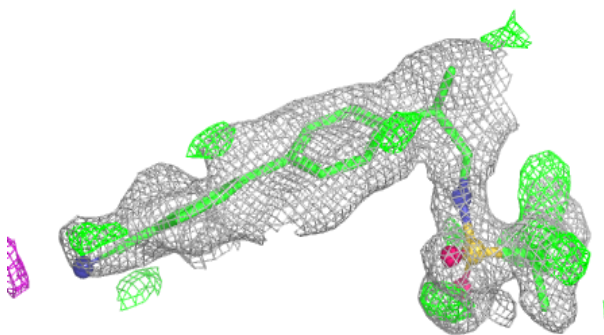


Electron density around 1YV C 804 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 1YV B 805:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.