



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 PM GMT

PDB ID : 4LZ5  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

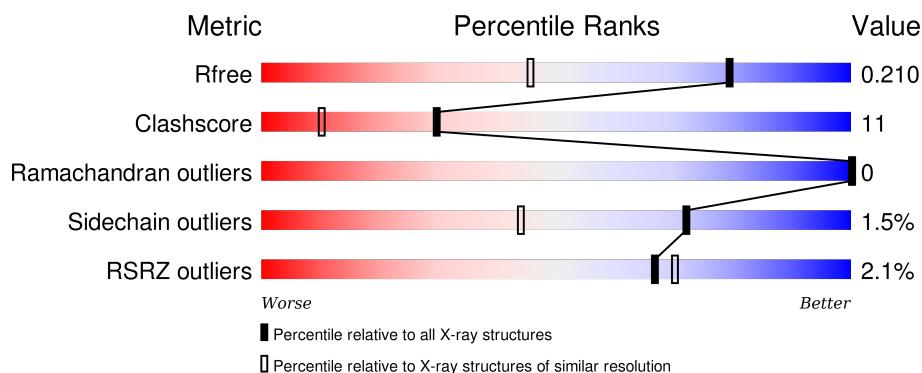
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	275	
1	C	275	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	1YV	B	805	-	-	-	X
4	1YV	C	804[A]	-	-	-	X
4	1YV	C	804[B]	-	-	-	X

## 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

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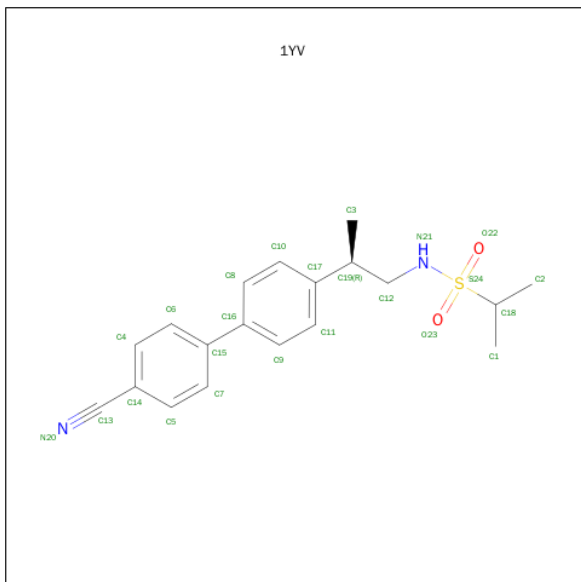
Chain	Residue	Modelled	Actual	Comment	Reference
C	381	MET	-	EXPRESSION TAG	UNP P19491
C	382	GLY	-	EXPRESSION TAG	UNP P19491
C	389	ARG	GLY	ENGINEERED MUTATION	UNP P19491
C	390	GLY	LEU	ENGINEERED MUTATION	UNP P19491
C	391	ALA	GLU	ENGINEERED MUTATION	UNP P19491
C	507	GLY	-	LINKER	UNP P19491
C	508	THR	-	LINKER	UNP P19491

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- Chemical structure of L-glutamate (GLU) is shown. The structure includes the following labels:
- GLU**: Label for the entire molecule.
  - O**: Oxygen atom of the carboxyl group.
  - OXT**: Label for the hydroxyl group of the carboxyl group.
  - C**: Carbon atom of the carboxyl group.
  - CA(S)**: Chiral center (C-alpha).
  - N**: Nitrogen atom of the amino group.
  - NH<sub>2</sub>**: Amino group.
  - CB**: Carbon atom (C-beta).
  - CG**: Carbon atom (C-gamma).
  - CD**: Carbon atom (C-delta).
  - OE1**: Oxygen atom of the carboxyl group.
  - OE2**: Hydroxyl group of the carboxyl group.

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

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

- Molecule 4 is N-[(2R)-2-(4'-CYANOBIIPHENYL-4-YL)PROPYL]PROPANE-2-SULFONAMIDE (three-letter code: 1YV) (formula: C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>S).



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		

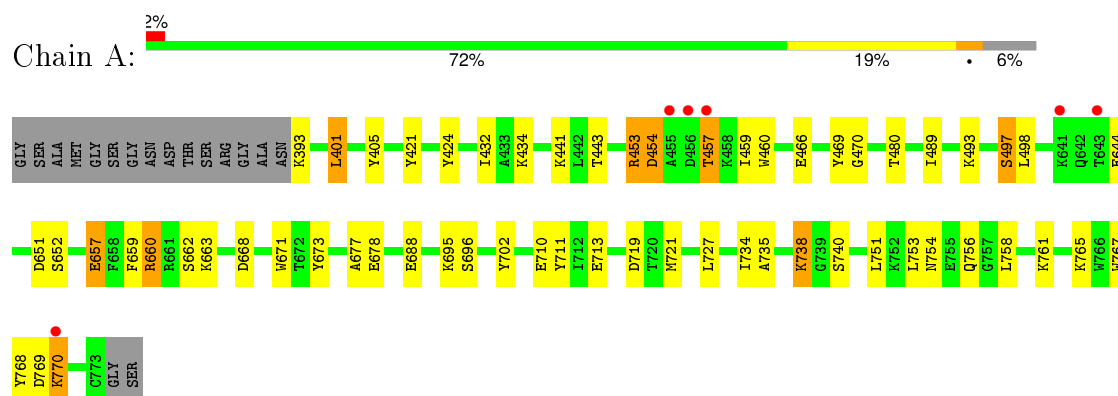
- Molecule 5 is water.

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		

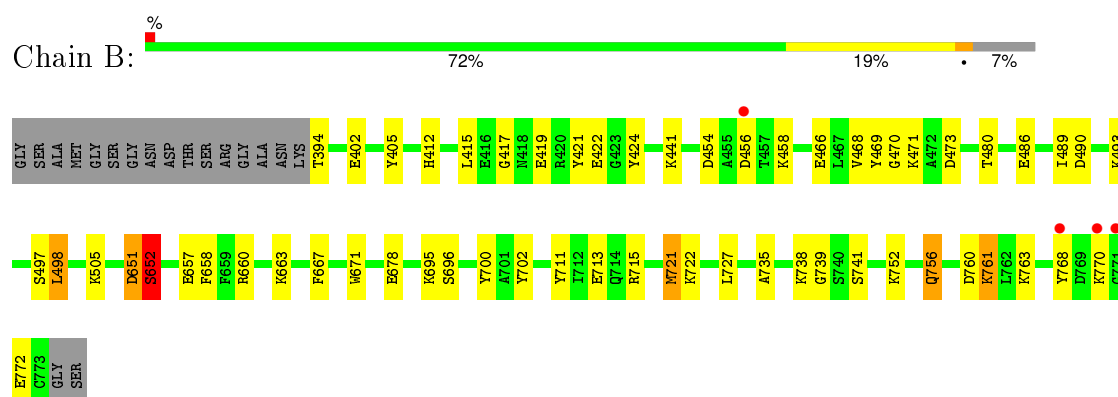
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

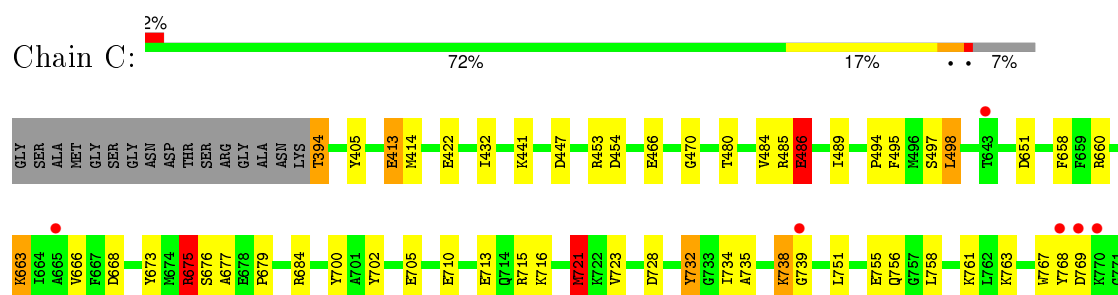
#### • Molecule 1: Glutamate receptor 2



#### • 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, $\alpha$ , $\beta$ , $\gamma$	114.75Å 164.54Å 47.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.07 – 1.50 41.11 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (94.07-1.50) 98.1 (41.11-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 141629 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.76	38/2054 (1.9%)	1.49	21/2762 (0.8%)
1	B	1.73	35/2045 (1.7%)	1.55	28/2751 (1.0%)
1	C	1.61	21/2044 (1.0%)	1.39	19/2749 (0.7%)
All	All	1.70	94/6143 (1.5%)	1.48	68/8262 (0.8%)

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 (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	GLU	CD-OE1	14.22	1.41	1.25
1	A	710	GLU	CG-CD	12.74	1.71	1.51
1	B	678	GLU	CD-OE1	11.04	1.37	1.25
1	B	738	LYS	CB-CG	-10.00	1.25	1.52
1	B	696	SER	CB-OG	9.85	1.55	1.42
1	C	738	LYS	CB-CG	-9.51	1.26	1.52
1	B	405	TYR	CZ-OH	9.09	1.53	1.37
1	B	711	TYR	CE1-CZ	-9.08	1.26	1.38
1	A	405	TYR	CD2-CE2	8.69	1.52	1.39
1	B	678	GLU	CB-CG	-8.61	1.35	1.52
1	B	713	GLU	CD-OE1	-8.09	1.16	1.25
1	B	761	LYS	CE-NZ	7.91	1.68	1.49
1	A	713	GLU	CD-OE2	-7.85	1.17	1.25
1	C	405	TYR	CD2-CE2	7.73	1.50	1.39
1	A	644	GLU	CD-OE1	7.70	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	TYR	CZ-OH	7.63	1.50	1.37
1	B	702	TYR	CE1-CZ	-7.49	1.28	1.38
1	C	772	GLU	CB-CG	-7.43	1.38	1.52
1	A	696	SER	CB-OG	7.35	1.51	1.42
1	C	768	TYR	CD1-CE1	7.09	1.50	1.39
1	A	657	GLU	CD-OE1	7.09	1.33	1.25
1	B	493	LYS	CG-CD	-7.05	1.28	1.52
1	B	405	TYR	CD2-CE2	7.02	1.49	1.39
1	C	422	GLU	CG-CD	6.96	1.62	1.51
1	B	493	LYS	CB-CG	6.94	1.71	1.52
1	A	688	GLU	CG-CD	6.90	1.62	1.51
1	B	497	SER	CB-OG	-6.77	1.33	1.42
1	B	711	TYR	CZ-OH	6.76	1.49	1.37
1	B	721	MET	SD-CE	-6.72	1.40	1.77
1	A	671	TRP	CG-CD1	6.68	1.46	1.36
1	B	752	LYS	CE-NZ	6.51	1.65	1.49
1	C	466	GLU	CD-OE2	6.50	1.32	1.25
1	C	405	TYR	CZ-OH	6.31	1.48	1.37
1	C	673	TYR	CD2-CE2	-6.26	1.29	1.39
1	B	721	MET	CA-CB	6.24	1.67	1.53
1	B	763	LYS	CD-CE	6.22	1.66	1.51
1	A	710	GLU	CD-OE2	-6.21	1.18	1.25
1	C	710	GLU	CD-OE2	6.17	1.32	1.25
1	B	657	GLU	CD-OE2	6.16	1.32	1.25
1	C	486	GLU	CB-CG	6.06	1.63	1.52
1	C	484	VAL	CB-CG1	6.02	1.65	1.52
1	A	441	LYS	CB-CG	-5.98	1.36	1.52
1	A	768	TYR	CG-CD1	5.92	1.46	1.39
1	A	767	TRP	CB-CG	5.91	1.60	1.50
1	A	668	ASP	CB-CG	5.91	1.64	1.51
1	C	702	TYR	CZ-OH	5.87	1.47	1.37
1	A	469	TYR	CB-CG	-5.86	1.42	1.51
1	A	434	LYS	CB-CG	-5.86	1.36	1.52
1	A	673	TYR	CD2-CE2	-5.80	1.30	1.39
1	B	738	LYS	CA-C	-5.80	1.37	1.52
1	A	740	SER	CA-CB	5.74	1.61	1.52
1	B	768	TYR	CB-CG	5.71	1.60	1.51
1	C	702	TYR	CE2-CZ	-5.71	1.31	1.38
1	B	756	GLN	CB-CG	-5.71	1.37	1.52
1	B	711	TYR	CD2-CE2	5.70	1.47	1.39
1	A	651	ASP	C-O	5.67	1.34	1.23
1	B	421	TYR	CE2-CZ	-5.66	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	ALA	CA-CB	5.62	1.64	1.52
1	B	652	SER	N-CA	5.59	1.57	1.46
1	A	711	TYR	CE2-CZ	-5.59	1.31	1.38
1	A	721	MET	CB-CG	-5.56	1.33	1.51
1	B	402	GLU	CD-OE2	5.55	1.31	1.25
1	A	711	TYR	CD1-CE1	5.53	1.47	1.39
1	C	702	TYR	CE1-CZ	-5.53	1.31	1.38
1	B	468	VAL	CB-CG1	5.47	1.64	1.52
1	A	678	GLU	CD-OE1	-5.46	1.19	1.25
1	B	505	LYS	CE-NZ	5.40	1.62	1.49
1	B	652	SER	CA-C	5.39	1.67	1.52
1	A	405	TYR	CG-CD1	-5.37	1.32	1.39
1	C	767	TRP	CB-CG	5.36	1.59	1.50
1	A	710	GLU	CB-CG	-5.35	1.42	1.52
1	B	722	LYS	C-O	5.31	1.33	1.23
1	A	713	GLU	CG-CD	5.31	1.59	1.51
1	C	684	ARG	CG-CD	5.31	1.65	1.51
1	A	662	SER	CB-OG	-5.30	1.35	1.42
1	A	460	TRP	CZ3-CH2	-5.28	1.31	1.40
1	A	424	TYR	CG-CD2	5.28	1.46	1.39
1	C	658	PHE	CD1-CE1	5.26	1.49	1.39
1	A	770	LYS	CB-CG	5.25	1.66	1.52
1	B	469	TYR	CG-CD1	5.20	1.46	1.39
1	B	658	PHE	CE2-CZ	5.20	1.47	1.37
1	A	702	TYR	CE2-CZ	-5.19	1.31	1.38
1	A	644	GLU	CG-CD	5.16	1.59	1.51
1	B	505	LYS	CD-CE	5.15	1.64	1.51
1	A	662	SER	N-CA	-5.15	1.36	1.46
1	B	671	TRP	CD1-NE1	-5.12	1.29	1.38
1	C	700	TYR	CE2-CZ	-5.10	1.31	1.38
1	B	756	GLN	CG-CD	5.10	1.62	1.51
1	A	497	SER	CB-OG	-5.09	1.35	1.42
1	A	405	TYR	CE2-CZ	-5.08	1.31	1.38
1	A	644	GLU	CD-OE2	5.05	1.31	1.25
1	C	394	THR	N-CA	5.04	1.56	1.46
1	C	495	PHE	CE2-CZ	-5.03	1.27	1.37
1	C	663	LYS	CE-NZ	5.01	1.61	1.49

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	660	ARG	NE-CZ-NH1	13.25	126.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	660	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	B	678	GLU	OE1-CD-OE2	-12.74	108.01	123.30
1	A	660	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	C	675	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	C	721	MET	CG-SD-CE	-11.03	82.55	100.20
1	A	678	GLU	OE1-CD-OE2	8.86	133.93	123.30
1	C	422	GLU	OE1-CD-OE2	8.86	133.93	123.30
1	A	421	TYR	CB-CG-CD1	-8.82	115.71	121.00
1	B	405	TYR	CG-CD2-CE2	-8.54	114.47	121.30
1	B	721	MET	CG-SD-CE	-8.53	86.55	100.20
1	A	405	TYR	CG-CD2-CE2	-8.45	114.54	121.30
1	B	660	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	727	LEU	CB-CG-CD1	7.99	124.58	111.00
1	C	660	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	651	ASP	CB-CG-OD1	7.88	125.39	118.30
1	B	678	GLU	CG-CD-OE1	7.63	133.56	118.30
1	B	658	PHE	CB-CG-CD2	7.56	126.09	120.80
1	A	727	LEU	CB-CG-CD1	7.38	123.56	111.00
1	C	684	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	761	LYS	CD-CE-NZ	7.21	128.28	111.70
1	A	453	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	B	419	GLU	OE1-CD-OE2	7.13	131.85	123.30
1	A	769	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	405	TYR	CG-CD1-CE1	7.07	126.96	121.30
1	B	652	SER	CB-CA-C	-7.03	96.74	110.10
1	B	424	TYR	CB-CG-CD1	7.00	125.20	121.00
1	B	422	GLU	OE1-CD-OE2	6.70	131.34	123.30
1	A	651	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	711	TYR	CG-CD2-CE2	-6.56	116.05	121.30
1	A	738	LYS	CD-CE-NZ	6.47	126.58	111.70
1	C	405	TYR	CG-CD2-CE2	-6.43	116.16	121.30
1	A	651	ASP	CB-CG-OD1	6.43	124.08	118.30
1	B	405	TYR	CD1-CE1-CZ	-6.37	114.07	119.80
1	A	696	SER	CB-CA-C	6.34	122.14	110.10
1	A	660	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	490	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	447	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	A	424	TYR	CB-CG-CD1	6.22	124.73	121.00
1	C	684	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	675	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	454	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	453	ARG	NE-CZ-NH2	5.98	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	B	473	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	763	LYS	CD-CE-NZ	5.86	125.17	111.70
1	C	769	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	728	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	454	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	700	TYR	CB-CG-CD1	5.58	124.35	121.00
1	B	402	GLU	CG-CD-OE1	5.56	129.41	118.30
1	B	498	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	719	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	659	PHE	CB-CG-CD1	5.46	124.62	120.80
1	B	405	TYR	CE1-CZ-CE2	5.37	128.39	119.80
1	A	434	LYS	CD-CE-NZ	5.30	123.89	111.70
1	A	421	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	B	493	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	A	401	LEU	CB-CG-CD2	5.14	119.74	111.00
1	B	667	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	C	675	ARG	CD-NE-CZ	5.13	130.79	123.60
1	B	772	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	B	738	LYS	CB-CA-C	-5.13	100.14	110.40
1	B	667	PHE	CB-CG-CD1	5.11	124.38	120.80
1	C	732	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	C	485	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	760	ASP	O-C-N	5.02	130.73	122.70
1	C	732	TYR	CB-CG-CD1	5.01	124.00	121.00

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	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2009	0	2037	36	0
1	C	2008	0	2033	52	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	10	0	5	1	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	26	0
5	B	475	0	0	29	0
5	C	373	0	0	28	0
All	All	7405	0	6201	138	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 (138) 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: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
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:466:GLU:CD	5:A:1292:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OG	1:A:652:SER:O	1.96	0.80
1:C:414:MET:HE2	5:C:1244:HOH:O	1.78	0.79
1:C:432:ILE:HD13	1:C:734:ILE:CD1	2.10	0.79
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:C:432:ILE:CD1	1:C:734:ILE:HD11	2.14	0.75
1:A:432:ILE:CD1	1:A:734:ILE:HD11	2.17	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: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:A:770:LYS:NZ	5:A:1265:HOH:O	2.20	0.62
1:C:432:ILE:CD1	1:C:734:ILE:HD13	2.18	0.62
1:A:393:LYS:N	5:A:1253:HOH:O	2.33	0.61
1:A:761:LYS:HE3	5:A:1031:HOH:O	2.00	0.61
1:C:758:LEU:CD2	1:C:761:LYS:HE2	2.33	0.59
4:B:805:1YV:O23	5:B:1252:HOH:O	2.15	0.58
1:C:738:LYS:NZ	5:C:1239:HOH:O	2.30	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:A:493:LYS:NZ	1:C:486:GLU:OE2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:ASP:CA	5:C:1034:HOH:O	2.53	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:C:713:GLU:CD	5:C:1227:HOH:O	2.43	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: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:C:668:ASP:OD1	5:C:1261:HOH:O	2.19	0.51
1:A:663:LYS:NZ	5:A:1279:HOH:O	2.42	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:A:756:GLN:CD	5:A:1101:HOH:O	2.51	0.48
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
4:B:805:1YV:C2	5:B:1252:HOH:O	2.00	0.48
1:B:770:LYS:CB	5:B:1346:HOH:O	2.62	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:LYS:CG	5:B:1025:HOH:O	2.44	0.46
1:A:480:THR:HG1	2:A:801:GLU:N	2.13	0.45
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:B:480:THR:HG1	2:B:804:GLU:N	2.15	0.45
1:A:457:THR:HG23	1:A:459:ILE:HG13	1.99	0.45
1:A:453:ARG:NH2	5:A:1264:HOH:O	2.50	0.45
1:B:770:LYS:C	5:B:1346:HOH:O	2.55	0.45
1:C:716:LYS:HG3	1:C:772:GLU:HG3	1.99	0.45
1:A:657:GLU:HG2	5:A:1004:HOH:O	2.17	0.45
1:C:721:MET:HE3	1:C:721:MET:HB3	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:C:480:THR:HG1	2:C:803:GLU:N	2.15	0.44
1:C:721:MET:HE2	1:C:721:MET:HB2	1.25	0.44
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:721:MET:HB2	1:B:721:MET:HE2	1.17	0.42
1:B:761:LYS:HB2	1:B:761:LYS:HE3	1.85	0.42
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.01	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:HD3	1:B:695:LYS:HA	1.80	0.41
1:C:675:ARG:NE	5:C:1240:HOH:O	2.49	0.41
1:B:471:LYS:HG2	5:B:1333:HOH:O	2.19	0.41
1:C:414:MET:HE3	5:C:1244:HOH:O	2.05	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
1:A:470:GLY:HA2	5:A:955:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 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	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

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%)	214 (99%)	3 (1%)	74	47
1	B	216/227 (95%)	214 (99%)	2 (1%)	84	65
1	C	216/227 (95%)	211 (98%)	5 (2%)	58	24
All	All	649/681 (95%)	639 (98%)	10 (2%)	72	44

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

Mol	Chain	Res	Type
1	A	457	THR
1	A	498	LEU
1	A	738	LYS
1	B	498	LEU
1	B	652	SER

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Mol	Chain	Res	Type
1	C	413	GLU
1	C	486	GLU
1	C	498	LEU
1	C	675	ARG
1	C	721	MET

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

Mol	Chain	Res	Type
1	B	744	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	3,9,9	0.59	0	2,11,11	1.08	0
2	GLU	B	804	-	3,9,9	0.18	0	2,11,11	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1YV	B	805	-	24,25,25	1.90	5 (20%)	25,35,35	1.83	4 (16%)
2	GLU	C	803	-	3,9,9	0.42	0	2,11,11	0.92	0
4	1YV	C	804[A]	-	24,25,25	1.71	5 (20%)	25,35,35	1.97	4 (16%)
4	1YV	C	804[B]	-	24,25,25	1.96	2 (8%)	25,35,35	1.73	2 (8%)

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	-	-	0/3/9/9	0/0/0/0
2	GLU	B	804	-	-	0/3/9/9	0/0/0/0
4	1YV	B	805	-	-	0/20/22/22	0/2/2/2
2	GLU	C	803	-	-	0/3/9/9	0/0/0/0
4	1YV	C	804[A]	-	-	0/20/22/22	0/2/2/2
4	1YV	C	804[B]	-	-	0/20/22/22	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	1YV	C14-C13	-6.60	1.28	1.44
4	C	804[B]	1YV	C14-C13	-6.21	1.29	1.44
4	C	804[A]	1YV	C14-C13	-5.13	1.31	1.44
4	C	804[A]	1YV	S24-N21	-2.12	1.55	1.61
4	C	804[A]	1YV	C12-C19	2.09	1.58	1.54
4	B	805	1YV	C2-C18	2.19	1.57	1.52
4	C	804[A]	1YV	C6-C15	2.27	1.44	1.39
4	B	805	1YV	C11-C17	2.39	1.42	1.39
4	B	805	1YV	O22-S24	3.03	1.47	1.43
4	B	805	1YV	O23-S24	3.70	1.47	1.43
4	C	804[A]	1YV	O23-S24	4.03	1.48	1.43
4	C	804[B]	1YV	O23-S24	5.75	1.50	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804[B]	1YV	O22-S24-O23	-7.47	107.07	119.34
4	C	804[A]	1YV	O22-S24-O23	-6.14	109.26	119.34
4	B	805	1YV	C10-C17-C11	-4.77	112.23	118.31
4	C	804[A]	1YV	C1-C18-C2	-3.02	106.67	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804[B]	1YV	C10-C17-C11	-2.25	115.45	118.31
4	C	804[A]	1YV	C14-C13-N20	-2.17	172.74	177.99
4	B	805	1YV	C3-C19-C17	2.18	117.83	112.12
4	B	805	1YV	C8-C16-C15	2.46	125.81	121.39
4	B	805	1YV	C9-C11-C17	3.75	125.05	121.20
4	C	804[A]	1YV	C19-C12-N21	4.52	119.39	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GLU	1	0
2	B	804	GLU	1	0
4	B	805	1YV	3	0
2	C	803	GLU	1	0
4	C	804[A]	1YV	3	0
4	C	804[B]	1YV	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	258/275 (93%)	-0.03	6 (2%) 64 67	8, 15, 29, 49	0
1	B	257/275 (93%)	-0.15	4 (1%) 74 78	7, 13, 27, 46	0
1	C	257/275 (93%)	0.07	6 (2%) 64 67	9, 17, 33, 45	0
All	All	772/825 (93%)	-0.04	16 (2%) 67 70	7, 15, 31, 49	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	770	LYS	6.5
1	A	456	ASP	5.6
1	B	456	ASP	4.6
1	B	768	TYR	4.5
1	A	455	ALA	3.5
1	B	770	LYS	3.5
1	A	457	THR	3.3
1	C	739	GLY	3.3
1	C	768	TYR	3.0
1	A	770	LYS	2.9
1	C	643	THR	2.6
1	A	643	THR	2.4
1	C	769	ASP	2.4
1	C	665	ALA	2.1
1	A	641	LYS	2.0
1	B	771	GLY	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	1YV	C	804[B]	24/24	0.93	0.22	8.18	8,15,23,27	24
4	1YV	C	804[A]	24/24	0.93	0.22	6.58	9,14,19,25	24
4	1YV	B	805	24/24	0.93	0.15	4.79	9,13,23,25	24
2	GLU	C	803	10/10	0.97	0.09	0.02	8,12,14,15	0
2	GLU	B	804	10/10	0.98	0.07	-0.77	7,8,10,10	0
2	GLU	A	801	10/10	0.98	0.07	-1.06	8,10,13,14	0
3	ZN	B	802	1/1	0.99	0.04	-1.48	18,18,18,18	0
3	ZN	C	801	1/1	0.98	0.04	-1.86	19,19,19,19	0
3	ZN	B	801	1/1	0.99	0.05	-1.91	14,14,14,14	0
3	ZN	B	803	1/1	0.99	0.04	-2.89	14,14,14,14	0
3	ZN	C	802	1/1	0.98	0.10	-	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.