



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2018 – 07:55 AM EST

PDB ID : 5UN1  
Title : Crystal structure of GluN1/GluN2B delta-ATD NMDA receptor  
Authors : Song, X.; Gouaux, E.  
Deposited on : 2017-01-30  
Resolution : 3.60 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:

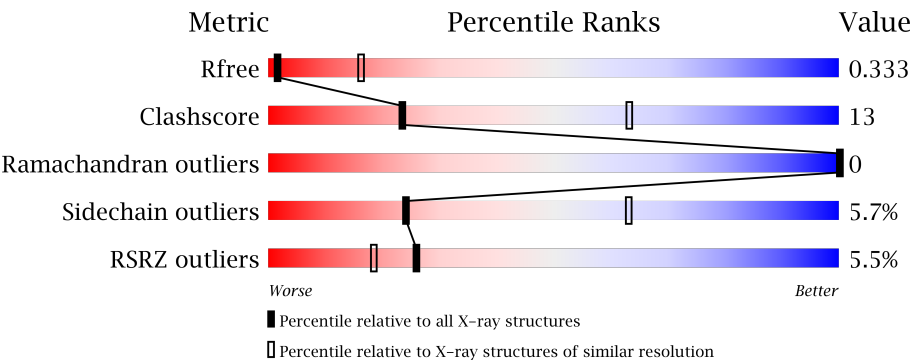
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

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 3.60 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 <sub>free</sub>	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	451	<div><div>0.1%</div><div><div></div><div>78%</div><div>13%</div><div>8%</div></div></div>
1	C	451	<div><div>3%</div><div><div></div><div>74%</div><div>18%</div><div>8%</div></div></div>
1	E	451	<div><div>8%</div><div><div></div><div>76%</div><div>15%</div><div>9%</div></div></div>
1	G	451	<div><div>2%</div><div><div></div><div>73%</div><div>19%</div><div>6%</div></div></div>
2	B	448	<div><div>5%</div><div><div></div><div>74%</div><div>14%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	448	
2	F	448	
2	H	448	

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
3	GLY	G	1001	-	-	X	-
5	TRS	G	1003	-	-	-	X
6	GLU	B	1001	-	-	X	-
6	GLU	D	1002	-	-	X	X
6	GLU	H	1001	-	-	X	-
7	BMK	G	1005	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20143 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 N-methyl-D-aspartate receptor subunit NR1-3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	424	Total	C	N	O	S	0	0	0
			2753	1727	499	512	15			
1	A	416	Total	C	N	O	S	0	0	0
			2643	1655	466	508	14			
1	E	412	Total	C	N	O	S	0	0	0
			2486	1549	448	477	12			
1	C	415	Total	C	N	O	S	0	0	0
			2591	1629	461	487	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	440	ASP	ASN	conflict	UNP C0KD15
G	469	ASP	ASN	conflict	UNP C0KD15
G	493	ALA	LYS	conflict	UNP C0KD15
G	494	ALA	LYS	conflict	UNP C0KD15
G	495	ALA	GLU	conflict	UNP C0KD15
G	?	-	LYS	deletion	UNP C0KD15
G	?	-	VAL	deletion	UNP C0KD15
G	?	-	ASN	deletion	UNP C0KD15
G	?	-	SER	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	?	-	GLU	deletion	UNP C0KD15
G	602	ARG	GLY	conflict	UNP C0KD15
G	609	LEU	ILE	conflict	UNP C0KD15
G	648	ARG	ASP	conflict	UNP C0KD15
G	761	GLU	ASN	conflict	UNP C0KD15
G	829	SER	-	expression tag	UNP C0KD15
G	830	ARG	-	expression tag	UNP C0KD15
G	831	ALA	-	expression tag	UNP C0KD15
G	832	GLU	-	expression tag	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
G	833	ALA	-	expression tag	UNP C0KD15
G	834	LYS	-	expression tag	UNP C0KD15
G	835	ARG	-	expression tag	UNP C0KD15
G	836	MET	-	expression tag	UNP C0KD15
G	837	LYS	-	expression tag	UNP C0KD15
G	838	GLY	-	expression tag	UNP C0KD15
G	839	LEU	-	expression tag	UNP C0KD15
G	840	GLU	-	expression tag	UNP C0KD15
G	841	VAL	-	expression tag	UNP C0KD15
G	842	LEU	-	expression tag	UNP C0KD15
G	843	PHE	-	expression tag	UNP C0KD15
G	844	GLN	-	expression tag	UNP C0KD15
A	440	ASP	ASN	conflict	UNP C0KD15
A	469	ASP	ASN	conflict	UNP C0KD15
A	493	ALA	LYS	conflict	UNP C0KD15
A	494	ALA	LYS	conflict	UNP C0KD15
A	495	ALA	GLU	conflict	UNP C0KD15
A	?	-	LYS	deletion	UNP C0KD15
A	?	-	VAL	deletion	UNP C0KD15
A	?	-	ASN	deletion	UNP C0KD15
A	?	-	SER	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	?	-	GLU	deletion	UNP C0KD15
A	602	ARG	GLY	conflict	UNP C0KD15
A	609	LEU	ILE	conflict	UNP C0KD15
A	648	ARG	ASP	conflict	UNP C0KD15
A	761	GLU	ASN	conflict	UNP C0KD15
A	829	SER	-	expression tag	UNP C0KD15
A	830	ARG	-	expression tag	UNP C0KD15
A	831	ALA	-	expression tag	UNP C0KD15
A	832	GLU	-	expression tag	UNP C0KD15
A	833	ALA	-	expression tag	UNP C0KD15
A	834	LYS	-	expression tag	UNP C0KD15
A	835	ARG	-	expression tag	UNP C0KD15
A	836	MET	-	expression tag	UNP C0KD15
A	837	LYS	-	expression tag	UNP C0KD15
A	838	GLY	-	expression tag	UNP C0KD15
A	839	LEU	-	expression tag	UNP C0KD15
A	840	GLU	-	expression tag	UNP C0KD15
A	841	VAL	-	expression tag	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	842	LEU	-	expression tag	UNP C0KD15
A	843	PHE	-	expression tag	UNP C0KD15
A	844	GLN	-	expression tag	UNP C0KD15
E	440	ASP	ASN	conflict	UNP C0KD15
E	469	ASP	ASN	conflict	UNP C0KD15
E	493	ALA	LYS	conflict	UNP C0KD15
E	494	ALA	LYS	conflict	UNP C0KD15
E	495	ALA	GLU	conflict	UNP C0KD15
E	?	-	LYS	deletion	UNP C0KD15
E	?	-	VAL	deletion	UNP C0KD15
E	?	-	ASN	deletion	UNP C0KD15
E	?	-	SER	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	?	-	GLU	deletion	UNP C0KD15
E	602	ARG	GLY	conflict	UNP C0KD15
E	609	LEU	ILE	conflict	UNP C0KD15
E	648	ARG	ASP	conflict	UNP C0KD15
E	761	GLU	ASN	conflict	UNP C0KD15
E	829	SER	-	expression tag	UNP C0KD15
E	830	ARG	-	expression tag	UNP C0KD15
E	831	ALA	-	expression tag	UNP C0KD15
E	832	GLU	-	expression tag	UNP C0KD15
E	833	ALA	-	expression tag	UNP C0KD15
E	834	LYS	-	expression tag	UNP C0KD15
E	835	ARG	-	expression tag	UNP C0KD15
E	836	MET	-	expression tag	UNP C0KD15
E	837	LYS	-	expression tag	UNP C0KD15
E	838	GLY	-	expression tag	UNP C0KD15
E	839	LEU	-	expression tag	UNP C0KD15
E	840	GLU	-	expression tag	UNP C0KD15
E	841	VAL	-	expression tag	UNP C0KD15
E	842	LEU	-	expression tag	UNP C0KD15
E	843	PHE	-	expression tag	UNP C0KD15
E	844	GLN	-	expression tag	UNP C0KD15
C	440	ASP	ASN	conflict	UNP C0KD15
C	469	ASP	ASN	conflict	UNP C0KD15
C	493	ALA	LYS	conflict	UNP C0KD15
C	494	ALA	LYS	conflict	UNP C0KD15
C	495	ALA	GLU	conflict	UNP C0KD15
C	?	-	LYS	deletion	UNP C0KD15

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP C0KD15
C	?	-	ASN	deletion	UNP C0KD15
C	?	-	SER	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	?	-	GLU	deletion	UNP C0KD15
C	602	ARG	GLY	conflict	UNP C0KD15
C	609	LEU	ILE	conflict	UNP C0KD15
C	648	ARG	ASP	conflict	UNP C0KD15
C	761	GLU	ASN	conflict	UNP C0KD15
C	829	SER	-	expression tag	UNP C0KD15
C	830	ARG	-	expression tag	UNP C0KD15
C	831	ALA	-	expression tag	UNP C0KD15
C	832	GLU	-	expression tag	UNP C0KD15
C	833	ALA	-	expression tag	UNP C0KD15
C	834	LYS	-	expression tag	UNP C0KD15
C	835	ARG	-	expression tag	UNP C0KD15
C	836	MET	-	expression tag	UNP C0KD15
C	837	LYS	-	expression tag	UNP C0KD15
C	838	GLY	-	expression tag	UNP C0KD15
C	839	LEU	-	expression tag	UNP C0KD15
C	840	GLU	-	expression tag	UNP C0KD15
C	841	VAL	-	expression tag	UNP C0KD15
C	842	LEU	-	expression tag	UNP C0KD15
C	843	PHE	-	expression tag	UNP C0KD15
C	844	GLN	-	expression tag	UNP C0KD15

- Molecule 2 is a protein called Ionotropic glutamate receptor subunit NR2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	397	Total	C	N	O	S	0	0	0
			2328	1452	427	440	9			
2	H	409	Total	C	N	O	S	0	0	0
			2382	1460	443	466	13			
2	F	416	Total	C	N	O	S	0	0	0
			2319	1436	430	445	8			
2	D	405	Total	C	N	O	S	0	0	0
			2413	1502	439	461	11			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	486	VAL	THR	conflict	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	CYS	deletion	UNP A7XY94
B	?	-	LEU	deletion	UNP A7XY94
B	?	-	ALA	deletion	UNP A7XY94
B	?	-	ASP	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	?	-	ARG	deletion	UNP A7XY94
B	?	-	GLU	deletion	UNP A7XY94
B	?	-	PRO	deletion	UNP A7XY94
B	?	-	GLY	deletion	UNP A7XY94
B	601	LEU	VAL	conflict	UNP A7XY94
B	640	ARG	GLU	conflict	UNP A7XY94
B	641	ARG	GLU	conflict	UNP A7XY94
B	826	TYR	-	expression tag	UNP A7XY94
B	827	LYS	-	expression tag	UNP A7XY94
B	828	SER	-	expression tag	UNP A7XY94
B	829	ARG	-	expression tag	UNP A7XY94
B	830	ALA	-	expression tag	UNP A7XY94
B	831	GLU	-	expression tag	UNP A7XY94
B	832	ALA	-	expression tag	UNP A7XY94
B	833	LYS	-	expression tag	UNP A7XY94
B	834	ARG	-	expression tag	UNP A7XY94
B	835	MET	-	expression tag	UNP A7XY94
B	836	LYS	-	expression tag	UNP A7XY94
B	837	GLY	-	expression tag	UNP A7XY94
B	838	LEU	-	expression tag	UNP A7XY94
B	839	GLU	-	expression tag	UNP A7XY94
B	840	VAL	-	expression tag	UNP A7XY94
B	841	LEU	-	expression tag	UNP A7XY94
B	842	PHE	-	expression tag	UNP A7XY94
B	843	GLN	-	expression tag	UNP A7XY94
H	486	VAL	THR	conflict	UNP A7XY94
H	?	-	ARG	deletion	UNP A7XY94
H	?	-	CYS	deletion	UNP A7XY94
H	?	-	LEU	deletion	UNP A7XY94
H	?	-	ALA	deletion	UNP A7XY94
H	?	-	ASP	deletion	UNP A7XY94
H	?	-	GLY	deletion	UNP A7XY94
H	?	-	ARG	deletion	UNP A7XY94
H	?	-	GLU	deletion	UNP A7XY94
H	?	-	PRO	deletion	UNP A7XY94
H	?	-	GLY	deletion	UNP A7XY94

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Chain	Residue	Modelled	Actual	Comment	Reference
H	601	LEU	VAL	conflict	UNP A7XY94
H	640	ARG	GLU	conflict	UNP A7XY94
H	641	ARG	GLU	conflict	UNP A7XY94
H	826	TYR	-	expression tag	UNP A7XY94
H	827	LYS	-	expression tag	UNP A7XY94
H	828	SER	-	expression tag	UNP A7XY94
H	829	ARG	-	expression tag	UNP A7XY94
H	830	ALA	-	expression tag	UNP A7XY94
H	831	GLU	-	expression tag	UNP A7XY94
H	832	ALA	-	expression tag	UNP A7XY94
H	833	LYS	-	expression tag	UNP A7XY94
H	834	ARG	-	expression tag	UNP A7XY94
H	835	MET	-	expression tag	UNP A7XY94
H	836	LYS	-	expression tag	UNP A7XY94
H	837	GLY	-	expression tag	UNP A7XY94
H	838	LEU	-	expression tag	UNP A7XY94
H	839	GLU	-	expression tag	UNP A7XY94
H	840	VAL	-	expression tag	UNP A7XY94
H	841	LEU	-	expression tag	UNP A7XY94
H	842	PHE	-	expression tag	UNP A7XY94
H	843	GLN	-	expression tag	UNP A7XY94
F	486	VAL	THR	conflict	UNP A7XY94
F	?	-	ARG	deletion	UNP A7XY94
F	?	-	CYS	deletion	UNP A7XY94
F	?	-	LEU	deletion	UNP A7XY94
F	?	-	ALA	deletion	UNP A7XY94
F	?	-	ASP	deletion	UNP A7XY94
F	?	-	GLY	deletion	UNP A7XY94
F	?	-	ARG	deletion	UNP A7XY94
F	?	-	GLU	deletion	UNP A7XY94
F	?	-	PRO	deletion	UNP A7XY94
F	?	-	GLY	deletion	UNP A7XY94
F	601	LEU	VAL	conflict	UNP A7XY94
F	640	ARG	GLU	conflict	UNP A7XY94
F	641	ARG	GLU	conflict	UNP A7XY94
F	826	TYR	-	expression tag	UNP A7XY94
F	827	LYS	-	expression tag	UNP A7XY94
F	828	SER	-	expression tag	UNP A7XY94
F	829	ARG	-	expression tag	UNP A7XY94
F	830	ALA	-	expression tag	UNP A7XY94
F	831	GLU	-	expression tag	UNP A7XY94
F	832	ALA	-	expression tag	UNP A7XY94

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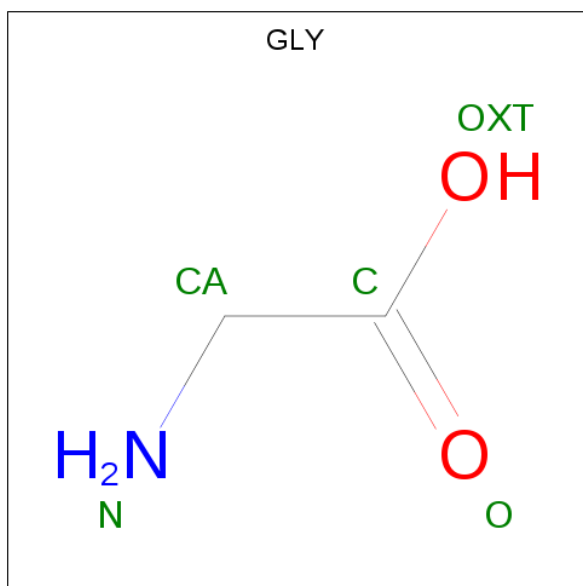
Chain	Residue	Modelled	Actual	Comment	Reference
F	833	LYS	-	expression tag	UNP A7XY94
F	834	ARG	-	expression tag	UNP A7XY94
F	835	MET	-	expression tag	UNP A7XY94
F	836	LYS	-	expression tag	UNP A7XY94
F	837	GLY	-	expression tag	UNP A7XY94
F	838	LEU	-	expression tag	UNP A7XY94
F	839	GLU	-	expression tag	UNP A7XY94
F	840	VAL	-	expression tag	UNP A7XY94
F	841	LEU	-	expression tag	UNP A7XY94
F	842	PHE	-	expression tag	UNP A7XY94
F	843	GLN	-	expression tag	UNP A7XY94
D	486	VAL	THR	conflict	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	CYS	deletion	UNP A7XY94
D	?	-	LEU	deletion	UNP A7XY94
D	?	-	ALA	deletion	UNP A7XY94
D	?	-	ASP	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	?	-	ARG	deletion	UNP A7XY94
D	?	-	GLU	deletion	UNP A7XY94
D	?	-	PRO	deletion	UNP A7XY94
D	?	-	GLY	deletion	UNP A7XY94
D	601	LEU	VAL	conflict	UNP A7XY94
D	640	ARG	GLU	conflict	UNP A7XY94
D	641	ARG	GLU	conflict	UNP A7XY94
D	826	TYR	-	expression tag	UNP A7XY94
D	827	LYS	-	expression tag	UNP A7XY94
D	828	SER	-	expression tag	UNP A7XY94
D	829	ARG	-	expression tag	UNP A7XY94
D	830	ALA	-	expression tag	UNP A7XY94
D	831	GLU	-	expression tag	UNP A7XY94
D	832	ALA	-	expression tag	UNP A7XY94
D	833	LYS	-	expression tag	UNP A7XY94
D	834	ARG	-	expression tag	UNP A7XY94
D	835	MET	-	expression tag	UNP A7XY94
D	836	LYS	-	expression tag	UNP A7XY94
D	837	GLY	-	expression tag	UNP A7XY94
D	838	LEU	-	expression tag	UNP A7XY94
D	839	GLU	-	expression tag	UNP A7XY94
D	840	VAL	-	expression tag	UNP A7XY94
D	841	LEU	-	expression tag	UNP A7XY94
D	842	PHE	-	expression tag	UNP A7XY94

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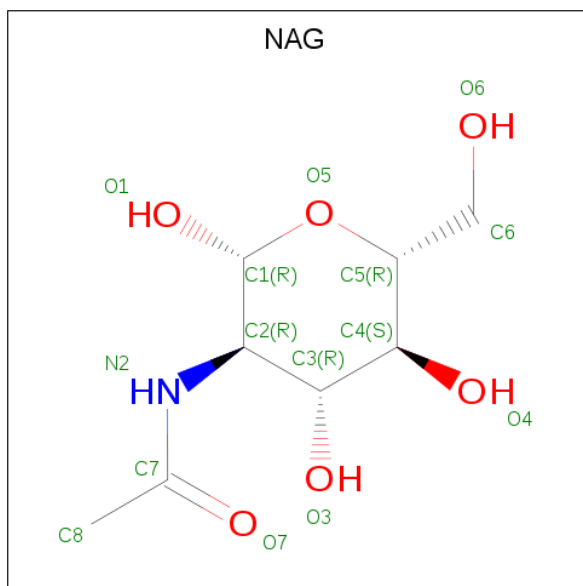
Chain	Residue	Modelled	Actual	Comment	Reference
D	843	GLN	-	expression tag	UNP A7XY94

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



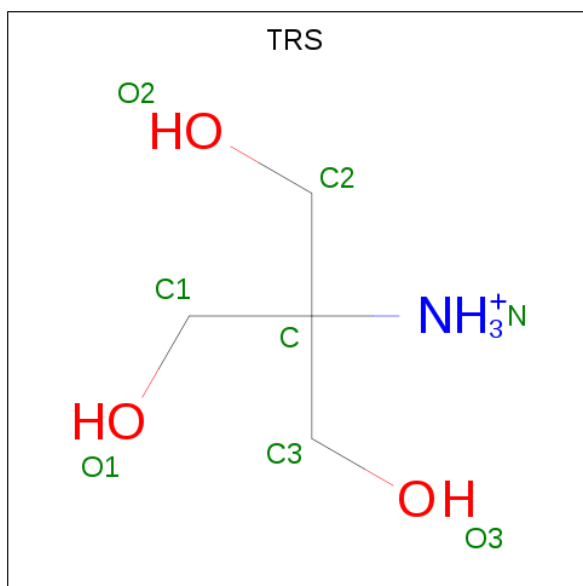
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



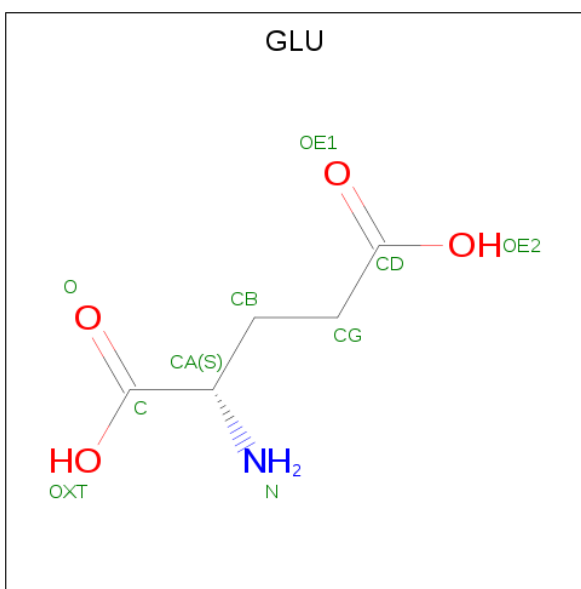
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	F	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



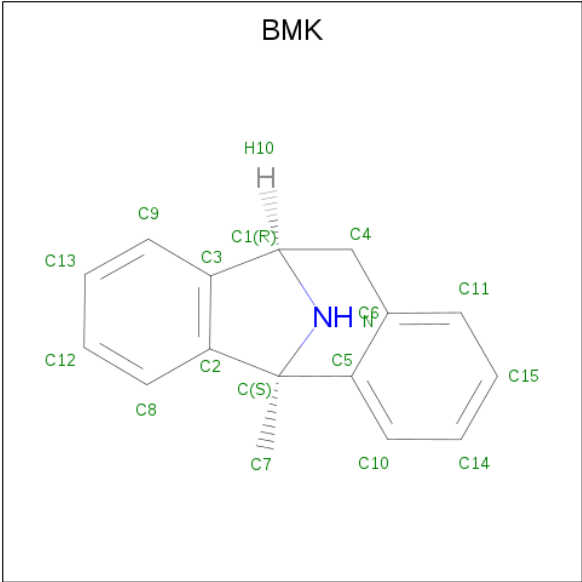
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	B	1	Total	C	N	O	0	0
			10	5	1	4		
6	H	1	Total	C	N	O	0	0
			10	5	1	4		
6	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 7 is (5S,10R)-5-methyl-10,11-dihydro-5H-5,10-epiminodibenzo[a,d][7]annulene (three-letter code: BMK) (formula: C<sub>16</sub>H<sub>15</sub>N).

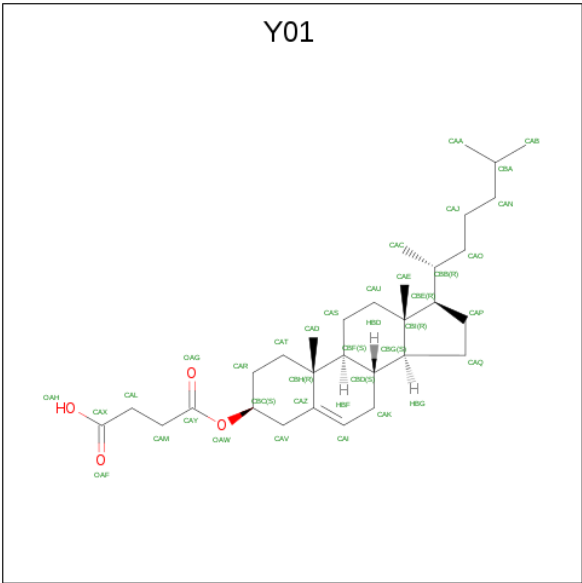


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	N	0	0
			17	16	1		
7	B	1	Total	C	N	0	0
			17	16	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).

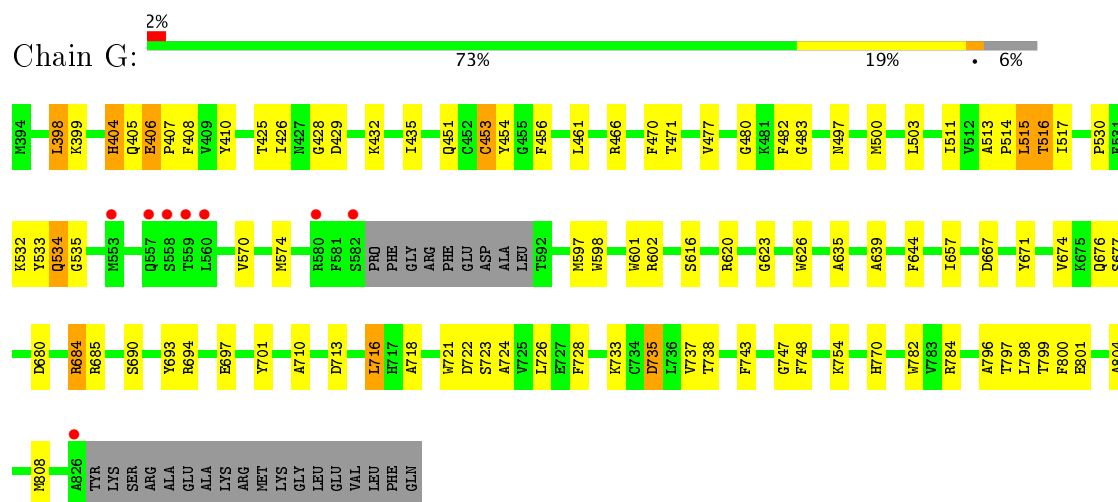


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			35	31	4		

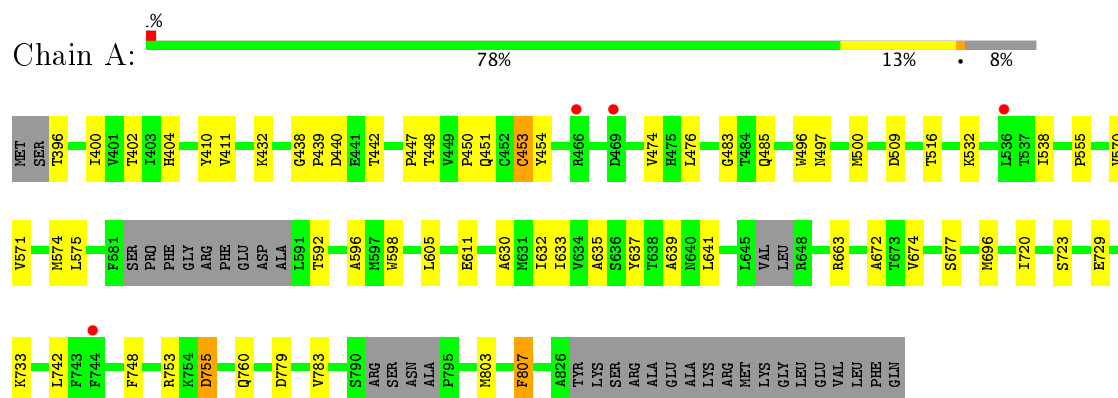
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

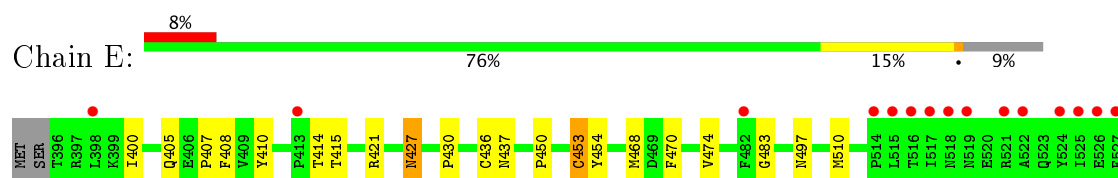
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a



- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a

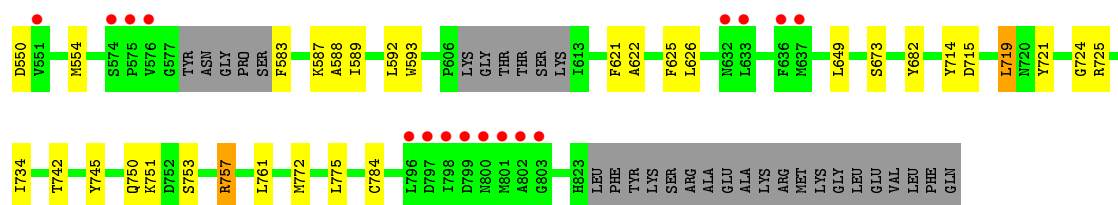


- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a

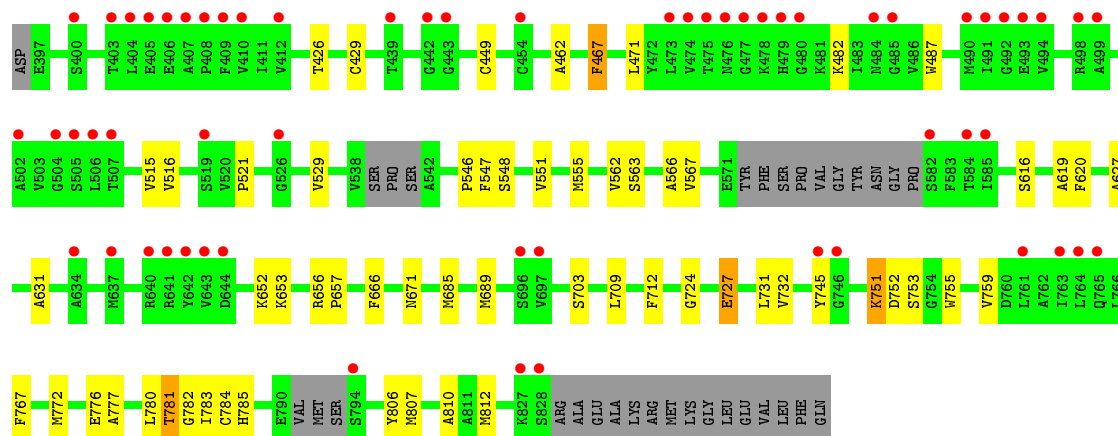
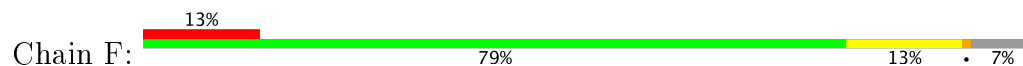




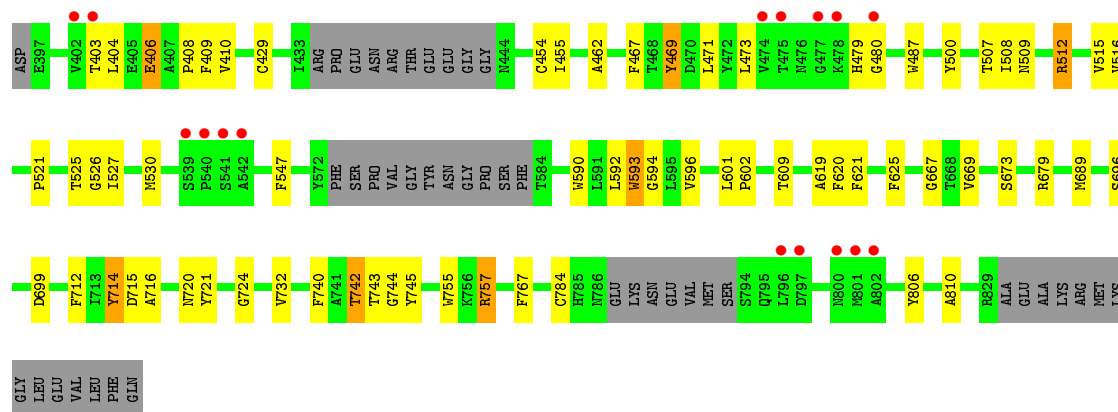
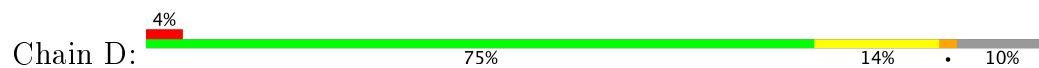




• Molecule 2: Ionotropic glutamate receptor subunit NR2B



• Molecule 2: Ionotropic glutamate receptor subunit NR2B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.57Å 108.47Å 182.46Å 90.00° 111.44° 90.00°	Depositor
Resolution (Å)	49.99 – 3.60 169.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.99-3.60) 78.8 (169.83-3.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.41Å)	Xtriage
Refinement program	PHENIX (dev_2597: ???)	Depositor
R, $R_{free}$	0.288 , 0.316 0.306 , 0.333	Depositor DCC
$R_{free}$ test set	3563 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.11 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.117 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	20143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, 0.333 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: BMK, MG, Y01, TRS, NAG

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	0.28	0/2694	0.45	0/3703
1	C	0.31	0/2647	0.44	0/3648
1	E	0.28	0/2529	0.45	0/3491
1	G	0.37	0/2808	0.50	0/3848
2	B	0.27	0/2363	0.44	0/3260
2	D	0.28	0/2452	0.48	0/3384
2	F	0.30	0/2344	0.49	0/3245
2	H	0.29	0/2409	0.47	0/3317
All	All	0.30	0/20246	0.46	0/27896

There are no bond length outliers.

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	A	2643	0	1928	44	0
1	C	2591	0	1819	70	0
1	E	2486	0	1710	46	0
1	G	2753	0	2092	85	0
2	B	2328	0	1521	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2413	0	1600	63	0
2	F	2319	0	1436	58	0
2	H	2382	0	1585	35	0
3	A	5	0	2	1	0
3	G	5	0	2	5	0
4	B	15	0	15	3	0
4	D	30	0	30	0	0
4	F	15	0	15	0	0
4	G	15	0	15	0	0
4	H	15	0	15	0	0
5	G	8	0	12	2	0
6	B	10	0	5	4	0
6	D	10	0	5	8	0
6	G	20	0	10	2	0
6	H	10	0	5	4	0
7	B	17	0	0	0	0
7	G	17	0	0	0	0
8	A	1	0	0	0	0
9	E	35	0	42	5	0
All	All	20143	0	13864	433	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 13.

All (433) 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)
9:E:1001:Y01:CAQ	9:E:1001:Y01:CAP	1.82	1.51
1:C:624:MET:CB	2:D:593:TRP:HE1	1.33	1.41
1:C:624:MET:CB	2:D:593:TRP:NE1	1.90	1.31
2:D:512:ARG:NH2	6:D:1002:GLU:OXT	1.73	1.20
1:C:624:MET:CB	2:D:593:TRP:CD1	2.31	1.13
2:D:509:ASN:ND2	2:D:512:ARG:HD2	1.59	1.13
1:E:547:SER:CB	1:E:802:ASN:CB	2.30	1.09
1:A:483:GLY:HA2	1:A:497:ASN:O	1.59	1.03
2:D:507:THR:HG1	6:D:1002:GLU:N	1.58	1.01
2:D:509:ASN:HD21	2:D:512:ARG:HD2	0.88	1.01
2:F:724:GLY:HA2	2:F:784:CYS:HB3	1.43	1.00
2:D:509:ASN:HD21	2:D:512:ARG:CD	1.76	0.99
2:B:657:PRO:HB3	2:B:664:PHE:CE1	1.99	0.97
1:G:701:TYR:HE2	1:G:716:LEU:CD1	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:516:THR:OG1	3:G:1001:GLY:OXT	1.85	0.94
2:D:716:ALA:O	2:D:720:ASN:HB2	1.70	0.92
2:F:562:VAL:O	2:F:566:ALA:HB3	1.72	0.90
1:C:568:VAL:HA	1:C:626:TRP:CZ2	2.08	0.89
1:G:657:ILE:HD12	1:G:743:PHE:CE2	2.09	0.87
2:H:505:SER:O	6:H:1001:GLU:N	2.08	0.86
2:H:479:HIS:O	2:H:490:MET:N	2.09	0.85
1:G:799:THR:O	1:G:801:GLU:O	1.96	0.84
1:A:611:GLU:HA	2:B:602:PRO:HB2	1.60	0.84
1:A:516:THR:HG1	3:A:902:GLY:N	1.75	0.84
1:C:483:GLY:HA2	1:C:497:ASN:O	1.77	0.83
1:C:568:VAL:HA	1:C:626:TRP:CH2	2.12	0.83
1:A:410:TYR:O	1:A:453:CYS:HA	1.79	0.83
1:C:770:HIS:CB	2:D:742:THR:OG1	2.27	0.83
2:B:671:ASN:ND2	4:B:1002:NAG:O5	2.12	0.82
2:F:751:LYS:HD3	2:F:752:ASP:CB	2.10	0.82
1:G:797:THR:CB	2:F:547:PHE:C	2.48	0.82
2:H:550:ASP:O	2:H:554:MET:HB2	1.78	0.82
1:C:410:TYR:HB2	1:C:454:TYR:O	1.80	0.81
2:F:776:GLU:CB	2:F:780:LEU:HD12	2.12	0.79
2:D:429:CYS:HA	2:D:471:LEU:HD11	1.64	0.77
1:G:534:GLN:HG2	1:G:723:SER:HB3	1.65	0.77
2:F:777:ALA:O	2:F:781:THR:OG1	2.04	0.76
2:D:715:ASP:OD2	2:D:745:TYR:OH	2.02	0.76
2:F:777:ALA:HA	2:F:781:THR:OG1	1.85	0.76
2:F:731:LEU:O	2:F:732:VAL:HG12	1.83	0.76
1:C:632:ILE:O	1:C:636:SER:CB	2.34	0.76
1:G:701:TYR:HE2	1:G:716:LEU:HD12	1.50	0.76
1:G:404:HIS:HE1	1:G:406:GLU:HG2	1.49	0.76
2:D:406:GLU:H	2:D:410:VAL:CG1	1.99	0.75
2:D:509:ASN:ND2	2:D:512:ARG:CD	2.43	0.75
1:G:516:THR:HG1	3:G:1001:GLY:C	1.89	0.75
1:C:631:MET:O	1:C:635:ALA:HB3	1.87	0.74
2:H:497:LYS:NZ	2:H:497:LYS:O	2.20	0.74
1:G:770:HIS:ND1	2:H:742:THR:OG1	2.21	0.73
2:H:515:VAL:HG23	2:H:516:VAL:HG13	1.67	0.73
2:F:727:GLU:OE1	2:F:727:GLU:N	2.18	0.73
1:G:701:TYR:CE2	1:G:716:LEU:HD12	2.22	0.73
2:D:404:LEU:O	2:D:410:VAL:HG11	1.90	0.72
2:F:563:SER:O	2:F:567:VAL:CB	2.38	0.71
1:G:797:THR:CB	2:F:547:PHE:O	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:667:GLY:HA2	2:D:689:MET:HG2	1.72	0.70
2:F:562:VAL:O	2:F:566:ALA:CB	2.38	0.70
2:B:657:PRO:CB	2:B:664:PHE:CE1	2.75	0.70
2:B:590:TRP:HH2	2:B:602:PRO:HD2	1.56	0.70
1:G:517:ILE:HG13	1:G:747:GLY:O	1.92	0.70
2:D:673:SER:HG	6:D:1002:GLU:N	1.89	0.70
2:H:507:THR:OG1	6:H:1001:GLU:HA	1.93	0.69
2:D:526:GLY:O	2:D:716:ALA:N	2.26	0.69
2:H:434:ARG:HA	2:H:442:GLY:HA2	1.75	0.69
1:C:631:MET:O	1:C:635:ALA:CB	2.40	0.68
2:D:724:GLY:HA2	2:D:784:CYS:HB2	1.74	0.68
1:G:534:GLN:HG2	1:G:535:GLY:H	1.59	0.68
2:B:657:PRO:HG3	2:B:664:PHE:HE1	1.56	0.68
2:B:665:ARG:O	2:B:710:ASP:N	2.26	0.68
2:F:731:LEU:O	2:F:732:VAL:CG1	2.41	0.68
1:G:532:LYS:HB3	1:G:748:PHE:HB2	1.76	0.67
2:D:507:THR:OG1	6:D:1002:GLU:O	2.13	0.67
1:G:796:ALA:O	1:G:797:THR:C	2.32	0.67
2:B:657:PRO:HB3	2:B:664:PHE:CD1	2.30	0.67
2:B:515:VAL:HG23	2:B:516:VAL:HG13	1.76	0.67
2:D:480:GLY:O	2:D:512:ARG:NH1	2.27	0.67
1:G:701:TYR:CE2	1:G:716:LEU:CD1	2.71	0.67
2:B:724:GLY:HA2	2:B:785:HIS:CB	2.26	0.66
1:E:483:GLY:HA2	1:E:497:ASN:O	1.95	0.65
1:C:532:LYS:HB3	1:C:748:PHE:HB2	1.78	0.65
2:B:550:ASP:O	2:B:553:VAL:N	2.29	0.65
1:G:722:ASP:OD2	3:G:1001:GLY:N	2.31	0.64
1:G:534:GLN:OE1	1:G:723:SER:N	2.30	0.64
1:C:598:TRP:O	1:C:602:ARG:CB	2.45	0.64
1:G:796:ALA:O	1:G:798:LEU:N	2.30	0.64
2:H:512:ARG:NH2	6:H:1001:GLU:OXT	2.29	0.64
1:C:600:SER:HA	1:C:626:TRP:NE1	2.12	0.64
2:H:622:ALA:O	2:H:626:LEU:CB	2.46	0.64
2:B:521:PRO:HB3	2:B:744:GLY:HA3	1.80	0.64
1:C:562:LEU:O	1:C:566:LEU:CB	2.46	0.64
1:E:541:LYS:HA	1:E:735:ASP:O	1.96	0.64
2:B:508:ILE:HD11	2:B:746:GLY:HA3	1.80	0.64
1:G:516:THR:OG1	3:G:1001:GLY:C	2.34	0.63
2:D:406:GLU:H	2:D:410:VAL:HG12	1.62	0.63
1:G:799:THR:O	1:G:800:PHE:C	2.36	0.63
2:F:515:VAL:HG23	2:F:516:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:ALA:O	1:E:639:ALA:HB2	1.98	0.63
1:E:657:ILE:HB	1:E:743:PHE:HB3	1.79	0.63
1:C:533:TYR:CE2	2:D:742:THR:O	2.52	0.62
2:B:550:ASP:O	2:B:552:TRP:N	2.33	0.62
2:D:512:ARG:HH22	6:D:1002:GLU:C	1.92	0.62
2:D:716:ALA:O	2:D:720:ASN:CB	2.46	0.62
1:G:674:VAL:O	1:G:677:SER:OG	2.16	0.61
1:G:410:TYR:HB2	1:G:454:TYR:O	2.00	0.61
2:B:550:ASP:O	2:B:551:VAL:C	2.37	0.61
1:C:735:ASP:N	1:C:735:ASP:OD1	2.34	0.61
1:E:427:ASN:OD1	1:E:427:ASN:N	2.34	0.61
1:G:570:VAL:O	1:G:574:MET:CB	2.48	0.61
2:B:548:SER:O	2:B:549:ALA:HB3	2.00	0.60
1:C:563:LEU:O	1:C:567:SER:CB	2.49	0.60
1:E:618:SER:O	1:E:622:LEU:HG	2.01	0.60
2:F:727:GLU:CD	2:F:727:GLU:H	2.04	0.60
2:F:777:ALA:CA	2:F:781:THR:OG1	2.49	0.60
2:H:715:ASP:OD2	2:H:745:TYR:OH	2.19	0.60
2:H:772:MET:SD	2:H:772:MET:N	2.75	0.60
2:B:673:SER:OG	6:B:1001:GLU:OE2	2.20	0.60
2:D:512:ARG:NH2	6:D:1002:GLU:C	2.52	0.60
1:E:571:VAL:HG11	1:E:626:TRP:HB2	1.84	0.60
1:A:611:GLU:HA	2:B:602:PRO:CB	2.31	0.60
2:B:773:GLU:O	2:B:777:ALA:HB3	2.02	0.59
1:C:522:ALA:O	2:D:757:ARG:NH2	2.34	0.59
2:H:429:CYS:HB3	2:H:471:LEU:HD23	1.83	0.59
2:H:521:PRO:HA	2:H:745:TYR:O	2.01	0.59
1:A:485:GLN:HB3	1:A:496:TRP:CE2	2.37	0.59
1:A:532:LYS:HB3	1:A:748:PHE:HB2	1.84	0.59
1:E:802:ASN:O	1:E:805:GLY:N	2.35	0.59
1:G:426:ILE:HG23	6:G:1004:GLU:OE1	2.02	0.59
2:B:657:PRO:CG	2:B:664:PHE:HE1	2.15	0.59
2:B:767:PHE:CD1	2:B:772:MET:HG3	2.38	0.59
2:F:751:LYS:O	2:F:753:SER:N	2.25	0.59
1:C:539:LEU:O	1:C:718:ALA:HA	2.03	0.59
1:A:483:GLY:CA	1:A:497:ASN:O	2.45	0.58
2:B:665:ARG:CB	2:B:710:ASP:H	2.16	0.58
1:E:637:TYR:O	1:E:641:LEU:CB	2.51	0.58
2:B:773:GLU:O	2:B:777:ALA:CB	2.51	0.58
2:F:777:ALA:C	2:F:781:THR:OG1	2.41	0.58
1:C:568:VAL:CA	1:C:626:TRP:CH2	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:777:ALA:C	2:F:781:THR:HG1	2.03	0.58
1:G:671:TYR:HB3	1:G:718:ALA:HB3	1.85	0.58
1:A:439:PRO:HG2	1:A:442:THR:HA	1.84	0.58
1:C:567:SER:O	1:C:626:TRP:CH2	2.56	0.58
2:F:782:GLY:C	2:F:784:CYS:N	2.55	0.58
2:B:611:SER:O	2:B:615:VAL:CB	2.52	0.58
1:C:758:TRP:O	1:C:762:VAL:HB	2.04	0.58
2:F:731:LEU:C	2:F:732:VAL:CG1	2.71	0.58
1:G:516:THR:N	3:G:1001:GLY:OXT	2.22	0.58
1:C:616:SER:O	1:C:620:ARG:N	2.26	0.57
2:D:515:VAL:HG23	2:D:516:VAL:HG13	1.85	0.57
1:G:735:ASP:N	1:G:735:ASP:OD1	2.26	0.57
2:H:583:PHE:O	2:H:587:LYS:N	2.37	0.57
2:H:772:MET:O	2:H:775:LEU:N	2.37	0.57
1:G:534:GLN:HG2	1:G:535:GLY:N	2.18	0.57
1:A:396:THR:HA	1:E:430:PRO:HG2	1.87	0.57
2:B:547:PHE:O	2:B:548:SER:CB	2.52	0.57
2:B:657:PRO:CG	2:B:664:PHE:CE1	2.88	0.57
1:C:569:HIS:CD2	1:C:601:TRP:HE1	2.22	0.57
1:A:402:THR:HG23	1:A:476:LEU:HD23	1.87	0.56
1:A:803:MET:CB	2:D:547:PHE:HE1	2.17	0.56
1:A:438:GLY:O	1:A:448:THR:HA	2.05	0.56
1:E:570:VAL:O	1:E:574:MET:CB	2.53	0.56
1:C:600:SER:HA	1:C:626:TRP:CD1	2.41	0.56
2:F:782:GLY:O	2:F:783:ILE:C	2.44	0.56
1:E:674:VAL:O	1:E:677:SER:OG	2.23	0.56
2:B:526:GLY:O	2:B:716:ALA:N	2.38	0.56
1:E:665:PRO:HB3	1:E:692:MET:HA	1.88	0.56
2:F:652:LYS:O	2:F:656:ARG:N	2.34	0.55
1:G:398:LEU:HD11	1:G:470:PHE:CD1	2.41	0.55
1:E:421:ARG:HH12	9:E:1001:Y01:CAY	2.20	0.55
1:G:797:THR:HA	2:F:546:PRO:O	2.05	0.55
2:B:487:TRP:HD1	2:B:492:GLY:HA2	1.72	0.55
1:C:569:HIS:N	1:C:569:HIS:CD2	2.74	0.55
1:E:410:TYR:O	1:E:453:CYS:HA	2.06	0.55
1:E:468:MET:HB2	1:E:470:PHE:CD1	2.42	0.55
2:F:529:VAL:HA	2:F:712:PHE:O	2.07	0.55
1:G:754:LYS:HE3	2:H:757:ARG:HH11	1.72	0.55
2:D:410:VAL:HG23	2:D:455:ILE:HD11	1.89	0.55
2:H:589:ILE:O	2:H:593:TRP:CB	2.55	0.55
1:G:721:TRP:CG	1:G:722:ASP:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:685:MET:O	2:F:689:MET:CB	2.55	0.54
2:B:512:ARG:H	2:B:512:ARG:HD2	1.72	0.54
1:A:611:GLU:CA	2:B:602:PRO:HB2	2.36	0.54
2:F:731:LEU:C	2:F:732:VAL:HG13	2.28	0.54
2:F:782:GLY:O	2:F:784:CYS:N	2.40	0.54
1:G:503:LEU:HD22	1:G:511:ILE:HD13	1.90	0.54
2:D:526:GLY:H	2:D:716:ALA:HB3	1.72	0.53
1:G:693:TYR:O	1:G:697:GLU:N	2.34	0.53
1:G:667:ASP:OD1	5:G:1003:TRS:O2	2.26	0.53
1:G:797:THR:CA	2:F:546:PRO:O	2.56	0.53
1:G:399:LYS:H	1:G:399:LYS:HD2	1.73	0.53
1:G:513:ALA:HB1	1:G:514:PRO:HD2	1.90	0.53
1:A:442:THR:HG22	1:A:476:LEU:HD13	1.91	0.53
1:C:568:VAL:CA	1:C:626:TRP:CZ2	2.87	0.53
1:C:567:SER:C	1:C:626:TRP:HH2	2.11	0.53
1:E:541:LYS:CB	1:E:736:LEU:HD23	2.17	0.53
1:E:690:SER:O	1:E:693:TYR:HB3	2.08	0.53
1:A:570:VAL:O	1:A:574:MET:CB	2.57	0.53
1:A:555:PRO:O	2:B:796:LEU:N	2.41	0.53
1:G:483:GLY:HA3	1:G:500:MET:HB2	1.90	0.53
2:B:673:SER:HB3	6:B:1001:GLU:HG3	1.91	0.52
1:C:688:GLU:O	1:C:691:THR:HG22	2.09	0.52
2:H:529:VAL:O	2:H:734:ILE:N	2.40	0.52
1:C:690:SER:O	1:C:693:TYR:HB3	2.09	0.52
2:F:551:VAL:O	2:F:555:MET:CB	2.57	0.52
1:G:398:LEU:HD12	1:G:471:THR:O	2.10	0.52
1:G:800:PHE:O	1:G:804:ALA:N	2.38	0.52
1:C:437:ASN:H	1:C:475:HIS:HA	1.74	0.52
2:H:715:ASP:O	2:H:719:LEU:HB2	2.09	0.52
2:B:671:ASN:HD22	4:B:1002:NAG:H62	1.73	0.52
2:B:477:GLY:HA3	2:B:489:GLY:HA2	1.91	0.52
2:F:482:LYS:HA	2:F:487:TRP:HA	1.91	0.52
2:D:673:SER:HB3	6:D:1002:GLU:HA	1.93	0.51
2:F:653:LYS:HA	2:F:657:PRO:HA	1.92	0.51
2:F:703:SER:O	2:F:709:LEU:N	2.42	0.51
1:G:425:THR:O	1:G:428:GLY:N	2.29	0.51
1:A:760:GLN:HA	1:A:760:GLN:OE1	2.10	0.51
2:H:714:TYR:CG	2:H:715:ASP:N	2.78	0.51
1:E:532:LYS:O	1:E:747:GLY:HA2	2.09	0.51
1:C:743:PHE:HD1	1:C:743:PHE:H	1.59	0.51
1:E:536:LEU:HD12	1:E:721:TRP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:ARG:HE	6:B:1001:GLU:N	2.09	0.50
2:H:397:GLU:O	2:H:468:THR:OG1	2.17	0.50
2:B:806:TYR:O	2:B:810:ALA:CB	2.59	0.50
1:C:723:SER:O	1:C:727:GLU:HB2	2.10	0.50
9:E:1001:Y01:HAE2	9:E:1001:Y01:HAC1	1.94	0.50
2:H:621:PHE:O	2:H:625:PHE:CB	2.60	0.50
1:A:450:PRO:O	1:A:451:GLN:HG3	2.10	0.50
1:G:721:TRP:HB3	1:G:726:LEU:HD11	1.93	0.50
1:G:533:TYR:CE2	2:H:742:THR:O	2.65	0.50
1:C:538:ILE:O	1:C:739:THR:N	2.36	0.50
2:B:657:PRO:HG3	2:B:664:PHE:CE1	2.42	0.50
2:D:403:THR:HG23	2:D:473:LEU:HD12	1.93	0.50
1:G:410:TYR:O	1:G:453:CYS:HA	2.11	0.50
2:B:506:LEU:HD12	6:B:1001:GLU:HB3	1.92	0.49
1:G:435:ILE:HA	1:G:451:GLN:O	2.12	0.49
1:G:616:SER:O	1:G:620:ARG:N	2.35	0.49
1:A:637:TYR:O	1:A:641:LEU:CB	2.60	0.49
1:A:538:ILE:HA	1:A:720:ILE:HA	1.94	0.49
1:E:622:LEU:HD23	2:F:812:MET:HA	1.94	0.49
1:G:405:GLN:HE21	1:G:482:PHE:HZ	1.59	0.49
1:E:468:MET:HB2	1:E:470:PHE:HD1	1.76	0.49
1:G:432:LYS:HD2	1:G:432:LYS:H	1.76	0.49
1:G:532:LYS:HE2	1:G:724:ALA:HB2	1.95	0.49
1:C:569:HIS:NE2	1:C:601:TRP:HZ2	2.10	0.49
2:F:776:GLU:HA	2:F:780:LEU:HB2	1.94	0.49
1:E:765:ASN:O	1:E:769:SER:N	2.37	0.49
1:A:439:PRO:HA	1:A:447:PRO:O	2.13	0.49
1:E:436:CYS:O	1:E:450:PRO:HA	2.13	0.49
2:F:627:ALA:O	2:F:631:ALA:N	2.45	0.49
2:D:410:VAL:O	2:D:410:VAL:HG13	2.13	0.48
2:D:525:THR:O	2:D:743:THR:O	2.31	0.48
1:G:597:MET:O	1:G:601:TRP:HB2	2.13	0.48
2:F:666:PHE:CZ	2:F:685:MET:HA	2.49	0.48
1:C:624:MET:CA	2:D:593:TRP:NE1	2.71	0.48
1:E:571:VAL:O	1:E:575:LEU:CB	2.62	0.48
1:C:769:SER:O	1:C:772:ASN:ND2	2.46	0.48
1:G:796:ALA:C	1:G:798:LEU:N	2.66	0.48
2:D:590:TRP:HE1	2:D:602:PRO:HD2	1.78	0.48
1:C:567:SER:C	1:C:626:TRP:CH2	2.86	0.48
2:H:509:ASN:OD1	2:H:510:GLU:N	2.47	0.48
1:E:400:ILE:HB	1:E:474:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:ARG:CB	2:B:710:ASP:N	2.77	0.48
1:G:497:ASN:HB3	1:G:676:GLN:HE22	1.78	0.47
1:A:571:VAL:O	1:A:575:LEU:CB	2.62	0.47
2:F:562:VAL:O	2:F:566:ALA:N	2.46	0.47
1:A:672:ALA:HA	1:A:696:MET:HG2	1.96	0.47
1:A:509:ASP:HA	1:A:753:ARG:HH21	1.79	0.47
2:B:590:TRP:CH2	2:B:602:PRO:HD2	2.42	0.47
1:G:408:PHE:HA	1:G:456:PHE:HB3	1.96	0.47
1:G:534:GLN:HE21	1:G:534:GLN:HB3	1.35	0.47
1:C:627:ALA:O	1:C:630:ALA:N	2.44	0.47
1:G:690:SER:O	1:G:694:ARG:N	2.41	0.47
2:B:462:ALA:HA	2:B:467:PHE:HE1	1.80	0.47
1:C:626:TRP:O	1:C:627:ALA:C	2.50	0.47
1:G:797:THR:CB	2:F:548:SER:N	2.78	0.47
1:E:541:LYS:CB	1:E:736:LEU:CD2	2.84	0.47
2:F:776:GLU:O	2:F:781:THR:N	2.48	0.47
1:E:400:ILE:HD13	1:E:510:MET:HB3	1.96	0.47
1:E:654:ILE:CB	1:E:739:THR:HA	2.43	0.47
2:B:657:PRO:CB	2:B:664:PHE:HE1	2.27	0.46
1:C:600:SER:CA	1:C:626:TRP:NE1	2.77	0.46
2:D:479:HIS:NE2	6:D:1002:GLU:OE2	2.48	0.46
1:E:535:GLY:HA2	1:E:745:ARG:HA	1.97	0.46
1:E:693:TYR:O	1:E:697:GLU:N	2.49	0.46
2:F:666:PHE:HZ	2:F:685:MET:HA	1.80	0.46
1:E:407:PRO:HG2	1:E:408:PHE:CD2	2.51	0.46
1:G:497:ASN:HB3	1:G:676:GLN:NE2	2.30	0.46
1:C:407:PRO:HB3	1:C:728:PHE:CD2	2.50	0.46
2:F:776:GLU:O	2:F:780:LEU:HB2	2.14	0.46
1:C:569:HIS:HD2	1:C:601:TRP:HE1	1.62	0.46
2:B:671:ASN:HD21	4:B:1002:NAG:C1	2.29	0.46
2:B:818:THR:O	2:B:822:GLU:CB	2.64	0.46
1:C:570:VAL:O	1:C:574:MET:CB	2.64	0.46
2:B:774:GLU:H	2:B:774:GLU:HG3	1.57	0.46
2:F:429:CYS:HB3	2:F:471:LEU:HB3	1.98	0.46
2:H:470:ASP:N	2:H:470:ASP:OD1	2.47	0.46
1:A:404:HIS:CE1	1:A:411:VAL:H	2.34	0.45
1:G:733:LYS:HB3	1:G:735:ASP:OD1	2.16	0.45
1:G:737:VAL:HG12	1:G:738:THR:N	2.32	0.45
1:G:514:PRO:HB2	1:G:748:PHE:CZ	2.51	0.45
1:E:628:GLY:O	1:E:632:ILE:HG13	2.16	0.45
1:A:592:THR:O	1:A:596:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:508:ILE:HG12	2:D:744:GLY:O	2.17	0.45
1:G:530:PRO:HB2	1:G:533:TYR:CE1	2.51	0.45
2:B:472:TYR:HE1	2:B:499:ALA:HB2	1.82	0.45
2:H:482:LYS:NZ	2:H:515:VAL:HG21	2.32	0.45
1:C:786:GLN:HA	1:C:786:GLN:OE1	2.16	0.45
2:D:409:PHE:HB3	2:D:454:CYS:SG	2.57	0.45
2:F:806:TYR:O	2:F:810:ALA:HB2	2.17	0.45
1:A:410:TYR:HB2	1:A:454:TYR:O	2.17	0.45
1:C:672:ALA:HA	1:C:696:MET:HG2	1.98	0.45
2:D:593:TRP:CE3	2:D:593:TRP:O	2.70	0.45
2:F:751:LYS:C	2:F:753:SER:H	2.15	0.45
1:C:721:TRP:HB3	1:C:726:LEU:HG	1.99	0.45
2:D:714:TYR:CD1	2:D:715:ASP:N	2.85	0.45
1:E:414:THR:OG1	1:E:415:THR:N	2.50	0.45
1:C:427:ASN:HD21	1:C:781:THR:HG22	1.82	0.44
1:C:573:VAL:HA	1:C:576:TYR:HB3	1.99	0.44
1:G:466:ARG:HD3	1:A:755:ASP:HB3	1.99	0.44
2:H:588:ALA:O	2:H:592:LEU:CB	2.65	0.44
1:A:630:ALA:HA	1:A:633:ILE:HG22	2.00	0.44
1:C:398:LEU:HB2	1:C:509:ASP:HB2	2.00	0.44
1:E:410:TYR:HB2	1:E:454:TYR:O	2.17	0.44
1:A:400:ILE:HB	1:A:474:VAL:HA	1.99	0.44
1:A:496:TRP:CZ3	1:A:500:MET:HE2	2.53	0.44
1:C:436:CYS:O	1:C:450:PRO:HA	2.18	0.44
2:B:525:THR:O	2:B:743:THR:N	2.45	0.44
2:B:548:SER:O	2:B:549:ALA:CB	2.66	0.44
1:C:624:MET:CA	2:D:593:TRP:HE1	2.15	0.44
1:A:779:ASP:HA	1:A:783:VAL:HG12	2.00	0.44
2:F:784:CYS:O	2:F:785:HIS:CB	2.66	0.44
1:G:515:LEU:O	1:G:748:PHE:HA	2.18	0.44
2:H:724:GLY:HA2	2:H:784:CYS:HB2	2.00	0.44
1:C:407:PRO:HB3	1:C:728:PHE:CG	2.53	0.43
2:D:593:TRP:HA	2:D:593:TRP:CE3	2.53	0.43
2:D:527:ILE:HB	2:D:740:PHE:CB	2.47	0.43
1:G:710:ALA:HB1	1:G:716:LEU:HB2	2.00	0.43
2:B:506:LEU:O	2:B:745:TYR:HA	2.18	0.43
2:D:462:ALA:HA	2:D:467:PHE:CE1	2.53	0.43
2:D:593:TRP:HE3	2:D:593:TRP:HA	1.83	0.43
1:A:632:ILE:HG21	2:B:804:VAL:HG21	2.00	0.43
1:E:538:ILE:HA	1:E:720:ILE:HA	2.01	0.43
1:E:635:ALA:O	1:E:639:ALA:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:426:THR:CB	2:F:449:CYS:HB3	2.48	0.43
1:G:782:TRP:CZ3	6:G:1004:GLU:HG2	2.53	0.43
1:A:807:PHE:HB2	2:D:621:PHE:HE1	1.84	0.43
2:F:521:PRO:HA	2:F:745:TYR:O	2.18	0.43
2:H:408:PRO:HG3	2:H:721:TYR:CG	2.53	0.43
2:B:803:GLY:O	2:B:807:MET:HG2	2.18	0.43
1:C:403:ILE:HG13	1:C:477:VAL:HG11	2.01	0.43
1:C:569:HIS:NE2	1:C:601:TRP:CZ2	2.87	0.43
1:A:598:TRP:HZ2	2:D:609:THR:HA	1.84	0.43
2:B:755:TRP:HB2	2:B:759:VAL:HG23	2.01	0.43
1:C:634:VAL:O	1:C:638:THR:HG23	2.18	0.43
1:E:540:VAL:O	1:E:737:VAL:N	2.38	0.43
2:F:755:TRP:O	2:F:759:VAL:HG23	2.18	0.43
1:G:680:ASP:O	1:G:684:ARG:CB	2.67	0.43
2:D:806:TYR:O	2:D:810:ALA:HB2	2.18	0.43
1:E:405:GLN:HG3	1:E:407:PRO:HD2	2.00	0.43
1:E:797:THR:O	1:E:799:THR:N	2.51	0.43
2:D:469:TYR:H	2:D:469:TYR:HD1	1.67	0.43
1:C:619:ALA:O	1:C:623:GLY:N	2.52	0.43
1:C:637:TYR:CD1	1:C:637:TYR:C	2.91	0.43
2:H:509:ASN:HB3	2:H:512:ARG:HG3	2.00	0.43
2:H:751:LYS:O	2:H:753:SER:N	2.44	0.43
1:G:477:VAL:HG13	1:G:480:GLY:H	1.83	0.42
2:B:716:ALA:O	2:B:720:ASN:HB2	2.19	0.42
1:G:515:LEU:HA	1:G:515:LEU:HD12	1.89	0.42
2:D:594:GLY:HA3	2:D:601:LEU:CB	2.49	0.42
1:A:605:LEU:O	2:D:619:ALA:HB1	2.19	0.42
1:E:421:ARG:HH12	9:E:1001:Y01:CAM	2.32	0.42
9:E:1001:Y01:HAB2	9:E:1001:Y01:HAJ2	1.80	0.42
2:B:775:LEU:O	2:B:779:TRP:HD1	2.02	0.42
2:F:782:GLY:C	2:F:784:CYS:H	2.22	0.42
1:G:534:GLN:NE2	1:G:748:PHE:CZ	2.87	0.42
1:G:534:GLN:OE1	1:G:722:ASP:HB3	2.19	0.42
2:H:757:ARG:O	2:H:761:LEU:HG	2.19	0.42
1:C:624:MET:O	1:C:627:ALA:HB3	2.20	0.42
1:C:526:GLU:HB2	1:C:754:LYS:HA	2.01	0.42
2:F:616:SER:O	2:F:619:ALA:HB3	2.20	0.42
1:A:635:ALA:O	1:A:639:ALA:HB2	2.19	0.42
2:B:714:TYR:CG	2:B:715:ASP:N	2.85	0.42
1:E:437:ASN:HA	1:E:450:PRO:HA	2.02	0.42
1:G:623:GLY:HA2	1:G:626:TRP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:VAL:O	1:C:572:ALA:HB2	2.19	0.42
2:D:408:PRO:HD3	2:D:721:TYR:CD2	2.54	0.42
2:F:467:PHE:N	2:F:467:PHE:CD1	2.87	0.42
1:G:635:ALA:O	1:G:639:ALA:HB2	2.19	0.42
1:C:439:PRO:HA	1:C:447:PRO:O	2.19	0.42
1:E:421:ARG:HH11	1:E:421:ARG:HG3	1.85	0.42
1:E:539:LEU:O	1:E:719:PHE:N	2.53	0.42
2:F:776:GLU:CA	2:F:780:LEU:HD12	2.50	0.42
1:G:461:LEU:HD22	1:G:461:LEU:O	2.20	0.42
1:G:598:TRP:O	1:G:602:ARG:CB	2.68	0.42
1:G:667:ASP:OD1	5:G:1003:TRS:H11	2.20	0.42
1:A:432:LYS:H	1:A:432:LYS:HG2	1.73	0.42
2:D:530:MET:HA	2:D:732:VAL:O	2.20	0.42
1:G:404:HIS:CE1	1:G:406:GLU:HG2	2.40	0.42
1:G:407:PRO:HG3	1:G:728:PHE:CD2	2.55	0.42
1:G:804:ALA:O	1:G:808:MET:CB	2.68	0.42
2:H:673:SER:H	6:H:1001:GLU:HG3	1.85	0.42
1:A:663:ARG:HD2	1:A:663:ARG:HA	1.74	0.41
1:C:532:LYS:O	1:C:747:GLY:CA	2.68	0.41
1:G:407:PRO:HG3	1:G:728:PHE:CG	2.55	0.41
1:C:626:TRP:O	1:C:629:PHE:N	2.53	0.41
2:D:592:LEU:O	2:D:596:VAL:HG23	2.21	0.41
2:D:755:TRP:CD1	2:D:755:TRP:N	2.88	0.41
2:B:407:ALA:HA	2:B:408:PRO:HA	1.82	0.41
1:C:530:PRO:HB2	1:C:533:TYR:HE1	1.85	0.41
2:D:714:TYR:CG	2:D:715:ASP:N	2.88	0.41
2:B:522:PHE:N	2:B:745:TYR:O	2.44	0.41
2:D:500:TYR:CE2	2:D:755:TRP:NE1	2.88	0.41
1:E:725:VAL:O	1:E:729:GLU:HG2	2.20	0.41
2:F:767:PHE:HA	2:F:772:MET:HG2	2.02	0.41
1:C:687:VAL:O	1:C:690:SER:CB	2.68	0.41
1:C:533:TYR:OH	2:D:521:PRO:HG3	2.20	0.41
1:A:440:ASP:N	1:A:447:PRO:O	2.40	0.41
1:C:534:GLN:OE1	1:C:722:ASP:HB3	2.21	0.41
1:G:797:THR:CB	2:F:546:PRO:O	2.69	0.41
1:A:674:VAL:O	1:A:677:SER:OG	2.36	0.41
2:B:806:TYR:O	2:B:810:ALA:HB2	2.21	0.41
2:D:696:SER:O	2:D:699:ASP:N	2.54	0.41
2:F:671:ASN:N	2:F:671:ASN:HD22	2.19	0.41
1:G:425:THR:N	1:G:429:ASP:O	2.27	0.41
1:C:517:ILE:HD12	1:C:530:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:530:PRO:HB2	1:G:533:TYR:HE1	1.86	0.41
2:B:526:GLY:H	2:B:716:ALA:HB3	1.86	0.41
2:D:471:LEU:C	2:D:471:LEU:HD12	2.41	0.41
2:D:669:VAL:HG23	2:D:712:PHE:HZ	1.85	0.40
1:A:729:GLU:O	1:A:733:LYS:N	2.40	0.40
2:F:462:ALA:HA	2:F:467:PHE:CE1	2.56	0.40
2:F:807:MET:SD	2:F:807:MET:N	2.94	0.40
1:A:723:SER:HB3	1:A:742:LEU:HD11	2.04	0.40
2:H:416:ASP:O	2:H:420:GLY:N	2.53	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	408/451 (90%)	388 (95%)	20 (5%)	0	100	100
1	C	407/451 (90%)	385 (95%)	22 (5%)	0	100	100
1	E	404/451 (90%)	387 (96%)	17 (4%)	0	100	100
1	G	420/451 (93%)	400 (95%)	20 (5%)	0	100	100
2	B	387/448 (86%)	350 (90%)	37 (10%)	0	100	100
2	D	397/448 (89%)	376 (95%)	21 (5%)	0	100	100
2	F	408/448 (91%)	377 (92%)	31 (8%)	0	100	100
2	H	401/448 (90%)	369 (92%)	32 (8%)	0	100	100
All	All	3232/3596 (90%)	3032 (94%)	200 (6%)	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	163/387 (42%)	160 (98%)	3 (2%)	64	87
1	C	145/387 (38%)	142 (98%)	3 (2%)	59	85
1	E	130/387 (34%)	125 (96%)	5 (4%)	38	74
1	G	176/387 (46%)	162 (92%)	14 (8%)	14	50
2	B	99/383 (26%)	93 (94%)	6 (6%)	22	61
2	D	114/383 (30%)	102 (90%)	12 (10%)	8	39
2	F	78/383 (20%)	73 (94%)	5 (6%)	20	59
2	H	110/383 (29%)	101 (92%)	9 (8%)	13	49
All	All	1015/3080 (33%)	958 (94%)	57 (6%)	24	63

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	398	LEU
1	G	404	HIS
1	G	406	GLU
1	G	453	CYS
1	G	515	LEU
1	G	516	THR
1	G	534	GLN
1	G	644	PHE
1	G	684	ARG
1	G	685	ARG
1	G	713	ASP
1	G	716	LEU
1	G	735	ASP
1	G	784	ARG
1	A	453	CYS
1	A	755	ASP
1	A	807	PHE
2	B	467	PHE
2	B	666	PHE

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Mol	Chain	Res	Type
2	B	682	TYR
2	B	755	TRP
2	B	774	GLU
2	B	784	CYS
2	H	470	ASP
2	H	488	ASN
2	H	497	LYS
2	H	649	LEU
2	H	682	TYR
2	H	719	LEU
2	H	725	ARG
2	H	750	GLN
2	H	757	ARG
1	E	427	ASN
1	E	453	CYS
1	E	736	LEU
1	E	784	ARG
1	E	788	CYS
2	F	467	PHE
2	F	620	PHE
2	F	727	GLU
2	F	751	LYS
2	F	781	THR
1	C	436	CYS
1	C	693	TYR
1	C	743	PHE
2	D	406	GLU
2	D	469	TYR
2	D	487	TRP
2	D	512	ARG
2	D	593	TRP
2	D	620	PHE
2	D	625	PHE
2	D	679	ARG
2	D	714	TYR
2	D	742	THR
2	D	757	ARG
2	D	767	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	404	HIS
1	C	569	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z  > 2$
3	GLY	A	902	-	1,4,4	0.43	0	0,4,4	0.00	-
6	GLU	B	1001	-	1,9,9	0.38	0	1,11,11	0.52	0
4	NAG	B	1002	-	15,15,15	0.19	0	21,21,21	0.30	0
7	BMK	B	1003	-	16,20,20	2.26	3 (18%)	18,31,31	1.26	2 (11%)
4	NAG	D	1001	-	15,15,15	0.11	0	21,21,21	0.16	0
6	GLU	D	1002	-	1,9,9	0.23	0	1,11,11	1.49	0
4	NAG	D	1003	-	15,15,15	0.09	0	21,21,21	0.14	0
9	Y01	E	1001	-	35,38,38	8.19	26 (74%)	54,57,57	2.74	22 (40%)
4	NAG	F	1001	-	15,15,15	0.14	0	21,21,21	0.14	0
3	GLY	G	1001	-	1,4,4	0.42	0	0,4,4	0.00	-
4	NAG	G	1002	-	15,15,15	0.22	0	21,21,21	0.21	0
5	TRS	G	1003	-	7,7,7	0.39	0	9,9,9	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GLU	G	1004	-	1,9,9	0.07	0	1,11,11	0.73	0
7	BMK	G	1005	-	16,20,20	2.24	3 (18%)	18,31,31	1.34	2 (11%)
6	GLU	G	1006	-	1,9,9	0.10	0	1,11,11	0.39	0
6	GLU	H	1001	-	1,9,9	0.47	0	1,11,11	0.28	0
4	NAG	H	1002	-	15,15,15	0.12	0	21,21,21	0.13	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	GLY	A	902	-	-	0/0/2/2	0/0/0/0
6	GLU	B	1001	-	-	0/3/9/9	0/0/0/0
4	NAG	B	1002	-	-	0/6/26/26	0/1/1/1
7	BMK	B	1003	-	-	0/0/25/25	0/2/4/4
4	NAG	D	1001	-	-	0/6/26/26	0/1/1/1
6	GLU	D	1002	-	-	0/3/9/9	0/0/0/0
4	NAG	D	1003	-	-	0/6/26/26	0/1/1/1
9	Y01	E	1001	-	-	0/17/77/77	0/4/4/4
4	NAG	F	1001	-	-	0/6/26/26	0/1/1/1
3	GLY	G	1001	-	-	0/0/2/2	0/0/0/0
4	NAG	G	1002	-	-	0/6/26/26	0/1/1/1
5	TRS	G	1003	-	-	0/9/9/9	0/0/0/0
6	GLU	G	1004	-	-	0/3/9/9	0/0/0/0
7	BMK	G	1005	-	-	0/0/25/25	0/2/4/4
6	GLU	G	1006	-	-	0/3/9/9	0/0/0/0
6	GLU	H	1001	-	-	0/3/9/9	0/0/0/0
4	NAG	H	1002	-	-	0/6/26/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1001	Y01	CBD-CBG	-27.10	1.00	1.53
9	E	1001	Y01	CAU-CAS	-16.89	1.17	1.53
9	E	1001	Y01	CAU-CBI	-15.58	1.24	1.54
9	E	1001	Y01	CAK-CBD	-14.90	1.27	1.53
9	E	1001	Y01	CBH-CAZ	-11.42	1.29	1.52
9	E	1001	Y01	CBD-CBF	-8.37	1.37	1.53
9	E	1001	Y01	CBB-CBE	-6.64	1.42	1.54
9	E	1001	Y01	CAR-CBC	-5.10	1.38	1.51
7	G	1005	BMK	C-C5	-2.81	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1003	BMK	C-C5	-2.54	1.49	1.53
9	E	1001	Y01	CAS-CBF	2.01	1.57	1.53
9	E	1001	Y01	CAV-CBC	2.06	1.57	1.52
9	E	1001	Y01	CAM-CAY	2.11	1.56	1.50
9	E	1001	Y01	OAW-CBC	2.28	1.52	1.46
9	E	1001	Y01	CAE-CBI	2.43	1.58	1.54
9	E	1001	Y01	CAC-CBB	2.75	1.60	1.53
9	E	1001	Y01	CAV-CAZ	3.08	1.58	1.51
9	E	1001	Y01	CAO-CBB	3.49	1.63	1.54
9	E	1001	Y01	OAW-CAY	3.71	1.45	1.34
9	E	1001	Y01	CAI-CAZ	3.76	1.41	1.32
9	E	1001	Y01	CAP-CBE	4.24	1.63	1.54
7	G	1005	BMK	C3-C2	5.06	1.46	1.39
7	B	1003	BMK	C3-C2	5.23	1.46	1.39
9	E	1001	Y01	CBI-CBG	5.76	1.66	1.55
7	G	1005	BMK	C6-C5	6.52	1.49	1.40
7	B	1003	BMK	C6-C5	6.65	1.49	1.40
9	E	1001	Y01	CAT-CBH	7.02	1.67	1.54
9	E	1001	Y01	CAQ-CBG	7.96	1.71	1.54
9	E	1001	Y01	CAK-CAI	8.51	1.67	1.50
9	E	1001	Y01	CBH-CBF	8.60	1.70	1.56
9	E	1001	Y01	CBI-CBE	9.66	1.73	1.55
9	E	1001	Y01	CAQ-CAP	10.17	1.82	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1001	Y01	CAS-CBF-CBH	-5.55	105.43	113.10
9	E	1001	Y01	CBH-CAZ-CAI	-5.49	114.05	122.92
9	E	1001	Y01	CAE-CBI-CBG	-5.12	102.03	111.73
9	E	1001	Y01	CAK-CAI-CAZ	-4.79	115.75	125.06
9	E	1001	Y01	CAM-CAL-CAX	-4.00	105.83	112.66
7	G	1005	BMK	C13-C9-C3	-3.68	116.29	121.01
9	E	1001	Y01	CAD-CBH-CBF	-3.67	107.14	111.68
7	B	1003	BMK	C13-C9-C3	-3.53	116.48	121.01
9	E	1001	Y01	CAC-CBB-CAO	-2.75	106.02	110.35
9	E	1001	Y01	CAD-CBH-CAT	-2.50	105.39	109.41
9	E	1001	Y01	CAV-CAZ-CAI	-2.46	116.84	120.59
9	E	1001	Y01	CAQ-CBG-CBI	-2.36	100.93	103.83
9	E	1001	Y01	CAP-CBE-CBI	-2.22	101.09	103.83
7	G	1005	BMK	C12-C8-C2	-2.13	116.05	119.95
7	B	1003	BMK	C12-C8-C2	-2.06	116.18	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1001	Y01	OAW-CBC-CAR	2.12	113.58	108.38
9	E	1001	Y01	CAK-CBD-CBG	2.24	114.33	110.92
9	E	1001	Y01	CBI-CBE-CBB	2.50	123.48	119.47
9	E	1001	Y01	CAS-CAU-CBI	3.03	118.08	112.80
9	E	1001	Y01	CAU-CBI-CBG	3.20	112.29	107.27
9	E	1001	Y01	CBG-CBI-CBE	3.34	104.06	100.07
9	E	1001	Y01	CAK-CBD-CBF	3.95	114.68	109.72
9	E	1001	Y01	CBF-CBD-CBG	5.10	116.00	109.09
9	E	1001	Y01	OAW-CAY-CAM	5.26	122.47	111.55
9	E	1001	Y01	CAT-CBH-CAZ	5.43	119.07	108.78
9	E	1001	Y01	CAC-CBB-CBE	6.72	123.47	112.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GLY	1	0
6	B	1001	GLU	4	0
4	B	1002	NAG	3	0
6	D	1002	GLU	8	0
9	E	1001	Y01	5	0
3	G	1001	GLY	5	0
5	G	1003	TRS	2	0
6	G	1004	GLU	2	0
6	H	1001	GLU	4	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

### 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, 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	416/451 (92%)	-0.68	4 (0%) 82 70	39, 115, 206, 238	0
1	C	415/451 (92%)	-0.51	14 (3%) 46 33	64, 138, 201, 264	0
1	E	412/451 (91%)	-0.14	38 (9%) 10 7	74, 186, 251, 316	0
1	G	424/451 (94%)	-0.67	8 (1%) 67 53	13, 73, 214, 287	0
2	B	397/448 (88%)	-0.31	22 (5%) 26 18	43, 137, 209, 244	0
2	D	405/448 (90%)	-0.54	16 (3%) 39 28	46, 123, 197, 225	0
2	F	416/448 (92%)	0.26	59 (14%) 3 3	92, 167, 216, 273	0
2	H	409/448 (91%)	-0.44	20 (4%) 30 21	22, 119, 215, 251	0
All	All	3294/3596 (91%)	-0.38	181 (5%) 26 18	13, 140, 220, 316	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	796	ALA	14.6
2	F	477	GLY	14.3
2	F	405	GLU	13.7
2	H	797	ASP	12.1
2	H	799	ASP	11.7
2	F	505	SER	11.6
2	D	540	PRO	11.3
2	F	828	SER	11.1
2	H	800	ASN	11.0
2	B	541	SER	10.8
2	F	404	LEU	10.7
2	B	542	ALA	9.4
2	F	642	TYR	9.1
2	H	575	PRO	8.5
2	F	479	HIS	8.5
2	F	504	GLY	8.0

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Mol	Chain	Res	Type	RSRZ
2	D	539	SER	7.8
1	E	676	GLN	7.7
1	C	548	THR	7.7
1	C	797	THR	7.7
2	F	473	LEU	7.7
2	F	480	GLY	7.3
2	D	541	SER	7.2
1	E	516	THR	7.2
1	E	746	SER	6.8
2	H	802	ALA	6.8
1	E	747	GLY	6.7
2	F	643	VAL	6.6
1	E	526	GLU	6.4
2	F	641	ARG	6.4
2	H	633	LEU	6.2
2	F	478	LYS	6.2
2	D	800	ASN	6.2
2	F	476	ASN	6.1
1	E	517	ILE	6.0
1	C	826	ALA	6.0
2	F	474	VAL	5.9
2	H	798	ILE	5.8
2	H	576	VAL	5.6
2	H	801	MET	5.5
2	B	581	PRO	5.5
2	B	605	ASN	5.4
2	B	604	GLN	5.3
1	E	521	ARG	5.3
2	F	493	GLU	5.2
2	B	606	PRO	5.2
1	G	559	THR	5.1
2	F	403	THR	5.1
2	F	485	GLY	5.0
2	F	582	SER	5.0
2	F	506	LEU	5.0
2	D	801	MET	4.9
2	F	406	GLU	4.9
2	F	409	PHE	4.9
1	G	560	LEU	4.8
1	G	826	ALA	4.8
2	F	499	ALA	4.7
2	D	797	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	796	LEU	4.6
2	H	636	PHE	4.6
1	E	751	GLY	4.6
2	F	644	ASP	4.5
1	E	527	PHE	4.5
1	C	549	LEU	4.5
1	E	677	SER	4.5
2	H	632	ASN	4.5
2	F	494	VAL	4.4
1	E	794	ALA	4.4
2	F	410	VAL	4.3
2	F	764	LEU	4.3
1	C	489	ASN	4.3
1	E	518	ASN	4.3
2	H	544	LEU	4.3
1	E	548	THR	4.2
2	F	498	ARG	4.2
2	H	803	GLY	4.1
2	F	400	SER	4.0
1	E	752	MET	4.0
1	A	744	PHE	4.0
2	B	548	SER	4.0
2	D	403	THR	3.8
1	G	582	SER	3.8
2	F	454	CYS	3.8
1	E	529	LYS	3.8
1	G	580	ARG	3.7
2	D	796	LEU	3.7
2	B	607	LYS	3.7
1	E	614	PRO	3.7
2	F	585	ILE	3.6
1	E	650	PRO	3.6
1	E	525	ILE	3.6
2	F	407	ALA	3.5
2	F	475	THR	3.5
1	C	546	ARG	3.4
1	E	514	PRO	3.4
2	H	574	SER	3.4
1	G	553	MET	3.4
1	C	550	ASP	3.4
2	F	794	SER	3.3
1	E	413	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	482	PHE	3.2
2	F	745	TYR	3.2
2	F	490	MET	3.0
1	E	682	TYR	3.0
1	C	488	VAL	3.0
2	B	547	PHE	3.0
2	F	763	ILE	3.0
2	F	761	LEU	2.9
2	F	408	PRO	2.9
2	F	827	LYS	2.9
1	E	524	TYR	2.9
2	F	697	VAL	2.9
2	F	640	ARG	2.9
1	G	558	SER	2.9
2	F	442	GLY	2.8
1	E	641	LEU	2.8
2	D	542	ALA	2.8
2	B	670	PRO	2.8
2	B	549	ALA	2.8
2	F	412	VAL	2.8
2	D	402	VAL	2.8
2	B	412	VAL	2.7
2	F	443	GLY	2.7
2	B	582	SER	2.7
1	E	612	GLY	2.7
2	D	477	GLY	2.7
2	B	671	ASN	2.7
2	B	636	PHE	2.7
1	C	500	MET	2.6
1	E	678	SER	2.6
2	H	637	MET	2.5
2	B	669	VAL	2.5
2	B	800	ASN	2.5
1	C	545	PRO	2.5
2	F	507	THR	2.5
1	G	557	GLN	2.5
1	E	796	ALA	2.5
2	D	802	ALA	2.5
2	F	696	SER	2.4
1	E	701	TYR	2.4
2	H	546	PRO	2.4
2	B	633	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	2.3
2	F	637	MET	2.3
1	C	510	MET	2.3
2	F	484	ASN	2.3
2	F	526	GLY	2.3
1	E	613	ALA	2.3
2	F	502	ALA	2.3
2	F	634	ALA	2.2
2	B	799	ASP	2.2
1	A	466	ARG	2.2
2	H	547	PHE	2.2
2	H	545	GLU	2.2
2	B	635	ALA	2.2
2	F	439	THR	2.2
1	E	679	VAL	2.2
2	B	543	PHE	2.2
1	E	704	ALA	2.1
1	E	519	ASN	2.1
1	A	469	ASP	2.1
2	F	491	ILE	2.1
2	F	765	GLN	2.1
2	F	492	GLY	2.1
1	E	674	VAL	2.1
2	F	746	GLY	2.1
2	F	519	SER	2.1
1	E	522	ALA	2.1
2	B	691	LYS	2.1
2	F	584	THR	2.1
1	C	799	THR	2.0
1	E	515	LEU	2.0
2	D	478	LYS	2.0
1	C	825	ILE	2.0
2	D	475	THR	2.0
2	H	551	VAL	2.0
1	E	644	PHE	2.0
2	D	480	GLY	2.0
1	E	398	LEU	2.0
1	E	649	ARG	2.0
2	D	474	VAL	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( $\text{\AA}^2$ )	Q<0.9
5	TRS	G	1003	8/8	0.95	0.26	4.00	6,17,56,81	0
7	BMK	G	1005	17/17	0.78	0.41	2.07	128,155,191,209	0
6	GLU	D	1002	10/10	0.81	0.47	1.33	84,114,139,149	0
6	GLU	G	1006	10/10	0.90	0.26	0.60	71,97,108,112	0
6	GLU	G	1004	10/10	0.73	0.20	0.33	58,86,122,166	0
4	NAG	G	1002	15/15	0.86	0.13	0.14	90,111,144,148	0
6	GLU	H	1001	10/10	0.96	0.14	-0.33	28,77,102,104	0
6	GLU	B	1001	10/10	0.89	0.21	-0.44	57,87,105,131	0
4	NAG	F	1001	15/15	0.88	0.36	-0.47	113,149,175,194	0
9	Y01	E	1001	35/35	0.85	0.14	-0.52	66,152,172,179	0
3	GLY	A	902	5/5	0.90	0.17	-0.71	67,67,79,81	0
7	BMK	B	1003	17/17	0.90	0.11	-0.82	111,153,186,199	0
3	GLY	G	1001	5/5	0.98	0.10	-1.40	28,30,42,59	0
4	NAG	H	1002	15/15	0.95	0.11	-	96,119,134,145	0
4	NAG	B	1002	15/15	0.92	0.75	-	109,152,165,169	0
4	NAG	D	1001	15/15	0.87	0.13	-	101,150,172,201	0
4	NAG	D	1003	15/15	0.90	0.20	-	128,160,180,195	0
8	MG	A	901	1/1	0.98	0.25	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.