



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:00 PM UTC

PDB ID : 5UN1 / pdb_00005un1
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

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

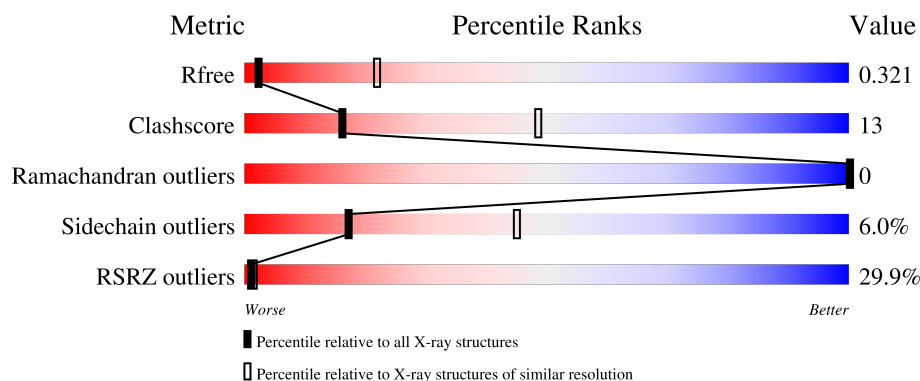
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	451	26% 78% 14% 8%
1	C	451	28% 73% 17% 8%
1	E	451	31% 75% 16% 9%
1	G	451	19% 71% 20% 6%
2	B	448	28% 74% 13% 11%

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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	-
6	GLU	B	1001	-	-	X	-
6	GLU	D	1002	-	-	X	-
6	GLU	H	1001	-	-	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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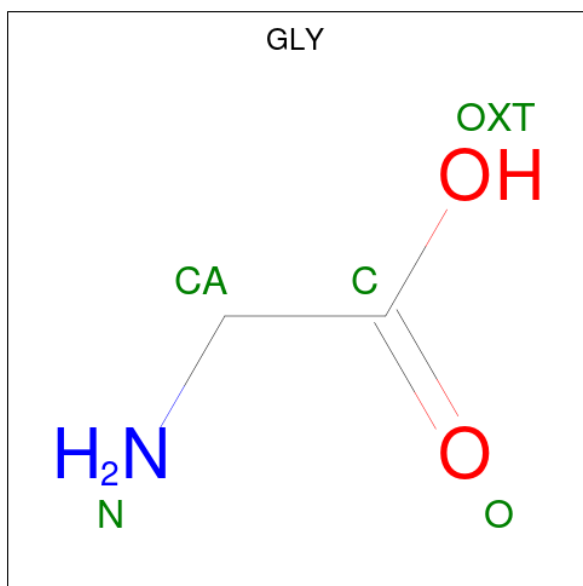
Chain	Residue	Modelled	Actual	Comment	Reference
F	833	LYS	-	expression tag	UNP A7XY94
F	834	ARG	-	expression tag	UNP A7XY94
F	835	MET	-	expression tag	UNP A7XY94
F	836	LYS	-	expression tag	UNP A7XY94
F	837	GLY	-	expression tag	UNP A7XY94
F	838	LEU	-	expression tag	UNP A7XY94
F	839	GLU	-	expression tag	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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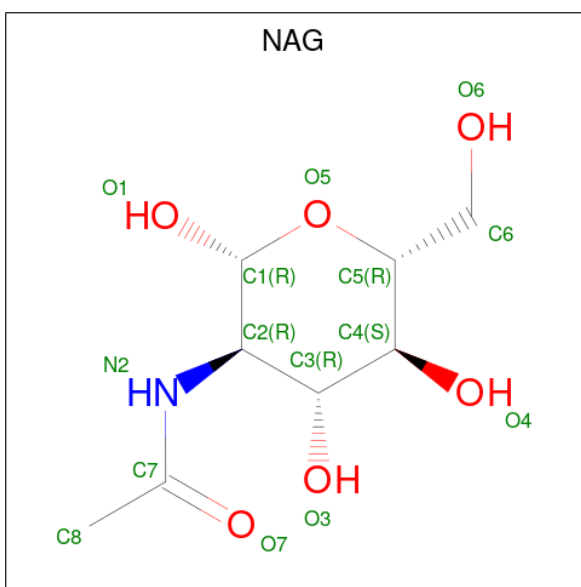
Chain	Residue	Modelled	Actual	Comment	Reference
D	843	GLN	-	expression tag	UNP A7XY94

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



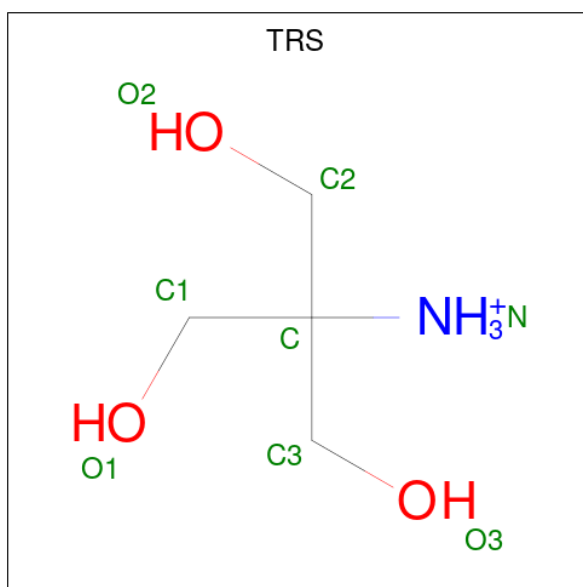
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



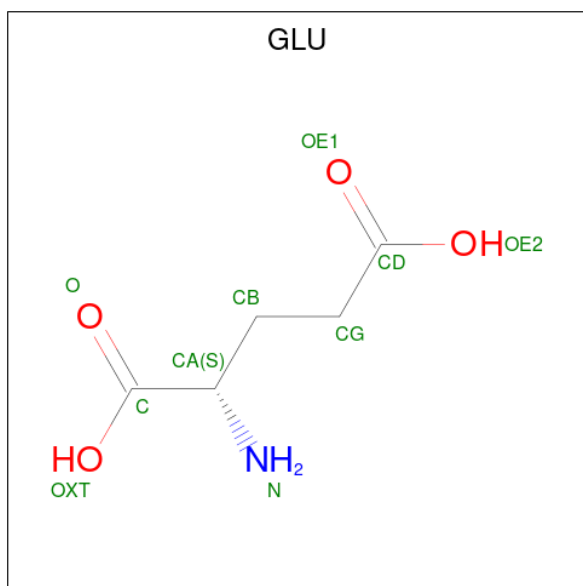
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	H	1	Total	C	N	O	0	0
			15	8	1	6		
4	F	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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 (CCD ID: GLU) (formula: C₅H₉NO₄).



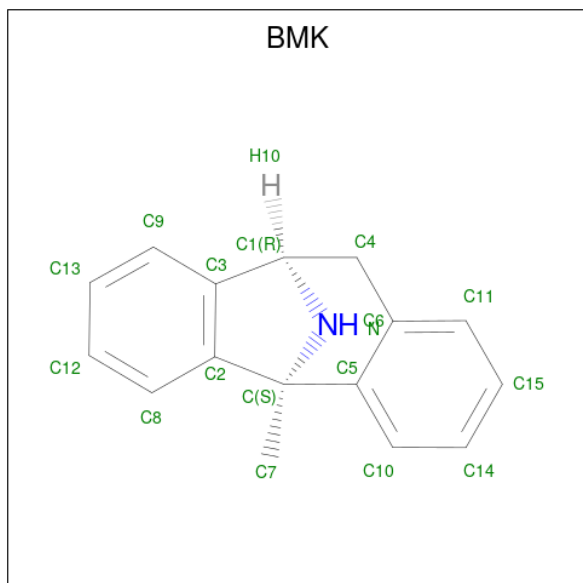
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	G	1	Total	C	N	O	0	0
			10	5	1	4		
6	B	1	Total	C	N	O	0	0
			10	5	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (CCD ID: BMK) (formula: C₁₆H₁₅N).

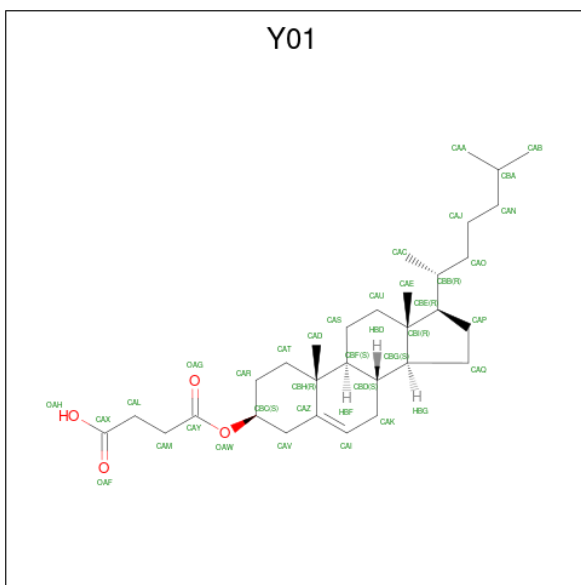


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	N	0	0
			17	16	1		
7	B	1	Total	C	N	0	0
			17	16	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).

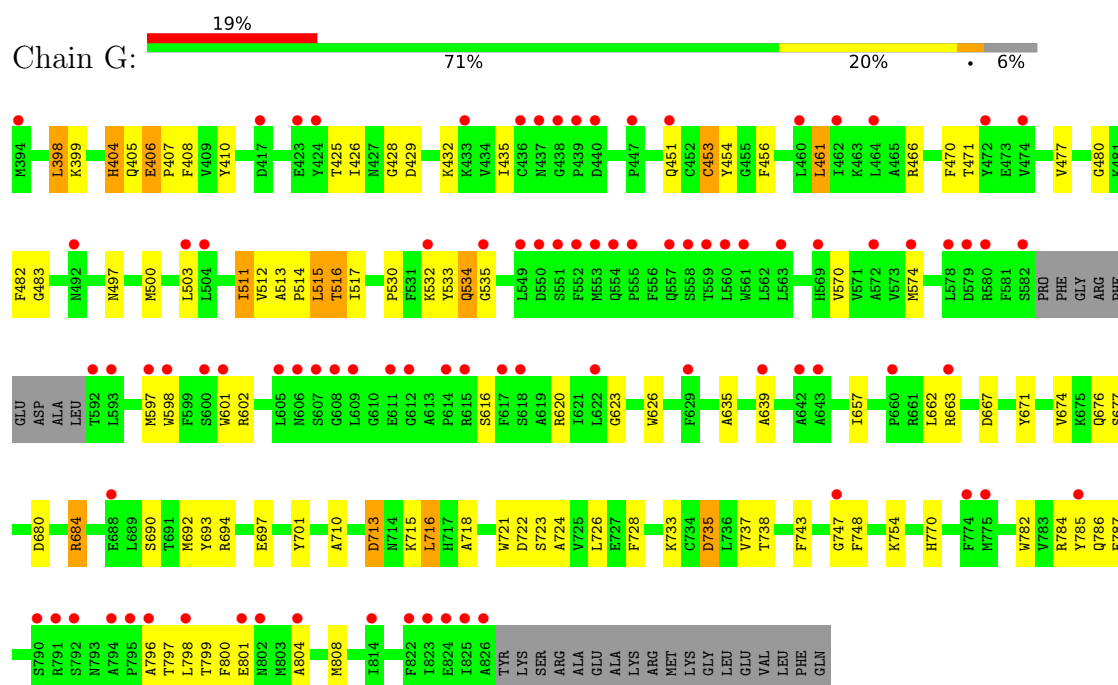


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			35	31	4		

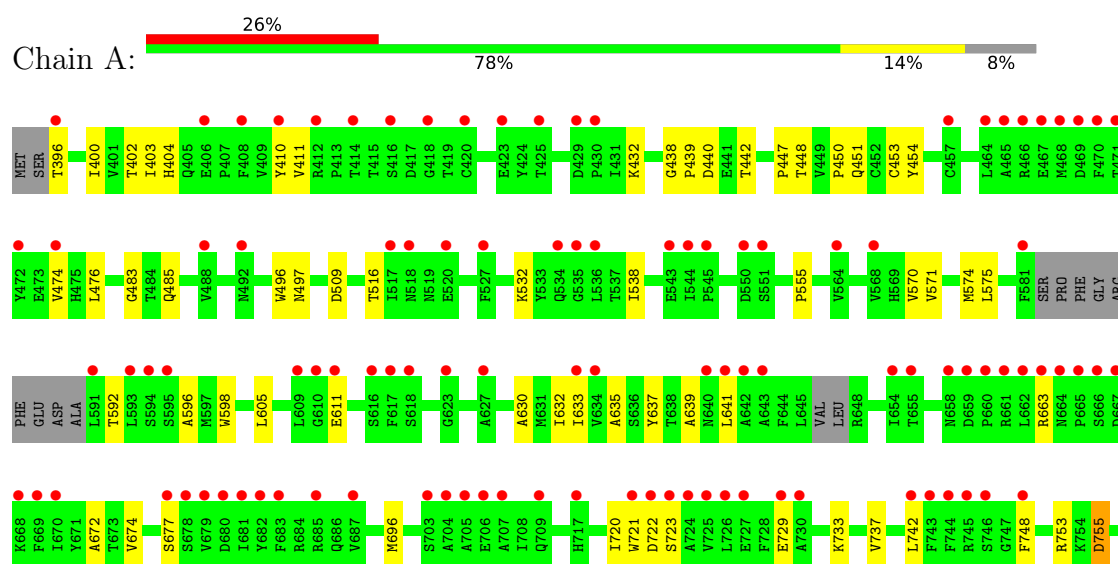
3 Residue-property plots

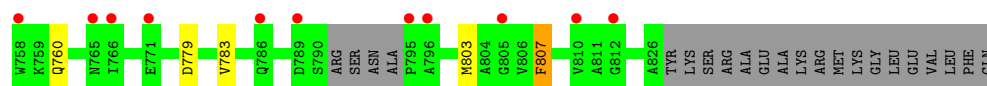
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-methyl-D-aspartate receptor subunit NR1-3a

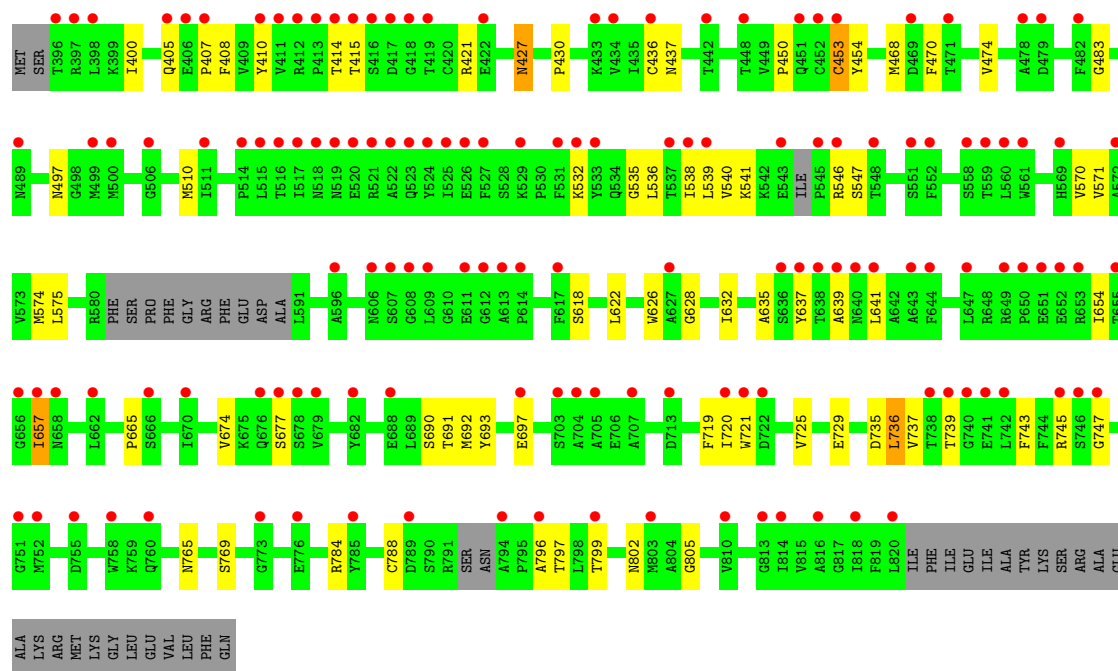
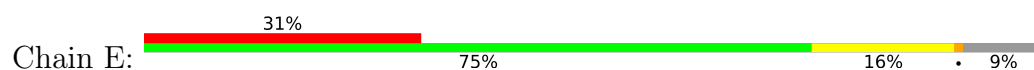


- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a

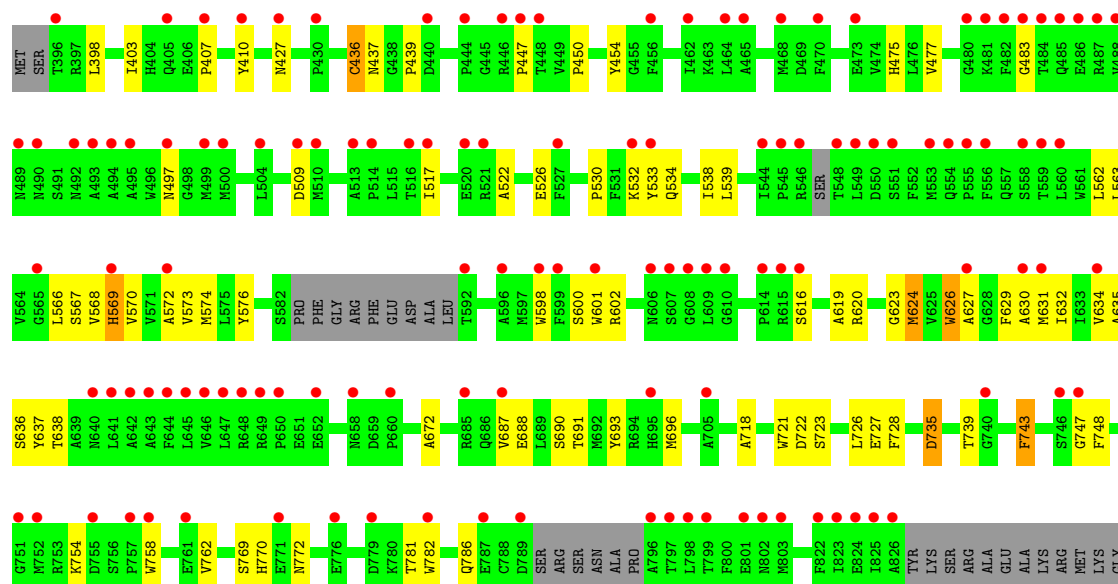
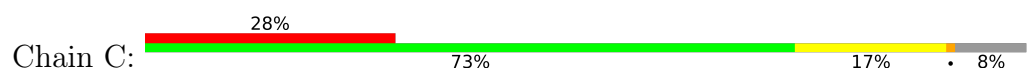




- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a



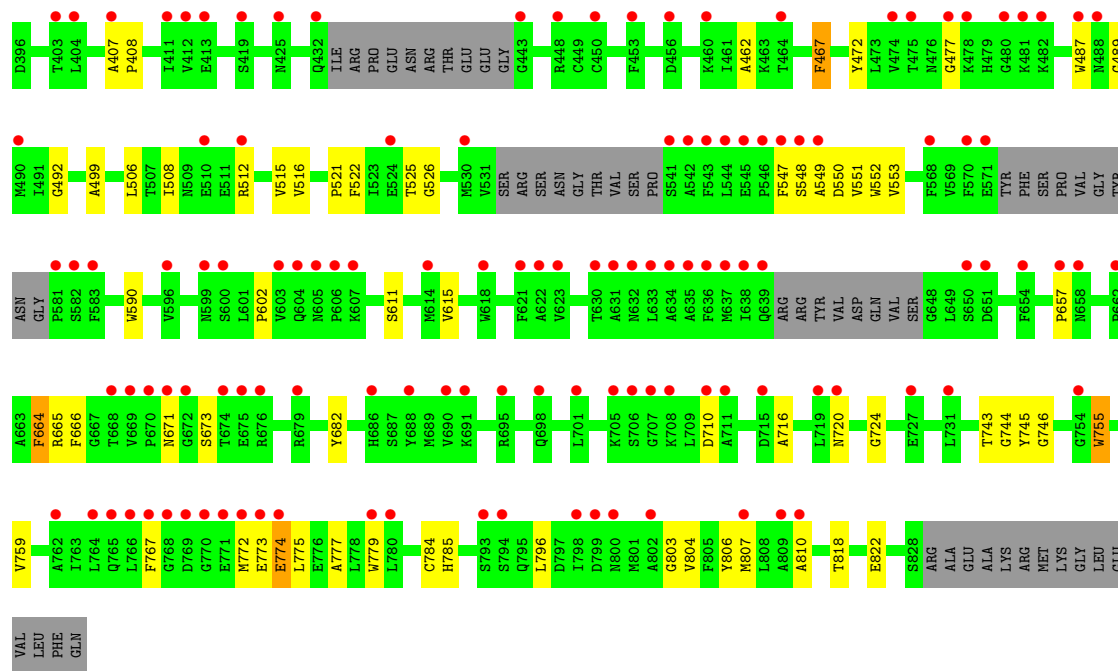
- Molecule 1: N-methyl-D-aspartate receptor subunit NR1-3a



LEU
GLU
VAL
LEU
PHE
GLN

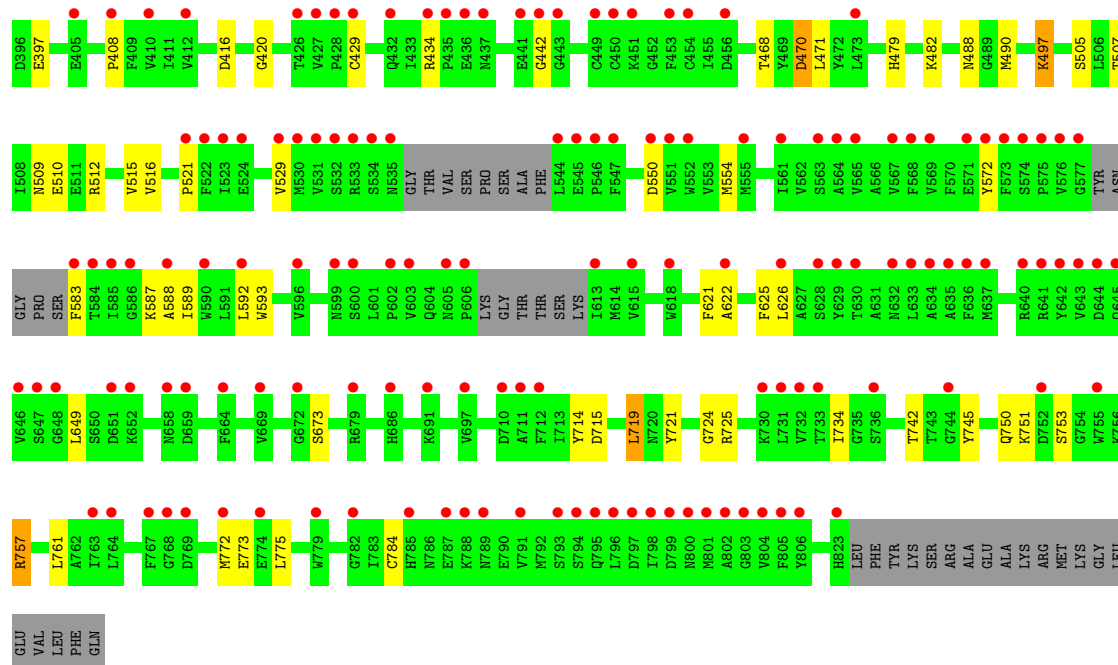
● Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain B: 28% 74% 13% 11%



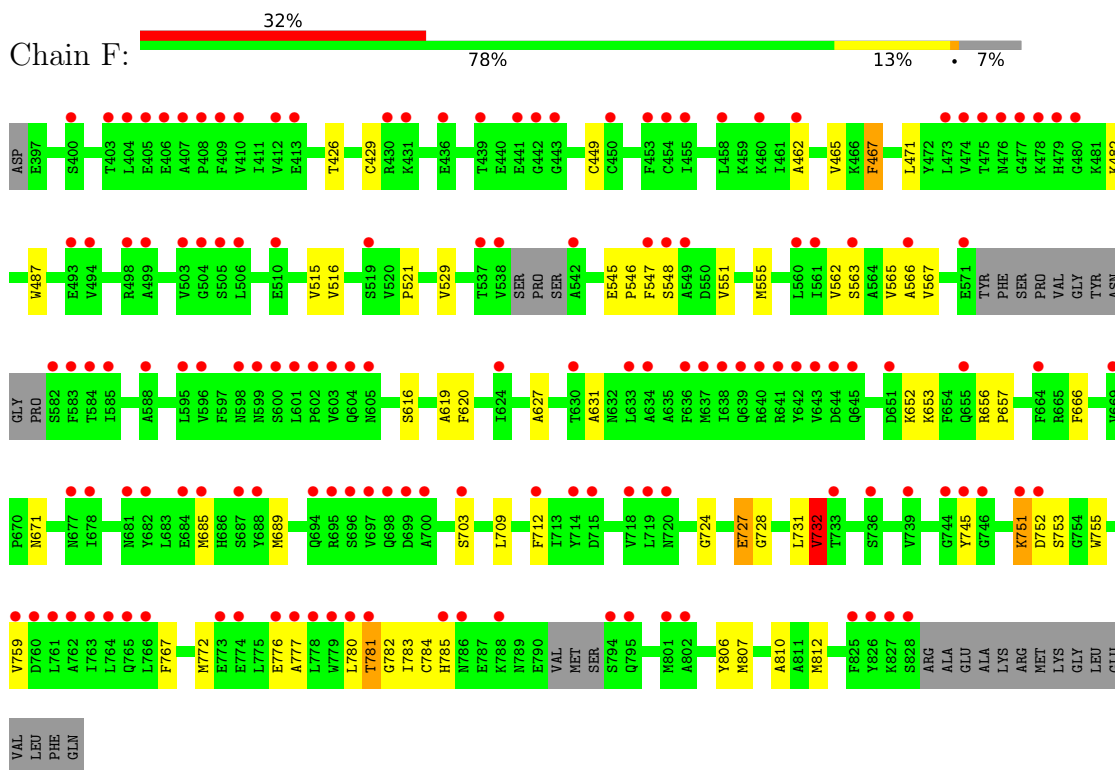
● Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain H: 32% 79% 12% 9%



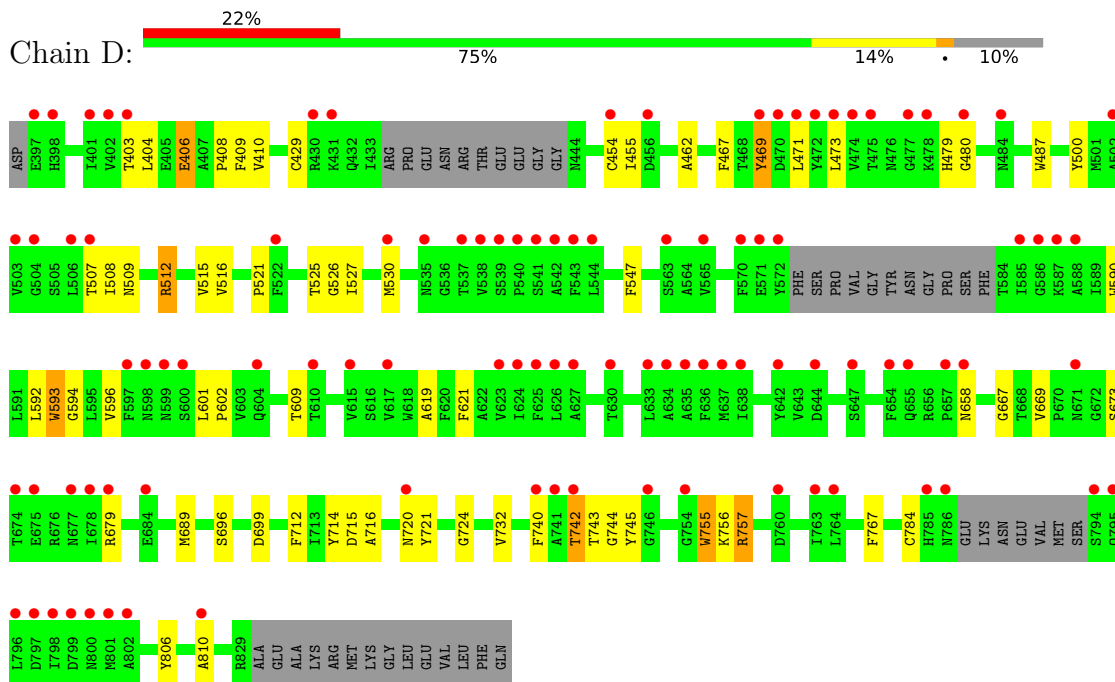
- Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain F:



- Molecule 2: Ionotropic glutamate receptor subunit NR2B

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	181.57Å 108.47Å 182.46Å 90.00° 111.44° 90.00°	Depositor
Resolution (Å)	49.99 – 3.60 49.99 – 3.60	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.99-3.60) 91.0 (49.99-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.41Å)	Xtriage
Refinement program	PHENIX (dev_2597: ???)	Depositor
R, R_{free}	0.288 , 0.316 0.291 , 0.321	Depositor DCC
R_{free} test set	3670 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	104.5	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.117 for l,-k,h	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	20143	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: MG, TRS, BMK, NAG, Y01

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	0.22	0/2694	0.34	0/3703
1	C	0.26	0/2647	0.42	2/3648 (0.1%)
1	E	0.20	0/2529	0.41	2/3491 (0.1%)
1	G	0.35	0/2808	0.51	1/3848 (0.0%)
2	B	0.19	0/2363	0.42	1/3260 (0.0%)
2	D	0.24	0/2452	0.49	3/3384 (0.1%)
2	F	0.28	0/2344	0.58	6/3245 (0.2%)
2	H	0.24	0/2409	0.43	1/3317 (0.0%)
All	All	0.25	0/20246	0.45	16/27896 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	728	GLY	N-CA-C	-7.50	105.39	115.36
2	H	572	TYR	CB-CA-C	-6.15	109.50	116.63
2	F	565	VAL	CA-C-N	6.08	128.74	120.54
2	F	565	VAL	C-N-CA	6.08	128.74	120.54
1	E	546	ARG	N-CA-C	6.07	117.90	111.28
2	D	755	TRP	N-CA-C	-5.95	104.80	111.28
1	G	786	GLN	N-CA-C	-5.91	101.54	110.70
1	C	624	MET	N-CA-C	-5.89	104.86	111.28
2	F	545	GLU	CA-C-N	5.84	125.31	119.24
2	F	545	GLU	C-N-CA	5.84	125.31	119.24
2	D	756	LYS	CB-CA-C	-5.76	109.95	116.63
2	D	658	ASN	N-CA-C	5.48	117.34	111.36
1	E	796	ALA	CB-CA-C	-5.48	110.27	116.63
1	C	626	TRP	N-CA-C	-5.47	105.21	111.07
2	F	732	VAL	N-CA-C	5.14	115.05	107.75
2	B	664	PHE	N-CA-C	5.01	116.55	108.08

There are no chirality outliers.

There are no planarity outliers.

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	2643	0	1928	44	0
1	C	2591	0	1819	73	0
1	E	2486	0	1710	46	0
1	G	2753	0	2092	91	0
2	B	2328	0	1521	60	0
2	D	2413	0	1600	64	0
2	F	2319	0	1436	59	0
2	H	2382	0	1585	37	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	447	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 (447) 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:CAP	9:E:1001:Y01:CAQ	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: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
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
1:G:797:THR:CB	2:F:547:PHE:C	2.48	0.86
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: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:H:550:ASP:O	2:H:554:MET:HB2	1.78	0.82
2:F:751:LYS:HD3	2:F:752:ASP:CB	2.10	0.82
1:C:410:TYR:HB2	1:C:454:TYR:O	1.80	0.81
1:A:516:THR:HG1	3:A:902:GLY:N	1.78	0.80
1:G:516:THR:HG1	3:G:1001:GLY:C	1.89	0.79
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:D:512:ARG:HH22	6:D:1002:GLU:C	1.92	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:G:701:TYR:HE2	1:G:716:LEU:HD12	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:ILE:O	1:C:636:SER:CB	2.34	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: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
1:G:796:ALA:O	1:G:797:THR:C	2.32	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
2:F:562:VAL:O	2:F:566:ALA:CB	2.38	0.70
2:D:667:GLY:HA2	2:D:689:MET:HG2	1.72	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: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:516:THR:OG1	3:G:1001:GLY:C	2.34	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
1:G:799:THR:O	1:G:800:PHE:C	2.36	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: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
1:G:701:TYR:CE2	1:G:716:LEU:CD1	2.71	0.67
2:D:480:GLY:O	2:D:512:ARG:NH1	2.27	0.67
2:B:724:GLY:HA2	2:B:785:HIS:CB	2.26	0.66
2:B:550:ASP:O	2:B:551:VAL:C	2.37	0.66
2:F:777:ALA:C	2:F:781:THR:HG1	2.02	0.66
1:E:483:GLY:HA2	1:E:497:ASN:O	1.95	0.65
2:F:727:GLU:H	2:F:727:GLU:CD	2.04	0.65
1:C:532:LYS:HB3	1:C:748:PHE:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:512:ARG:NH2	6:D:1002:GLU:C	2.52	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:G:796:ALA:O	1:G:798:LEU:N	2.30	0.64
1:C:598:TRP:O	1:C:602:ARG:CB	2.45	0.64
2:H:512:ARG:NH2	6:H:1001:GLU:OXT	2.29	0.64
2:H:622:ALA:O	2:H:626:LEU:CB	2.46	0.64
1:C:600:SER:HA	1:C:626:TRP:NE1	2.12	0.64
2:B:521:PRO:HB3	2:B:744:GLY:HA3	1.80	0.64
1:E:541:LYS:HA	1:E:735:ASP:O	1.96	0.64
1:C:562:LEU:O	1:C:566:LEU:CB	2.46	0.64
2:B:508:ILE:HD11	2:B:746:GLY:HA3	1.80	0.64
2:D:406:GLU:H	2:D:410:VAL:HG12	1.62	0.63
1:G:721:TRP:CG	1:G:722:ASP:H	2.16	0.63
2:F:777:ALA:C	2:F:781:THR:OG1	2.41	0.63
2:F:515:VAL:HG23	2:F:516:VAL:HG13	1.81	0.63
2:F:731:LEU:C	2:F:732:VAL:CG1	2.71	0.63
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: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:D:507:THR:OG1	6:D:1002:GLU:O	2.13	0.61
1:C:735:ASP:OD1	1:C:735:ASP:N	2.34	0.61
1:G:570:VAL:O	1:G:574:MET:CB	2.48	0.61
1:E:427:ASN:OD1	1:E:427:ASN:N	2.34	0.61
2:F:782:GLY:O	2:F:783:ILE:C	2.44	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: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
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
1:G:663:ARG:HA	1:G:692:MET:HE2	1.82	0.59
2:B:773:GLU:O	2:B:777:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:522:ALA:O	2:D:757:ARG:NH2	2.34	0.59
2:D:673:SER:HG	6:D:1002:GLU:N	1.99	0.59
1:G:426:ILE:HG23	6:G:1004:GLU:OE1	2.02	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
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
2:F:731:LEU:C	2:F:732:VAL:HG13	2.28	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
1:C:568:VAL:CA	1:C:626:TRP:CH2	2.86	0.58
1:G:671:TYR:HB3	1:G:718:ALA:HB3	1.85	0.58
2:H:397:GLU:O	2:H:468:THR:OG1	2.17	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
1:G:516:THR:N	3:G:1001:GLY:OXT	2.22	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
1:G:735:ASP:OD1	1:G:735:ASP:N	2.26	0.57
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:C:567:SER:C	1:C:626:TRP:HH2	2.11	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
2:D:507:THR:OG1	6:D:1002:GLU: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:SER:HA	1:C:626:TRP:CD1	2.41	0.56
2:F:782:GLY:C	2:F:784:CYS:N	2.55	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
1:G:398:LEU:HD11	1:G:470:PHE:CD1	2.41	0.55
2:F:652:LYS:O	2:F:656:ARG:N	2.34	0.55
1:G:797:THR:HA	2:F:546:PRO:O	2.05	0.55
1:E:421:ARG:HH12	9:E:1001:Y01:CAY	2.20	0.55
2:B:487:TRP:HD1	2:B:492:GLY:HA2	1.72	0.55
1:C:569:HIS:CD2	1:C:569:HIS:N	2.74	0.55
1:G:754:LYS:HE3	2:H:757:ARG:HH11	1.72	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
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
2:D:755:TRP:H	2:D:755:TRP:CD1	2.25	0.54
2:B:755:TRP:H	2:B:755:TRP:CD1	2.23	0.54
2:F:685:MET:O	2:F:689:MET:CB	2.55	0.54
1:A:611:GLU:CA	2:B:602:PRO:HB2	2.36	0.54
2:B:512:ARG:H	2:B:512:ARG:HD2	1.72	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
1:G:693:TYR:O	1:G:697:GLU:N	2.34	0.53
2:D:526:GLY:H	2:D:716:ALA:HB3	1.72	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:G:796:ALA:C	1:G:798:LEU:N	2.66	0.53
1:C:781:THR:HG1	1:C:782:TRP:CD1	2.26	0.53
1:A:442:THR:HG22	1:A:476:LEU:HD13	1.91	0.53
1:E:541:LYS:CB	1:E:736:LEU:HD23	2.17	0.53
1:C:568:VAL:CA	1:C:626:TRP:CZ2	2.87	0.53
1:E:690:SER:O	1:E:693:TYR:HB3	2.08	0.53
1:G:483:GLY:HA3	1:G:500:MET:HB2	1.90	0.53
1:A:555:PRO:O	2:B:796:LEU:N	2.41	0.53
1:A:570:VAL:O	1:A:574:MET:CB	2.57	0.53
1:C:567:SER:C	1:C:626:TRP:CH2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:673:SER:HB3	6:B:1001:GLU:HG3	1.91	0.52
2:H:529:VAL:O	2:H:734:ILE:N	2.40	0.52
1:C:688:GLU:O	1:C:691:THR:HG22	2.09	0.52
1:C:690:SER:O	1:C:693:TYR:HB3	2.09	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
2:F:551:VAL:O	2:F:555:MET:CB	2.57	0.52
1:C:721:TRP:CG	1:C:722:ASP:H	2.27	0.52
2:H:715:ASP:O	2:H:719:LEU:HB2	2.09	0.52
1:C:437:ASN:H	1:C:475:HIS:HA	1.74	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
1:G:425:THR:O	1:G:428:GLY:N	2.29	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:C:626:TRP:O	1:C:627:ALA:C	2.50	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:E:536:LEU:HD12	1:E:721:TRP:O	2.11	0.51
1:C:743:PHE:H	1:C:743:PHE:HD1	1.59	0.51
2:B:512:ARG:HE	6:B:1001:GLU:N	2.09	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
2:H:621:PHE:O	2:H:625:PHE:CB	2.60	0.50
9:E:1001:Y01:HAE2	9:E:1001:Y01:HAC1	1.94	0.50
1:G:533:TYR:CE2	2:H:742:THR:O	2.65	0.50
1:G:721:TRP:HB3	1:G:726:LEU:HD11	1.93	0.50
1:A:450:PRO:O	1:A:451:GLN:HG3	2.10	0.50
1:C:538:ILE:O	1:C:739:THR:N	2.36	0.50
1:G:410:TYR:O	1:G:453:CYS:HA	2.11	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: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:G:662:LEU:O	1:G:671:TYR:OH	2.25	0.49
2:B:506:LEU:HD12	6:B:1001:GLU:HB3	1.92	0.49
1:A:538:ILE:HA	1:A:720:ILE:HA	1.94	0.49
1:A:637:TYR:O	1:A:641:LEU:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:LEU:HD23	2:F:812:MET:HA	1.94	0.49
2:F:751:LYS:C	2:F:753:SER:H	2.15	0.49
1:G:405:GLN:HE21	1:G:482:PHE:HZ	1.59	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:E:468:MET:HB2	1:E:470:PHE:HD1	1.76	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
1:G:597:MET:O	1:G:601:TRP:HB2	2.13	0.48
2:D:525:THR:O	2:D:743:THR:O	2.31	0.48
2:F:666:PHE:CZ	2:F:685:MET:HA	2.49	0.48
1:E:571:VAL:O	1:E:575:LEU:CB	2.62	0.48
1:C:624:MET:CA	2:D:593:TRP:NE1	2.71	0.48
1:C:769:SER:O	1:C:772:ASN:ND2	2.46	0.48
2:D:590:TRP:HE1	2:D:602:PRO:HD2	1.78	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
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
1:C:637:TYR:C	1:C:637:TYR:CD1	2.91	0.47
2:F:562:VAL:O	2:F:566:ALA:N	2.46	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:A:509:ASP:HA	1:A:753:ARG:HH21	1.79	0.47
1:A:672:ALA:HA	1:A:696:MET:HG2	1.96	0.47
2:B:590:TRP:CH2	2:B:602:PRO:HD2	2.42	0.47
1:G:690:SER:O	1:G:694:ARG:N	2.41	0.47
1:C:627:ALA:O	1:C:630:ALA:N	2.44	0.47
2:B:462:ALA:HA	2:B:467:PHE:HE1	1.80	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
2:F:782:GLY:C	2:F:784:CYS:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:657:PRO:CB	2:B:664:PHE:HE1	2.27	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
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
2:F:666:PHE:HZ	2:F:685:MET:HA	1.80	0.46
1:G:497:ASN:HB3	1:G:676:GLN:NE2	2.30	0.46
1:E:407:PRO:HG2	1:E:408:PHE:CD2	2.51	0.46
2:F:776:GLU:O	2:F:780:LEU:HB2	2.14	0.46
1:C:407:PRO:HB3	1:C:728:PHE:CD2	2.50	0.46
1:C:569:HIS:HD2	1:C:601:TRP:HE1	1.62	0.46
1:A:721:TRP:CG	1:A:722:ASP:H	2.34	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:H:470:ASP:OD1	2:H:470:ASP:N	2.47	0.46
2:F:429:CYS:HB3	2:F:471:LEU:HB3	1.98	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
2:D:471:LEU:C	2:D:471:LEU:HD12	2.41	0.45
1:G:514:PRO:HB2	1:G:748:PHE:CZ	2.51	0.45
1:G:737:VAL:HG12	1:G:738:THR:N	2.32	0.45
1:C:600:SER:C	1:C:626:TRP:HE1	2.22	0.45
1:G:785:TYR:C	1:G:787:GLU:H	2.25	0.45
1:E:628:GLY:O	1:E:632:ILE:HG13	2.16	0.45
1:G:530:PRO:HB2	1:G:533:TYR:CE1	2.51	0.45
1:A:592:THR:O	1:A:596:ALA:N	2.50	0.45
2:D:508:ILE:HG12	2:D:744:GLY:O	2.17	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
2:F:806:TYR:O	2:F:810:ALA:HB2	2.17	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
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
1:G:785:TYR:C	1:G:787:GLU:N	2.75	0.45
1:E:414:THR:OG1	1:E:415:THR:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:550:ASP:C	2:B:552:TRP:N	2.75	0.44
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: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
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
2:F:784:CYS:O	2:F:785:HIS:CB	2.66	0.44
1:G:710:ALA:HB1	1:G:716:LEU:HB2	2.00	0.43
1:C:407:PRO:HB3	1:C:728:PHE:CG	2.53	0.43
2:D:527:ILE:HB	2:D:740:PHE:CB	2.47	0.43
2:D:593:TRP:CE3	2:D:593:TRP:HA	2.53	0.43
2:B:506:LEU:O	2:B:745:TYR:HA	2.18	0.43
2:F:727:GLU:N	2:F:727:GLU:CD	2.73	0.43
2:D:462:ALA:HA	2:D:467:PHE:CE1	2.53	0.43
2:D:593:TRP:HA	2:D:593:TRP:HE3	1.83	0.43
1:G:782:TRP:CZ3	6:G:1004:GLU:HG2	2.53	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
2:F:426:THR:CB	2:F:449:CYS:HB3	2.48	0.43
1:A:807:PHE:HB2	2:D:621:PHE:HE1	1.84	0.43
2:H:408:PRO:HG3	2:H:721:TYR:CG	2.53	0.43
2:F:521:PRO:HA	2:F:745:TYR:O	2.18	0.43
1:A:598:TRP:HZ2	2:D:609:THR:HA	1.84	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:G:680:ASP:O	1:G:684:ARG:CB	2.67	0.43
2:B:755:TRP:HB2	2:B:759:VAL:HG23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:VAL:O	1:C:638:THR:HG23	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:806:TYR:O	2:D:810:ALA:HB2	2.18	0.43
2:D:469:TYR:HD1	2:D:469:TYR:H	1.67	0.43
2:H:482:LYS:HZ1	2:H:515:VAL:HG21	1.84	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:C:619:ALA:O	1:C:623:GLY:N	2.52	0.43
1:G:477:VAL:HG13	1:G:480:GLY:H	1.83	0.42
1:G:515:LEU:HD12	1:G:515:LEU:HA	1.89	0.42
2:B:716:ALA:O	2:B:720:ASN:HB2	2.19	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:D:594:GLY:HA3	2:D:601:LEU:CB	2.49	0.42
1:G:534:GLN:OE1	1:G:722:ASP:HB3	2.19	0.42
1:G:534:GLN:NE2	1:G:748:PHE:CZ	2.87	0.42
2:B:775:LEU:O	2:B:779:TRP:HD1	2.02	0.42
2:H:757:ARG:O	2:H:761:LEU:HG	2.19	0.42
2:F:616:SER:O	2:F:619:ALA:HB3	2.20	0.42
1:C:526:GLU:HB2	1:C:754:LYS:HA	2.01	0.42
1:C:624:MET:O	1:C:627:ALA:HB3	2.20	0.42
1:G:623:GLY:HA2	1:G:626:TRP:HB3	2.00	0.42
1:A:635:ALA:O	1:A:639:ALA:HB2	2.19	0.42
1:E:437:ASN:HA	1:E:450:PRO:HA	2.02	0.42
1:G:635:ALA:O	1:G:639:ALA:HB2	2.19	0.42
2:F:467:PHE:N	2:F:467:PHE:CD1	2.87	0.42
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
1:G:461:LEU:O	1:G:461:LEU:HD22	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:E:421:ARG:HG3	1:E:421:ARG:HH11	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:C:439:PRO:HA	1:C:447:PRO:O	2.19	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
1:A:432:LYS:H	1:A:432:LYS:HG2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:673:SER:H	6:H:1001:GLU:HG3	1.85	0.42
2:H:772:MET:O	2:H:773:GLU:C	2.63	0.42
2:D:530:MET:HA	2:D:732:VAL:O	2.20	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
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
2:D:500:TYR:CE2	2:D:755:TRP:NE1	2.88	0.41
1:C:533:TYR:OH	2:D:521:PRO:HG3	2.20	0.41
1:C:687:VAL:O	1:C:690:SER:CB	2.68	0.41
1:G:797:THR:CB	2:F:546:PRO:O	2.69	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:425:THR:N	1:G:429:ASP:O	2.27	0.41
1:G:530:PRO:HB2	1:G:533:TYR:HE1	1.86	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:F:671:ASN:N	2:F:671:ASN:HD22	2.19	0.41
1:C:517:ILE:HD12	1:C:530:PRO:HG3	2.02	0.41
2:D:696:SER:O	2:D:699:ASP:N	2.54	0.41
1:G:713:ASP:C	1:G:715:LYS:H	2.29	0.41
2:B:526:GLY:H	2:B:716:ALA:HB3	1.86	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:N	2:F:807:MET:SD	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%)	159 (98%)	4 (2%)	42	63
1	C	145/387 (38%)	141 (97%)	4 (3%)	38	60
1	E	130/387 (34%)	123 (95%)	7 (5%)	20	47
1	G	176/387 (46%)	161 (92%)	15 (8%)	10	35
2	B	99/383 (26%)	93 (94%)	6 (6%)	17	45
2	D	114/383 (30%)	105 (92%)	9 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	78/383 (20%)	71 (91%)	7 (9%)	9	33
2	H	110/383 (29%)	102 (93%)	8 (7%)	13	40
All	All	1015/3080 (33%)	955 (94%)	60 (6%)	17	45

All (60) 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	461	LEU
1	G	511	ILE
1	G	512	VAL
1	G	515	LEU
1	G	516	THR
1	G	534	GLN
1	G	684	ARG
1	G	713	ASP
1	G	716	LEU
1	G	735	ASP
1	G	784	ARG
1	A	403	ILE
1	A	737	VAL
1	A	755	ASP
1	A	807	PHE
2	B	467	PHE
2	B	666	PHE
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	719	LEU
2	H	725	ARG
2	H	750	GLN
2	H	757	ARG
1	E	427	ASN

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Mol	Chain	Res	Type
1	E	453	CYS
1	E	657	ILE
1	E	691	THR
1	E	736	LEU
1	E	784	ARG
1	E	788	CYS
2	F	465	VAL
2	F	467	PHE
2	F	620	PHE
2	F	727	GLU
2	F	732	VAL
2	F	751	LYS
2	F	781	THR
1	C	436	CYS
1	C	569	HIS
1	C	735	ASP
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	679	ARG
2	D	742	THR
2	D	757	ARG
2	D	767	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	404	HIS
1	G	405	GLN
2	B	671	ASN
2	B	680	ASN
1	E	497	ASN
1	C	507	GLN
1	C	569	HIS
2	D	681	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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$
4	NAG	G	1002	-	15,15,15	0.22	0	21,21,21	0.21	0
7	BMK	B	1003	-	17,20,20	2.46	4 (23%)	18,31,31	1.58	3 (16%)
4	NAG	F	1001	-	15,15,15	0.14	0	21,21,21	0.13	0
5	TRS	G	1003	-	7,7,7	0.40	0	9,9,9	0.63	0
6	GLU	H	1001	-	8,9,9	1.10	1 (12%)	8,11,11	1.34	3 (37%)
4	NAG	B	1002	-	15,15,15	0.18	0	21,21,21	0.27	0
4	NAG	D	1003	-	15,15,15	0.08	0	21,21,21	0.13	0
6	GLU	D	1002	-	8,9,9	1.13	0	8,11,11	1.42	2 (25%)
7	BMK	G	1005	-	17,20,20	2.43	4 (23%)	18,31,31	1.55	4 (22%)
6	GLU	B	1001	-	8,9,9	1.11	1 (12%)	8,11,11	1.24	1 (12%)
3	GLY	A	902	-	4,4,4	1.17	1 (25%)	3,4,4	1.69	2 (66%)
4	NAG	D	1001	-	15,15,15	0.12	0	21,21,21	0.16	0
6	GLU	G	1004	-	8,9,9	1.06	1 (12%)	8,11,11	1.34	1 (12%)
9	Y01	E	1001	-	38,38,38	8.30	26 (68%)	57,57,57	2.84	26 (45%)
3	GLY	G	1001	-	4,4,4	1.18	1 (25%)	3,4,4	1.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GLU	G	1006	-	8,9,9	1.10	1 (12%)	8,11,11	1.23	1 (12%)
4	NAG	H	1002	-	15,15,15	0.13	0	21,21,21	0.12	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
4	NAG	G	1002	-	-	2/6/26/26	0/1/1/1
7	BMK	B	1003	-	-	-	0/5/4/4
4	NAG	F	1001	-	-	2/6/26/26	0/1/1/1
5	TRS	G	1003	-	-	8/9/9/9	-
6	GLU	H	1001	-	-	3/9/9/9	-
4	NAG	B	1002	-	-	1/6/26/26	0/1/1/1
4	NAG	D	1003	-	-	2/6/26/26	0/1/1/1
6	GLU	D	1002	-	-	3/9/9/9	-
7	BMK	G	1005	-	-	-	0/5/4/4
6	GLU	B	1001	-	-	1/9/9/9	-
3	GLY	A	902	-	-	0/2/2/2	-
4	NAG	D	1001	-	-	2/6/26/26	0/1/1/1
6	GLU	G	1004	-	-	2/9/9/9	-
9	Y01	E	1001	-	-	12/19/77/77	0/4/4/4
3	GLY	G	1001	-	-	0/2/2/2	-
6	GLU	G	1006	-	-	3/9/9/9	-
4	NAG	H	1002	-	-	2/6/26/26	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1001	Y01	CBD-CBG	-28.13	1.00	1.53
9	E	1001	Y01	CAU-CAS	-18.25	1.17	1.53
9	E	1001	Y01	CAU-CBI	-16.77	1.24	1.54
9	E	1001	Y01	CAK-CBD	-16.03	1.27	1.53
9	E	1001	Y01	CBH-CAZ	-12.16	1.29	1.52
9	E	1001	Y01	CAQ-CAP	10.38	1.82	1.54
9	E	1001	Y01	CBI-CBE	10.29	1.73	1.55
9	E	1001	Y01	CBH-CBF	9.17	1.70	1.56
9	E	1001	Y01	CBD-CBF	-8.69	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1001	Y01	CAK-CAI	8.60	1.67	1.50
9	E	1001	Y01	CAQ-CBG	8.30	1.71	1.54
9	E	1001	Y01	CAT-CBH	7.32	1.67	1.54
9	E	1001	Y01	CBB-CBE	-6.97	1.42	1.54
7	B	1003	BMK	C6-C5	6.89	1.49	1.40
7	G	1005	BMK	C6-C5	6.76	1.49	1.40
9	E	1001	Y01	CBI-CBG	6.14	1.66	1.55
7	B	1003	BMK	C3-C2	5.48	1.46	1.39
7	G	1005	BMK	C3-C2	5.30	1.46	1.39
9	E	1001	Y01	CAR-CBC	-4.92	1.38	1.51
9	E	1001	Y01	CAP-CBE	4.42	1.63	1.54
9	E	1001	Y01	CAI-CAZ	4.18	1.41	1.33
9	E	1001	Y01	CAO-CBB	3.83	1.63	1.54
9	E	1001	Y01	OAW-CAY	3.82	1.45	1.34
9	E	1001	Y01	CAV-CAZ	3.43	1.58	1.51
7	B	1003	BMK	C3-C1	-3.30	1.47	1.51
7	G	1005	BMK	C3-C1	-3.12	1.47	1.51
7	G	1005	BMK	C-C5	-2.98	1.48	1.53
9	E	1001	Y01	CAC-CBB	2.75	1.60	1.53
7	B	1003	BMK	C-C5	-2.68	1.49	1.53
9	E	1001	Y01	CAE-CBI	2.67	1.58	1.54
9	E	1001	Y01	OAW-CBC	2.51	1.52	1.46
9	E	1001	Y01	CAV-CBC	2.38	1.57	1.52
6	B	1001	GLU	OXT-C	-2.29	1.23	1.30
3	A	902	GLY	OXT-C	-2.23	1.23	1.30
6	G	1004	GLU	OXT-C	-2.23	1.23	1.30
3	G	1001	GLY	OXT-C	-2.22	1.23	1.30
6	H	1001	GLU	OXT-C	-2.19	1.23	1.30
6	G	1006	GLU	OXT-C	-2.15	1.23	1.30
9	E	1001	Y01	CAS-CBF	2.11	1.57	1.53
9	E	1001	Y01	CAM-CAY	2.10	1.56	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1001	Y01	CAC-CBB-CBE	7.05	123.47	112.88
9	E	1001	Y01	CAS-CBF-CBH	-6.21	105.43	113.08
9	E	1001	Y01	CBH-CAZ-CAI	-6.08	114.05	122.93
9	E	1001	Y01	CAT-CBH-CAZ	5.99	119.07	108.74
9	E	1001	Y01	CAK-CAI-CAZ	-5.49	115.75	125.02
9	E	1001	Y01	CAE-CBI-CBG	-5.32	102.03	111.68
9	E	1001	Y01	CBF-CBD-CBG	5.29	116.00	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1001	Y01	OAW-CAY-CAM	5.08	122.47	111.48
9	E	1001	Y01	CAK-CBD-CBF	4.29	114.68	109.72
9	E	1001	Y01	CAD-CBH-CBF	-4.02	107.14	111.66
7	G	1005	BMK	C13-C9-C3	-3.92	116.29	120.99
7	B	1003	BMK	C13-C9-C3	-3.77	116.48	120.99
7	B	1003	BMK	C3-C1-N	-3.61	98.90	101.74
9	E	1001	Y01	CBG-CBI-CBE	3.45	104.06	100.10
9	E	1001	Y01	CAU-CBI-CBG	3.37	112.29	107.25
9	E	1001	Y01	CAS-CAU-CBI	3.17	118.08	112.74
9	E	1001	Y01	CAM-CAL-CAX	-2.95	105.83	113.67
6	G	1006	GLU	OXT-C-O	-2.81	117.70	124.08
9	E	1001	Y01	CAC-CBB-CAO	-2.79	106.02	110.34
6	G	1004	GLU	OXT-C-O	-2.79	117.76	124.08
9	E	1001	Y01	CAV-CAZ-CAI	-2.75	116.84	120.57
7	G	1005	BMK	C3-C1-N	-2.67	99.64	101.74
9	E	1001	Y01	CAD-CBH-CAT	-2.66	105.39	109.43
6	B	1001	GLU	OXT-C-O	-2.64	118.09	124.08
9	E	1001	Y01	CBI-CBE-CBB	2.58	123.48	119.50
6	D	1002	GLU	OE1-CD-CG	-2.53	115.07	123.09
9	E	1001	Y01	CAQ-CBG-CBI	-2.47	100.93	103.84
9	E	1001	Y01	CAK-CBD-CBG	2.40	114.33	110.93
9	E	1001	Y01	CAP-CBE-CBI	-2.34	101.09	103.84
6	H	1001	GLU	OXT-C-O	-2.31	118.84	124.08
9	E	1001	Y01	OAH-CAX-CAL	2.24	121.08	114.00
6	D	1002	GLU	OE2-CD-OE1	2.24	129.09	123.33
9	E	1001	Y01	OAW-CBC-CAR	2.20	113.58	108.37
7	G	1005	BMK	C12-C8-C2	-2.19	116.05	119.99
7	G	1005	BMK	C12-C13-C9	2.18	122.92	120.24
9	E	1001	Y01	CAV-CAZ-CBH	-2.13	113.70	116.42
9	E	1001	Y01	OAW-CAY-OAG	-2.12	118.76	123.70
7	B	1003	BMK	C12-C8-C2	-2.12	116.18	119.99
3	A	902	GLY	OXT-C-O	-2.07	118.01	123.33
6	H	1001	GLU	OE2-CD-CG	2.05	120.49	114.00
9	E	1001	Y01	CAE-CBI-CBE	-2.05	107.97	111.68
3	A	902	GLY	OXT-C-CA	2.02	121.42	113.38
6	H	1001	GLU	OE1-CD-CG	-2.02	116.68	123.09

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1003	TRS	C3-C-C1-O1

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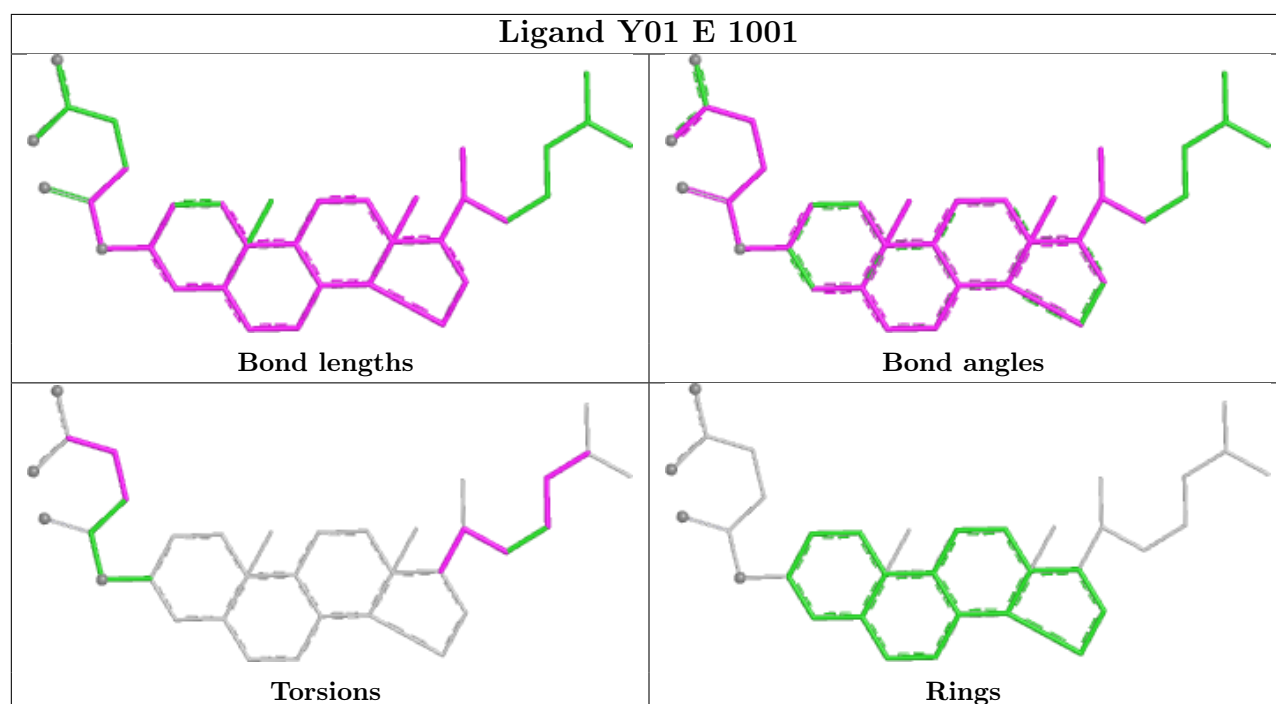
Mol	Chain	Res	Type	Atoms
5	G	1003	TRS	C2-C-C3-O3
6	H	1001	GLU	N-CA-CB-CG
9	E	1001	Y01	CAO-CBB-CBE-CAP
9	E	1001	Y01	CAO-CBB-CBE-CBI
9	E	1001	Y01	CAC-CBB-CBE-CBI
9	E	1001	Y01	CAC-CBB-CBE-CAP
4	H	1002	NAG	O5-C5-C6-O6
4	G	1002	NAG	O5-C5-C6-O6
9	E	1001	Y01	CAJ-CAO-CBB-CBE
4	D	1003	NAG	C4-C5-C6-O6
4	D	1003	NAG	O5-C5-C6-O6
4	F	1001	NAG	O5-C5-C6-O6
4	B	1002	NAG	O5-C5-C6-O6
9	E	1001	Y01	CAO-CAJ-CAN-CBA
4	G	1002	NAG	C4-C5-C6-O6
4	H	1002	NAG	C4-C5-C6-O6
5	G	1003	TRS	C2-C-C1-O1
5	G	1003	TRS	C1-C-C3-O3
4	D	1001	NAG	O5-C5-C6-O6
6	D	1002	GLU	CA-CB-CG-CD
9	E	1001	Y01	CAX-CAL-CAM-CAY
4	F	1001	NAG	C4-C5-C6-O6
5	G	1003	TRS	N-C-C1-O1
5	G	1003	TRS	N-C-C3-O3
6	H	1001	GLU	C-CA-CB-CG
6	B	1001	GLU	CA-CB-CG-CD
6	D	1002	GLU	OE1-CD-CG-CB
6	G	1006	GLU	OXT-C-CA-N
9	E	1001	Y01	CAJ-CAO-CBB-CAC
6	D	1002	GLU	OE2-CD-CG-CB
4	D	1001	NAG	C1-C2-N2-C7
6	G	1006	GLU	OE2-CD-CG-CB
6	G	1004	GLU	OE2-CD-CG-CB
6	H	1001	GLU	OXT-C-CA-CB
6	G	1006	GLU	OE1-CD-CG-CB
5	G	1003	TRS	C1-C-C2-O2
6	G	1004	GLU	OE1-CD-CG-CB
9	E	1001	Y01	CAM-CAL-CAX-OAF
9	E	1001	Y01	CAM-CAL-CAX-OAH
9	E	1001	Y01	CAJ-CAN-CBA-CAB
5	G	1003	TRS	N-C-C2-O2
9	E	1001	Y01	CAJ-CAN-CBA-CAA

There are no ring outliers.

9 monomers are involved in 34 short contacts:

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



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	416/451 (92%)	1.45	116 (27%) 1 1	39, 115, 206, 238	0
1	C	415/451 (92%)	1.83	127 (30%) 1 1	64, 138, 201, 264	0
1	E	412/451 (91%)	1.91	142 (34%) 1 1	74, 186, 251, 316	0
1	G	424/451 (94%)	0.99	87 (20%) 2 3	13, 73, 214, 287	0
2	B	397/448 (88%)	1.83	125 (31%) 1 1	43, 137, 209, 244	0
2	D	405/448 (90%)	1.60	100 (24%) 2 2	46, 123, 197, 225	0
2	F	416/448 (92%)	2.09	144 (34%) 1 1	92, 167, 216, 273	0
2	H	409/448 (91%)	1.96	144 (35%) 1 1	22, 119, 215, 251	0
All	All	3294/3596 (91%)	1.70	985 (29%) 1 1	13, 140, 220, 316	0

All (985) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	799	ASP	33.9
2	F	405	GLU	30.4
2	D	539	SER	30.2
2	D	540	PRO	28.7
1	C	796	ALA	28.6
2	H	797	ASP	22.5
2	H	575	PRO	22.0
1	C	548	THR	21.9
1	C	797	THR	20.7
1	C	826	ALA	19.6
2	H	800	ASN	19.5
2	F	642	TYR	19.3
2	H	636	PHE	18.9
2	D	800	ASN	18.8
2	H	802	ALA	17.5
1	A	469	ASP	17.1

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Mol	Chain	Res	Type	RSRZ
2	H	801	MET	16.5
2	D	541	SER	16.5
2	B	605	ASN	16.4
2	F	404	LEU	16.3
1	E	526	GLU	15.3
2	D	797	ASP	15.1
2	F	477	GLY	14.7
2	D	796	LEU	14.5
2	F	505	SER	14.2
2	F	504	GLY	14.0
2	H	576	VAL	13.6
2	B	636	PHE	13.5
2	H	803	GLY	13.1
2	B	606	PRO	13.1
2	H	798	ILE	13.0
1	E	521	ARG	12.9
1	E	516	THR	12.9
2	B	541	SER	12.8
2	B	604	GLN	12.8
1	C	825	ILE	12.5
1	C	549	LEU	12.5
2	B	542	ALA	12.5
1	E	747	GLY	12.4
2	D	538	VAL	12.0
2	H	633	LEU	11.8
1	C	550	ASP	11.2
1	A	466	ARG	11.0
2	F	643	VAL	10.9
1	E	746	SER	10.9
2	F	406	GLU	10.9
2	B	548	SER	10.8
2	D	802	ALA	10.7
2	B	549	ALA	10.5
1	G	559	THR	10.5
2	D	801	MET	10.5
1	E	413	PRO	10.5
1	A	744	PHE	10.3
2	F	473	LEU	10.3
2	F	640	ARG	10.3
2	H	632	ASN	10.2
1	C	645	LEU	10.2
2	F	407	ALA	10.2

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Mol	Chain	Res	Type	RSRZ
2	F	641	ARG	10.1
2	B	607	LYS	9.8
1	E	525	ILE	9.8
2	F	644	ASP	9.6
1	C	776	GLU	9.6
2	H	544	LEU	9.6
1	E	641	LEU	9.5
2	D	542	ALA	9.5
2	F	409	PHE	9.5
2	F	697	VAL	9.5
2	H	796	LEU	9.4
1	E	751	GLY	9.4
2	B	581	PRO	9.4
2	D	799	ASP	9.4
1	C	643	ALA	9.3
2	B	545	GLU	9.3
1	E	527	PHE	9.2
2	H	637	MET	9.1
1	C	500	MET	9.1
1	C	823	ILE	9.1
2	F	696	SER	9.0
2	F	403	THR	9.0
1	C	642	ALA	9.0
2	B	547	PHE	8.9
2	D	403	THR	8.9
2	B	799	ASP	8.8
2	H	634	ALA	8.8
2	F	474	VAL	8.8
1	E	517	ILE	8.7
2	B	634	ALA	8.7
1	G	560	LEU	8.6
2	B	633	LEU	8.6
1	C	554	GLN	8.5
2	F	585	ILE	8.4
2	B	770	GLY	8.3
1	G	580	ARG	8.3
1	E	752	MET	8.3
1	C	483	GLY	8.0
1	A	682	TYR	8.0
2	D	504	GLY	8.0
1	C	758	TRP	7.9
1	A	685	ARG	7.9

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Mol	Chain	Res	Type	RSRZ
2	B	670	PRO	7.9
1	C	510	MET	7.9
2	F	637	MET	7.8
2	H	679	ARG	7.8
2	F	634	ALA	7.8
2	B	635	ALA	7.7
2	F	410	VAL	7.7
1	C	489	ASN	7.7
1	C	755	ASP	7.7
1	A	703	SER	7.7
2	D	402	VAL	7.6
1	G	563	LEU	7.6
1	C	555	PRO	7.6
1	E	678	SER	7.6
2	H	635	ALA	7.6
1	E	453	CYS	7.5
2	H	574	SER	7.5
2	B	802	ALA	7.5
1	A	743	PHE	7.5
2	B	768	GLY	7.4
2	B	769	ASP	7.3
2	H	545	GLU	7.3
1	A	535	GLY	7.2
2	B	767	PHE	7.2
2	D	798	ILE	7.1
1	A	465	ALA	7.1
2	D	472	TYR	7.0
1	G	826	ALA	7.0
2	H	767	PHE	6.9
1	C	647	LEU	6.9
1	E	677	SER	6.9
1	C	801	GLU	6.8
2	B	771	GLU	6.8
1	A	722	ASP	6.7
2	D	503	VAL	6.7
1	G	825	ILE	6.7
1	A	724	ALA	6.6
2	F	493	GLU	6.6
1	G	582	SER	6.6
1	C	545	PRO	6.6
2	H	630	THR	6.5
1	G	607	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	518	ASN	6.5
1	E	524	TYR	6.5
2	B	691	LYS	6.4
2	D	786	ASN	6.4
1	E	644	PHE	6.4
1	E	434	VAL	6.4
2	D	507	THR	6.4
1	C	799	THR	6.3
2	F	599	ASN	6.3
2	B	582	SER	6.3
1	E	417	ASP	6.3
2	B	637	MET	6.2
1	A	683	PHE	6.2
1	A	467	GLU	6.2
1	E	452	CYS	6.2
2	F	715	ASP	6.2
1	A	406	GLU	6.1
2	F	478	LYS	6.1
2	D	470	ASP	6.1
1	C	824	GLU	6.1
1	A	536	LEU	6.0
1	E	613	ALA	6.0
2	D	478	LYS	6.0
2	D	636	PHE	6.0
2	D	506	LEU	5.9
2	F	695	ARG	5.9
2	B	412	VAL	5.9
2	B	480	GLY	5.9
1	E	412	ARG	5.9
1	A	468	MET	5.9
2	B	544	LEU	5.8
2	F	794	SER	5.8
2	B	765	GLN	5.8
2	H	547	PHE	5.8
2	B	669	VAL	5.8
2	F	773	GLU	5.7
1	G	796	ALA	5.7
1	A	518	ASN	5.7
1	G	790	SER	5.7
2	B	639	GLN	5.7
2	F	764	LEU	5.6
2	D	480	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
2	D	543	PHE	5.6
1	E	785	TYR	5.6
2	F	761	LEU	5.6
2	F	408	PRO	5.6
2	B	688	TYR	5.6
2	H	645	GLN	5.6
2	D	401	ILE	5.6
2	H	658	ASN	5.5
2	D	675	GLU	5.5
1	C	490	ASN	5.5
1	C	798	LEU	5.5
1	G	804	ALA	5.5
2	B	464	THR	5.5
2	H	752	ASP	5.4
1	A	420	CYS	5.4
1	C	488	VAL	5.4
2	F	762	ALA	5.4
1	E	482	PHE	5.4
2	B	807	MET	5.4
2	D	637	MET	5.4
1	C	757	PRO	5.4
1	E	451	GLN	5.4
2	F	698	GLN	5.4
2	F	700	ALA	5.3
2	F	584	THR	5.3
1	G	639	ALA	5.3
2	D	544	LEU	5.3
1	A	627	ALA	5.3
1	A	664	ASN	5.3
2	H	450	CYS	5.2
1	E	548	THR	5.2
2	H	522	PHE	5.2
1	A	492	ASN	5.2
1	A	727	GLU	5.2
2	H	534	SER	5.2
1	E	519	ASN	5.2
1	A	534	GLN	5.1
2	B	583	PHE	5.1
1	E	649	ARG	5.1
1	G	438	GLY	5.1
2	H	551	VAL	5.1
1	G	802	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	479	HIS	5.1
1	A	745	ARG	5.1
1	G	605	LEU	5.0
2	F	745	TYR	5.0
2	D	473	LEU	5.0
1	E	514	PRO	5.0
2	D	397	GLU	5.0
1	C	606	ASN	5.0
2	B	546	PRO	5.0
1	E	614	PRO	5.0
2	F	638	ILE	5.0
2	F	454	CYS	5.0
1	E	414	THR	4.9
2	F	763	ILE	4.9
1	C	641	LEU	4.9
1	E	658	ASN	4.9
2	H	449	CYS	4.9
1	C	546	ARG	4.9
1	E	612	GLY	4.9
1	E	704	ALA	4.9
2	H	710	ASP	4.8
2	B	631	ALA	4.8
1	A	470	PHE	4.8
2	B	460	LYS	4.8
1	G	606	ASN	4.8
2	H	535	ASN	4.8
1	E	416	SER	4.8
1	C	649	ARG	4.8
1	E	796	ALA	4.8
2	H	646	VAL	4.8
2	D	570	PHE	4.8
2	B	772	MET	4.8
1	E	676	GLN	4.8
1	E	522	ALA	4.8
1	E	794	ALA	4.8
2	H	606	PRO	4.8
1	A	706	GLU	4.8
2	H	441	GLU	4.8
1	A	429	ASP	4.8
1	A	704	ALA	4.8
2	B	638	ILE	4.8
2	B	456	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	644	ASP	4.7
2	H	546	PRO	4.7
1	E	546	ARG	4.7
1	A	643	ALA	4.7
1	G	663	ARG	4.7
1	C	802	ASN	4.7
2	F	718	VAL	4.7
1	C	468	MET	4.7
2	F	412	VAL	4.6
2	F	828	SER	4.6
1	C	499	MET	4.6
1	A	396	THR	4.6
2	D	477	GLY	4.6
2	D	678	ILE	4.6
1	A	611	GLU	4.6
1	E	741	GLU	4.6
2	B	671	ASN	4.6
2	F	633	LEU	4.6
1	C	521	ARG	4.6
2	H	524	GLU	4.5
1	C	644	PHE	4.5
2	B	404	LEU	4.5
2	H	768	GLY	4.5
1	E	650	PRO	4.5
2	F	498	ARG	4.5
1	A	723	SER	4.5
2	D	674	THR	4.5
1	G	550	ASP	4.5
2	F	538	VAL	4.5
1	A	795	PRO	4.5
2	B	524	GLU	4.5
1	C	560	LEU	4.4
1	E	607	SER	4.4
2	D	600	SER	4.4
1	C	650	PRO	4.4
1	A	765	ASN	4.4
2	D	615	VAL	4.4
1	G	504	LEU	4.4
1	E	722	ASP	4.4
1	G	592	THR	4.4
2	B	432	GLN	4.4
1	C	822	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	805	PHE	4.4
1	E	611	GLU	4.4
2	F	802	ALA	4.4
1	C	646	VAL	4.3
1	E	419	THR	4.3
1	E	657	ILE	4.3
2	B	800	ASN	4.3
2	D	638	ILE	4.3
2	H	652	LYS	4.3
2	D	586	GLY	4.3
2	B	662	PRO	4.3
1	G	601	TRP	4.2
2	B	766	LEU	4.2
2	F	760	ASP	4.2
2	F	645	GLN	4.2
2	B	706	SER	4.2
1	C	648	ARG	4.2
2	D	746	GLY	4.2
1	A	680	ASP	4.2
1	A	418	GLY	4.2
1	C	482	PHE	4.2
2	H	408	PRO	4.2
2	D	474	VAL	4.2
2	D	617	VAL	4.2
1	G	553	MET	4.2
2	D	677	ASN	4.2
1	G	557	GLN	4.1
2	F	639	GLN	4.1
1	G	394	MET	4.1
2	H	643	VAL	4.1
2	F	494	VAL	4.1
2	F	598	ASN	4.1
1	G	558	SER	4.1
2	H	736	SER	4.1
1	E	398	LEU	4.1
1	A	681	ILE	4.1
1	A	725	VAL	4.1
1	A	551	SER	4.1
1	E	647	LEU	4.1
1	E	529	LYS	4.1
2	H	669	VAL	4.1
1	E	415	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	764	LEU	4.1
1	C	640	ASN	4.1
1	A	661	ARG	4.0
1	A	642	ALA	4.0
1	C	462	ILE	4.0
1	A	678	SER	4.0
2	H	523	ILE	4.0
1	A	705	ALA	4.0
1	C	631	MET	4.0
1	E	662	LEU	4.0
2	H	615	VAL	4.0
1	A	758	TRP	4.0
2	H	552	TRP	4.0
1	A	520	GLU	4.0
1	E	418	GLY	4.0
1	E	740	GLY	4.0
2	H	806	TYR	4.0
1	A	726	LEU	4.0
2	F	506	LEU	4.0
1	C	492	ASN	4.0
2	D	598	ASN	4.0
2	D	597	PHE	3.9
2	F	795	GLN	3.9
1	E	543	GLU	3.9
1	G	792	SER	3.9
1	E	406	GLU	3.9
2	D	572	TYR	3.9
1	G	554	GLN	3.9
1	G	474	VAL	3.9
1	A	729	GLU	3.9
2	B	530	MET	3.9
2	H	521	PRO	3.9
1	A	550	ASP	3.9
1	C	405	GLN	3.9
2	H	432	GLN	3.9
1	A	805	GLY	3.9
2	H	672	GLY	3.9
1	G	451	GLN	3.8
1	E	810	VAL	3.8
2	D	647	SER	3.8
1	G	642	ALA	3.8
2	B	754	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	785	HIS	3.8
1	E	533	TYR	3.8
2	F	682	TYR	3.8
1	E	478	ALA	3.8
1	C	495	ALA	3.8
2	H	568	PHE	3.8
2	F	774	GLU	3.8
2	F	826	TYR	3.8
2	H	410	VAL	3.8
2	H	794	SER	3.8
1	A	640	ASN	3.8
2	F	719	LEU	3.8
2	B	679	ARG	3.8
1	A	581	PHE	3.8
2	F	655	GLN	3.8
1	G	549	LEU	3.8
1	C	609	LEU	3.8
1	E	442	THR	3.8
2	F	455	ILE	3.7
2	D	469	TYR	3.7
2	F	475	THR	3.7
1	E	499	MET	3.7
2	H	533	ARG	3.7
2	D	794	SER	3.7
1	C	464	LEU	3.7
2	B	675	GLU	3.7
2	F	600	SER	3.7
2	F	801	MET	3.7
1	C	556	PHE	3.7
2	B	707	GLY	3.7
2	H	586	GLY	3.7
1	A	746	SER	3.7
1	E	397	ARG	3.7
1	C	514	PRO	3.7
1	C	685	ARG	3.7
2	H	642	TYR	3.7
2	F	604	GLN	3.7
1	A	667	ASP	3.7
2	B	478	LYS	3.7
2	D	657	PRO	3.7
1	E	469	ASP	3.7
2	H	731	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	742	LEU	3.6
1	A	665	PRO	3.6
1	C	430	PRO	3.6
2	H	772	MET	3.6
2	B	477	GLY	3.6
2	F	636	PHE	3.6
1	E	640	ASN	3.6
2	H	596	VAL	3.6
1	G	824	GLU	3.6
1	G	798	LEU	3.6
2	F	733	THR	3.6
1	E	637	TYR	3.6
2	H	626	LEU	3.6
2	F	442	GLY	3.6
1	E	656	GLY	3.5
1	E	703	SER	3.5
1	E	742	LEU	3.5
2	D	654	PHE	3.5
2	B	658	ASN	3.5
2	B	705	LYS	3.5
2	H	789	ASN	3.5
2	F	476	ASN	3.5
1	E	407	PRO	3.5
1	C	444	PRO	3.5
1	C	660	PRO	3.5
1	A	544	ILE	3.5
1	E	411	VAL	3.5
1	E	636	SER	3.5
1	G	614	PRO	3.5
1	E	666	SER	3.5
2	B	482	LYS	3.5
1	C	803	MET	3.5
1	E	515	LEU	3.5
1	C	497	ASN	3.5
2	D	599	ASN	3.5
2	H	787	GLU	3.5
2	B	708	LYS	3.5
2	F	759	VAL	3.5
1	G	608	GLY	3.5
1	C	559	THR	3.5
2	F	765	GLN	3.5
2	H	435	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	405	GLU	3.4
1	E	655	THR	3.4
1	E	799	THR	3.4
1	G	660	PRO	3.4
1	A	543	GLU	3.4
1	G	822	PHE	3.4
1	E	745	ARG	3.4
1	C	487	ARG	3.4
2	B	720	ASN	3.4
2	D	634	ALA	3.4
2	B	623	VAL	3.4
2	H	628	SER	3.4
1	C	601	TRP	3.4
2	H	795	GLN	3.4
2	H	530	MET	3.4
2	B	603	VAL	3.4
1	E	755	ASP	3.4
1	C	751	GLY	3.3
2	H	590	TRP	3.3
2	F	779	TRP	3.3
1	A	679	VAL	3.3
1	A	663	ARG	3.3
2	D	430	ARG	3.3
1	G	801	GLU	3.3
1	A	662	LEU	3.3
2	H	456	ASP	3.3
1	G	643	ALA	3.3
2	H	453	PHE	3.3
1	E	396	THR	3.3
1	E	643	ALA	3.3
2	B	632	ASN	3.3
1	E	739	THR	3.3
1	C	592	THR	3.3
2	H	686	HIS	3.3
1	E	433	LYS	3.3
2	D	740	PHE	3.3
1	E	721	TRP	3.3
1	C	396	THR	3.3
1	G	552	PHE	3.2
1	A	609	LEU	3.2
2	D	585	ILE	3.2
2	F	699	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	787	GLU	3.2
1	E	820	LEU	3.2
2	B	407	ALA	3.2
1	C	789	ASP	3.2
1	C	446	ARG	3.2
2	D	763	ILE	3.2
2	H	564	ALA	3.2
1	A	416	SER	3.2
2	B	710	ASP	3.2
1	A	410	TYR	3.2
2	F	549	ALA	3.2
2	B	793	SER	3.2
1	G	472	TYR	3.2
2	F	688	TYR	3.2
1	A	771	GLU	3.2
2	F	519	SER	3.2
2	D	431	LYS	3.2
2	H	785	HIS	3.2
1	C	470	PHE	3.2
1	E	653	ARG	3.2
1	C	516	THR	3.2
2	D	530	MET	3.2
1	G	578	LEU	3.2
1	E	551	SER	3.1
2	B	690	VAL	3.1
2	F	462	ALA	3.1
1	A	796	ALA	3.1
2	D	454	CYS	3.1
1	G	551	SER	3.1
1	E	682	TYR	3.1
2	B	450	CYS	3.1
2	H	428	PRO	3.1
2	H	641	ARG	3.1
2	F	827	LYS	3.1
2	H	744	GLY	3.1
2	B	630	THR	3.1
2	D	471	LEU	3.1
2	B	475	THR	3.1
2	H	569	VAL	3.1
2	H	647	SER	3.1
2	D	741	ALA	3.1
2	F	684	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	592	LEU	3.1
2	D	537	THR	3.1
1	E	816	ALA	3.0
1	E	606	ASN	3.0
2	B	543	PHE	3.0
2	D	720	ASN	3.0
2	D	764	LEU	3.0
2	F	583	PHE	3.0
2	H	648	GLY	3.0
2	D	624	ILE	3.0
1	A	730	ALA	3.0
2	F	450	CYS	3.0
2	H	640	ARG	3.0
2	B	571	GLU	3.0
2	D	795	GLN	3.0
1	A	677	SER	3.0
1	C	607	SER	3.0
1	A	707	ALA	3.0
2	F	499	ALA	3.0
1	A	660	PRO	3.0
1	A	659	ASP	3.0
1	E	639	ALA	3.0
2	B	810	ALA	3.0
2	F	430	ARG	3.0
1	G	795	PRO	3.0
1	E	545	PRO	3.0
1	C	440	ASP	3.0
2	F	458	LEU	2.9
2	H	659	ASP	2.9
1	C	517	ILE	2.9
1	A	593	LEU	2.9
1	E	552	PHE	2.9
2	D	475	THR	2.9
2	F	651	ASP	2.9
1	C	569	HIS	2.9
2	H	473	LEU	2.9
1	C	779	ASP	2.9
2	D	522	PHE	2.9
2	D	398	HIS	2.9
2	D	484	ASN	2.9
1	G	747	GLY	2.9
1	A	666	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	812	GLY	2.9
1	A	471	THR	2.9
2	B	403	THR	2.9
2	H	451	LYS	2.9
2	H	622	ALA	2.9
1	C	407	PRO	2.9
1	E	688	GLU	2.9
1	C	509	ASP	2.9
1	C	565	GLY	2.9
2	H	567	VAL	2.9
2	H	791	VAL	2.9
2	F	687	SER	2.9
1	C	598	TRP	2.9
1	C	465	ALA	2.9
2	F	664	PHE	2.9
1	E	569	HIS	2.8
1	C	634	VAL	2.8
2	H	563	SER	2.8
1	G	823	ILE	2.8
1	E	760	GLN	2.8
2	B	698	GLN	2.8
1	G	572	ALA	2.8
1	E	627	ALA	2.8
2	B	764	LEU	2.8
1	G	791	ARG	2.8
1	A	616	SER	2.8
2	H	585	ILE	2.8
2	F	752	ASP	2.8
2	D	502	ALA	2.8
1	E	758	TRP	2.8
2	H	618	TRP	2.8
2	B	568	PHE	2.8
2	B	621	PHE	2.8
2	H	572	TYR	2.8
1	A	594	SER	2.8
1	C	558	SER	2.8
1	C	480	GLY	2.8
2	B	686	HIS	2.8
1	C	627	ALA	2.8
2	F	537	THR	2.8
2	F	560	LEU	2.8
1	A	414	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	588	ALA	2.8
2	B	657	PRO	2.8
2	H	732	VAL	2.8
1	G	611	GLU	2.8
1	C	652	GLU	2.8
1	C	747	GLY	2.8
2	B	727	GLU	2.8
2	H	436	GLU	2.8
2	D	671	ASN	2.8
2	F	781	THR	2.8
1	A	789	ASP	2.8
1	G	503	LEU	2.8
1	G	555	PRO	2.8
2	F	602	PRO	2.8
1	G	424	TYR	2.8
1	C	533	TYR	2.8
2	H	573	PHE	2.8
2	F	547	PHE	2.8
2	F	746	GLY	2.8
2	B	411	ILE	2.7
1	A	527	PHE	2.7
2	F	460	LYS	2.7
2	B	510	GLU	2.7
2	H	733	THR	2.7
1	G	609	LEU	2.7
2	F	739	VAL	2.7
1	A	430	PRO	2.7
2	H	602	PRO	2.7
2	H	691	LYS	2.7
2	D	642	TYR	2.7
1	E	560	LEU	2.7
1	C	494	ALA	2.7
2	F	677	ASN	2.7
2	F	786	ASN	2.7
1	G	532	LYS	2.7
2	H	600	SER	2.7
1	A	810	VAL	2.7
2	B	780	LEU	2.7
1	E	405	GLN	2.7
2	H	442	GLY	2.7
2	F	480	GLY	2.7
2	F	566	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	436	CYS	2.7
1	A	595	SER	2.7
2	F	736	SER	2.7
2	D	604	GLN	2.7
2	H	774	GLU	2.7
2	H	429	CYS	2.7
1	E	500	MET	2.7
1	G	569	HIS	2.6
2	F	596	VAL	2.6
2	B	488	ASN	2.6
2	D	785	HIS	2.6
1	A	709	GLN	2.6
1	G	417	ASP	2.6
2	H	769	ASP	2.6
2	B	419	SER	2.6
2	B	448	ARG	2.6
2	B	512	ARG	2.6
1	G	794	ALA	2.6
1	A	721	TRP	2.6
1	G	460	LEU	2.6
1	E	738	THR	2.6
1	C	761	GLU	2.6
2	D	625	PHE	2.6
2	F	548	SER	2.6
1	G	447	PRO	2.6
2	D	627	ALA	2.6
1	A	748	PHE	2.6
2	H	779	TRP	2.6
1	G	437	ASN	2.6
2	F	431	LYS	2.6
2	F	601	LEU	2.6
2	F	744	GLY	2.6
2	F	825	PHE	2.6
1	E	559	THR	2.6
1	E	532	LYS	2.6
2	F	681	ASN	2.6
2	F	777	ALA	2.6
1	E	422	GLU	2.5
2	B	774	GLU	2.5
1	E	679	VAL	2.5
1	G	579	ASP	2.5
1	A	545	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	707	ALA	2.5
1	C	572	ALA	2.5
1	C	610	GLY	2.5
2	B	672	GLY	2.5
1	A	717	HIS	2.5
1	E	511	ILE	2.5
1	E	561	TRP	2.5
1	C	782	TRP	2.5
2	H	532	SER	2.5
2	H	565	VAL	2.5
2	B	731	LEU	2.5
1	A	617	PHE	2.5
1	C	493	ALA	2.5
2	B	668	THR	2.5
2	D	610	THR	2.5
1	G	423	GLU	2.5
1	E	652	GLU	2.5
1	A	655	THR	2.5
1	C	484	THR	2.5
1	C	410	TYR	2.5
2	D	633	LEU	2.5
2	B	474	VAL	2.5
2	F	571	GLU	2.5
1	A	669	PHE	2.5
2	H	437	ASN	2.5
1	E	479	ASP	2.5
2	F	630	THR	2.5
2	F	603	VAL	2.5
1	C	520	GLU	2.5
1	G	617	PHE	2.5
1	G	629	PHE	2.5
1	E	489	ASN	2.5
2	H	577	GLY	2.5
1	E	537	THR	2.5
2	D	742	THR	2.5
2	H	793	SER	2.5
2	F	400	SER	2.5
1	E	697	GLU	2.4
1	C	513	ALA	2.4
2	B	711	ALA	2.4
1	E	608	GLY	2.4
1	E	436	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	584	THR	2.4
2	H	529	VAL	2.4
1	E	531	PHE	2.4
2	F	751	LYS	2.4
1	C	544	ILE	2.4
2	F	776	GLU	2.4
2	F	542	ALA	2.4
2	B	676	ARG	2.4
2	D	754	GLY	2.4
2	H	651	ASP	2.4
1	A	408	PHE	2.4
1	C	481	LYS	2.4
2	F	788	LYS	2.4
1	E	818	ILE	2.4
1	G	598	TRP	2.4
2	B	487	TRP	2.4
2	B	695	ARG	2.4
1	A	658	ASN	2.4
1	C	740	GLY	2.4
2	B	443	GLY	2.4
2	H	697	VAL	2.4
1	E	776	GLU	2.4
2	D	810	ALA	2.4
1	G	597	MET	2.4
1	A	668	LYS	2.4
2	F	582	SER	2.4
2	D	587	LYS	2.4
1	E	410	TYR	2.4
1	E	520	GLU	2.4
2	H	711	ALA	2.4
2	D	588	ALA	2.4
1	A	564	VAL	2.4
1	A	568	VAL	2.4
1	C	448	THR	2.4
2	B	719	LEU	2.4
1	G	775	MET	2.4
1	E	705	ALA	2.4
1	C	771	GLU	2.4
2	B	622	ALA	2.4
2	B	773	GLU	2.4
2	D	655	GLN	2.3
1	C	599	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	720	ILE	2.3
2	B	618	TRP	2.3
2	B	701	LEU	2.3
2	B	596	VAL	2.3
2	H	804	VAL	2.3
1	E	789	ASP	2.3
1	E	651	GLU	2.3
1	C	486	GLU	2.3
2	F	436	GLU	2.3
2	B	425	ASN	2.3
2	H	443	GLY	2.3
2	D	456	ASP	2.3
1	G	439	PRO	2.3
1	G	612	GLY	2.3
1	C	427	ASN	2.3
2	D	535	ASN	2.3
2	D	623	VAL	2.3
2	B	481	LYS	2.3
2	F	685	MET	2.3
1	A	464	LEU	2.3
1	C	504	LEU	2.3
1	A	766	ILE	2.3
1	E	670	ILE	2.3
1	E	814	ILE	2.3
2	H	571	GLU	2.3
2	F	510	GLU	2.3
2	F	561	ILE	2.3
2	D	644	ASP	2.3
1	C	746	SER	2.3
1	A	610	GLY	2.3
1	E	773	GLY	2.3
2	H	823	HIS	2.3
1	C	615	ARG	2.3
2	B	779	TRP	2.3
1	A	591	LEU	2.3
1	C	473	GLU	2.3
1	G	600	SER	2.3
2	F	563	SER	2.3
1	A	474	VAL	2.3
1	C	532	LYS	2.3
1	A	412	ARG	2.3
1	C	553	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	599	ASN	2.3
2	H	755	TRP	2.3
2	F	766	LEU	2.3
1	E	813	GLY	2.3
1	C	687	VAL	2.3
2	F	443	GLY	2.3
1	G	574	MET	2.3
1	A	633	ILE	2.2
1	A	654	ILE	2.2
2	B	809	ALA	2.2
2	F	694	GLN	2.2
1	G	615	ARG	2.2
1	A	687	VAL	2.2
2	H	531	VAL	2.2
2	F	669	VAL	2.2
1	E	638	THR	2.2
2	F	439	THR	2.2
2	F	778	LEU	2.2
1	A	517	ILE	2.2
1	A	786	GLN	2.2
2	B	614	MET	2.2
2	D	571	GLU	2.2
2	D	679	ARG	2.2
2	H	599	ASN	2.2
2	H	763	ILE	2.2
1	G	774	PHE	2.2
2	H	730	LYS	2.2
1	A	472	TYR	2.2
1	C	551	SER	2.2
2	B	650	SER	2.2
2	D	563	SER	2.2
1	G	688	GLU	2.2
1	A	623	GLY	2.2
2	H	782	GLY	2.2
2	F	441	GLU	2.2
1	C	527	PHE	2.2
1	G	492	ASN	2.2
1	E	713	ASP	2.2
1	E	572	ALA	2.2
1	C	630	ALA	2.2
1	A	618	SER	2.2
1	E	523	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	785	TYR	2.2
2	F	714	TYR	2.2
1	A	634	VAL	2.2
2	F	503	VAL	2.2
2	D	565	VAL	2.2
1	A	670	ILE	2.2
1	C	614	PRO	2.2
2	H	583	PHE	2.2
2	F	453	PHE	2.2
1	A	457	CYS	2.2
2	F	605	ASN	2.2
1	G	618	SER	2.2
1	G	535	GLY	2.2
1	C	608	GLY	2.2
2	H	426	THR	2.2
1	A	488	VAL	2.1
2	F	678	ILE	2.1
2	H	712	PHE	2.1
1	G	593	LEU	2.1
1	E	539	LEU	2.1
2	H	434	ARG	2.1
2	H	613	ILE	2.1
2	F	595	LEU	2.1
2	B	762	ALA	2.1
2	H	605	ASN	2.1
2	F	588	ALA	2.1
2	D	658	ASN	2.1
2	B	798	ILE	2.1
1	G	433	LYS	2.1
2	B	654	PHE	2.1
2	H	412	VAL	2.1
1	G	622	LEU	2.1
1	A	423	GLU	2.1
2	B	413	GLU	2.1
1	E	448	THR	2.1
1	E	471	THR	2.1
2	B	490	MET	2.1
2	B	600	SER	2.1
1	C	485	GLN	2.1
2	B	453	PHE	2.1
2	H	603	VAL	2.1
2	H	629	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	803	MET	2.1
1	C	752	MET	2.1
1	C	596	ALA	2.1
2	F	703	SER	2.1
1	E	617	PHE	2.1
1	C	658	ASN	2.1
2	H	664	PHE	2.1
2	F	720	ASN	2.1
2	D	626	LEU	2.1
1	C	695	HIS	2.1
1	G	440	ASP	2.1
1	E	506	GLY	2.1
2	H	555	MET	2.1
1	C	447	PRO	2.1
2	B	715	ASP	2.1
1	A	425	THR	2.1
2	B	674	THR	2.1
2	D	684	GLU	2.1
2	H	454	CYS	2.1
1	E	596	ALA	2.1
2	B	794	SER	2.1
2	D	635	ALA	2.1
1	C	456	PHE	2.1
2	B	570	PHE	2.1
1	G	561	TRP	2.0
1	G	462	ILE	2.0
1	G	814	ILE	2.0
1	E	538	ILE	2.0
2	H	788	LYS	2.0
1	C	616	SER	2.0
2	F	712	PHE	2.0
1	A	641	LEU	2.0
1	E	609	LEU	2.0
2	H	561	ILE	2.0
2	F	624	ILE	2.0
2	H	550	ASP	2.0
2	F	413	GLU	2.0
1	G	464	LEU	2.0
2	F	780	LEU	2.0
2	D	630	THR	2.0
1	E	558	SER	2.0
1	C	705	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	651	ASP	2.0
2	D	760	ASP	2.0
2	H	427	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 oligosaccharides in this entry.

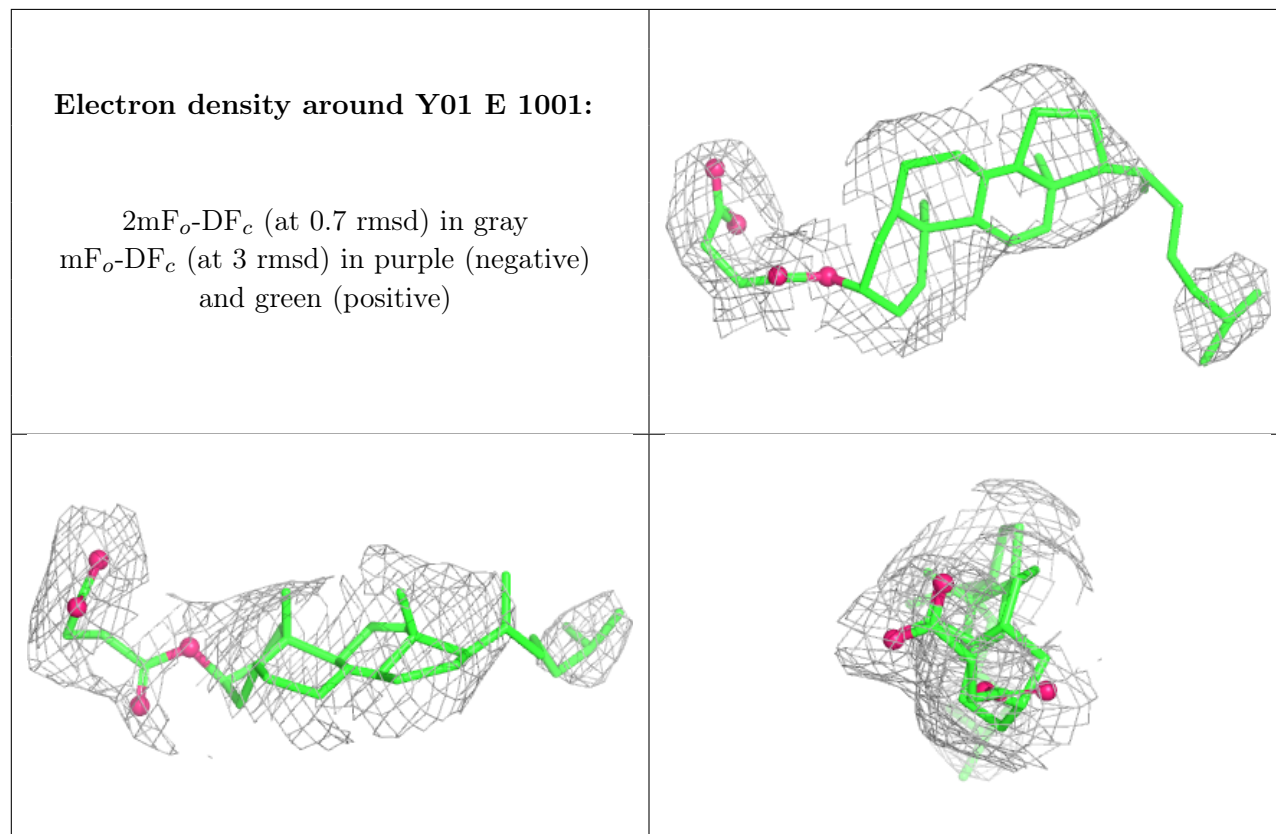
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GLU	D	1002	10/10	0.54	0.20	84,114,139,149	0
9	Y01	E	1001	35/35	0.70	0.18	66,152,172,179	0
7	BMK	G	1005	17/17	0.74	0.30	128,155,191,209	0
4	NAG	D	1001	15/15	0.77	0.15	101,150,172,201	0
4	NAG	F	1001	15/15	0.78	0.09	113,149,175,194	0
4	NAG	D	1003	15/15	0.78	0.14	128,160,180,195	0
6	GLU	G	1004	10/10	0.78	0.18	58,86,122,166	0
4	NAG	G	1002	15/15	0.85	0.12	90,111,144,148	0
4	NAG	B	1002	15/15	0.85	0.09	109,152,165,169	0
6	GLU	B	1001	10/10	0.85	0.15	57,87,105,131	0
7	BMK	B	1003	17/17	0.89	0.21	111,153,186,199	0
5	TRS	G	1003	8/8	0.89	0.23	6,17,56,81	0
3	GLY	A	902	5/5	0.90	0.16	67,67,79,81	0
6	GLU	G	1006	10/10	0.92	0.20	71,97,108,112	0
4	NAG	H	1002	15/15	0.94	0.08	96,119,134,145	0
6	GLU	H	1001	10/10	0.94	0.12	28,77,102,104	0
3	GLY	G	1001	5/5	0.97	0.07	28,30,42,59	0
8	MG	A	901	1/1	0.98	0.21	37,37,37,37	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.