



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:22 PM UTC

PDB ID : 5L1B / pdb_00005l1b
Title : AMPA subtype ionotropic glutamate receptor GluA2 in Apo state
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.
Deposited on : 2016-07-28
Resolution : 4.00 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
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

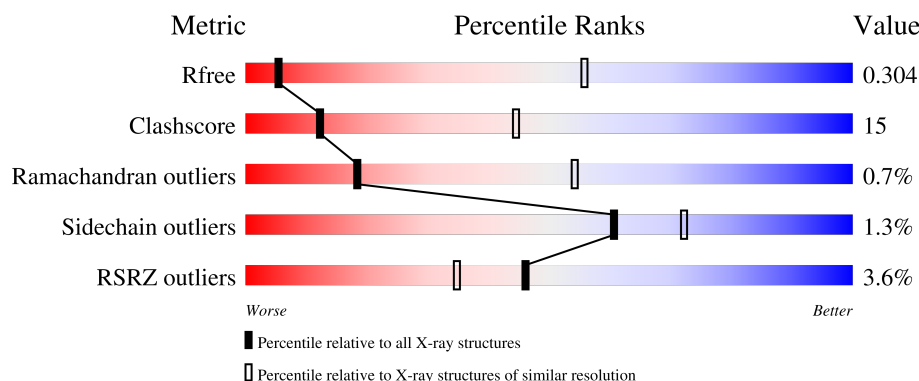
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	803	 4% 71% 23% ..
1	B	803	 2% 71% 23% ..
1	C	803	 2% 74% 20% ...
1	D	803	 5% 73% 22% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2, Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	0	0
			6017	3865	995	1128	29			
1	B	780	Total	C	N	O	S	0	0	0
			6022	3868	995	1130	29			
1	C	780	Total	C	N	O	S	0	0	0
			6023	3868	995	1131	29			
1	D	783	Total	C	N	O	S	0	0	0
			6038	3875	998	1136	29			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	744	THR	ASN	engineered mutation	UNP P19491
A	745	PRO	ALA	engineered mutation	UNP P19491
A	754	SER	ASN	engineered mutation	UNP P19491
A	758	VAL	LEU	engineered mutation	UNP P19491
A	775	ALA	SER	engineered mutation	UNP P19491
A	776	LYS	GLY	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	ASP	GLY	engineered mutation	UNP P19491
A	778	SER	GLY	engineered mutation	UNP P19491
A	779	GLY	ASP	engineered mutation	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	744	THR	ASN	engineered mutation	UNP P19491
B	745	PRO	ALA	engineered mutation	UNP P19491
B	754	SER	ASN	engineered mutation	UNP P19491
B	758	VAL	LEU	engineered mutation	UNP P19491
B	775	ALA	SER	engineered mutation	UNP P19491
B	776	LYS	GLY	engineered mutation	UNP P19491
B	777	ASP	GLY	engineered mutation	UNP P19491
B	778	SER	GLY	engineered mutation	UNP P19491
B	779	GLY	ASP	engineered mutation	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491

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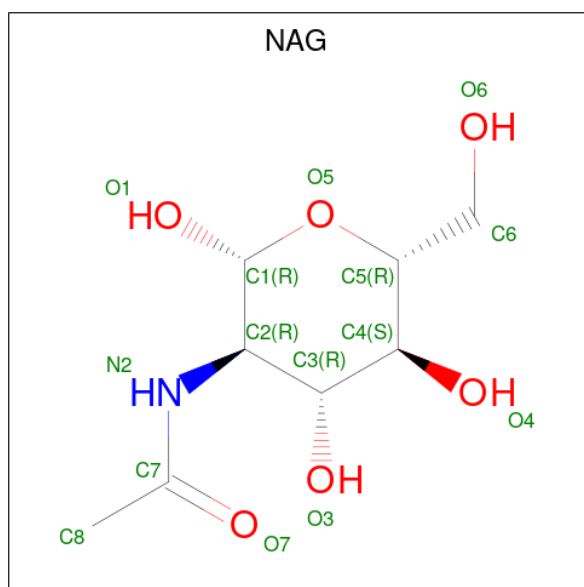
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
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C	745	PRO	ALA	engineered mutation	UNP P19491
C	754	SER	ASN	engineered mutation	UNP P19491
C	758	VAL	LEU	engineered mutation	UNP P19491
C	775	ALA	SER	engineered mutation	UNP P19491
C	776	LYS	GLY	engineered mutation	UNP P19491
C	777	ASP	GLY	engineered mutation	UNP P19491
C	778	SER	GLY	engineered mutation	UNP P19491
C	779	GLY	ASP	engineered mutation	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	545	ASP	-	linker	UNP P19491
D	546	THR	-	linker	UNP P19491
D	547	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	744	THR	ASN	engineered mutation	UNP P19491
D	745	PRO	ALA	engineered mutation	UNP P19491
D	754	SER	ASN	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	758	VAL	LEU	engineered mutation	UNP P19491
D	775	ALA	SER	engineered mutation	UNP P19491
D	776	LYS	GLY	engineered mutation	UNP P19491
D	777	ASP	GLY	engineered mutation	UNP P19491
D	778	SER	GLY	engineered mutation	UNP P19491
D	779	GLY	ASP	engineered mutation	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

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

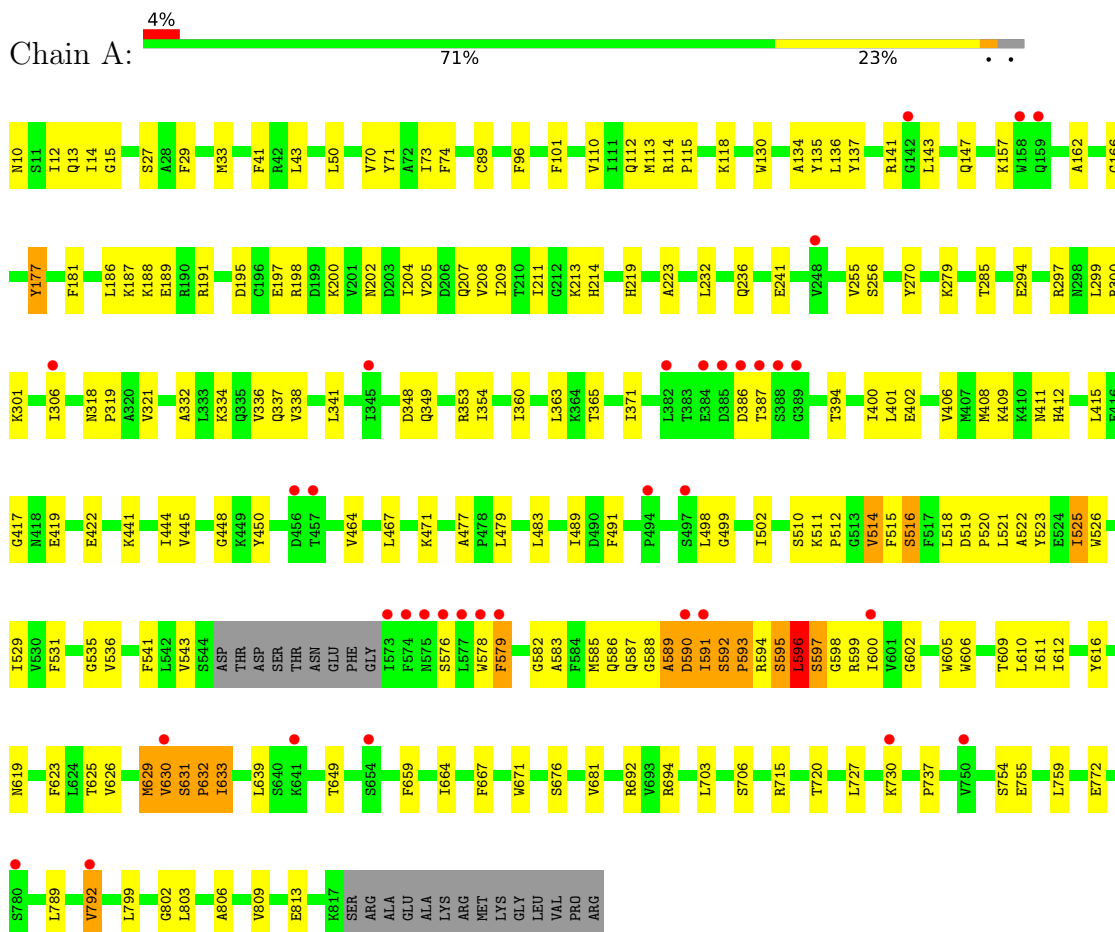


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

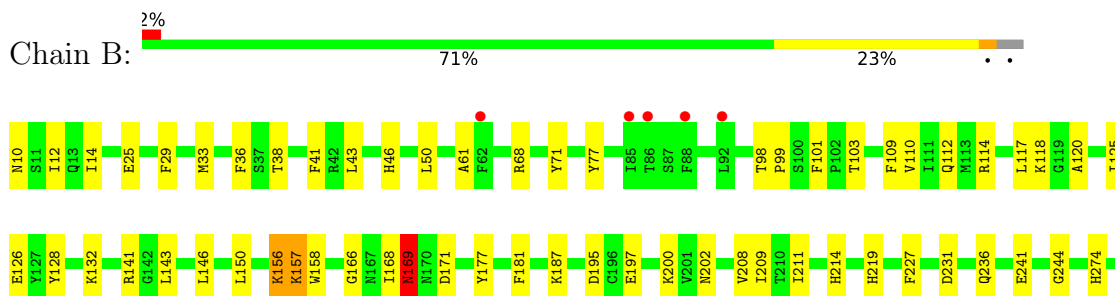
3 Residue-property plots

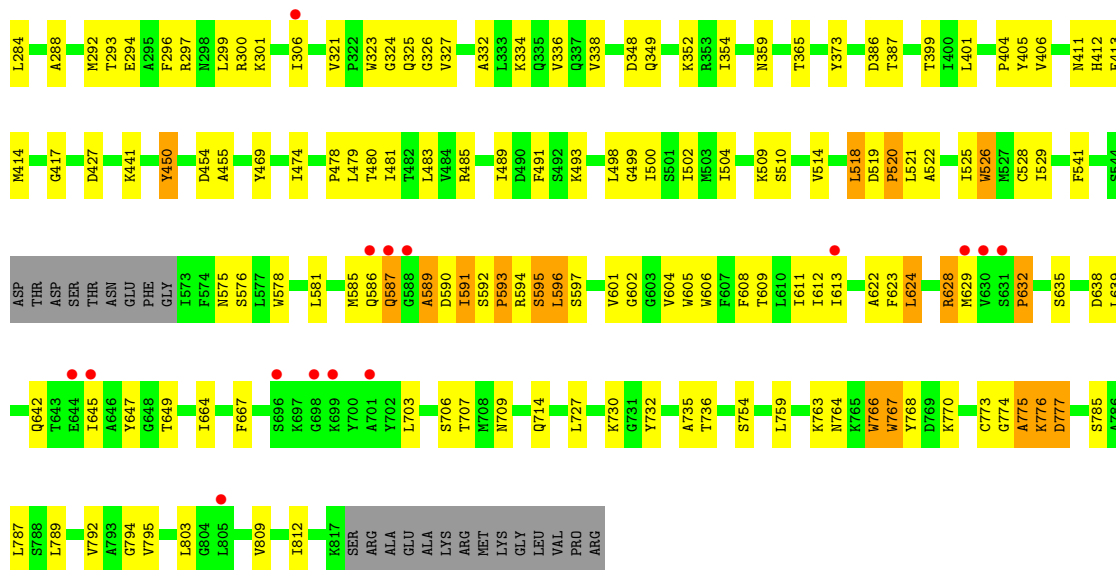
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor 2, Glutamate receptor 2

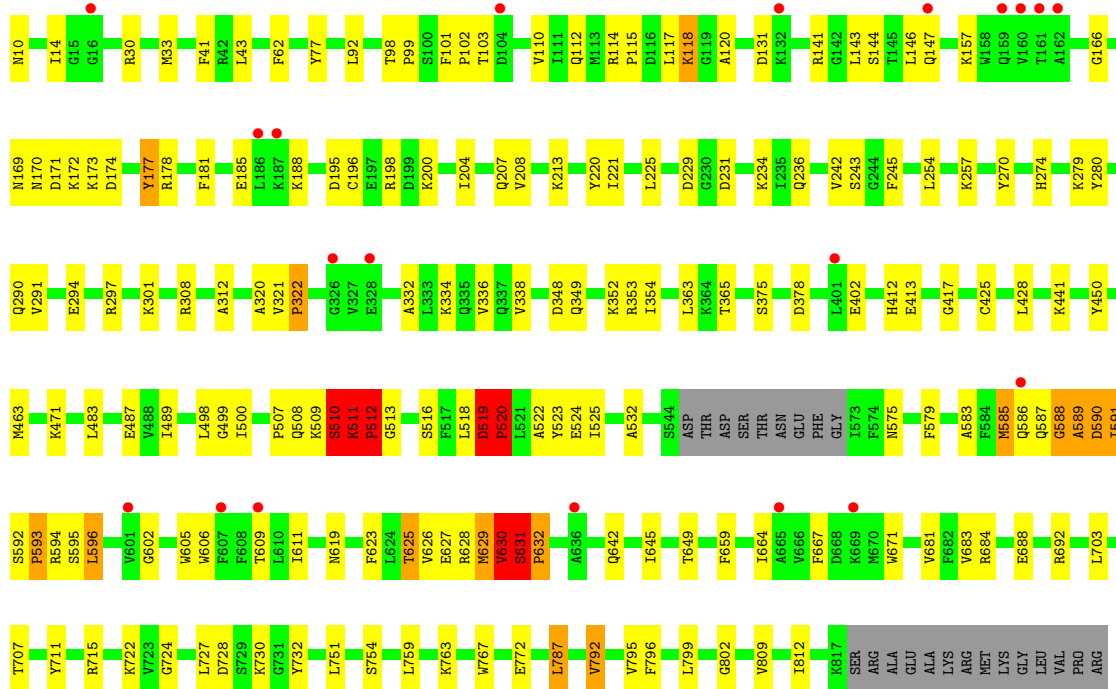
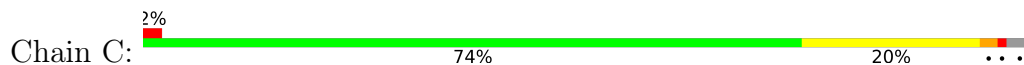


- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

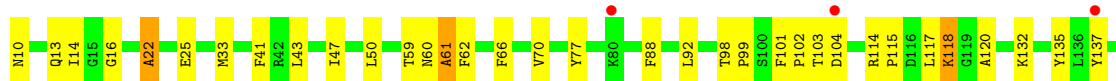
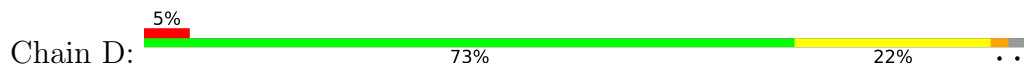


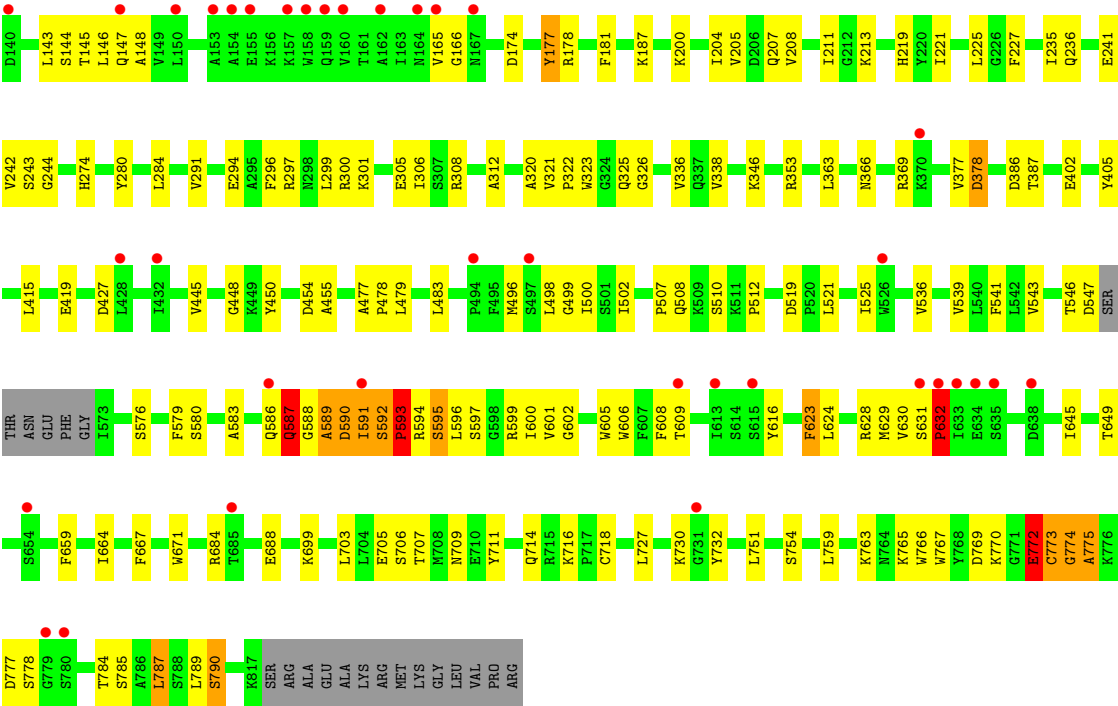


- Molecule 1: Glutamate receptor 2, Glutamate receptor 2



- Molecule 1: Glutamate receptor 2, Glutamate receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.05Å 309.39Å 110.02Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	48.55 – 4.00 48.55 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.55-4.00) 97.7 (48.55-4.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.265 , 0.292 0.289 , 0.304	Depositor DCC
R_{free} test set	2522 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	175.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24156	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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:
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	0.29	2/6143 (0.0%)	0.70	21/8319 (0.3%)
1	B	0.32	3/6148 (0.0%)	0.96	37/8326 (0.4%)
1	C	0.51	6/6149 (0.1%)	0.80	37/8327 (0.4%)
1	D	0.41	4/6164 (0.1%)	0.74	26/8349 (0.3%)
All	All	0.39	15/24604 (0.1%)	0.81	121/33321 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	22.87	1.79	1.47
1	D	632	PRO	N-CD	22.49	1.79	1.47
1	A	632	PRO	N-CD	18.38	1.73	1.47
1	C	322	PRO	N-CD	-17.25	1.23	1.47
1	C	630	VAL	CA-C	16.97	1.74	1.52
1	B	520	PRO	N-CD	15.47	1.69	1.47
1	C	632	PRO	N-CD	14.12	1.67	1.47
1	D	631	SER	CA-C	11.94	1.67	1.52
1	D	587	GLN	C-N	-11.09	1.20	1.33
1	B	623	PHE	CA-C	9.66	1.67	1.52
1	B	632	PRO	N-CD	7.82	1.58	1.47
1	C	519	ASP	CA-C	7.49	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	631	SER	C-N	5.53	1.40	1.33
1	A	631	SER	C-N	5.50	1.40	1.33
1	D	593	PRO	N-CD	5.37	1.55	1.47

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	775	ALA	N-CA-C	35.80	159.61	111.28
1	B	450	TYR	N-CA-C	29.02	143.25	111.03
1	C	589	ALA	N-CA-C	28.06	149.97	111.24
1	D	589	ALA	N-CA-C	27.55	149.26	111.24
1	A	589	ALA	N-CA-C	27.36	149.00	111.24
1	B	589	ALA	N-CA-C	22.31	141.82	111.92
1	D	589	ALA	CB-CA-C	-21.27	79.33	112.09
1	C	589	ALA	CB-CA-C	-20.78	80.09	112.09
1	B	595	SER	N-CA-C	19.85	141.08	108.73
1	A	589	ALA	CB-CA-C	-19.39	82.23	112.09
1	D	790	SER	O-C-N	18.69	141.93	122.12
1	B	775	ALA	CB-CA-C	-18.55	85.03	112.11
1	B	595	SER	CB-CA-C	-18.12	80.84	110.19
1	B	596	LEU	N-CA-CB	-17.92	80.03	110.50
1	C	510	SER	N-CA-C	16.71	130.46	110.91
1	A	595	SER	N-CA-C	16.60	136.16	109.76
1	A	596	LEU	N-CA-CB	-15.58	84.02	110.50
1	A	597	SER	N-CA-C	-15.43	92.66	111.33
1	C	588	GLY	N-CA-C	14.68	131.50	111.54
1	B	589	ALA	CB-CA-C	-13.93	92.68	111.63
1	A	595	SER	CB-CA-C	-13.86	87.25	109.84
1	C	595	SER	N-CA-C	13.32	130.95	109.24
1	B	776	LYS	N-CA-CB	-13.31	87.86	110.50
1	C	595	SER	CB-CA-C	-13.28	87.84	109.75
1	C	596	LEU	N-CA-CB	-13.05	88.31	110.50
1	B	776	LYS	N-CA-C	11.95	144.45	111.00
1	B	450	TYR	CB-CA-C	-11.86	92.56	110.95
1	D	588	GLY	N-CA-C	11.81	129.37	111.18
1	D	590	ASP	N-CA-CB	-11.80	93.46	110.45
1	C	322	PRO	CA-N-CD	11.76	128.46	112.00
1	C	520	PRO	CA-N-CD	-11.65	95.69	112.00
1	B	622	ALA	N-CA-C	11.44	124.86	111.71
1	C	520	PRO	N-CA-CB	11.25	115.06	103.25
1	D	632	PRO	CA-N-CD	-11.24	95.76	111.50
1	B	624	LEU	N-CA-CB	11.06	126.04	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	VAL	CA-C-O	11.01	134.54	120.78
1	B	156	LYS	N-CA-C	-10.59	92.02	109.07
1	C	518	LEU	N-CA-C	10.57	124.51	112.57
1	A	630	VAL	N-CA-C	10.57	126.84	112.04
1	C	322	PRO	N-CA-CB	-10.42	93.29	103.19
1	A	632	PRO	CA-N-CD	-10.11	97.85	112.00
1	D	590	ASP	N-CA-C	9.89	125.22	109.79
1	C	590	ASP	N-CA-CB	-9.64	94.20	110.49
1	B	623	PHE	CA-C-O	9.51	130.68	119.56
1	A	590	ASP	N-CA-CB	-9.48	94.46	110.49
1	B	623	PHE	CB-CA-C	-8.91	95.50	110.56
1	D	790	SER	CA-C-N	-8.68	109.16	120.44
1	D	790	SER	C-N-CA	-8.68	109.16	120.44
1	B	520	PRO	CA-N-CD	-8.55	100.03	112.00
1	C	632	PRO	CA-N-CD	-8.53	100.06	112.00
1	D	61	ALA	N-CA-C	-8.49	102.11	111.36
1	B	590	ASP	N-CA-CB	-8.35	94.96	110.07
1	D	592	SER	C-N-CD	8.31	138.88	120.60
1	B	324	GLY	N-CA-C	8.24	122.06	112.50
1	B	590	ASP	N-CA-C	8.19	122.80	109.94
1	A	629	MET	N-CA-C	8.16	123.06	113.18
1	A	632	PRO	N-CA-CB	8.13	110.91	103.34
1	B	777	ASP	N-CA-C	-8.13	102.82	114.12
1	D	632	PRO	N-CA-CB	8.01	111.41	102.60
1	B	628	ARG	N-CA-C	7.92	119.55	111.07
1	C	627	GLU	N-CA-C	-7.85	102.80	111.36
1	B	766	TRP	N-CA-C	7.82	121.69	112.93
1	D	103	THR	N-CA-C	7.69	119.87	110.41
1	D	587	GLN	O-C-N	-7.63	108.92	121.20
1	C	630	VAL	CB-CA-C	-7.59	98.85	111.29
1	D	104	ASP	N-CA-C	7.54	121.67	108.56
1	A	597	SER	N-CA-CB	-7.52	98.78	110.06
1	D	61	ALA	N-CA-CB	7.36	121.05	110.16
1	A	632	PRO	N-CA-C	-7.32	99.70	111.19
1	B	767	TRP	CB-CA-C	-7.28	99.60	109.28
1	D	144	SER	N-CA-C	-7.22	102.80	111.69
1	D	59	THR	N-CA-C	7.19	119.74	111.11
1	D	587	GLN	CA-C-N	7.15	127.73	121.58
1	D	587	GLN	C-N-CA	7.15	127.73	121.58
1	C	518	LEU	CB-CA-C	-6.89	100.38	111.06
1	A	631	SER	CA-C-N	-6.89	112.87	119.76
1	A	631	SER	C-N-CA	-6.89	112.87	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	510	SER	CB-CA-C	-6.88	100.24	112.27
1	B	624	LEU	N-CA-C	-6.81	105.26	113.97
1	C	632	PRO	N-CA-CB	6.71	109.57	103.33
1	A	514	VAL	N-CA-C	6.70	117.45	110.62
1	C	590	ASP	N-CA-C	6.62	124.90	110.80
1	C	625	THR	N-CA-C	6.61	118.57	111.36
1	C	593	PRO	CA-C-N	6.53	133.45	121.70
1	C	593	PRO	C-N-CA	6.53	133.45	121.70
1	B	520	PRO	N-CA-C	-6.51	104.04	113.75
1	C	630	VAL	N-CA-C	6.51	122.88	109.34
1	B	593	PRO	CA-C-N	6.45	133.31	121.70
1	B	593	PRO	C-N-CA	6.45	133.31	121.70
1	A	593	PRO	CA-C-N	6.38	133.19	121.70
1	A	593	PRO	C-N-CA	6.38	133.19	121.70
1	C	631	SER	CA-C-N	-6.38	113.41	119.85
1	C	631	SER	C-N-CA	-6.38	113.41	119.85
1	D	630	VAL	N-CA-C	6.37	119.13	108.81
1	B	767	TRP	N-CA-C	6.32	121.82	114.62
1	C	519	ASP	CB-CA-C	-6.31	97.74	110.17
1	C	787	LEU	N-CA-C	6.28	119.45	110.10
1	B	518	LEU	N-CA-C	6.19	119.30	111.69
1	A	590	ASP	N-CA-C	6.06	123.71	110.80
1	C	520	PRO	N-CA-C	-5.93	100.26	112.47
1	C	144	SER	N-CA-C	-5.88	104.95	111.36
1	D	772	GLU	N-CA-C	-5.86	104.80	111.07
1	B	623	PHE	N-CA-C	5.71	119.94	112.92
1	D	587	GLN	CB-CA-C	-5.70	110.02	116.63
1	C	627	GLU	N-CA-CB	5.66	118.54	110.16
1	D	774	GLY	N-CA-C	-5.66	108.45	114.67
1	A	630	VAL	CB-CA-C	-5.61	99.04	111.77
1	A	631	SER	C-N-CD	5.54	147.72	125.00
1	D	631	SER	CB-CA-C	5.46	120.94	110.17
1	B	596	LEU	N-CA-C	5.43	126.20	111.00
1	B	450	TYR	CA-C-N	5.36	131.91	121.41
1	B	450	TYR	C-N-CA	5.36	131.91	121.41
1	C	320	ALA	N-CA-C	-5.33	101.76	109.59
1	D	775	ALA	N-CA-C	-5.33	105.47	111.28
1	B	773	CYS	CB-CA-C	-5.31	98.63	109.94
1	C	519	ASP	N-CA-C	5.28	121.48	109.81
1	B	768	TYR	N-CA-CB	5.26	119.48	110.34
1	C	511	LYS	CA-C-N	-5.20	113.34	119.84
1	C	511	LYS	C-N-CA	-5.20	113.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	SER	N-CA-C	-5.11	105.89	111.82
1	C	628	ARG	N-CA-C	-5.06	106.96	113.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	TYR	Peptide
1	D	587	GLN	Mainchain
1	D	595	SER	Peptide
1	D	772	GLU	Peptide

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	6017	0	5899	220	1
1	B	6022	0	5906	217	1
1	C	6023	0	5907	182	0
1	D	6038	0	5907	223	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
All	All	24156	0	23671	740	1

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 15.

All (740) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLN:HE22	1:C:586:GLN:CB	1.01	1.55
1:D:711:TYR:HB2	1:D:767:TRP:CZ3	1.49	1.45
1:C:587:GLN:HE22	1:D:586:GLN:CB	1.29	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:PRO:CD	1:A:632:PRO:N	1.73	1.41
1:B:587:GLN:NE2	1:C:586:GLN:CB	1.74	1.41
1:B:520:PRO:CD	1:B:520:PRO:N	1.69	1.40
1:C:587:GLN:NE2	1:D:586:GLN:HB3	1.16	1.40
1:D:632:PRO:N	1:D:632:PRO:CD	1.79	1.39
1:C:632:PRO:CD	1:C:632:PRO:N	1.67	1.38
1:A:578:TRP:CB	1:D:596:LEU:CD1	2.02	1.36
1:A:578:TRP:CB	1:D:596:LEU:CD2	2.04	1.35
1:C:711:TYR:HB2	1:C:767:TRP:CZ3	1.60	1.35
1:C:520:PRO:N	1:C:520:PRO:CD	1.79	1.35
1:B:763:LYS:HE3	1:B:767:TRP:CZ3	1.60	1.33
1:B:126:GLU:OE2	1:B:156:LYS:NZ	1.65	1.29
1:C:587:GLN:NE2	1:D:586:GLN:CB	1.90	1.26
1:A:186:LEU:HB3	1:B:157:LYS:NZ	1.48	1.25
1:A:596:LEU:CD2	1:B:578:TRP:CB	2.15	1.24
1:B:587:GLN:NE2	1:C:586:GLN:HB2	1.31	1.23
1:D:594:ARG:O	1:D:596:LEU:HD12	1.08	1.20
1:C:626:VAL:HA	1:C:629:MET:HB2	1.23	1.17
1:A:623:PHE:CE1	1:B:785:SER:O	1.97	1.16
1:B:587:GLN:NE2	1:C:586:GLN:HB3	1.51	1.16
1:D:594:ARG:O	1:D:596:LEU:HA	1.44	1.15
1:A:619:ASN:ND2	1:A:623:PHE:HE2	1.40	1.14
1:B:763:LYS:HE3	1:B:767:TRP:CE3	1.84	1.11
1:D:716:LYS:N	1:D:772:GLU:OE1	1.82	1.11
1:A:578:TRP:CB	1:D:596:LEU:HD13	1.76	1.09
1:C:587:GLN:HE22	1:D:586:GLN:CA	1.65	1.08
1:A:578:TRP:CB	1:D:596:LEU:HD22	1.78	1.06
1:B:126:GLU:CD	1:B:156:LYS:NZ	2.13	1.06
1:A:596:LEU:HD21	1:B:578:TRP:CB	1.86	1.06
1:D:143:LEU:HD12	1:D:143:LEU:O	1.53	1.06
1:A:186:LEU:CB	1:B:157:LYS:NZ	2.17	1.05
1:A:186:LEU:CB	1:B:157:LYS:HZ1	1.68	1.05
1:D:594:ARG:C	1:D:596:LEU:HD12	1.79	1.05
1:D:711:TYR:CB	1:D:767:TRP:HZ3	1.69	1.05
1:D:594:ARG:O	1:D:596:LEU:CD1	2.05	1.04
1:D:579:PHE:CZ	1:D:590:ASP:HB3	1.91	1.04
1:A:578:TRP:CB	1:D:596:LEU:HD21	1.87	1.04
1:A:587:GLN:HE22	1:B:586:GLN:HA	1.22	1.03
1:A:186:LEU:HB3	1:B:157:LYS:HZ1	0.86	1.02
1:A:578:TRP:CA	1:D:596:LEU:HD21	1.90	1.02
1:A:633:ILE:H	1:A:633:ILE:HD12	1.17	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TRP:CB	1:D:596:LEU:HD11	1.85	1.00
1:D:595:SER:HA	1:D:596:LEU:HD13	1.43	1.00
1:C:510:SER:C	1:C:512:PRO:HD3	1.86	1.00
1:C:763:LYS:O	1:C:767:TRP:HD1	1.43	0.99
1:C:711:TYR:CB	1:C:767:TRP:HZ3	1.76	0.98
1:C:143:LEU:HD12	1:C:143:LEU:O	1.64	0.97
1:A:578:TRP:CA	1:D:596:LEU:HD11	1.94	0.97
1:A:595:SER:HA	1:A:596:LEU:HD22	1.47	0.97
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.44	0.96
1:D:579:PHE:HZ	1:D:590:ASP:HB3	1.23	0.96
1:A:619:ASN:ND2	1:A:623:PHE:CE2	2.33	0.95
1:A:578:TRP:HA	1:D:596:LEU:HD21	1.46	0.95
1:C:630:VAL:HG12	1:C:630:VAL:O	1.67	0.95
1:C:623:PHE:HE1	1:D:785:SER:CB	1.80	0.95
1:A:578:TRP:CB	1:D:596:LEU:CG	2.45	0.94
1:D:711:TYR:CB	1:D:767:TRP:CZ3	2.45	0.93
1:A:619:ASN:HD21	1:A:623:PHE:HE2	1.05	0.93
1:C:198:ARG:HD3	1:C:279:LYS:HD2	1.49	0.92
1:A:578:TRP:C	1:D:596:LEU:HD11	1.95	0.91
1:A:596:LEU:HD23	1:B:578:TRP:CB	1.96	0.91
1:A:587:GLN:NE2	1:B:586:GLN:HA	1.85	0.91
1:A:623:PHE:HE1	1:B:785:SER:O	1.52	0.90
1:A:518:LEU:CD1	1:A:523:TYR:CZ	2.54	0.90
1:C:510:SER:O	1:C:512:PRO:HD3	1.72	0.89
1:B:157:LYS:O	1:B:158:TRP:CD1	2.25	0.89
1:B:763:LYS:CE	1:B:767:TRP:CE3	2.55	0.89
1:A:518:LEU:HD11	1:A:523:TYR:CZ	2.08	0.89
1:D:595:SER:HA	1:D:596:LEU:CD1	2.02	0.88
1:A:596:LEU:HD13	1:A:599:ARG:CB	2.05	0.86
1:A:498:LEU:HD11	1:A:730:LYS:CD	2.06	0.86
1:C:626:VAL:CA	1:C:629:MET:HB2	2.06	0.86
1:A:596:LEU:HD21	1:B:578:TRP:C	2.01	0.86
1:C:711:TYR:CB	1:C:767:TRP:CZ3	2.52	0.86
1:A:596:LEU:O	1:A:599:ARG:N	2.09	0.85
1:C:587:GLN:HE21	1:D:586:GLN:HB3	1.07	0.85
1:D:143:LEU:CD1	1:D:147:GLN:HG3	2.07	0.85
1:B:510:SER:N	1:B:629:MET:SD	2.52	0.83
1:B:126:GLU:CD	1:B:156:LYS:HZ2	1.83	0.83
1:B:763:LYS:CE	1:B:767:TRP:CZ3	2.55	0.83
1:C:763:LYS:O	1:C:767:TRP:CD1	2.31	0.83
1:B:518:LEU:HD12	1:B:519:ASP:N	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLY:HA2	1:C:200:LYS:HZ3	1.45	0.82
1:B:143:LEU:CD2	1:B:146:LEU:HD23	2.10	0.81
1:A:518:LEU:CD1	1:A:523:TYR:CE1	2.64	0.81
1:A:596:LEU:CG	1:B:578:TRP:CB	2.58	0.81
1:C:143:LEU:HD21	1:D:143:LEU:HD21	1.60	0.81
1:A:578:TRP:O	1:D:596:LEU:HD11	1.81	0.80
1:C:711:TYR:HB2	1:C:767:TRP:HZ3	1.00	0.80
1:C:623:PHE:CE1	1:D:785:SER:HB3	2.16	0.80
1:B:714:GLN:HE22	1:B:775:ALA:HB3	1.45	0.80
1:D:143:LEU:O	1:D:143:LEU:CD1	2.30	0.80
1:D:592:SER:HB3	1:D:594:ARG:H	1.46	0.80
1:D:579:PHE:HZ	1:D:590:ASP:C	1.90	0.79
1:D:592:SER:HB3	1:D:594:ARG:N	1.98	0.79
1:C:587:GLN:HE22	1:D:586:GLN:HA	1.46	0.78
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.14	0.78
1:A:596:LEU:HG	1:B:578:TRP:CB	2.13	0.78
1:C:623:PHE:CE1	1:D:785:SER:CB	2.65	0.77
1:D:579:PHE:HZ	1:D:590:ASP:CB	1.98	0.77
1:A:510:SER:HB3	1:A:511:LYS:HA	1.66	0.77
1:A:518:LEU:HD13	1:A:523:TYR:CE1	2.19	0.77
1:C:630:VAL:O	1:C:631:SER:O	2.03	0.77
1:B:587:GLN:HE21	1:C:586:GLN:HB3	1.46	0.77
1:B:169:ASN:H	1:B:169:ASN:ND2	1.83	0.77
1:D:592:SER:N	1:D:593:PRO:HA	1.97	0.76
1:C:198:ARG:CD	1:C:279:LYS:HD2	2.14	0.76
1:A:518:LEU:HD13	1:A:523:TYR:CZ	2.21	0.76
1:B:132:LYS:NZ	1:B:187:LYS:HB3	2.02	0.75
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.68	0.75
1:B:454:ASP:OD1	1:B:455:ALA:N	2.20	0.75
1:D:221:ILE:HG12	1:D:243:SER:HB2	1.66	0.74
1:C:166:GLY:HA2	1:C:200:LYS:NZ	2.03	0.73
1:A:602:GLY:HA2	1:A:605:TRP:HB3	1.70	0.73
1:C:498:LEU:HD12	1:C:499:GLY:N	2.02	0.73
1:D:579:PHE:CZ	1:D:590:ASP:C	2.66	0.73
1:D:763:LYS:O	1:D:767:TRP:HD1	1.72	0.73
1:A:623:PHE:CZ	1:B:785:SER:O	2.41	0.73
1:D:590:ASP:O	1:D:591:ILE:HG22	1.88	0.72
1:D:166:GLY:HA2	1:D:200:LYS:HZ1	1.55	0.72
1:A:498:LEU:HD11	1:A:730:LYS:HD2	1.70	0.72
1:A:498:LEU:HD12	1:A:730:LYS:HG3	1.69	0.72
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLY:HA2	1:D:200:LYS:NZ	2.05	0.72
1:C:143:LEU:O	1:C:143:LEU:CD1	2.37	0.72
1:C:498:LEU:CD2	1:C:732:TYR:CE2	2.72	0.72
1:A:600:ILE:HG12	1:B:581:LEU:HD11	1.71	0.72
1:A:498:LEU:CD1	1:A:730:LYS:HD2	2.20	0.71
1:B:166:GLY:HA2	1:B:200:LYS:NZ	2.05	0.71
1:D:519:ASP:CG	1:D:623:PHE:HE2	1.98	0.71
1:D:602:GLY:HA2	1:D:605:TRP:HB3	1.72	0.71
1:D:774:GLY:O	1:D:778:SER:N	2.20	0.71
1:C:510:SER:HA	1:C:511:LYS:CB	2.20	0.71
1:D:583:ALA:HB1	1:D:589:ALA:H	1.55	0.71
1:B:404:PRO:HG3	1:B:767:TRP:CD1	2.26	0.70
1:A:166:GLY:HA2	1:A:200:LYS:NZ	2.06	0.70
1:B:334:LYS:NZ	1:B:349:GLN:O	2.24	0.70
1:A:625:THR:O	1:A:629:MET:HG3	1.91	0.70
1:D:50:LEU:C	1:D:50:LEU:HD12	2.16	0.70
1:A:415:LEU:HD13	1:A:419:GLU:HB3	1.74	0.70
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.70
1:C:579:PHE:HE2	1:C:590:ASP:HB3	1.56	0.70
1:C:498:LEU:CD1	1:C:730:LYS:HG3	2.21	0.69
1:C:510:SER:C	1:C:512:PRO:CD	2.65	0.69
1:C:143:LEU:CD2	1:D:143:LEU:HD21	2.21	0.69
1:A:755:GLU:OE2	1:D:483:LEU:N	2.26	0.69
1:B:404:PRO:CG	1:B:767:TRP:HE1	2.06	0.69
1:C:185:GLU:OE1	1:C:213:LYS:NZ	2.24	0.69
1:A:600:ILE:HG12	1:B:581:LEU:CD1	2.22	0.68
1:C:522:ALA:H	1:D:787:LEU:HD12	1.58	0.68
1:A:166:GLY:HA2	1:A:200:LYS:HZ3	1.57	0.68
1:C:198:ARG:HE	1:C:229:ASP:HB3	1.58	0.68
1:B:157:LYS:O	1:B:158:TRP:HD1	1.75	0.68
1:C:619:ASN:OD1	1:D:624:LEU:HD13	1.93	0.68
1:C:213:LYS:O	1:C:220:TYR:OH	2.12	0.68
1:A:595:SER:HA	1:A:596:LEU:CD2	2.21	0.68
1:A:498:LEU:CD1	1:A:730:LYS:CD	2.72	0.67
1:B:103:THR:O	1:B:352:LYS:NZ	2.21	0.67
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.75	0.67
1:B:498:LEU:HD21	1:B:732:TYR:CZ	2.29	0.67
1:B:766:TRP:O	1:B:767:TRP:HD1	1.77	0.67
1:D:60:ASN:OD1	1:D:61:ALA:N	2.28	0.67
1:D:366:ASN:HD21	1:D:369:ARG:HH11	1.43	0.67
1:B:38:THR:HG21	1:B:297:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LEU:HD12	1:D:143:LEU:C	2.19	0.67
1:D:628:ARG:N	1:D:629:MET:HA	2.10	0.67
1:A:519:ASP:HB2	1:A:520:PRO:HD3	1.76	0.66
1:C:626:VAL:HA	1:C:629:MET:CB	2.15	0.66
1:A:498:LEU:HD12	1:A:730:LYS:CG	2.25	0.66
1:C:587:GLN:NE2	1:D:586:GLN:HA	2.07	0.66
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.77	0.66
1:A:498:LEU:CD1	1:A:730:LYS:CG	2.74	0.66
1:B:498:LEU:CD1	1:B:730:LYS:HG3	2.25	0.65
1:C:623:PHE:HE1	1:D:785:SER:CA	2.08	0.65
1:A:596:LEU:CD1	1:A:599:ARG:CB	2.74	0.65
1:B:498:LEU:HD11	1:B:730:LYS:HD2	1.79	0.65
1:B:14:ILE:HD13	1:B:43:LEU:HD23	1.79	0.65
1:C:498:LEU:HD12	1:C:730:LYS:HG3	1.76	0.65
1:D:763:LYS:O	1:D:767:TRP:CD1	2.49	0.65
1:A:676:SER:OG	1:B:770:LYS:NZ	2.29	0.65
1:B:587:GLN:HE22	1:C:586:GLN:HB2	0.49	0.65
1:C:763:LYS:HD2	1:C:767:TRP:NE1	2.11	0.65
1:D:143:LEU:HD11	1:D:147:GLN:HE21	1.61	0.65
1:D:594:ARG:C	1:D:596:LEU:CD1	2.64	0.65
1:A:498:LEU:HD12	1:A:499:GLY:N	2.12	0.65
1:B:541:PHE:HD1	1:B:576:SER:HB3	1.62	0.65
1:C:498:LEU:HD11	1:C:730:LYS:CD	2.26	0.65
1:D:143:LEU:HD12	1:D:147:GLN:HG3	1.78	0.65
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.79	0.65
1:C:587:GLN:NE2	1:D:586:GLN:CA	2.40	0.65
1:A:596:LEU:HD21	1:B:578:TRP:CA	2.27	0.64
1:B:498:LEU:HD11	1:B:730:LYS:CD	2.27	0.64
1:B:50:LEU:C	1:B:50:LEU:HD12	2.22	0.64
1:A:50:LEU:HD12	1:A:50:LEU:C	2.22	0.64
1:D:498:LEU:HD22	1:D:707:THR:CG2	2.28	0.64
1:D:763:LYS:HD2	1:D:767:TRP:CD1	2.32	0.64
1:B:589:ALA:HB2	1:B:602:GLY:HA3	1.80	0.64
1:D:308:ARG:HE	1:D:312:ALA:HB2	1.63	0.64
1:C:763:LYS:HD2	1:C:767:TRP:CD1	2.32	0.63
1:C:590:ASP:O	1:C:591:ILE:HG22	1.98	0.63
1:C:143:LEU:HD12	1:C:143:LEU:C	2.23	0.63
1:D:143:LEU:HB2	1:D:146:LEU:HB3	1.79	0.63
1:B:38:THR:CG2	1:B:297:ARG:NH2	2.61	0.63
1:D:498:LEU:CD2	1:D:707:THR:CG2	2.75	0.63
1:A:518:LEU:HD11	1:A:523:TYR:OH	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.26	0.62
1:C:417:GLY:HA2	1:C:441:LYS:NZ	2.14	0.62
1:B:294:GLU:HG3	1:B:338:VAL:HG11	1.82	0.62
1:A:522:ALA:H	1:B:787:LEU:HD12	1.64	0.62
1:B:169:ASN:H	1:B:169:ASN:HD22	1.47	0.62
1:C:583:ALA:HB1	1:C:589:ALA:HA	1.82	0.62
1:C:498:LEU:HD23	1:C:732:TYR:CE2	2.35	0.61
1:A:596:LEU:O	1:A:597:SER:C	2.42	0.61
1:D:323:TRP:CZ3	1:D:326:GLY:N	2.68	0.61
1:B:586:GLN:HG3	1:B:586:GLN:O	2.00	0.61
1:A:181:PHE:HE2	1:A:208:VAL:HG22	1.64	0.61
1:A:595:SER:CA	1:A:596:LEU:HD22	2.28	0.61
1:A:518:LEU:HD11	1:A:523:TYR:CE1	2.34	0.61
1:B:587:GLN:CD	1:C:586:GLN:HB2	2.18	0.60
1:B:132:LYS:HZ1	1:B:187:LYS:HB3	1.65	0.60
1:B:404:PRO:HG3	1:B:767:TRP:NE1	2.16	0.60
1:A:596:LEU:HD21	1:B:578:TRP:O	2.00	0.60
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.36	0.60
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.81	0.60
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.66	0.60
1:D:498:LEU:CD2	1:D:707:THR:HG23	2.31	0.60
1:B:498:LEU:HD12	1:B:730:LYS:CG	2.32	0.60
1:B:498:LEU:CD2	1:B:732:TYR:CZ	2.85	0.60
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.83	0.60
1:D:519:ASP:OD1	1:D:623:PHE:HE2	1.84	0.60
1:B:166:GLY:HA2	1:B:200:LYS:HZ1	1.65	0.60
1:B:604:VAL:HG11	1:C:802:GLY:HA3	1.84	0.60
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.84	0.60
1:A:236:GLN:NE2	1:A:365:THR:O	2.32	0.60
1:A:143:LEU:O	1:A:143:LEU:HD12	2.02	0.60
1:A:543:VAL:HG11	1:A:597:SER:HB3	1.83	0.59
1:A:633:ILE:H	1:A:633:ILE:CD1	1.96	0.59
1:B:323:TRP:HZ3	1:B:325:GLN:HB2	1.66	0.59
1:D:498:LEU:HD22	1:D:707:THR:HG23	1.83	0.59
1:B:498:LEU:HD21	1:B:732:TYR:CE1	2.37	0.59
1:B:99:PRO:HB3	1:B:284:LEU:HB2	1.84	0.59
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.84	0.59
1:C:579:PHE:CE2	1:C:590:ASP:HB3	2.37	0.59
1:C:722:LYS:NZ	1:C:724:GLY:O	2.35	0.59
1:D:323:TRP:HZ3	1:D:325:GLN:HB2	1.68	0.59
1:A:630:VAL:HG12	1:A:630:VAL:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG12	1:B:112:GLN:HG3	1.85	0.58
1:D:519:ASP:OD1	1:D:623:PHE:CE2	2.55	0.58
1:A:587:GLN:HE22	1:B:586:GLN:CA	2.05	0.58
1:B:236:GLN:NE2	1:B:365:THR:O	2.29	0.58
1:B:502:ILE:O	1:B:709:ASN:ND2	2.36	0.58
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.86	0.58
1:B:274:HIS:O	1:B:274:HIS:ND1	2.35	0.58
1:D:765:LYS:O	1:D:770:LYS:HG2	2.04	0.58
1:A:143:LEU:HD12	1:A:143:LEU:C	2.29	0.58
1:A:334:LYS:HZ3	1:A:349:GLN:C	2.12	0.58
1:D:402:GLU:OE1	1:D:450:TYR:OH	2.20	0.58
1:D:498:LEU:HD23	1:D:707:THR:HG21	1.86	0.57
1:A:141:ARG:NH2	1:A:195:ASP:OD1	2.23	0.57
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.86	0.57
1:A:510:SER:HB3	1:A:512:PRO:HD3	1.85	0.57
1:C:520:PRO:O	1:D:787:LEU:HG	2.05	0.57
1:B:498:LEU:HD12	1:B:730:LYS:HG3	1.84	0.57
1:B:586:GLN:O	1:B:587:GLN:C	2.46	0.57
1:D:308:ARG:NH2	1:D:323:TRP:NE1	2.52	0.57
1:A:143:LEU:HD22	1:B:143:LEU:HD22	1.85	0.57
1:D:118:LYS:HD2	1:D:148:ALA:HB2	1.87	0.57
1:B:202:ASN:HD21	1:B:231:ASP:H	1.52	0.57
1:B:498:LEU:CD1	1:B:730:LYS:CG	2.82	0.57
1:C:33:MET:HE1	1:C:43:LEU:HB2	1.85	0.57
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.85	0.57
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.87	0.57
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.39	0.57
1:A:543:VAL:CG1	1:A:597:SER:HB3	2.34	0.56
1:C:498:LEU:HD12	1:C:730:LYS:CG	2.35	0.56
1:B:707:THR:HB	1:B:767:TRP:CH2	2.41	0.56
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.87	0.56
1:D:579:PHE:CE2	1:D:591:ILE:HG22	2.41	0.56
1:A:464:VAL:HG13	1:A:489:ILE:HG12	1.87	0.56
1:B:412:HIS:CE1	1:B:413:GLU:HG3	2.40	0.56
1:D:132:LYS:HZ1	1:D:187:LYS:HB3	1.71	0.56
1:D:498:LEU:HD12	1:D:499:GLY:N	2.21	0.56
1:A:186:LEU:HB2	1:B:157:LYS:NZ	2.15	0.56
1:A:590:ASP:O	1:A:591:ILE:HG22	2.06	0.56
1:A:681:VAL:HA	1:A:692:ARG:HH12	1.71	0.56
1:B:606:TRP:HA	1:B:609:THR:HG22	1.87	0.56
1:C:274:HIS:O	1:C:274:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:GLN:OE1	1:B:586:GLN:HB3	2.05	0.56
1:B:529:ILE:HD12	1:B:612:ILE:HG21	1.87	0.56
1:C:626:VAL:O	1:C:626:VAL:HG12	2.06	0.56
1:D:521:LEU:HD23	1:D:616:TYR:HD1	1.71	0.56
1:A:134:ALA:HB2	1:A:189:GLU:HG2	1.87	0.56
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.86	0.56
1:D:454:ASP:OD1	1:D:455:ALA:N	2.39	0.56
1:C:143:LEU:HB2	1:C:146:LEU:HB3	1.88	0.56
1:A:633:ILE:HD12	1:A:633:ILE:N	2.02	0.56
1:A:754:SER:HB2	1:A:759:LEU:HD12	1.88	0.56
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.87	0.56
1:D:628:ARG:H	1:D:629:MET:HA	1.70	0.56
1:A:583:ALA:HB1	1:A:589:ALA:H	1.71	0.55
1:A:626:VAL:O	1:A:630:VAL:HG23	2.06	0.55
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.88	0.55
1:B:10:ASN:HB3	1:B:300:ARG:HH22	1.72	0.55
1:D:579:PHE:CZ	1:D:590:ASP:CB	2.76	0.55
1:D:102:PRO:HD3	1:D:114:ARG:HD2	1.87	0.55
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.88	0.55
1:A:15:GLY:HA3	1:A:73:ILE:HG12	1.87	0.55
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.87	0.55
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.87	0.55
1:D:99:PRO:HB3	1:D:284:LEU:HB2	1.88	0.55
1:C:110:VAL:HG12	1:C:112:GLN:HG3	1.89	0.55
1:A:12:ILE:HG23	1:A:71:TYR:HD2	1.70	0.55
1:D:219:HIS:HA	1:D:241:GLU:O	2.06	0.55
1:D:579:PHE:CE2	1:D:590:ASP:O	2.60	0.55
1:D:592:SER:OG	1:D:595:SER:C	2.50	0.54
1:B:480:THR:O	1:B:485:ARG:NH1	2.40	0.54
1:C:177:TYR:CD2	1:C:207:GLN:HG3	2.43	0.54
1:C:181:PHE:HE2	1:C:208:VAL:HG22	1.73	0.54
1:D:10:ASN:HB3	1:D:300:ARG:HH22	1.72	0.54
1:D:496:MET:HE2	1:D:763:LYS:HD3	1.90	0.54
1:C:498:LEU:HD12	1:C:498:LEU:C	2.33	0.54
1:C:10:ASN:HB2	1:C:41:PHE:HA	1.89	0.54
1:C:157:LYS:HD2	1:D:187:LYS:HE3	1.89	0.54
1:B:498:LEU:CD1	1:B:730:LYS:HD2	2.38	0.54
1:C:174:ASP:O	1:C:178:ARG:NH1	2.41	0.54
1:D:583:ALA:HB1	1:D:589:ALA:N	2.22	0.54
1:C:498:LEU:CD1	1:C:730:LYS:CG	2.86	0.53
1:C:510:SER:CA	1:C:511:LYS:CB	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.42	0.53
1:D:580:SER:HA	1:D:583:ALA:HB3	1.89	0.53
1:D:594:ARG:HA	1:D:599:ARG:CB	2.38	0.53
1:B:504:ILE:HD12	1:B:632:PRO:HD2	1.89	0.53
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.73	0.53
1:D:323:TRP:CZ3	1:D:325:GLN:C	2.86	0.53
1:A:186:LEU:CB	1:B:157:LYS:HZ3	2.18	0.53
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.90	0.53
1:A:529:ILE:HD12	1:A:612:ILE:HG21	1.90	0.53
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.43	0.53
1:C:103:THR:N	1:C:112:GLN:OE1	2.34	0.53
1:A:579:PHE:HE1	1:A:590:ASP:HB3	1.72	0.53
1:D:711:TYR:HB2	1:D:767:TRP:CE3	2.29	0.53
1:C:623:PHE:HE1	1:D:785:SER:HA	1.73	0.53
1:B:323:TRP:CZ3	1:B:326:GLY:N	2.77	0.53
1:D:498:LEU:CD2	1:D:707:THR:HG21	2.38	0.53
1:A:595:SER:CA	1:A:596:LEU:CD2	2.86	0.53
1:D:594:ARG:C	1:D:596:LEU:HA	2.29	0.53
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.90	0.53
1:B:404:PRO:CG	1:B:767:TRP:NE1	2.72	0.53
1:C:498:LEU:CD1	1:C:499:GLY:N	2.72	0.53
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.91	0.53
1:C:334:LYS:NZ	1:C:349:GLN:O	2.42	0.53
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.90	0.53
1:B:595:SER:HB2	1:C:575:ASN:HA	1.91	0.52
1:D:498:LEU:HD21	1:D:732:TYR:CZ	2.45	0.52
1:D:784:THR:HA	1:D:785:SER:HB2	1.90	0.52
1:C:498:LEU:CD1	1:C:730:LYS:CD	2.87	0.52
1:D:14:ILE:HD13	1:D:43:LEU:HD23	1.90	0.52
1:D:219:HIS:HD2	1:D:241:GLU:O	1.91	0.52
1:C:532:ALA:HB1	1:C:605:TRP:HZ3	1.73	0.52
1:B:36:PHE:HB3	1:B:293:THR:HG21	1.91	0.52
1:C:728:ASP:OD2	1:C:730:LYS:HE3	2.10	0.52
1:A:181:PHE:CE2	1:A:208:VAL:HG22	2.44	0.52
1:D:770:LYS:N	1:D:770:LYS:CE	2.73	0.52
1:A:498:LEU:HD11	1:A:730:LYS:CG	2.40	0.52
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.75	0.52
1:B:498:LEU:HD12	1:B:498:LEU:C	2.35	0.52
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.92	0.52
1:B:775:ALA:HA	1:B:777:ASP:H	1.75	0.52
1:B:50:LEU:CD2	1:B:61:ALA:CB	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:CD2	1:B:61:ALA:HB2	2.40	0.52
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.92	0.51
1:A:587:GLN:OE1	1:B:586:GLN:CB	2.58	0.51
1:A:610:LEU:HD21	1:B:613:ILE:HG21	1.91	0.51
1:B:33:MET:HE1	1:B:43:LEU:HB2	1.90	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.46	0.51
1:D:132:LYS:NZ	1:D:187:LYS:HB3	2.25	0.51
1:A:29:PHE:O	1:A:33:MET:HG2	2.11	0.51
1:B:639:LEU:O	1:B:639:LEU:HD23	2.10	0.51
1:B:707:THR:HA	1:B:767:TRP:CH2	2.46	0.51
1:B:775:ALA:N	1:B:777:ASP:H	2.08	0.51
1:A:188:LYS:NZ	1:A:471:LYS:NZ	2.59	0.51
1:B:132:LYS:HZ3	1:B:187:LYS:HB3	1.75	0.51
1:D:498:LEU:HD12	1:D:730:LYS:HG3	1.92	0.51
1:D:592:SER:N	1:D:593:PRO:CA	2.72	0.51
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.93	0.51
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.92	0.51
1:C:623:PHE:CE1	1:D:785:SER:HA	2.46	0.51
1:B:181:PHE:HD2	1:B:211:ILE:HD11	1.76	0.50
1:D:595:SER:CA	1:D:596:LEU:HD13	2.29	0.50
1:A:510:SER:HB3	1:A:511:LYS:CA	2.41	0.50
1:C:115:PRO:HA	1:C:353:ARG:HB2	1.93	0.50
1:B:707:THR:HB	1:B:767:TRP:HH2	1.76	0.50
1:D:498:LEU:HD23	1:D:707:THR:CG2	2.40	0.50
1:D:770:LYS:CA	1:D:770:LYS:HE2	2.41	0.50
1:C:291:VAL:HA	1:C:336:VAL:HG11	1.94	0.50
1:D:16:GLY:HA3	1:D:47:ILE:HD13	1.94	0.50
1:D:629:MET:O	1:D:629:MET:HG2	2.11	0.50
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.42	0.50
1:D:579:PHE:O	1:D:583:ALA:N	2.43	0.50
1:A:13:GLN:HG3	1:A:70:VAL:HG12	1.94	0.50
1:A:188:LYS:NZ	1:A:471:LYS:HZ3	2.10	0.50
1:A:337:GLN:NE2	2:A:901:NAG:O7	2.37	0.50
1:B:635:SER:OG	1:B:638:ASP:OD1	2.30	0.50
1:A:630:VAL:O	1:A:630:VAL:CG1	2.57	0.50
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.42	0.50
1:D:772:GLU:O	1:D:773:CYS:C	2.49	0.50
1:B:359:ASN:HA	1:B:373:TYR:HA	1.92	0.50
1:C:221:ILE:HG12	1:C:243:SER:HB2	1.93	0.50
1:C:602:GLY:HA2	1:C:605:TRP:HB3	1.93	0.50
1:B:763:LYS:HE2	1:B:767:TRP:CE3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:CE2	1:C:98:THR:HG21	2.47	0.49
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.94	0.49
1:D:592:SER:CB	1:D:594:ARG:N	2.73	0.49
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.94	0.49
1:D:716:LYS:HG3	1:D:772:GLU:OE1	2.11	0.49
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.94	0.49
1:B:348:ASP:HB3	1:B:354:ILE:HD13	1.93	0.49
1:C:188:LYS:NZ	1:C:471:LYS:NZ	2.61	0.49
1:C:625:THR:O	1:C:629:MET:N	2.45	0.49
1:D:236:GLN:HG3	1:D:363:LEU:HD11	1.95	0.49
1:B:586:GLN:C	1:B:587:GLN:HG2	2.37	0.49
1:B:639:LEU:CD2	1:B:647:TYR:CD1	2.96	0.49
1:D:62:PHE:HE2	1:D:92:LEU:HD12	1.77	0.49
1:A:592:SER:HB2	1:A:598:GLY:HA3	1.93	0.49
1:B:602:GLY:HA2	1:B:605:TRP:HB3	1.95	0.49
1:C:169:ASN:ND2	1:C:172:LYS:HD3	2.28	0.49
1:A:518:LEU:CD2	1:A:523:TYR:CE1	2.95	0.49
1:A:600:ILE:CG1	1:B:581:LEU:CD1	2.90	0.49
1:B:117:LEU:HD12	1:B:120:ALA:HB3	1.95	0.49
1:D:118:LYS:HG2	1:D:145:THR:HA	1.94	0.49
1:B:417:GLY:HA2	1:B:441:LYS:NZ	2.28	0.49
1:B:597:SER:O	1:B:601:VAL:HG23	2.13	0.49
1:B:405:TYR:CG	1:B:478:PRO:HG3	2.48	0.48
1:A:143:LEU:HD13	1:A:147:GLN:HG3	1.95	0.48
1:B:707:THR:CB	1:B:767:TRP:HH2	2.26	0.48
1:A:606:TRP:HA	1:A:609:THR:HG22	1.94	0.48
1:D:225:LEU:HB2	1:D:280:TYR:CD1	2.49	0.48
1:B:181:PHE:HE2	1:B:208:VAL:HG22	1.79	0.48
1:B:518:LEU:HD12	1:B:518:LEU:C	2.37	0.48
1:D:60:ASN:OD1	1:D:60:ASN:C	2.55	0.48
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.95	0.48
1:C:231:ASP:HB3	1:C:234:LYS:HE2	1.95	0.48
1:D:305:GLU:O	1:D:325:GLN:HG2	2.14	0.48
1:A:332:ALA:O	1:A:336:VAL:HG23	2.14	0.48
1:A:10:ASN:HB2	1:A:41:PHE:HA	1.96	0.48
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.30	0.48
1:C:711:TYR:CA	1:C:767:TRP:HZ3	2.26	0.48
1:A:600:ILE:O	1:A:600:ILE:HG22	2.13	0.48
1:B:526:TRP:HA	1:B:526:TRP:CE3	2.48	0.48
1:C:417:GLY:HA2	1:C:441:LYS:HZ2	1.79	0.48
1:D:512:PRO:HB3	1:D:790:SER:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:O	1:A:353:ARG:NH1	2.46	0.48
1:D:118:LYS:HB2	1:D:118:LYS:NZ	2.29	0.48
1:D:386:ASP:HA	1:D:387:THR:HA	1.61	0.48
1:C:707:THR:HG21	1:C:732:TYR:HE2	1.79	0.47
1:D:714:GLN:HA	1:D:773:CYS:HB2	1.96	0.47
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.95	0.47
1:A:181:PHE:HD2	1:A:211:ILE:HD11	1.78	0.47
1:A:792:VAL:HG21	1:D:525:ILE:HD13	1.96	0.47
1:C:242:VAL:HB	1:C:363:LEU:HB3	1.95	0.47
1:B:628:ARG:N	1:B:629:MET:HA	2.29	0.47
1:D:274:HIS:ND1	1:D:274:HIS:O	2.48	0.47
1:D:579:PHE:CZ	1:D:590:ASP:O	2.67	0.47
1:A:592:SER:OG	1:A:598:GLY:N	2.46	0.47
1:B:10:ASN:HB2	1:B:41:PHE:HA	1.96	0.47
1:C:62:PHE:HE2	1:C:92:LEU:HD12	1.80	0.47
1:D:415:LEU:HD13	1:D:419:GLU:HB3	1.97	0.47
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.96	0.47
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.79	0.47
1:C:236:GLN:NE2	1:C:365:THR:O	2.46	0.47
1:A:255:VAL:HG13	1:A:341:LEU:HD22	1.97	0.47
1:A:541:PHE:HD2	1:A:576:SER:HB3	1.80	0.47
1:A:593:PRO:HB2	1:A:594:ARG:CB	2.45	0.47
1:B:498:LEU:HD12	1:B:499:GLY:N	2.30	0.47
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.96	0.47
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.97	0.47
1:D:477:ALA:O	1:D:479:LEU:N	2.47	0.47
1:A:499:GLY:O	1:A:706:SER:N	2.48	0.47
1:D:291:VAL:HA	1:D:336:VAL:HG11	1.97	0.47
1:D:592:SER:H	1:D:593:PRO:HA	1.78	0.47
1:B:126:GLU:CG	1:B:156:LYS:NZ	2.78	0.47
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.96	0.47
1:D:377:VAL:HG23	1:D:378:ASP:OD1	2.15	0.47
1:A:181:PHE:CD2	1:A:213:LYS:HD2	2.50	0.47
1:D:205:VAL:HG13	1:D:235:ILE:HG23	1.98	0.46
1:A:204:ILE:O	1:A:208:VAL:HG23	2.15	0.46
1:C:308:ARG:HE	1:C:312:ALA:HB2	1.80	0.46
1:C:715:ARG:HH11	1:C:772:GLU:HG3	1.80	0.46
1:B:775:ALA:HA	1:B:776:LYS:HA	1.45	0.46
1:C:425:CYS:HA	1:C:428:LEU:HB3	1.97	0.46
1:A:188:LYS:HZ1	1:A:471:LYS:NZ	2.14	0.46
1:A:232:LEU:HB3	1:A:363:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ILE:HD13	1:B:792:VAL:HG21	1.98	0.46
1:C:498:LEU:HD21	1:C:732:TYR:CZ	2.51	0.46
1:D:235:ILE:HD12	1:D:242:VAL:HG21	1.97	0.46
1:D:308:ARG:NE	1:D:312:ALA:HB2	2.28	0.46
1:D:498:LEU:HD12	1:D:498:LEU:C	2.40	0.46
1:D:541:PHE:HD1	1:D:576:SER:HB3	1.80	0.46
1:A:521:LEU:HD22	1:A:526:TRP:CE2	2.51	0.46
1:C:715:ARG:NH1	1:C:772:GLU:HG3	2.31	0.46
1:D:165:VAL:HG21	1:D:204:ILE:HD11	1.98	0.46
1:D:579:PHE:HZ	1:D:590:ASP:CA	2.27	0.46
1:A:715:ARG:HH11	1:A:772:GLU:HG3	1.79	0.46
1:B:323:TRP:CZ3	1:B:325:GLN:HB2	2.49	0.46
1:C:103:THR:O	1:C:352:LYS:NZ	2.27	0.46
1:C:513:GLY:O	1:C:516:SER:OG	2.30	0.46
1:D:711:TYR:HB2	1:D:767:TRP:HZ3	0.81	0.46
1:D:62:PHE:CE2	1:D:88:PHE:HB3	2.51	0.46
1:A:583:ALA:HB1	1:A:589:ALA:N	2.30	0.46
1:B:528:CYS:HB3	1:C:796:PHE:CE2	2.51	0.46
1:C:290:GLN:HG2	1:C:338:VAL:HG21	1.98	0.46
1:A:348:ASP:HB3	1:A:354:ILE:HD13	1.97	0.45
1:B:209:ILE:HG23	1:B:214:HIS:NE2	2.32	0.45
1:B:386:ASP:HA	1:B:387:THR:HA	1.48	0.45
1:B:405:TYR:CD1	1:B:478:PRO:HG3	2.52	0.45
1:B:411:ASN:HB2	1:B:414:MET:HE2	1.99	0.45
1:C:198:ARG:NE	1:C:229:ASP:HB3	2.29	0.45
1:D:135:TYR:CE2	1:D:137:TYR:HB3	2.52	0.45
1:D:181:PHE:HD2	1:D:213:LYS:HD2	1.82	0.45
1:D:115:PRO:HA	1:D:353:ARG:HB2	1.99	0.45
1:D:502:ILE:O	1:D:709:ASN:ND2	2.47	0.45
1:A:514:VAL:O	1:A:515:PHE:C	2.57	0.45
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.98	0.45
1:B:593:PRO:HB2	1:B:594:ARG:CB	2.46	0.45
1:D:33:MET:HE1	1:D:43:LEU:HB2	1.98	0.45
1:D:498:LEU:CD1	1:D:730:LYS:HG3	2.47	0.45
1:A:619:ASN:O	1:A:623:PHE:HD2	1.99	0.45
1:C:118:LYS:HB2	1:C:118:LYS:NZ	2.32	0.45
1:D:297:ARG:HG2	1:D:301:LYS:HE3	1.99	0.45
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.46	0.45
1:D:770:LYS:N	1:D:770:LYS:HE2	2.31	0.45
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.52	0.45
1:B:766:TRP:O	1:B:767:TRP:CD1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:PRO:HD3	1:C:114:ARG:HD2	1.97	0.45
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.52	0.45
1:C:225:LEU:HB2	1:C:280:TYR:CD1	2.52	0.45
1:C:585:MET:HE3	1:C:586:GLN:HB3	1.98	0.45
1:D:211:ILE:HG13	1:D:213:LYS:HG3	1.98	0.45
1:D:597:SER:O	1:D:601:VAL:HG23	2.17	0.45
1:A:360:ILE:O	1:A:371:ILE:HG22	2.16	0.45
1:A:521:LEU:HD12	1:A:616:TYR:HB2	1.98	0.45
1:A:632:PRO:O	1:A:633:ILE:C	2.60	0.45
1:A:101:PHE:HA	1:A:114:ARG:HD2	1.99	0.45
1:C:606:TRP:HA	1:C:609:THR:HG22	1.99	0.45
1:D:507:PRO:HA	1:D:508:GLN:HA	1.57	0.45
1:D:541:PHE:HA	1:D:576:SER:OG	2.16	0.45
1:B:498:LEU:CD1	1:B:730:LYS:CD	2.94	0.44
1:C:348:ASP:HB3	1:C:354:ILE:HD13	1.99	0.44
1:A:386:ASP:HA	1:A:387:THR:HA	1.74	0.44
1:C:131:ASP:OD1	1:C:131:ASP:N	2.50	0.44
1:C:412:HIS:CE1	1:C:413:GLU:HG3	2.52	0.44
1:A:50:LEU:HD12	1:A:50:LEU:O	2.17	0.44
1:A:483:LEU:HD13	1:D:751:LEU:HB2	1.99	0.44
1:A:586:GLN:HA	1:D:587:GLN:OE1	2.17	0.44
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.47	0.44
1:D:579:PHE:CE1	1:D:590:ASP:HB3	2.49	0.44
1:B:227:PHE:CD2	1:B:244:GLY:HA3	2.53	0.44
1:C:117:LEU:HD11	1:C:245:PHE:CD1	2.51	0.44
1:D:645:ILE:HG12	1:D:699:LYS:HA	1.99	0.44
1:A:198:ARG:HH21	1:A:279:LYS:HD3	1.82	0.44
1:A:400:ILE:HG22	1:A:477:ALA:HB1	1.99	0.44
1:B:297:ARG:HG2	1:B:301:LYS:HE3	1.99	0.44
1:C:321:VAL:HA	1:C:322:PRO:HD3	1.39	0.44
1:A:143:LEU:CD1	1:A:147:GLN:HG3	2.48	0.44
1:B:525:ILE:HD13	1:C:792:VAL:HG21	1.99	0.44
1:A:186:LEU:HD13	1:B:157:LYS:NZ	2.32	0.44
1:B:521:LEU:HA	1:C:787:LEU:HD23	1.99	0.44
1:C:585:MET:O	1:C:586:GLN:C	2.55	0.44
1:D:320:ALA:O	1:D:322:PRO:HD3	2.18	0.44
1:A:515:PHE:CD1	1:A:518:LEU:HD21	2.52	0.44
1:A:518:LEU:HD12	1:A:518:LEU:O	2.18	0.44
1:B:474:ILE:HG13	1:B:736:THR:HG22	2.00	0.44
1:B:481:ILE:HG12	1:B:491:PHE:CD1	2.53	0.44
1:D:770:LYS:HE2	1:D:770:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.42	0.44
1:D:500:ILE:HB	1:D:727:LEU:HB2	2.00	0.44
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.53	0.43
1:A:498:LEU:CD1	1:A:499:GLY:N	2.80	0.43
1:C:143:LEU:HD11	1:C:147:GLN:HE21	1.83	0.43
1:C:204:ILE:O	1:C:208:VAL:HG23	2.18	0.43
1:A:582:GLY:HA2	1:A:585:MET:HE2	2.00	0.43
1:B:209:ILE:HG23	1:B:214:HIS:CE1	2.53	0.43
1:B:518:LEU:HB3	1:B:526:TRP:HE1	1.84	0.43
1:B:541:PHE:HA	1:B:576:SER:OG	2.18	0.43
1:C:579:PHE:O	1:C:583:ALA:N	2.52	0.43
1:D:774:GLY:O	1:D:777:ASP:N	2.51	0.43
1:A:297:ARG:HG2	1:A:301:LYS:HE3	2.01	0.43
1:B:25:GLU:OE1	1:B:25:GLU:N	2.49	0.43
1:C:297:ARG:HG2	1:C:301:LYS:HE3	2.00	0.43
1:C:684:ARG:N	1:C:688:GLU:OE1	2.44	0.43
1:D:227:PHE:CD2	1:D:244:GLY:HA3	2.53	0.43
1:D:579:PHE:CZ	1:D:591:ILE:HB	2.53	0.43
1:A:502:ILE:HD13	1:A:639:LEU:HD22	2.00	0.43
1:B:168:ILE:C	1:B:169:ASN:O	2.59	0.43
1:B:171:ASP:OD1	1:B:171:ASP:N	2.51	0.43
1:B:518:LEU:CB	1:B:526:TRP:HE1	2.31	0.43
1:D:181:PHE:CE2	1:D:208:VAL:HG22	2.54	0.43
1:A:408:MET:HE2	1:A:412:HIS:HB2	2.00	0.43
1:B:518:LEU:HD12	1:B:519:ASP:CA	2.48	0.43
1:C:500:ILE:O	1:C:727:LEU:N	2.46	0.43
1:D:593:PRO:C	1:D:595:SER:H	2.26	0.43
1:A:157:LYS:HD2	1:B:187:LYS:HE3	2.00	0.43
1:A:498:LEU:HD12	1:A:498:LEU:C	2.43	0.43
1:A:600:ILE:CG1	1:B:581:LEU:HD13	2.49	0.43
1:B:592:SER:N	1:B:593:PRO:HA	2.34	0.43
1:A:219:HIS:ND1	1:A:241:GLU:O	2.52	0.43
1:A:694:ARG:HE	1:A:720:THR:HG23	1.83	0.43
1:B:485:ARG:O	1:B:489:ILE:HG13	2.19	0.43
1:D:595:SER:CA	1:D:596:LEU:CD1	2.86	0.43
1:D:606:TRP:HA	1:D:609:THR:HG22	2.00	0.43
1:B:118:LYS:NZ	1:B:118:LYS:HB2	2.34	0.43
1:C:188:LYS:HZ1	1:C:471:LYS:NZ	2.16	0.43
1:B:608:PHE:CG	1:C:799:LEU:HD22	2.54	0.43
1:C:332:ALA:O	1:C:336:VAL:HG23	2.18	0.43
1:C:169:ASN:HB2	1:C:171:ASP:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:HA	1:B:510:SER:C	2.43	0.42
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.84	0.42
1:B:219:HIS:HD2	1:B:241:GLU:O	2.02	0.42
1:C:171:ASP:OD1	1:C:171:ASP:N	2.46	0.42
1:D:50:LEU:C	1:D:50:LEU:CD1	2.87	0.42
1:A:479:LEU:HG	1:A:491:PHE:HZ	1.85	0.42
1:A:715:ARG:NH1	1:A:772:GLU:HG3	2.34	0.42
1:B:296:PHE:HD1	1:B:299:LEU:HD12	1.84	0.42
1:B:639:LEU:HD21	1:B:647:TYR:CD1	2.55	0.42
1:C:174:ASP:HA	1:C:207:GLN:HE22	1.84	0.42
1:A:596:LEU:C	1:A:598:GLY:N	2.67	0.42
1:B:575:ASN:OD1	1:B:576:SER:N	2.50	0.42
1:C:588:GLY:HA3	1:C:605:TRP:HD1	1.84	0.42
1:C:684:ARG:HB3	1:C:688:GLU:OE2	2.19	0.42
1:D:546:THR:HA	1:D:547:ASP:C	2.43	0.42
1:D:716:LYS:CB	1:D:772:GLU:OE1	2.67	0.42
1:B:50:LEU:HD12	1:B:50:LEU:O	2.19	0.42
1:C:611:ILE:HD13	1:C:611:ILE:HA	1.92	0.42
1:D:13:GLN:HG3	1:D:70:VAL:HG12	2.00	0.42
1:D:705:GLU:CD	1:D:705:GLU:H	2.28	0.42
1:A:578:TRP:HA	1:D:596:LEU:CD2	2.33	0.42
1:C:30:ARG:HB2	1:C:270:TYR:HE2	1.84	0.42
1:D:602:GLY:O	1:D:606:TRP:N	2.41	0.42
1:B:168:ILE:HD11	1:B:200:LYS:HE2	2.02	0.42
1:C:507:PRO:O	1:C:509:LYS:N	2.52	0.42
1:A:209:ILE:HA	1:A:214:HIS:CE1	2.55	0.41
1:A:409:LYS:HG2	1:A:422:GLU:CD	2.45	0.41
1:B:624:LEU:HD23	1:B:624:LEU:HA	1.87	0.41
1:C:593:PRO:HB2	1:C:594:ARG:CB	2.50	0.41
1:D:499:GLY:O	1:D:706:SER:N	2.51	0.41
1:D:539:VAL:O	1:D:543:VAL:HG23	2.20	0.41
1:A:186:LEU:CD1	1:B:157:LYS:NZ	2.82	0.41
1:C:683:VAL:HB	1:C:688:GLU:HB2	2.01	0.41
1:D:323:TRP:HZ3	1:D:325:GLN:CB	2.31	0.41
1:A:181:PHE:CD2	1:A:211:ILE:HD11	2.54	0.41
1:A:195:ASP:HA	1:A:223:ALA:HB3	2.01	0.41
1:A:809:VAL:O	1:A:813:GLU:HG2	2.19	0.41
1:B:493:LYS:HD3	1:B:493:LYS:HA	1.90	0.41
1:C:498:LEU:HD21	1:C:732:TYR:CE2	2.55	0.41
1:D:10:ASN:HB2	1:D:41:PHE:HA	2.01	0.41
1:A:110:VAL:HG12	1:A:112:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.41
1:A:186:LEU:HB3	1:B:157:LYS:HZ2	1.67	0.41
1:B:498:LEU:HD11	1:B:730:LYS:CG	2.49	0.41
1:B:518:LEU:O	1:B:521:LEU:HG	2.20	0.41
1:B:591:ILE:HD12	1:B:591:ILE:HA	1.95	0.41
1:D:22:ALA:HB1	1:D:25:GLU:HB2	2.01	0.41
1:A:202:ASN:HA	1:A:205:VAL:HB	2.02	0.41
1:A:417:GLY:HA2	1:A:441:LYS:NZ	2.35	0.41
1:A:536:VAL:HG22	1:B:803:LEU:HD11	2.01	0.41
1:A:593:PRO:HD2	1:A:595:SER:N	2.36	0.41
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.01	0.41
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.41
1:B:125:ILE:H	1:B:125:ILE:HG13	1.72	0.41
1:B:611:ILE:HG21	1:C:795:VAL:HG21	2.02	0.41
1:C:196:CYS:HB3	1:C:200:LYS:HB3	2.03	0.41
1:D:174:ASP:O	1:D:178:ARG:HG3	2.21	0.41
1:D:405:TYR:CD1	1:D:478:PRO:HG3	2.56	0.41
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.56	0.41
1:B:12:ILE:HG23	1:B:71:TYR:HD1	1.85	0.41
1:B:109:PHE:HE2	1:B:327:VAL:HA	1.85	0.41
1:B:595:SER:HA	1:B:596:LEU:HA	1.96	0.41
1:B:754:SER:HB2	1:B:759:LEU:HD12	2.01	0.41
1:C:519:ASP:OD1	1:C:523:TYR:CE1	2.74	0.41
1:C:522:ALA:HB3	1:C:525:ILE:HG13	2.02	0.41
1:C:681:VAL:HA	1:C:692:ARG:HH12	1.86	0.41
1:D:684:ARG:HB3	1:D:688:GLU:OE2	2.21	0.41
1:A:89:CYS:SG	1:A:96:PHE:HB2	2.61	0.41
1:A:587:GLN:HB2	1:A:588:GLY:H	1.64	0.41
1:A:799:LEU:HD22	1:D:608:PHE:CG	2.56	0.41
1:B:639:LEU:HD23	1:B:647:TYR:CD1	2.56	0.41
1:C:596:LEU:O	1:C:596:LEU:HG	2.21	0.41
1:A:27:SER:HB3	1:A:270:TYR:HB3	2.02	0.41
1:A:135:TYR:CE2	1:A:137:TYR:HB3	2.56	0.41
1:A:589:ALA:HB3	1:B:585:MET:SD	2.61	0.41
1:A:596:LEU:O	1:A:598:GLY:N	2.53	0.41
1:B:29:PHE:O	1:B:33:MET:HG2	2.20	0.41
1:B:41:PHE:HZ	1:B:297:ARG:HB2	1.85	0.41
1:B:46:HIS:NE2	1:B:68:ARG:NH1	2.68	0.41
1:C:98:THR:HA	1:C:99:PRO:HD3	1.90	0.41
1:C:463:MET:HE3	1:C:463:MET:HB2	1.91	0.41
1:C:483:LEU:O	1:C:487:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:GLU:HB3	1:D:789:LEU:HD22	2.03	0.41
1:D:346:LYS:HZ2	2:D:901:NAG:H82	1.86	0.41
1:D:583:ALA:HB1	1:D:589:ALA:HA	2.02	0.41
1:D:769:ASP:C	1:D:770:LYS:HE2	2.46	0.41
1:A:802:GLY:O	1:A:806:ALA:N	2.46	0.41
1:B:401:LEU:HD23	1:B:406:VAL:HG12	2.02	0.41
1:B:483:LEU:HD13	1:C:751:LEU:HB2	2.02	0.41
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.86	0.41
1:D:296:PHE:HD1	1:D:299:LEU:HD12	1.86	0.41
1:D:718:CYS:HB3	1:D:775:ALA:HB2	2.03	0.41
1:A:401:LEU:HG	1:A:444:ILE:HD12	2.03	0.40
1:A:600:ILE:O	1:A:600:ILE:CG2	2.69	0.40
1:B:50:LEU:C	1:B:50:LEU:CD1	2.93	0.40
1:B:288:ALA:O	1:B:292:MET:HG3	2.21	0.40
1:B:489:ILE:HD13	1:B:735:ALA:HB1	2.02	0.40
1:A:10:ASN:HB3	1:A:300:ARG:HH22	1.85	0.40
1:A:162:ALA:HB3	1:B:150:LEU:HD22	2.04	0.40
1:A:402:GLU:OE1	1:A:450:TYR:OH	2.37	0.40
1:A:411:ASN:OD1	1:A:411:ASN:N	2.55	0.40
1:C:498:LEU:HD11	1:C:730:LYS:HG3	2.00	0.40
1:C:522:ALA:N	1:D:787:LEU:HD12	2.31	0.40
1:A:516:SER:HA	1:A:519:ASP:OD2	2.22	0.40
1:A:531:PHE:O	1:A:535:GLY:N	2.52	0.40
1:A:592:SER:N	1:A:593:PRO:HA	2.37	0.40
1:A:600:ILE:HG12	1:B:581:LEU:CD2	2.51	0.40
1:B:128:TYR:CE1	1:B:219:HIS:HE1	2.40	0.40
1:B:399:THR:OG1	1:B:406:VAL:HG21	2.21	0.40
1:C:630:VAL:O	1:C:631:SER:C	2.64	0.40
1:C:642:GLN:NE2	1:C:645:ILE:HB	2.35	0.40
1:D:66:PHE:CZ	1:D:312:ALA:HB1	2.57	0.40
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.86	0.40
1:A:50:LEU:C	1:A:50:LEU:CD1	2.93	0.40
1:A:136:LEU:HD11	1:A:181:PHE:HE1	1.86	0.40
1:A:187:LYS:HE3	1:B:157:LYS:HG2	2.03	0.40
1:A:318:ASN:HA	1:A:319:PRO:HA	1.95	0.40
1:B:332:ALA:O	1:B:336:VAL:HG23	2.21	0.40
1:C:257:LYS:HE3	1:C:257:LYS:HB3	1.96	0.40
1:C:623:PHE:CE1	1:D:785:SER:CA	2.95	0.40
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.87	0.40
1:B:479:LEU:HD12	1:B:479:LEU:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:OG	1:B:469:TYR:OH[1_556]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	776/803 (97%)	721 (93%)	51 (7%)	4 (0%)	24	60
1	B	776/803 (97%)	716 (92%)	56 (7%)	4 (0%)	24	60
1	C	776/803 (97%)	722 (93%)	43 (6%)	11 (1%)	9	39
1	D	779/803 (97%)	724 (93%)	52 (7%)	3 (0%)	30	65
All	All	3107/3212 (97%)	2883 (93%)	202 (6%)	22 (1%)	18	54

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	SER
1	C	511	LYS
1	C	585	MET
1	C	629	MET
1	C	631	SER
1	B	587	GLN
1	B	774	GLY
1	A	631	SER
1	B	169	ASN
1	C	508	GLN
1	D	591	ILE
1	D	22	ALA
1	D	510	SER
1	C	520	PRO
1	A	592	SER
1	C	512	PRO

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Mol	Chain	Res	Type
1	C	592	SER
1	C	630	VAL
1	A	591	ILE
1	B	591	ILE
1	C	519	ASP
1	C	591	ILE

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	631/683 (92%)	621 (98%)	10 (2%)	55	70
1	B	632/683 (92%)	625 (99%)	7 (1%)	65	74
1	C	633/683 (93%)	626 (99%)	7 (1%)	65	74
1	D	633/683 (93%)	624 (99%)	9 (1%)	59	71
All	All	2529/2732 (93%)	2496 (99%)	33 (1%)	61	72

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	177	TYR
1	A	197	GLU
1	A	321	VAL
1	A	394	THR
1	A	525	ILE
1	A	579	PHE
1	A	596	LEU
1	A	633	ILE
1	A	792	VAL
1	B	157	LYS
1	B	169	ASN
1	B	177	TYR
1	B	197	GLU
1	B	321	VAL

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Mol	Chain	Res	Type
1	B	526	TRP
1	B	764	ASN
1	C	118	LYS
1	C	177	TYR
1	C	254	LEU
1	C	489	ILE
1	C	510	SER
1	C	512	PRO
1	C	792	VAL
1	D	118	LYS
1	D	177	TYR
1	D	321	VAL
1	D	378	ASP
1	D	593	PRO
1	D	623	PHE
1	D	632	PRO
1	D	773	CYS
1	D	787	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	214	HIS
1	A	246	GLN
1	A	290	GLN
1	A	764	ASN
1	B	169	ASN
1	B	202	ASN
1	B	359	ASN
1	B	412	HIS
1	B	587	GLN
1	B	714	GLN
1	B	726	ASN
1	C	147	GLN
1	C	290	GLN
1	C	587	GLN
1	C	726	ASN
1	D	49	ASN
1	D	147	GLN
1	D	219	HIS
1	D	290	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	901	1	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	A	901	1	14,14,15	0.18	0	17,19,21	0.47	0
2	NAG	C	901	1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	D	901	1	14,14,15	0.20	0	17,19,21	0.45	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
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	2/6/23/26	0/1/1/1
2	NAG	D	901	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	NAG	C4-C5-C6-O6
2	C	901	NAG	O5-C5-C6-O6
2	D	901	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0
2	D	901	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	587:GLN	C	588:GLY	N	1.20

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	780/803 (97%)	0.06	34 (4%)	39	31	93, 169, 256, 282	0
1	B	780/803 (97%)	-0.04	20 (2%)	57	42	92, 148, 268, 287	0
1	C	780/803 (97%)	-0.06	20 (2%)	57	42	93, 180, 264, 285	0
1	D	783/803 (97%)	0.04	39 (4%)	34	28	94, 205, 257, 278	0
All	All	3123/3212 (97%)	0.00	113 (3%)	46	35	92, 170, 260, 287	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	ASN	10.5
1	C	159	GLN	6.5
1	A	576	SER	6.4
1	C	187	LYS	6.1
1	A	577	LEU	6.1
1	C	160	VAL	5.9
1	D	154	ALA	5.8
1	A	573	ILE	5.4
1	B	631	SER	5.3
1	B	698	GLY	5.2
1	D	167	ASN	5.1
1	B	306	ILE	4.9
1	A	456	ASP	4.9
1	A	384	GLU	4.8
1	B	699	LYS	4.3
1	A	385	ASP	4.2
1	D	631	SER	4.2
1	D	494	PRO	4.1
1	C	186	LEU	4.0
1	C	162	ALA	3.9
1	D	632	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	586	GLN	3.8
1	D	140	ASP	3.8
1	A	578	TRP	3.7
1	A	574	PHE	3.6
1	B	696	SER	3.6
1	B	630	VAL	3.5
1	C	161	THR	3.5
1	D	634	GLU	3.4
1	D	158	TRP	3.4
1	A	386	ASP	3.4
1	D	155	GLU	3.3
1	C	132	LYS	3.3
1	A	387	THR	3.2
1	D	609	THR	3.2
1	A	494	PRO	3.2
1	D	779	GLY	3.2
1	D	526	TRP	3.1
1	D	160	VAL	3.1
1	C	636	ALA	3.0
1	D	104	ASP	3.0
1	D	162	ALA	3.0
1	D	497	SER	3.0
1	B	644	GLU	3.0
1	C	147	GLN	3.0
1	C	665	ALA	3.0
1	C	401	LEU	2.9
1	C	607	PHE	2.9
1	B	587	GLN	2.9
1	A	159	GLN	2.9
1	C	601	VAL	2.9
1	B	62	PHE	2.8
1	A	457	THR	2.8
1	D	613	ILE	2.7
1	C	609	THR	2.7
1	A	591	ILE	2.7
1	D	633	ILE	2.7
1	B	701	ALA	2.7
1	A	306	ILE	2.7
1	A	750	VAL	2.7
1	A	382	LEU	2.7
1	D	635	SER	2.7
1	C	16	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	164	ASN	2.6
1	D	159	GLN	2.6
1	D	432	ILE	2.6
1	B	629	MET	2.6
1	D	157	LYS	2.6
1	D	165	VAL	2.6
1	A	579	PHE	2.6
1	A	142	GLY	2.6
1	D	685	THR	2.6
1	A	780	SER	2.5
1	A	345	ILE	2.5
1	C	328	GLU	2.5
1	D	153	ALA	2.5
1	D	428	LEU	2.5
1	A	388	SER	2.5
1	A	590	ASP	2.5
1	B	613	ILE	2.4
1	D	150	LEU	2.4
1	D	638	ASP	2.4
1	A	641	LYS	2.4
1	C	669	LYS	2.4
1	B	92	LEU	2.4
1	A	600	ILE	2.3
1	B	645	ILE	2.3
1	D	591	ILE	2.3
1	D	615	SER	2.3
1	A	248	VAL	2.3
1	C	104	ASP	2.3
1	D	586	GLN	2.3
1	D	370	LYS	2.3
1	A	158	TRP	2.3
1	A	654	SER	2.3
1	B	805	LEU	2.3
1	D	147	GLN	2.3
1	B	88	PHE	2.2
1	B	86	THR	2.2
1	A	497	SER	2.2
1	D	780	SER	2.2
1	A	389	GLY	2.2
1	D	731	GLY	2.2
1	C	586	GLN	2.2
1	D	137	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	85	ILE	2.1
1	A	792	VAL	2.1
1	D	654	SER	2.0
1	C	326	GLY	2.0
1	B	588	GLY	2.0
1	A	630	VAL	2.0
1	A	730	LYS	2.0
1	D	80	LYS	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
2	NAG	D	901	14/15	0.69	0.14	216,216,216,216	0
2	NAG	C	901	14/15	0.74	0.10	259,259,259,259	0
2	NAG	B	901	14/15	0.75	0.13	239,239,239,239	0
2	NAG	A	901	14/15	0.83	0.13	217,217,217,217	0

6.5 Other polymers [i](#)

There are no such residues in this entry.