



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BIW
Title : Crystal structure of the Neuroligin-1/Neurexin-1beta synaptic adhesion complex
Authors : Arac, D.; Boucard, A.A.; Ozkan, E.; Strop, P.; Newell, E.; Sudhof, T.C.; Brunger, A.T.
Deposited on : 2007-12-01
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

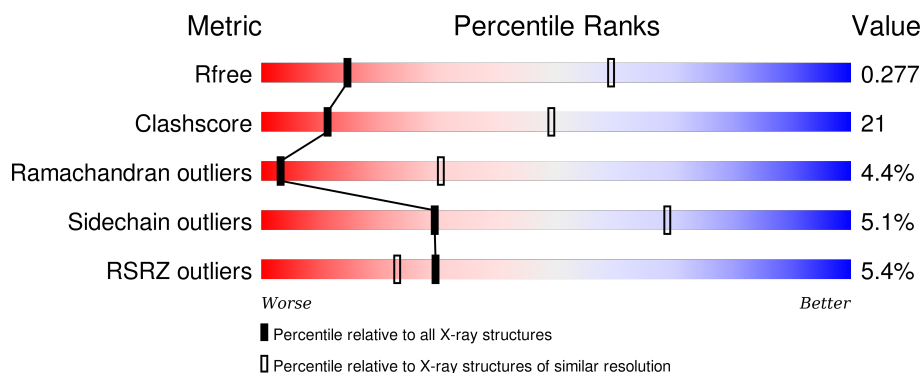
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	574	
1	B	574	
1	C	574	
1	D	574	
2	E	243	

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Mol	Chain	Length	Quality of chain
2	F	243	
2	G	243	
2	H	243	

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	NAG	D	702	-	-	-	X
4	NAG	E	306	-	-	X	-
4	NAG	F	306	-	-	X	-
4	NAG	G	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22438 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	B	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	C	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	D	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	-	EXPRESSION TAG	UNP Q62765
A	44	ASP	-	EXPRESSION TAG	UNP Q62765
A	45	PRO	-	EXPRESSION TAG	UNP Q62765
A	639	HIS	-	EXPRESSION TAG	UNP Q62765
A	640	HIS	-	EXPRESSION TAG	UNP Q62765
A	641	HIS	-	EXPRESSION TAG	UNP Q62765
A	642	HIS	-	EXPRESSION TAG	UNP Q62765
A	643	HIS	-	EXPRESSION TAG	UNP Q62765
A	644	HIS	-	EXPRESSION TAG	UNP Q62765
B	43	ALA	-	EXPRESSION TAG	UNP Q62765
B	44	ASP	-	EXPRESSION TAG	UNP Q62765
B	45	PRO	-	EXPRESSION TAG	UNP Q62765
B	639	HIS	-	EXPRESSION TAG	UNP Q62765
B	640	HIS	-	EXPRESSION TAG	UNP Q62765
B	641	HIS	-	EXPRESSION TAG	UNP Q62765
B	642	HIS	-	EXPRESSION TAG	UNP Q62765
B	643	HIS	-	EXPRESSION TAG	UNP Q62765
B	644	HIS	-	EXPRESSION TAG	UNP Q62765
C	43	ALA	-	EXPRESSION TAG	UNP Q62765
C	44	ASP	-	EXPRESSION TAG	UNP Q62765
C	45	PRO	-	EXPRESSION TAG	UNP Q62765

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Chain	Residue	Modelled	Actual	Comment	Reference
C	639	HIS	-	EXPRESSION TAG	UNP Q62765
C	640	HIS	-	EXPRESSION TAG	UNP Q62765
C	641	HIS	-	EXPRESSION TAG	UNP Q62765
C	642	HIS	-	EXPRESSION TAG	UNP Q62765
C	643	HIS	-	EXPRESSION TAG	UNP Q62765
C	644	HIS	-	EXPRESSION TAG	UNP Q62765
D	43	ALA	-	EXPRESSION TAG	UNP Q62765
D	44	ASP	-	EXPRESSION TAG	UNP Q62765
D	45	PRO	-	EXPRESSION TAG	UNP Q62765
D	639	HIS	-	EXPRESSION TAG	UNP Q62765
D	640	HIS	-	EXPRESSION TAG	UNP Q62765
D	641	HIS	-	EXPRESSION TAG	UNP Q62765
D	642	HIS	-	EXPRESSION TAG	UNP Q62765
D	643	HIS	-	EXPRESSION TAG	UNP Q62765
D	644	HIS	-	EXPRESSION TAG	UNP Q62765

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	F	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	G	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	H	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	GLY	-	EXPRESSION TAG	UNP Q63373
E	34	SER	-	EXPRESSION TAG	UNP Q63373
E	35	PRO	-	EXPRESSION TAG	UNP Q63373
E	36	GLY	-	EXPRESSION TAG	UNP Q63373
E	37	ILE	-	EXPRESSION TAG	UNP Q63373
E	38	SER	-	EXPRESSION TAG	UNP Q63373
E	39	GLY	-	EXPRESSION TAG	UNP Q63373
E	40	GLY	-	EXPRESSION TAG	UNP Q63373
E	41	GLY	-	EXPRESSION TAG	UNP Q63373
E	42	GLY	-	EXPRESSION TAG	UNP Q63373
E	43	GLY	-	EXPRESSION TAG	UNP Q63373

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Chain	Residue	Modelled	Actual	Comment	Reference
E	44	ILE	-	EXPRESSION TAG	UNP Q63373
E	45	LEU	-	EXPRESSION TAG	UNP Q63373
E	46	GLU	-	EXPRESSION TAG	UNP Q63373
E	300	HIS	-	EXPRESSION TAG	UNP Q63373
E	301	HIS	-	EXPRESSION TAG	UNP Q63373
E	302	HIS	-	EXPRESSION TAG	UNP Q63373
E	303	HIS	-	EXPRESSION TAG	UNP Q63373
E	304	HIS	-	EXPRESSION TAG	UNP Q63373
E	305	HIS	-	EXPRESSION TAG	UNP Q63373
F	33	GLY	-	EXPRESSION TAG	UNP Q63373
F	34	SER	-	EXPRESSION TAG	UNP Q63373
F	35	PRO	-	EXPRESSION TAG	UNP Q63373
F	36	GLY	-	EXPRESSION TAG	UNP Q63373
F	37	ILE	-	EXPRESSION TAG	UNP Q63373
F	38	SER	-	EXPRESSION TAG	UNP Q63373
F	39	GLY	-	EXPRESSION TAG	UNP Q63373
F	40	GLY	-	EXPRESSION TAG	UNP Q63373
F	41	GLY	-	EXPRESSION TAG	UNP Q63373
F	42	GLY	-	EXPRESSION TAG	UNP Q63373
F	43	GLY	-	EXPRESSION TAG	UNP Q63373
F	44	ILE	-	EXPRESSION TAG	UNP Q63373
F	45	LEU	-	EXPRESSION TAG	UNP Q63373
F	46	GLU	-	EXPRESSION TAG	UNP Q63373
F	300	HIS	-	EXPRESSION TAG	UNP Q63373
F	301	HIS	-	EXPRESSION TAG	UNP Q63373
F	302	HIS	-	EXPRESSION TAG	UNP Q63373
F	303	HIS	-	EXPRESSION TAG	UNP Q63373
F	304	HIS	-	EXPRESSION TAG	UNP Q63373
F	305	HIS	-	EXPRESSION TAG	UNP Q63373
G	33	GLY	-	EXPRESSION TAG	UNP Q63373
G	34	SER	-	EXPRESSION TAG	UNP Q63373
G	35	PRO	-	EXPRESSION TAG	UNP Q63373
G	36	GLY	-	EXPRESSION TAG	UNP Q63373
G	37	ILE	-	EXPRESSION TAG	UNP Q63373
G	38	SER	-	EXPRESSION TAG	UNP Q63373
G	39	GLY	-	EXPRESSION TAG	UNP Q63373
G	40	GLY	-	EXPRESSION TAG	UNP Q63373
G	41	GLY	-	EXPRESSION TAG	UNP Q63373
G	42	GLY	-	EXPRESSION TAG	UNP Q63373
G	43	GLY	-	EXPRESSION TAG	UNP Q63373
G	44	ILE	-	EXPRESSION TAG	UNP Q63373
G	45	LEU	-	EXPRESSION TAG	UNP Q63373

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Chain	Residue	Modelled	Actual	Comment	Reference
G	46	GLU	-	EXPRESSION TAG	UNP Q63373
G	300	HIS	-	EXPRESSION TAG	UNP Q63373
G	301	HIS	-	EXPRESSION TAG	UNP Q63373
G	302	HIS	-	EXPRESSION TAG	UNP Q63373
G	303	HIS	-	EXPRESSION TAG	UNP Q63373
G	304	HIS	-	EXPRESSION TAG	UNP Q63373
G	305	HIS	-	EXPRESSION TAG	UNP Q63373
H	33	GLY	-	EXPRESSION TAG	UNP Q63373
H	34	SER	-	EXPRESSION TAG	UNP Q63373
H	35	PRO	-	EXPRESSION TAG	UNP Q63373
H	36	GLY	-	EXPRESSION TAG	UNP Q63373
H	37	ILE	-	EXPRESSION TAG	UNP Q63373
H	38	SER	-	EXPRESSION TAG	UNP Q63373
H	39	GLY	-	EXPRESSION TAG	UNP Q63373
H	40	GLY	-	EXPRESSION TAG	UNP Q63373
H	41	GLY	-	EXPRESSION TAG	UNP Q63373
H	42	GLY	-	EXPRESSION TAG	UNP Q63373
H	43	GLY	-	EXPRESSION TAG	UNP Q63373
H	44	ILE	-	EXPRESSION TAG	UNP Q63373
H	45	LEU	-	EXPRESSION TAG	UNP Q63373
H	46	GLU	-	EXPRESSION TAG	UNP Q63373
H	300	HIS	-	EXPRESSION TAG	UNP Q63373
H	301	HIS	-	EXPRESSION TAG	UNP Q63373
H	302	HIS	-	EXPRESSION TAG	UNP Q63373
H	303	HIS	-	EXPRESSION TAG	UNP Q63373
H	304	HIS	-	EXPRESSION TAG	UNP Q63373
H	305	HIS	-	EXPRESSION TAG	UNP Q63373

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		

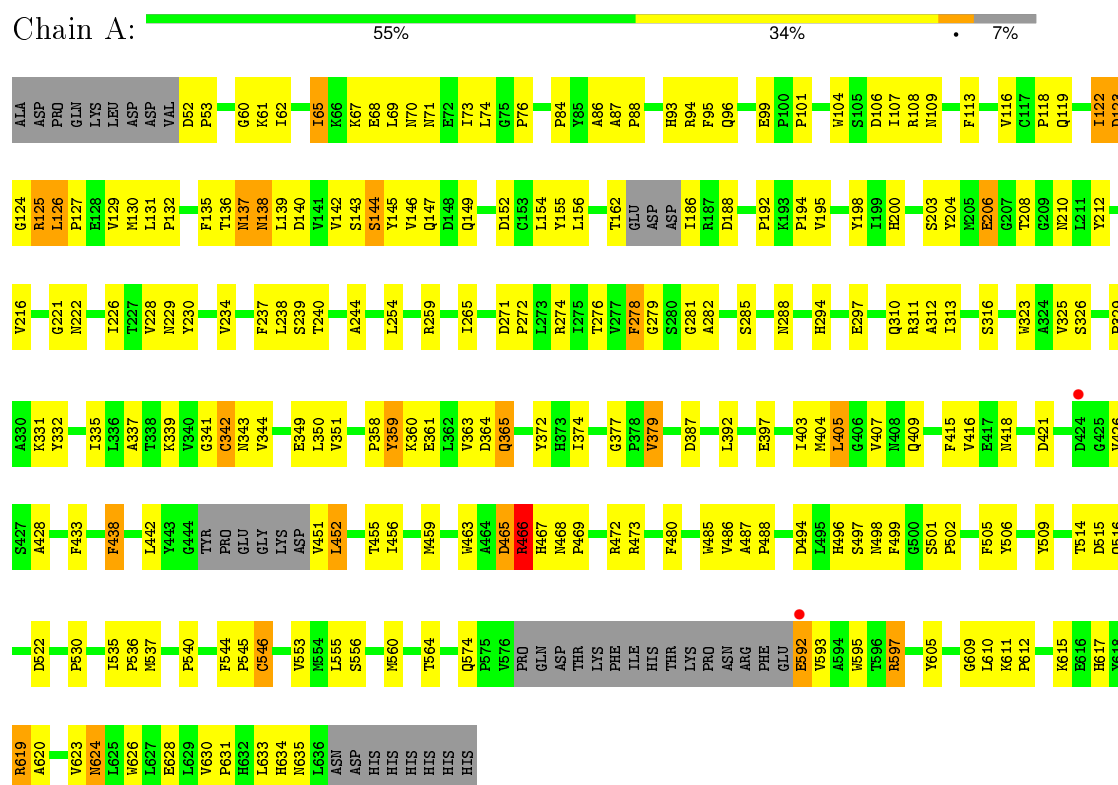
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		
5	E	2	Total	Ca	0	0
			2	2		

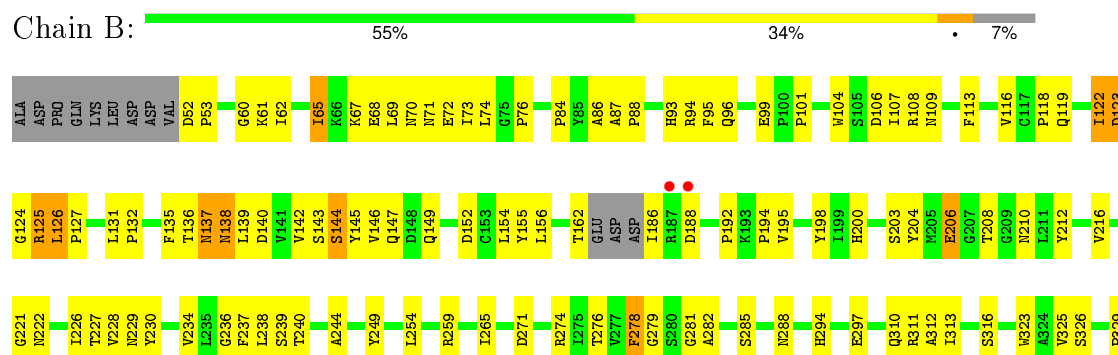
3 Residue-property plots

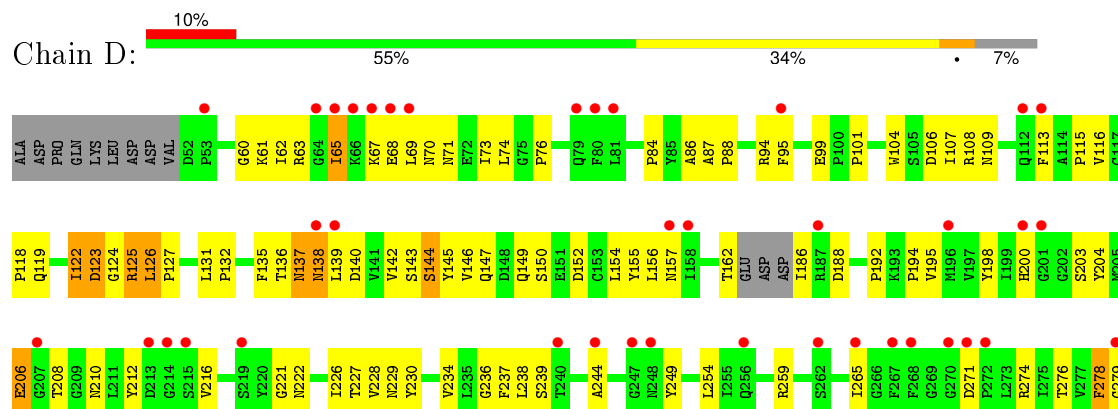
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

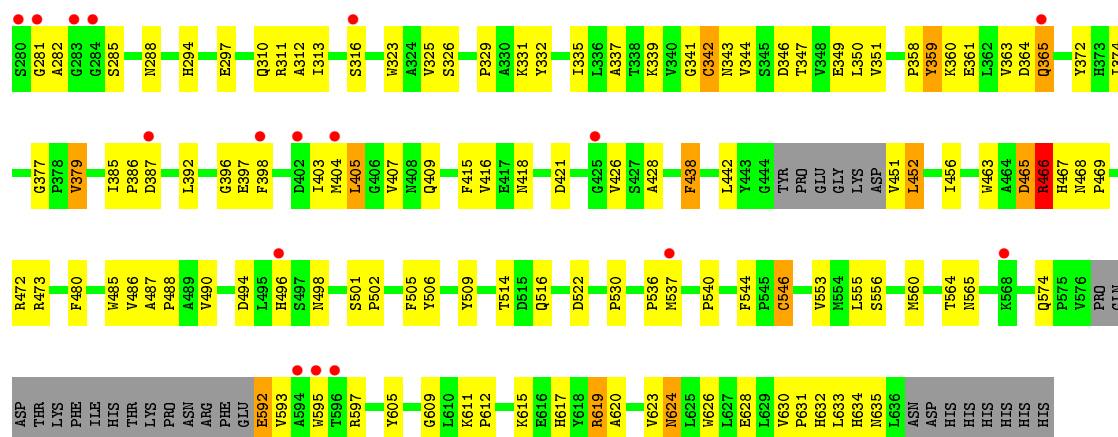
• Molecule 1: Neuroligin-1



• Molecule 1: Neuroligin-1

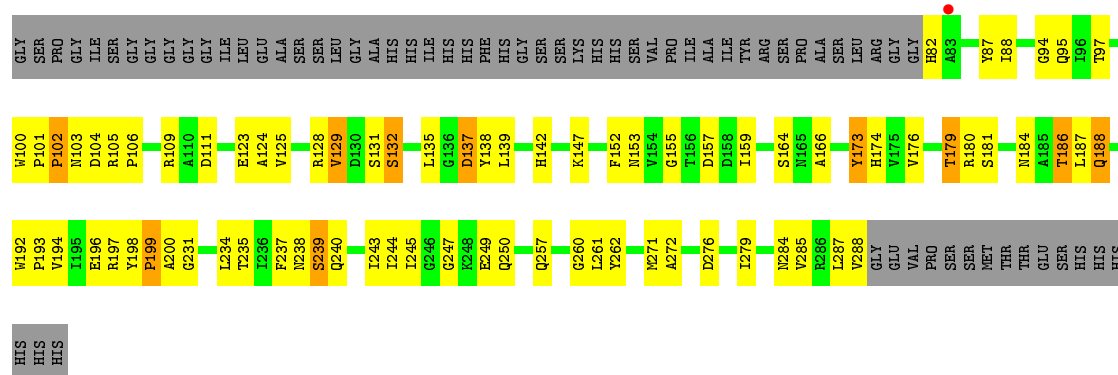






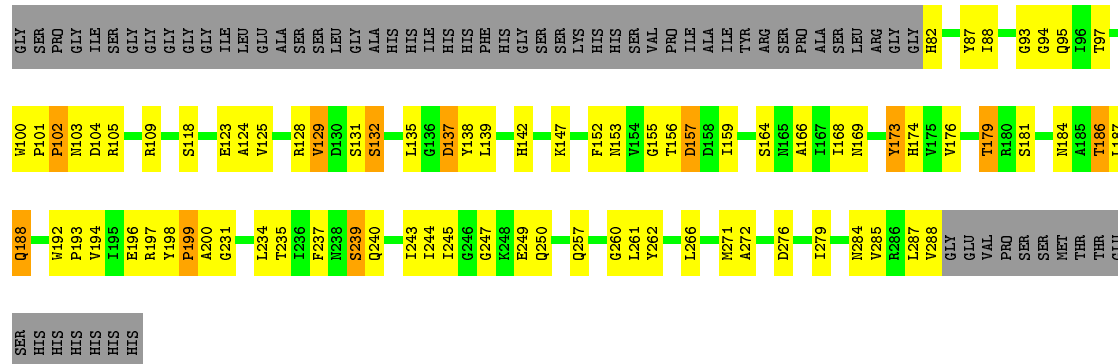
• Molecule 2: Neurexin-1-beta

Chain E: 41% 28% 27%



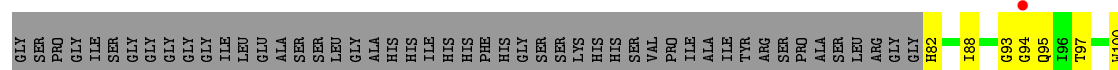
• Molecule 2: Neurexin-1-beta

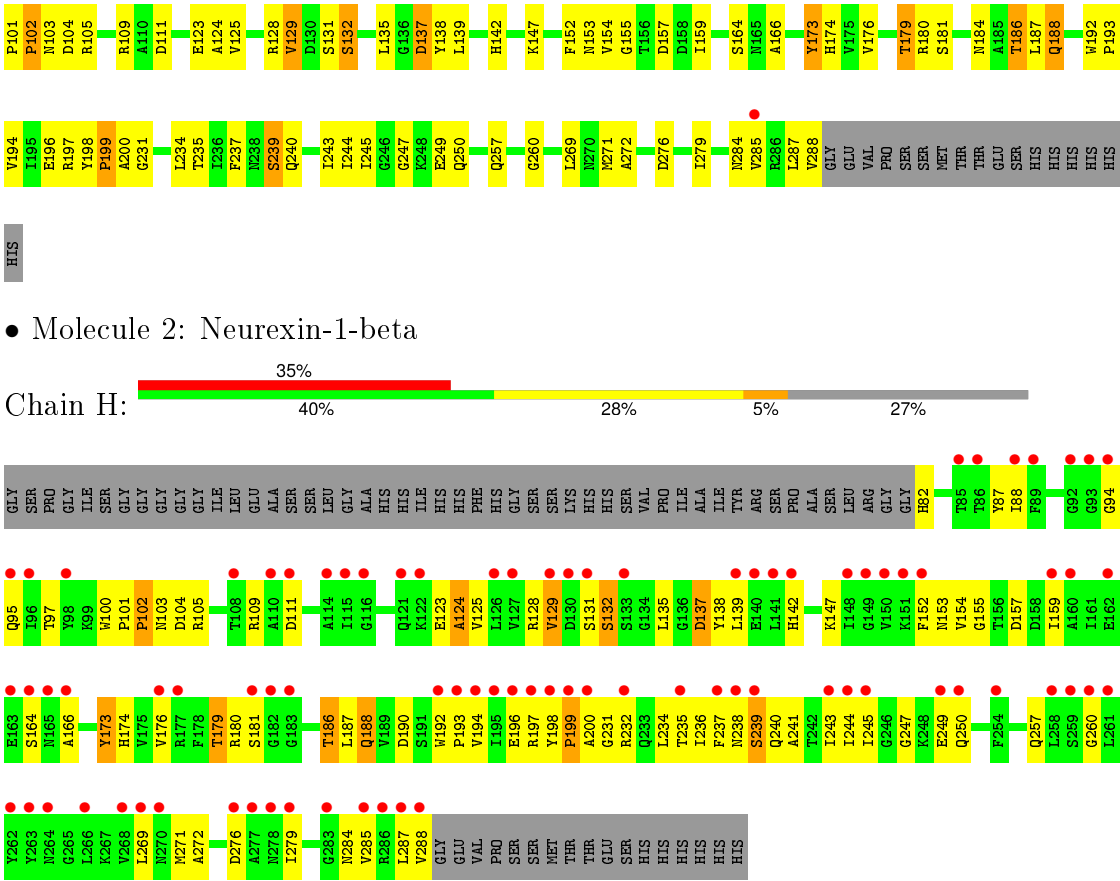
Chain F: 40% 28% 5% 27%



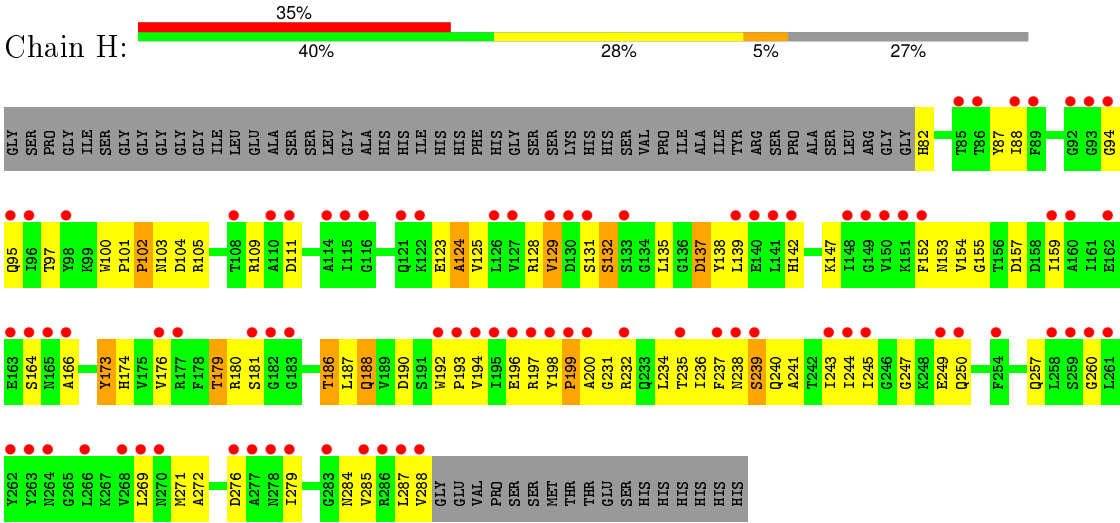
• Molecule 2: Neurexin-1-beta

Chain G: 42% 27% 27%





• Molecule 2: Neurexin-1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.83Å 148.80Å 123.60Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	45.90 – 3.50 45.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	94.9 (45.90-3.50) 92.4 (45.90-3.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.276 0.248 , 0.277	Depositor DCC
R_{free} test set	2538 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 53460 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22438	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 2.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.45	0/4302	0.65	1/5872 (0.0%)
1	B	0.45	0/4302	0.66	1/5872 (0.0%)
1	C	0.43	0/4302	0.65	0/5872
1	D	0.36	0/4302	0.63	1/5872 (0.0%)
2	E	0.44	0/1385	0.71	0/1877
2	F	0.48	0/1385	0.71	0/1877
2	G	0.47	0/1385	0.72	0/1877
2	H	0.34	0/1385	0.67	0/1877
All	All	0.42	0/22748	0.66	3/30996 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	452	LEU	N-CA-C	-5.23	96.87	111.00
1	A	452	LEU	N-CA-C	-5.09	97.24	111.00
1	B	452	LEU	N-CA-C	-5.07	97.31	111.00

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	4186	0	4046	176	0
1	B	4186	0	4046	175	0
1	C	4186	0	4046	175	0
1	D	4186	0	4045	173	0
2	E	1359	0	1345	54	1
2	F	1359	0	1345	59	0
2	G	1359	0	1345	53	0
2	H	1359	0	1347	58	0
3	A	42	0	39	3	0
3	B	42	0	39	3	0
3	C	42	0	39	3	0
3	D	42	0	39	2	0
4	E	28	0	25	7	0
4	F	28	0	25	7	0
4	G	28	0	25	7	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
All	All	22438	0	21796	916	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 21.

All (916) 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)
2:G:147:LYS:HD3	2:G:164:SER:HA	1.48	0.95
2:E:147:LYS:HD3	2:E:164:SER:HA	1.47	0.93
2:F:147:LYS:HD3	2:F:164:SER:HA	1.51	0.92
2:H:147:LYS:HD3	2:H:164:SER:HA	1.50	0.90
1:D:426:VAL:HG23	1:D:473:ARG:HB2	1.62	0.80
1:A:624:ASN:HD21	1:D:466:ARG:NH2	1.80	0.79
1:A:624:ASN:HD21	1:D:466:ARG:HH21	1.32	0.78
1:A:466:ARG:HH21	1:D:624:ASN:HD21	1.32	0.77
2:H:88:ILE:HG12	2:H:257:GLN:HG2	1.67	0.77
1:D:633:LEU:C	1:D:635:ASN:H	1.88	0.77
2:F:88:ILE:HG12	2:F:257:GLN:HG2	1.67	0.77
2:E:88:ILE:HG12	2:E:257:GLN:HG2	1.66	0.77
1:C:426:VAL:HG23	1:C:473:ARG:HB2	1.67	0.77
2:G:88:ILE:HG12	2:G:257:GLN:HG2	1.67	0.77
1:B:426:VAL:HG23	1:B:473:ARG:HB2	1.68	0.75
2:E:173:TYR:HD1	2:E:174:HIS:N	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:TYR:HD1	2:H:174:HIS:N	1.85	0.74
1:A:426:VAL:HG23	1:A:473:ARG:HB2	1.70	0.73
2:F:173:TYR:HD1	2:F:174:HIS:N	1.87	0.73
1:B:633:LEU:C	1:B:635:ASN:H	1.92	0.73
2:G:173:TYR:HD1	2:G:174:HIS:N	1.86	0.72
1:C:633:LEU:C	1:C:635:ASN:H	1.91	0.72
1:C:360:LYS:HE3	1:C:364:ASP:OD2	1.91	0.71
1:A:433:PHE:CE1	1:B:433:PHE:HB2	2.26	0.71
1:A:633:LEU:C	1:A:635:ASN:H	1.92	0.70
1:D:466:ARG:HH11	1:D:466:ARG:HG2	1.56	0.70
1:C:514:THR:HG22	1:C:546:CYS:SG	2.31	0.70
2:E:287:LEU:HD12	2:E:288:VAL:H	1.56	0.70
1:D:415:PHE:CD2	1:D:480:PHE:HB2	2.26	0.70
1:A:360:LYS:HE3	1:A:364:ASP:OD2	1.92	0.70
1:D:624:ASN:O	1:D:628:GLU:HB2	1.92	0.70
1:B:466:ARG:HH11	1:B:466:ARG:HG2	1.56	0.70
1:B:360:LYS:HE3	1:B:364:ASP:OD2	1.92	0.69
1:C:466:ARG:HG2	1:C:466:ARG:HH11	1.56	0.69
2:G:287:LEU:HD12	2:G:288:VAL:H	1.55	0.69
1:D:617:HIS:HB3	1:D:620:ALA:HB2	1.75	0.69
2:F:287:LEU:HD12	2:F:288:VAL:H	1.58	0.69
1:B:514:THR:HG22	1:B:546:CYS:SG	2.33	0.69
1:C:123:ASP:O	1:C:125:ARG:N	2.26	0.69
1:A:466:ARG:HG2	1:A:466:ARG:HH11	1.58	0.69
1:B:624:ASN:O	1:B:628:GLU:HB2	1.94	0.68
1:D:360:LYS:HE3	1:D:364:ASP:OD2	1.93	0.68
1:B:162:THR:O	1:B:186:ILE:HB	1.93	0.68
1:B:294:HIS:HA	2:F:109:ARG:NH2	2.07	0.68
2:H:287:LEU:HD12	2:H:288:VAL:H	1.58	0.68
1:A:162:THR:O	1:A:186:ILE:HB	1.94	0.67
1:C:162:THR:O	1:C:186:ILE:HB	1.94	0.67
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.76	0.67
1:B:123:ASP:O	1:B:125:ARG:N	2.27	0.67
1:D:123:ASP:O	1:D:125:ARG:N	2.28	0.67
2:G:147:LYS:HD3	2:G:164:SER:CA	2.22	0.67
1:A:123:ASP:O	1:A:125:ARG:N	2.27	0.67
1:D:514:THR:HG22	1:D:546:CYS:SG	2.34	0.67
1:D:487:ALA:HB3	1:D:488:PRO:HD3	1.76	0.66
1:B:415:PHE:CD2	1:B:480:PHE:HB2	2.30	0.66
1:C:415:PHE:CD2	1:C:480:PHE:HB2	2.30	0.66
1:A:76:PRO:HG2	1:A:162:THR:OG1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ALA:HB3	1:C:488:PRO:HD3	1.75	0.66
1:A:624:ASN:O	1:A:628:GLU:HB2	1.94	0.66
1:B:397:GLU:OE1	2:F:235:THR:HB	1.95	0.66
1:C:617:HIS:HB3	1:C:620:ALA:HB2	1.77	0.66
1:D:76:PRO:HG2	1:D:162:THR:OG1	1.96	0.66
2:H:147:LYS:HD3	2:H:164:SER:CA	2.24	0.66
1:C:624:ASN:O	1:C:628:GLU:HB2	1.95	0.65
2:E:147:LYS:HD3	2:E:164:SER:CA	2.22	0.65
1:D:162:THR:O	1:D:186:ILE:HB	1.96	0.65
1:C:259:ARG:HH11	1:C:259:ARG:HG3	1.60	0.65
1:D:259:ARG:HH11	1:D:259:ARG:HG3	1.61	0.65
1:B:76:PRO:HG2	1:B:162:THR:OG1	1.95	0.65
1:A:514:THR:HG22	1:A:546:CYS:SG	2.36	0.65
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.79	0.65
1:A:234:VAL:HG12	1:A:238:LEU:HD12	1.79	0.65
1:D:65:ILE:HD11	1:D:67:LYS:HE2	1.79	0.65
1:C:76:PRO:HG2	1:C:162:THR:OG1	1.97	0.65
1:D:234:VAL:HG12	1:D:238:LEU:HD12	1.78	0.65
1:C:502:PRO:HA	1:C:597:ARG:NH1	2.12	0.64
1:A:415:PHE:CD2	1:A:480:PHE:HB2	2.32	0.64
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.63	0.64
1:D:397:GLU:OE1	2:H:235:THR:HB	1.98	0.64
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.62	0.64
1:A:452:LEU:O	1:A:456:ILE:HG12	1.98	0.63
1:D:238:LEU:HD23	1:D:239:SER:N	2.12	0.63
2:G:272:ALA:N	2:G:279:ILE:HD12	2.14	0.63
2:F:101:PRO:HG2	2:F:104:ASP:HB2	1.80	0.63
1:D:452:LEU:O	1:D:456:ILE:HG12	1.99	0.63
2:H:101:PRO:HG2	2:H:104:ASP:HB2	1.79	0.63
1:C:65:ILE:HD11	1:C:67:LYS:HE2	1.79	0.63
1:B:487:ALA:HB3	1:B:488:PRO:HD3	1.79	0.63
1:C:452:LEU:O	1:C:456:ILE:HG12	1.98	0.63
2:F:147:LYS:HD3	2:F:164:SER:CA	2.25	0.63
2:H:272:ALA:N	2:H:279:ILE:HD12	2.14	0.63
1:B:238:LEU:HD23	1:B:239:SER:N	2.13	0.62
3:C:702:NAG:H83	3:C:702:NAG:O3	1.99	0.62
1:B:624:ASN:HD21	1:C:466:ARG:HH21	1.47	0.62
1:D:502:PRO:HA	1:D:597:ARG:NH1	2.14	0.62
1:B:502:PRO:HA	1:B:597:ARG:NH1	2.15	0.62
1:B:592:GLU:OE1	1:B:592:GLU:N	2.32	0.62
4:E:306:NAG:C3	4:E:307:NAG:H2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD11	1:A:67:LYS:HE2	1.80	0.62
3:B:702:NAG:H83	3:B:702:NAG:O3	1.99	0.62
1:A:238:LEU:HD23	1:A:239:SER:N	2.15	0.62
1:A:592:GLU:OE1	1:A:592:GLU:N	2.33	0.61
2:G:125:VAL:O	2:G:247:GLY:HA3	2.01	0.61
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.81	0.61
1:A:502:PRO:HA	1:A:597:ARG:NH1	2.15	0.61
1:B:238:LEU:HD23	1:B:238:LEU:C	2.20	0.61
2:E:101:PRO:HG2	2:E:104:ASP:HB2	1.82	0.61
1:C:238:LEU:HD23	1:C:239:SER:N	2.16	0.61
1:B:337:ALA:HB2	1:B:350:LEU:HD21	1.82	0.61
3:A:702:NAG:O3	3:A:702:NAG:H83	2.01	0.61
1:B:452:LEU:O	1:B:456:ILE:HG12	2.01	0.61
4:F:306:NAG:C3	4:F:307:NAG:H2	2.30	0.61
1:C:592:GLU:N	1:C:592:GLU:OE1	2.33	0.61
2:H:109:ARG:HG3	2:H:235:THR:CG2	2.31	0.61
1:A:294:HIS:HA	2:E:109:ARG:NH2	2.16	0.61
1:D:337:ALA:HB2	1:D:350:LEU:HD21	1.81	0.61
1:D:244:ALA:HB1	1:D:351:VAL:CG2	2.31	0.61
2:G:139:LEU:HD12	2:G:152:PHE:HB3	1.83	0.61
1:D:592:GLU:N	1:D:592:GLU:OE1	2.34	0.60
2:G:101:PRO:HG2	2:G:104:ASP:HB2	1.82	0.60
4:G:306:NAG:C3	4:G:307:NAG:H2	2.31	0.60
1:B:155:TYR:O	1:B:229:ASN:HB2	2.02	0.60
1:D:116:VAL:HG21	1:D:146:VAL:HA	1.83	0.60
2:F:139:LEU:HD12	2:F:152:PHE:HB3	1.84	0.60
2:F:125:VAL:O	2:F:247:GLY:HA3	2.02	0.60
2:F:82:HIS:HA	2:F:173:TYR:CE2	2.36	0.60
2:H:139:LEU:HD12	2:H:152:PHE:HB3	1.83	0.60
2:F:272:ALA:N	2:F:279:ILE:HD12	2.16	0.60
2:G:82:HIS:HA	2:G:173:TYR:CE2	2.37	0.60
1:B:234:VAL:HG12	1:B:238:LEU:HD12	1.84	0.60
1:B:65:ILE:HD11	1:B:67:LYS:HE2	1.83	0.60
1:D:238:LEU:C	1:D:238:LEU:HD23	2.22	0.59
4:E:306:NAG:H3	4:E:306:NAG:H83	1.84	0.59
2:F:184:ASN:ND2	4:F:306:NAG:H61	2.17	0.59
1:B:294:HIS:HB2	2:F:109:ARG:CZ	2.32	0.59
1:A:619:ARG:O	1:A:623:VAL:HG23	2.01	0.59
1:C:244:ALA:HB1	1:C:351:VAL:CG2	2.32	0.59
1:A:276:THR:HG23	1:A:311:ARG:HB2	1.84	0.59
1:C:234:VAL:HG12	1:C:238:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:184:ASN:ND2	4:E:306:NAG:H61	2.17	0.59
1:C:506:TYR:HB3	1:C:595:TRP:CZ2	2.37	0.59
1:C:238:LEU:HD23	1:C:238:LEU:C	2.22	0.59
2:F:188:GLN:HG3	2:F:194:VAL:HG22	1.84	0.59
1:B:619:ARG:O	1:B:623:VAL:HG23	2.03	0.59
2:G:188:GLN:HG3	2:G:194:VAL:HG22	1.85	0.59
1:B:506:TYR:HB3	1:B:595:TRP:CZ2	2.37	0.59
2:E:82:HIS:HA	2:E:173:TYR:CE2	2.37	0.59
1:C:350:LEU:O	1:C:350:LEU:HD23	2.03	0.59
1:B:131:LEU:HD12	1:B:131:LEU:N	2.17	0.59
2:E:139:LEU:HD12	2:E:152:PHE:HB3	1.84	0.59
2:H:188:GLN:HG3	2:H:194:VAL:HG22	1.85	0.59
1:A:506:TYR:HB3	1:A:595:TRP:CZ2	2.38	0.58
1:A:337:ALA:HB2	1:A:350:LEU:HD21	1.83	0.58
1:C:342:CYS:O	1:C:344:VAL:N	2.34	0.58
1:A:433:PHE:HE1	1:B:429:SER:O	1.85	0.58
1:A:342:CYS:O	1:A:344:VAL:N	2.36	0.58
1:D:633:LEU:C	1:D:635:ASN:N	2.56	0.58
1:C:244:ALA:HB1	1:C:351:VAL:HG21	1.84	0.58
1:D:342:CYS:O	1:D:344:VAL:N	2.35	0.58
1:B:329:PRO:HB3	1:B:379:VAL:HG11	1.85	0.58
1:B:244:ALA:HB1	1:B:351:VAL:HG21	1.86	0.58
2:E:125:VAL:O	2:E:247:GLY:HA3	2.03	0.58
1:D:466:ARG:NH1	1:D:466:ARG:HG2	2.19	0.58
1:B:132:PRO:HG2	1:B:135:PHE:HB2	1.86	0.58
1:B:244:ALA:HB1	1:B:351:VAL:CG2	2.34	0.58
1:D:426:VAL:O	1:D:472:ARG:HD2	2.03	0.58
1:C:71:ASN:OD1	1:C:73:ILE:HG13	2.03	0.58
2:F:109:ARG:HG3	2:F:235:THR:CG2	2.32	0.58
1:D:65:ILE:CD1	1:D:67:LYS:HE2	2.34	0.58
1:D:294:HIS:HA	2:H:109:ARG:NH2	2.19	0.58
1:C:466:ARG:HG2	1:C:466:ARG:NH1	2.19	0.58
1:A:244:ALA:HB1	1:A:351:VAL:CG2	2.34	0.58
4:G:306:NAG:H83	4:G:306:NAG:H3	1.86	0.58
1:B:198:TYR:CE1	1:B:279:GLY:HA2	2.39	0.58
1:D:244:ALA:HB1	1:D:351:VAL:HG21	1.85	0.57
1:C:337:ALA:HB2	1:C:350:LEU:HD21	1.85	0.57
2:E:272:ALA:N	2:E:279:ILE:HD12	2.18	0.57
1:A:238:LEU:HD23	1:A:238:LEU:C	2.23	0.57
1:D:329:PRO:HB3	1:D:379:VAL:HG11	1.84	0.57
1:C:155:TYR:O	1:C:229:ASN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:HD23	1:B:350:LEU:O	2.04	0.57
1:B:342:CYS:O	1:B:344:VAL:N	2.35	0.57
1:C:65:ILE:CD1	1:C:67:LYS:HE2	2.35	0.57
1:D:506:TYR:HB3	1:D:595:TRP:CZ2	2.40	0.57
1:A:540:PRO:HG3	1:A:546:CYS:O	2.05	0.57
4:F:306:NAG:H83	4:F:306:NAG:H3	1.86	0.57
2:E:188:GLN:HG3	2:E:194:VAL:HG22	1.84	0.57
2:H:196:GLU:HB3	2:H:198:TYR:HE1	1.70	0.57
1:A:409:GLN:OE1	1:A:522:ASP:HB3	2.05	0.57
2:H:82:HIS:HA	2:H:173:TYR:CE2	2.40	0.57
1:C:329:PRO:HB3	1:C:379:VAL:HG11	1.86	0.57
1:B:132:PRO:HG2	1:B:135:PHE:CB	2.35	0.57
1:A:329:PRO:HB3	1:A:379:VAL:HG11	1.85	0.57
1:D:203:SER:O	1:D:204:TYR:HB2	2.04	0.57
2:H:125:VAL:O	2:H:247:GLY:HA3	2.04	0.57
1:C:131:LEU:HD12	1:C:131:LEU:N	2.20	0.57
1:B:109:ASN:OD1	3:B:701:NAG:H2	2.05	0.57
1:C:116:VAL:HG21	1:C:146:VAL:HA	1.87	0.57
1:D:619:ARG:O	1:D:623:VAL:HG23	2.04	0.57
2:G:184:ASN:ND2	4:G:306:NAG:H61	2.19	0.57
1:A:244:ALA:HB1	1:A:351:VAL:HG21	1.86	0.57
1:A:132:PRO:HG2	1:A:135:PHE:HB2	1.86	0.57
1:A:155:TYR:O	1:A:229:ASN:HB2	2.05	0.57
1:A:87:ALA:HB3	1:A:99:GLU:HB2	1.86	0.57
1:D:132:PRO:HG2	1:D:135:PHE:HB2	1.87	0.56
1:C:132:PRO:HG2	1:C:135:PHE:HB2	1.87	0.56
1:C:87:ALA:HB3	1:C:99:GLU:HB2	1.86	0.56
2:H:137:ASP:HA	2:H:153:ASN:O	2.05	0.56
1:A:466:ARG:NH2	1:D:624:ASN:HD21	1.99	0.56
1:B:466:ARG:NH1	1:B:466:ARG:HG2	2.19	0.56
1:A:65:ILE:CD1	1:A:67:LYS:HE2	2.35	0.56
1:A:313:ILE:HA	1:A:404:MET:O	2.05	0.56
1:A:109:ASN:OD1	3:A:701:NAG:H2	2.05	0.56
1:D:155:TYR:O	1:D:229:ASN:HB2	2.05	0.56
1:A:624:ASN:ND2	1:D:466:ARG:NH2	2.51	0.56
1:A:466:ARG:NH1	1:A:466:ARG:HG2	2.20	0.56
1:A:433:PHE:CD1	1:B:433:PHE:HB2	2.40	0.56
1:A:131:LEU:HD12	1:A:131:LEU:N	2.21	0.56
1:A:71:ASN:OD1	1:A:73:ILE:HG13	2.05	0.56
1:D:74:LEU:HD13	1:D:216:VAL:HG13	1.87	0.56
1:C:540:PRO:HG3	1:C:546:CYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:109:ARG:HG3	2:E:235:THR:CG2	2.35	0.56
1:A:350:LEU:O	1:A:350:LEU:HD23	2.05	0.56
1:A:116:VAL:HG21	1:A:146:VAL:HA	1.87	0.56
1:B:116:VAL:HG21	1:B:146:VAL:HA	1.88	0.56
1:C:313:ILE:HA	1:C:404:MET:O	2.06	0.56
1:D:409:GLN:OE1	1:D:522:ASP:HB3	2.06	0.56
1:C:109:ASN:OD1	3:C:701:NAG:H2	2.05	0.56
1:A:132:PRO:HG2	1:A:135:PHE:CB	2.36	0.56
1:C:426:VAL:O	1:C:472:ARG:HD2	2.06	0.56
1:B:624:ASN:ND2	1:C:466:ARG:HH21	2.04	0.56
1:D:87:ALA:HB3	1:D:99:GLU:HB2	1.87	0.56
1:D:350:LEU:O	1:D:350:LEU:HD23	2.07	0.55
1:A:118:PRO:HA	1:A:149:GLN:OE1	2.06	0.55
1:D:74:LEU:CD1	1:D:216:VAL:HG13	2.36	0.55
2:G:128:ARG:HD2	2:G:250:GLN:HG2	1.88	0.55
1:A:62:ILE:HG22	1:A:108:ARG:HB3	1.89	0.55
2:H:173:TYR:HD1	2:H:174:HIS:H	1.55	0.55
1:B:276:THR:HG23	1:B:311:ARG:HB2	1.88	0.55
2:F:196:GLU:HB3	2:F:198:TYR:HE1	1.71	0.55
1:C:276:THR:HG23	1:C:311:ARG:HB2	1.88	0.55
1:B:71:ASN:OD1	1:B:73:ILE:HG13	2.06	0.55
1:A:125:ARG:O	1:A:125:ARG:HG3	2.05	0.55
2:G:196:GLU:HB3	2:G:198:TYR:HE1	1.71	0.55
1:C:118:PRO:HA	1:C:149:GLN:OE1	2.06	0.55
1:C:626:TRP:CE3	1:C:630:VAL:HG21	2.41	0.55
1:B:540:PRO:HG3	1:B:546:CYS:O	2.06	0.55
1:B:125:ARG:O	1:B:125:ARG:HG3	2.06	0.55
1:D:71:ASN:OD1	1:D:73:ILE:HG13	2.06	0.55
1:D:118:PRO:HA	1:D:149:GLN:OE1	2.06	0.55
1:A:230:TYR:CD1	1:A:254:LEU:HD21	2.42	0.55
1:B:372:TYR:HD2	1:B:442:LEU:CD2	2.20	0.55
1:D:313:ILE:HA	1:D:404:MET:O	2.06	0.55
4:E:306:NAG:O3	4:E:307:NAG:H2	2.06	0.55
1:D:131:LEU:HD12	1:D:131:LEU:N	2.21	0.55
1:D:62:ILE:HG22	1:D:108:ARG:HB3	1.88	0.55
1:D:372:TYR:HD2	1:D:442:LEU:CD2	2.19	0.55
1:B:65:ILE:CD1	1:B:67:LYS:HE2	2.36	0.55
1:A:198:TYR:CE1	1:A:279:GLY:HA2	2.42	0.55
1:A:372:TYR:HD2	1:A:442:LEU:CD2	2.19	0.55
1:B:203:SER:O	1:B:204:TYR:HB2	2.07	0.55
1:C:132:PRO:HG2	1:C:135:PHE:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLN:OE1	1:C:522:ASP:HB3	2.07	0.54
1:D:465:ASP:OD1	1:D:468:ASN:HB2	2.06	0.54
1:A:633:LEU:C	1:A:635:ASN:N	2.60	0.54
1:B:515:ASP:OD2	3:B:703:NAG:H62	2.07	0.54
1:C:515:ASP:OD2	3:C:703:NAG:H62	2.07	0.54
1:A:466:ARG:HH21	1:D:624:ASN:ND2	2.04	0.54
1:D:631:PRO:O	1:D:635:ASN:HB2	2.07	0.54
1:A:515:ASP:OD2	3:A:703:NAG:H62	2.08	0.54
1:B:192:PRO:HB2	1:B:271:ASP:HB2	1.89	0.54
2:E:128:ARG:HD2	2:E:250:GLN:HG2	1.88	0.54
1:B:465:ASP:OD1	1:B:468:ASN:HB2	2.07	0.54
1:C:387:ASP:HB3	1:C:392:LEU:HD21	1.90	0.54
1:C:631:PRO:O	1:C:635:ASN:HB2	2.07	0.54
1:D:259:ARG:NH1	1:D:259:ARG:HG3	2.22	0.54
4:E:306:NAG:C3	4:E:306:NAG:H83	2.38	0.54
1:C:372:TYR:HD2	1:C:442:LEU:CD2	2.20	0.54
1:C:192:PRO:HB2	1:C:271:ASP:HB2	1.90	0.54
1:A:192:PRO:HB2	1:A:271:ASP:HB2	1.90	0.54
2:H:173:TYR:CD1	2:H:174:HIS:N	2.72	0.54
1:C:125:ARG:HG3	1:C:125:ARG:O	2.06	0.54
1:C:62:ILE:HG22	1:C:108:ARG:HB3	1.90	0.54
1:C:203:SER:O	1:C:204:TYR:HB2	2.07	0.54
2:F:179:THR:HG22	2:F:186:THR:HB	1.89	0.54
2:E:196:GLU:HB3	2:E:198:TYR:HE1	1.73	0.54
1:D:398:PHE:N	2:H:236:ILE:HD12	2.23	0.54
2:E:137:ASP:HA	2:E:153:ASN:O	2.08	0.54
1:D:276:THR:HG23	1:D:311:ARG:HB2	1.88	0.54
1:C:346:ASP:HB2	1:D:346:ASP:HB2	1.89	0.54
2:G:173:TYR:CD1	2:G:174:HIS:N	2.73	0.54
1:D:125:ARG:O	1:D:125:ARG:HG3	2.08	0.54
1:A:426:VAL:O	1:A:472:ARG:HD2	2.08	0.53
1:B:118:PRO:HA	1:B:149:GLN:OE1	2.07	0.53
1:A:259:ARG:HG3	1:A:259:ARG:NH1	2.23	0.53
1:D:132:PRO:HG2	1:D:135:PHE:CB	2.38	0.53
1:B:407:VAL:HG21	1:B:486:VAL:HG22	1.91	0.53
1:A:221:GLY:O	1:A:222:ASN:HB3	2.09	0.53
1:A:203:SER:O	1:A:204:TYR:HB2	2.08	0.53
1:D:426:VAL:CG2	1:D:473:ARG:HB2	2.35	0.53
1:B:426:VAL:O	1:B:472:ARG:HD2	2.09	0.53
1:D:387:ASP:HB3	1:D:392:LEU:HD21	1.91	0.53
2:F:128:ARG:HD2	2:F:250:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HD13	1:C:216:VAL:HG13	1.90	0.53
1:C:230:TYR:CD1	1:C:254:LEU:HD21	2.44	0.53
1:B:87:ALA:HB3	1:B:99:GLU:HB2	1.89	0.53
1:A:387:ASP:HB3	1:A:392:LEU:HD21	1.91	0.53
1:C:259:ARG:NH1	1:C:259:ARG:HG3	2.22	0.53
1:B:313:ILE:HA	1:B:404:MET:O	2.08	0.53
1:B:611:LYS:HD2	1:B:611:LYS:N	2.23	0.53
1:B:62:ILE:HG22	1:B:108:ARG:HB3	1.91	0.53
2:G:173:TYR:HD1	2:G:174:HIS:H	1.55	0.53
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.24	0.53
1:A:631:PRO:O	1:A:635:ASN:HB2	2.09	0.53
2:F:109:ARG:HG3	2:F:235:THR:HG23	1.90	0.53
4:F:306:NAG:O3	4:F:307:NAG:H2	2.09	0.53
2:G:137:ASP:HA	2:G:153:ASN:O	2.09	0.53
1:D:230:TYR:CD1	1:D:254:LEU:HD21	2.43	0.53
2:F:179:THR:HB	2:F:186:THR:HG22	1.91	0.52
1:B:221:GLY:O	1:B:222:ASN:HB3	2.09	0.52
1:D:200:HIS:HB2	1:D:212:TYR:CE2	2.44	0.52
1:A:626:TRP:CE3	1:A:630:VAL:HG21	2.44	0.52
1:C:74:LEU:CD1	1:C:216:VAL:HG13	2.39	0.52
1:A:237:PHE:HB3	1:A:377:GLY:O	2.10	0.52
1:B:631:PRO:O	1:B:635:ASN:HB2	2.08	0.52
1:C:630:VAL:HB	1:C:631:PRO:HD3	1.92	0.52
1:B:294:HIS:HB2	2:F:109:ARG:NE	2.25	0.52
2:E:125:VAL:HG22	2:E:142:HIS:HB3	1.92	0.52
1:A:86:ALA:HA	1:A:101:PRO:HD3	1.90	0.52
1:C:409:GLN:HB2	1:C:509:TYR:CE2	2.44	0.52
1:B:409:GLN:OE1	1:B:522:ASP:HB3	2.10	0.52
2:H:128:ARG:HD2	2:H:250:GLN:HG2	1.91	0.52
1:C:537:MET:HG2	1:C:553:VAL:HG13	1.91	0.52
2:H:109:ARG:HG3	2:H:235:THR:HG23	1.92	0.52
1:A:409:GLN:HB2	1:A:509:TYR:CE2	2.45	0.52
2:F:137:ASP:HA	2:F:153:ASN:O	2.09	0.52
2:F:125:VAL:HG22	2:F:142:HIS:HB3	1.92	0.52
2:G:179:THR:HG22	2:G:186:THR:HB	1.92	0.52
1:A:574:GLN:HA	1:A:574:GLN:OE1	2.09	0.52
4:F:306:NAG:H83	4:F:307:NAG:H2	1.92	0.52
1:D:221:GLY:O	1:D:222:ASN:HB3	2.09	0.52
1:D:234:VAL:CG1	1:D:238:LEU:HD12	2.40	0.52
1:C:619:ARG:O	1:C:623:VAL:HG23	2.10	0.52
1:B:387:ASP:HB3	1:B:392:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:ARG:HG3	2:G:235:THR:CG2	2.39	0.52
1:C:198:TYR:CE1	1:C:279:GLY:HA2	2.45	0.51
1:C:221:GLY:O	1:C:222:ASN:HB3	2.10	0.51
1:A:465:ASP:OD1	1:A:468:ASN:HB2	2.11	0.51
1:C:86:ALA:HA	1:C:101:PRO:HD3	1.92	0.51
1:C:125:ARG:NH1	1:C:365:GLN:O	2.44	0.51
1:C:465:ASP:OD1	1:C:468:ASN:HB2	2.10	0.51
1:B:626:TRP:CE3	1:B:630:VAL:HG21	2.45	0.51
1:B:331:LYS:O	1:B:335:ILE:HG13	2.11	0.51
1:A:94:ARG:HG2	1:A:95:PHE:CD2	2.45	0.51
1:A:94:ARG:O	1:A:95:PHE:HB2	2.11	0.51
4:E:306:NAG:H83	4:E:307:NAG:H2	1.92	0.51
1:C:144:SER:HA	1:C:147:GLN:OE1	2.10	0.51
1:A:466:ARG:NH2	1:D:624:ASN:ND2	2.59	0.51
1:C:633:LEU:C	1:C:635:ASN:N	2.59	0.51
1:D:409:GLN:HB2	1:D:509:TYR:CE2	2.45	0.51
1:B:94:ARG:HG2	1:B:95:PHE:CD2	2.44	0.51
1:B:195:VAL:HG21	1:B:265:ILE:HG12	1.93	0.51
1:A:496:HIS:O	1:A:501:SER:HB2	2.11	0.51
2:F:173:TYR:HD1	2:F:174:HIS:H	1.56	0.51
1:D:540:PRO:HG3	1:D:546:CYS:O	2.10	0.51
4:F:306:NAG:H3	4:F:307:NAG:H2	1.93	0.51
1:B:409:GLN:HB2	1:B:509:TYR:CE2	2.46	0.51
1:B:86:ALA:HA	1:B:101:PRO:HD3	1.93	0.51
1:C:200:HIS:HB2	1:C:212:TYR:CE2	2.45	0.51
2:H:179:THR:HB	2:H:186:THR:HG22	1.92	0.51
1:D:144:SER:HA	1:D:147:GLN:OE1	2.11	0.51
4:G:306:NAG:C3	4:G:306:NAG:H83	2.41	0.51
2:F:196:GLU:HB3	2:F:198:TYR:CE1	2.46	0.51
1:D:86:ALA:HA	1:D:101:PRO:HD3	1.92	0.51
1:A:195:VAL:HG21	1:A:265:ILE:HG12	1.93	0.51
2:E:179:THR:HB	2:E:186:THR:HG22	1.93	0.51
1:B:630:VAL:HB	1:B:631:PRO:HD3	1.93	0.51
4:G:306:NAG:H3	4:G:307:NAG:H2	1.93	0.51
1:C:88:PRO:HG3	1:C:152:ASP:OD1	2.11	0.51
2:G:196:GLU:HB3	2:G:198:TYR:CE1	2.46	0.51
1:C:281:GLY:HA2	1:C:316:SER:O	2.10	0.51
1:C:226:ILE:HD11	1:C:265:ILE:HD13	1.92	0.51
1:D:198:TYR:CE1	1:D:279:GLY:HA2	2.46	0.50
2:H:196:GLU:HB3	2:H:198:TYR:CE1	2.46	0.50
2:F:179:THR:CG2	2:F:186:THR:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:HG2	1:C:95:PHE:CD2	2.46	0.50
1:B:119:GLN:OE1	1:B:206:GLU:HB2	2.11	0.50
1:A:281:GLY:HA2	1:A:316:SER:O	2.10	0.50
2:H:159:ILE:HD13	2:H:199:PRO:HG3	1.94	0.50
1:A:200:HIS:HB2	1:A:212:TYR:CE2	2.46	0.50
1:D:192:PRO:HB2	1:D:271:ASP:HB2	1.93	0.50
4:G:306:NAG:O3	4:G:307:NAG:H2	2.11	0.50
1:C:278:PHE:CB	1:C:313:ILE:HB	2.41	0.50
2:E:173:TYR:CD1	2:E:174:HIS:N	2.73	0.50
2:H:125:VAL:HG22	2:H:142:HIS:HB3	1.93	0.50
1:A:278:PHE:CB	1:A:313:ILE:HB	2.41	0.50
1:A:88:PRO:HG3	1:A:152:ASP:OD1	2.12	0.50
1:D:312:ALA:HB3	1:D:403:ILE:HD13	1.92	0.50
2:E:109:ARG:HG3	2:E:235:THR:HG23	1.93	0.50
2:F:173:TYR:CD1	2:F:174:HIS:N	2.74	0.50
1:A:234:VAL:CG1	1:A:238:LEU:HD12	2.41	0.50
1:A:74:LEU:CD1	1:A:216:VAL:HG13	2.42	0.50
1:C:574:GLN:OE1	1:C:574:GLN:HA	2.11	0.50
1:A:433:PHE:CE1	1:B:429:SER:O	2.65	0.50
1:A:125:ARG:NH1	1:A:365:GLN:O	2.45	0.50
1:C:195:VAL:HG21	1:C:265:ILE:HG12	1.94	0.50
1:B:237:PHE:HB3	1:B:377:GLY:O	2.12	0.50
1:B:609:GLY:O	1:B:612:PRO:HD3	2.11	0.50
1:C:94:ARG:O	1:C:95:PHE:HB2	2.12	0.50
1:D:574:GLN:OE1	1:D:574:GLN:HA	2.12	0.50
1:D:195:VAL:HG21	1:D:265:ILE:HG12	1.94	0.50
4:G:306:NAG:H83	4:G:307:NAG:H2	1.93	0.49
1:D:278:PHE:CB	1:D:313:ILE:HB	2.42	0.49
2:F:249:GLU:HB3	2:F:250:GLN:NE2	2.27	0.49
2:G:179:THR:CG2	2:G:186:THR:HB	2.42	0.49
1:D:226:ILE:HD11	1:D:265:ILE:HD13	1.94	0.49
1:D:88:PRO:HG3	1:D:152:ASP:OD1	2.11	0.49
2:G:287:LEU:HD12	2:G:288:VAL:N	2.26	0.49
1:A:278:PHE:HB2	1:A:313:ILE:HB	1.94	0.49
1:B:611:LYS:O	1:B:612:PRO:C	2.48	0.49
2:G:179:THR:HB	2:G:186:THR:HG22	1.94	0.49
2:E:179:THR:HG22	2:E:186:THR:HB	1.94	0.49
1:C:208:THR:C	1:C:210:ASN:H	2.14	0.49
1:A:556:SER:O	1:A:560:MET:HG3	2.12	0.49
1:C:556:SER:O	1:C:560:MET:HG3	2.13	0.49
1:A:294:HIS:HB2	2:E:109:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HD11	1:B:265:ILE:HD13	1.94	0.49
1:A:144:SER:HA	1:A:147:GLN:OE1	2.11	0.49
1:B:281:GLY:HA2	1:B:316:SER:O	2.12	0.49
1:D:137:ASN:HD22	1:D:516:GLN:HB3	1.78	0.49
2:G:125:VAL:HG22	2:G:142:HIS:HB3	1.93	0.49
4:F:306:NAG:C3	4:F:306:NAG:H83	2.42	0.49
1:B:230:TYR:CD1	1:B:254:LEU:HD21	2.48	0.49
1:D:119:GLN:OE1	1:D:206:GLU:HB2	2.13	0.49
1:B:208:THR:C	1:B:210:ASN:H	2.15	0.49
2:E:196:GLU:HB3	2:E:198:TYR:CE1	2.47	0.49
1:A:609:GLY:O	1:A:612:PRO:HD3	2.12	0.49
1:A:74:LEU:HD13	1:A:216:VAL:HG13	1.93	0.49
1:C:310:GLN:CD	1:C:310:GLN:N	2.66	0.49
1:D:94:ARG:HG2	1:D:95:PHE:CD2	2.48	0.49
1:B:574:GLN:HA	1:B:574:GLN:OE1	2.12	0.49
2:F:138:TYR:CD1	2:F:138:TYR:C	2.86	0.49
1:B:125:ARG:NH1	1:B:365:GLN:O	2.46	0.49
1:A:363:VAL:O	1:A:363:VAL:HG12	2.11	0.49
1:A:312:ALA:HB3	1:A:403:ILE:HD13	1.95	0.49
1:B:94:ARG:O	1:B:95:PHE:HB2	2.13	0.49
1:B:137:ASN:HD22	1:B:516:GLN:HB3	1.76	0.49
1:B:88:PRO:HG3	1:B:152:ASP:OD1	2.12	0.49
1:B:537:MET:HG2	1:B:553:VAL:HG13	1.94	0.49
1:A:143:SER:C	1:A:145:TYR:H	2.15	0.48
2:F:166:ALA:HB2	2:F:192:TRP:CE2	2.48	0.48
1:C:609:GLY:O	1:C:612:PRO:HD3	2.13	0.48
1:D:281:GLY:HA2	1:D:316:SER:O	2.13	0.48
1:A:630:VAL:HB	1:A:631:PRO:HD3	1.93	0.48
1:D:278:PHE:HB2	1:D:313:ILE:HB	1.95	0.48
2:F:97:THR:HG23	2:F:244:ILE:HG12	1.94	0.48
1:C:237:PHE:HB3	1:C:377:GLY:O	2.13	0.48
1:A:208:THR:C	1:A:210:ASN:H	2.15	0.48
1:D:143:SER:C	1:D:145:TYR:H	2.17	0.48
1:D:609:GLY:O	1:D:612:PRO:HD3	2.13	0.48
1:B:278:PHE:CB	1:B:313:ILE:HB	2.42	0.48
1:B:496:HIS:O	1:B:501:SER:HB2	2.13	0.48
1:D:537:MET:HG2	1:D:553:VAL:HG13	1.95	0.48
2:G:105:ARG:HB3	2:G:240:GLN:O	2.12	0.48
1:B:633:LEU:C	1:B:635:ASN:N	2.60	0.48
1:A:537:MET:HG2	1:A:553:VAL:HG13	1.95	0.48
1:D:415:PHE:HB2	1:D:480:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:THR:HG22	2:H:186:THR:HB	1.94	0.48
1:C:407:VAL:HG21	1:C:486:VAL:HG22	1.96	0.48
2:H:105:ARG:HB3	2:H:240:GLN:O	2.14	0.48
1:C:426:VAL:CG2	1:C:473:ARG:HB2	2.41	0.48
1:C:278:PHE:HB2	1:C:313:ILE:HB	1.95	0.48
1:C:118:PRO:CB	1:C:363:VAL:HG21	2.44	0.48
1:B:74:LEU:CD1	1:B:216:VAL:HG13	2.44	0.48
2:G:97:THR:HG23	2:G:244:ILE:HG12	1.96	0.48
1:B:325:VAL:C	1:B:374:ILE:HD11	2.34	0.48
1:D:331:LYS:O	1:D:335:ILE:HG13	2.14	0.48
2:H:166:ALA:HB2	2:H:192:TRP:CE2	2.49	0.48
3:D:702:NAG:O3	3:D:702:NAG:H83	2.14	0.48
1:B:69:LEU:N	1:B:69:LEU:HD12	2.29	0.48
1:A:137:ASN:HD22	1:A:516:GLN:HB3	1.79	0.48
1:D:237:PHE:HB3	1:D:377:GLY:O	2.14	0.48
1:B:200:HIS:HB2	1:B:212:TYR:CE2	2.48	0.48
2:E:173:TYR:HD1	2:E:174:HIS:H	1.55	0.48
2:G:197:ARG:C	2:G:198:TYR:HD1	2.17	0.48
1:C:611:LYS:N	1:C:611:LYS:HD2	2.28	0.48
1:D:496:HIS:O	1:D:501:SER:HB2	2.12	0.48
1:D:125:ARG:NH1	1:D:365:GLN:O	2.47	0.48
1:D:94:ARG:O	1:D:95:PHE:HB2	2.14	0.48
1:B:238:LEU:CD2	1:B:238:LEU:C	2.82	0.48
1:B:144:SER:HA	1:B:147:GLN:OE1	2.13	0.48
1:C:143:SER:C	1:C:145:TYR:H	2.18	0.48
1:A:310:GLN:CD	1:A:310:GLN:N	2.67	0.48
1:A:142:VAL:O	1:A:145:TYR:HB2	2.14	0.47
2:E:271:MET:HG2	2:E:276:ASP:OD2	2.14	0.47
2:G:129:VAL:HG13	2:G:243:ILE:HG12	1.96	0.47
1:B:556:SER:O	1:B:560:MET:HG3	2.14	0.47
1:B:228:VAL:HG12	1:B:229:ASN:N	2.29	0.47
1:B:131:LEU:HD12	1:B:131:LEU:H	1.79	0.47
1:B:405:LEU:N	1:B:405:LEU:HD23	2.28	0.47
1:D:633:LEU:O	1:D:635:ASN:N	2.47	0.47
1:D:142:VAL:O	1:D:145:TYR:HB2	2.14	0.47
2:H:135:LEU:CD1	2:H:239:SER:HB3	2.44	0.47
1:D:208:THR:C	1:D:210:ASN:H	2.17	0.47
2:F:135:LEU:CD1	2:F:239:SER:HB3	2.44	0.47
1:A:119:GLN:OE1	1:A:206:GLU:HB2	2.13	0.47
1:C:363:VAL:O	1:C:363:VAL:HG12	2.15	0.47
1:B:143:SER:C	1:B:145:TYR:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:129:VAL:HG13	2:E:243:ILE:HG12	1.96	0.47
1:B:198:TYR:HB2	1:B:278:PHE:CE2	2.50	0.47
2:G:109:ARG:HG3	2:G:235:THR:HG23	1.95	0.47
2:E:179:THR:CG2	2:E:186:THR:HB	2.45	0.47
2:E:131:SER:O	2:E:132:SER:C	2.52	0.47
1:D:630:VAL:HB	1:D:631:PRO:HD3	1.95	0.47
1:D:325:VAL:C	1:D:374:ILE:HD11	2.34	0.47
1:B:228:VAL:CG1	1:B:229:ASN:N	2.78	0.47
1:C:228:VAL:HG12	1:C:229:ASN:N	2.30	0.47
1:C:131:LEU:HD23	1:C:135:PHE:CE1	2.50	0.47
2:G:159:ILE:HD13	2:G:199:PRO:HG3	1.97	0.47
1:D:556:SER:O	1:D:560:MET:HG3	2.14	0.47
2:E:94:GLY:HA3	2:E:285:VAL:CG2	2.44	0.47
1:A:228:VAL:HG12	1:A:229:ASN:N	2.29	0.47
1:C:198:TYR:HB2	1:C:278:PHE:CE2	2.50	0.47
1:B:74:LEU:HD13	1:B:216:VAL:HG13	1.95	0.47
2:F:197:ARG:C	2:F:198:TYR:HD1	2.18	0.47
1:A:226:ILE:HD11	1:A:265:ILE:HD13	1.97	0.47
1:A:325:VAL:C	1:A:374:ILE:HD11	2.35	0.47
2:F:129:VAL:HG13	2:F:243:ILE:HG12	1.97	0.47
4:E:306:NAG:H3	4:E:307:NAG:H2	1.94	0.47
2:G:249:GLU:HB3	2:G:250:GLN:NE2	2.30	0.47
2:G:166:ALA:HB2	2:G:192:TRP:CE2	2.49	0.47
2:H:129:VAL:HG13	2:H:243:ILE:HG12	1.96	0.47
1:C:137:ASN:HD22	1:C:516:GLN:HB3	1.80	0.47
1:C:126:LEU:HD21	1:C:139:LEU:HD21	1.97	0.47
1:C:194:PRO:HG3	1:C:274:ARG:CZ	2.44	0.47
2:G:94:GLY:HA3	2:G:285:VAL:CG2	2.45	0.47
2:E:197:ARG:C	2:E:198:TYR:HD1	2.19	0.46
2:F:94:GLY:HA3	2:F:285:VAL:CG2	2.45	0.46
1:C:119:GLN:OE1	1:C:206:GLU:HB2	2.14	0.46
1:D:486:VAL:O	1:D:490:VAL:HG23	2.15	0.46
1:C:331:LYS:O	1:C:335:ILE:HG13	2.15	0.46
1:D:428:ALA:HA	1:D:472:ARG:HD3	1.97	0.46
1:B:84:PRO:HB3	1:B:155:TYR:CE2	2.51	0.46
1:C:228:VAL:CG1	1:C:229:ASN:N	2.78	0.46
1:B:142:VAL:O	1:B:145:TYR:HB2	2.14	0.46
2:H:271:MET:HG2	2:H:276:ASP:OD2	2.15	0.46
1:B:282:ALA:O	1:B:285:SER:HB2	2.14	0.46
1:D:238:LEU:CD2	1:D:238:LEU:C	2.84	0.46
2:E:97:THR:HG23	2:E:244:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:CB	1:A:363:VAL:HG21	2.45	0.46
1:B:312:ALA:HB3	1:B:403:ILE:HD13	1.97	0.46
2:E:105:ARG:HB3	2:E:240:GLN:O	2.15	0.46
1:A:52:ASP:HA	1:A:53:PRO:HD3	1.68	0.46
2:H:131:SER:O	2:H:132:SER:C	2.53	0.46
1:C:325:VAL:C	1:C:374:ILE:HD11	2.36	0.46
1:A:126:LEU:HD21	1:A:139:LEU:HD21	1.97	0.46
1:B:278:PHE:HB2	1:B:313:ILE:HB	1.97	0.46
1:A:228:VAL:CG1	1:A:229:ASN:N	2.79	0.46
1:C:415:PHE:HB2	1:C:480:PHE:CD2	2.51	0.46
2:H:197:ARG:C	2:H:198:TYR:HD1	2.19	0.46
1:D:198:TYR:HB2	1:D:278:PHE:CE2	2.51	0.46
1:D:372:TYR:CD2	1:D:442:LEU:CD2	2.98	0.46
1:D:611:LYS:N	1:D:611:LYS:HD2	2.30	0.46
2:H:94:GLY:HA3	2:H:285:VAL:CG2	2.46	0.46
2:G:123:GLU:O	2:G:124:ALA:HB2	2.16	0.46
1:C:156:LEU:HD12	1:C:156:LEU:C	2.35	0.46
2:F:179:THR:HB	2:F:186:THR:CG2	2.46	0.46
1:D:126:LEU:HD21	1:D:139:LEU:HD21	1.97	0.46
1:D:310:GLN:CD	1:D:310:GLN:N	2.69	0.46
1:C:240:THR:OG1	1:C:244:ALA:HB3	2.16	0.46
1:B:126:LEU:HD21	1:B:139:LEU:HD21	1.98	0.46
2:F:271:MET:HG2	2:F:276:ASP:OD2	2.16	0.46
2:F:131:SER:O	2:F:132:SER:C	2.53	0.46
1:B:310:GLN:N	1:B:310:GLN:CD	2.69	0.46
1:B:118:PRO:CB	1:B:363:VAL:HG21	2.46	0.46
2:H:179:THR:CG2	2:H:186:THR:HB	2.45	0.46
1:B:156:LEU:HD12	1:B:156:LEU:C	2.37	0.46
1:A:407:VAL:HG21	1:A:486:VAL:HG22	1.98	0.46
1:B:344:VAL:HG21	1:B:349:GLU:HB2	1.98	0.45
1:A:131:LEU:H	1:A:131:LEU:HD12	1.80	0.45
1:A:331:LYS:O	1:A:335:ILE:HG13	2.14	0.45
2:E:135:LEU:CD1	2:E:239:SER:HB3	2.45	0.45
2:G:131:SER:O	2:G:132:SER:C	2.54	0.45
1:D:203:SER:O	1:D:204:TYR:CB	2.63	0.45
1:A:238:LEU:C	1:A:238:LEU:CD2	2.85	0.45
1:C:239:SER:HB3	1:C:329:PRO:HB2	1.99	0.45
1:C:84:PRO:HB3	1:C:155:TYR:CE2	2.51	0.45
1:D:312:ALA:HB3	1:D:403:ILE:CD1	2.46	0.45
1:C:69:LEU:N	1:C:69:LEU:HD12	2.32	0.45
2:G:138:TYR:CD1	2:G:138:TYR:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:CG2	1:A:473:ARG:HB2	2.44	0.45
2:G:272:ALA:HA	2:G:279:ILE:HG21	1.99	0.45
2:H:272:ALA:HA	2:H:279:ILE:HG21	1.99	0.45
1:C:238:LEU:CD2	1:C:238:LEU:C	2.84	0.45
1:D:118:PRO:CB	1:D:363:VAL:HG21	2.46	0.45
1:D:611:LYS:O	1:D:612:PRO:C	2.54	0.45
2:E:192:TRP:HB3	2:E:193:PRO:HD2	1.98	0.45
2:G:271:MET:HG2	2:G:276:ASP:OD2	2.16	0.45
1:D:228:VAL:HG12	1:D:229:ASN:N	2.31	0.45
1:B:68:GLU:C	1:B:69:LEU:HD12	2.37	0.45
1:B:239:SER:HB3	1:B:329:PRO:HB2	1.98	0.45
1:C:344:VAL:HG21	1:C:349:GLU:HB2	1.98	0.45
1:A:198:TYR:HB2	1:A:278:PHE:CE2	2.51	0.45
1:A:372:TYR:CD2	1:A:442:LEU:CD2	2.99	0.45
1:B:363:VAL:HG12	1:B:363:VAL:O	2.17	0.45
2:G:111:ASP:OD2	2:G:180:ARG:NE	2.47	0.45
1:B:240:THR:OG1	1:B:244:ALA:HB3	2.16	0.45
2:F:272:ALA:HA	2:F:279:ILE:HG21	1.98	0.45
1:C:387:ASP:CB	1:C:392:LEU:HD21	2.47	0.45
2:E:179:THR:HB	2:E:186:THR:CG2	2.47	0.45
1:C:208:THR:C	1:C:210:ASN:N	2.70	0.45
2:G:192:TRP:HB3	2:G:193:PRO:HD2	1.99	0.45
1:A:530:PRO:HB3	1:A:544:PHE:CD1	2.52	0.45
1:B:576:VAL:O	1:B:576:VAL:HG12	2.16	0.45
2:F:266:LEU:HA	2:F:266:LEU:HD23	1.81	0.45
1:D:156:LEU:HD12	1:D:156:LEU:C	2.37	0.45
1:C:234:VAL:CG1	1:C:238:LEU:HD12	2.46	0.45
2:F:123:GLU:O	2:F:124:ALA:HB2	2.17	0.45
1:C:463:TRP:C	1:C:465:ASP:H	2.20	0.45
2:H:95:GLN:HA	2:H:245:ILE:O	2.17	0.45
2:F:105:ARG:HB3	2:F:240:GLN:O	2.17	0.45
2:H:123:GLU:O	2:H:124:ALA:HB2	2.17	0.45
1:A:428:ALA:HA	1:A:472:ARG:HD3	1.99	0.44
1:D:69:LEU:N	1:D:69:LEU:HD12	2.32	0.44
1:C:312:ALA:HB3	1:C:403:ILE:HD13	1.97	0.44
1:C:500:GLY:HA3	2:G:239:SER:HB2	1.99	0.44
1:C:52:ASP:HA	1:C:53:PRO:HD3	1.68	0.44
1:B:415:PHE:HB2	1:B:480:PHE:CD2	2.52	0.44
2:E:249:GLU:HB3	2:E:250:GLN:NE2	2.32	0.44
1:A:60:GLY:HA3	1:A:104:TRP:NE1	2.32	0.44
1:A:69:LEU:N	1:A:69:LEU:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:HIS:O	1:D:469:PRO:HD3	2.17	0.44
1:D:194:PRO:HG3	1:D:274:ARG:CZ	2.47	0.44
2:G:272:ALA:HB2	2:G:279:ILE:HD13	1.99	0.44
1:C:372:TYR:CD2	1:C:442:LEU:CD2	2.99	0.44
2:F:192:TRP:HB3	2:F:193:PRO:HD2	1.98	0.44
1:D:331:LYS:HE3	1:D:332:TYR:CZ	2.53	0.44
1:A:416:VAL:C	1:A:418:ASN:N	2.71	0.44
2:H:97:THR:HG23	2:H:244:ILE:HG12	1.99	0.44
1:D:136:THR:C	1:D:138:ASN:H	2.21	0.44
2:E:123:GLU:O	2:E:124:ALA:HB2	2.16	0.44
2:E:138:TYR:CD1	2:E:138:TYR:C	2.91	0.44
1:D:282:ALA:O	1:D:285:SER:HB2	2.18	0.44
1:A:456:ILE:HD12	1:A:626:TRP:CH2	2.53	0.44
1:C:428:ALA:HA	1:C:472:ARG:HD3	2.00	0.44
1:D:228:VAL:CG1	1:D:229:ASN:N	2.80	0.44
1:C:208:THR:O	1:C:208:THR:HG23	2.17	0.44
1:A:405:LEU:HD23	1:A:405:LEU:N	2.32	0.44
1:B:137:ASN:O	1:B:138:ASN:HB2	2.16	0.44
1:D:113:PHE:HB3	1:D:210:ASN:ND2	2.33	0.44
1:B:186:ILE:HD12	1:B:188:ASP:OD1	2.18	0.44
1:A:363:VAL:CG1	1:A:363:VAL:O	2.65	0.44
1:B:208:THR:HG23	1:B:208:THR:O	2.16	0.44
1:B:136:THR:C	1:B:138:ASN:H	2.21	0.44
2:G:135:LEU:CD1	2:G:239:SER:HB3	2.47	0.44
2:H:176:VAL:CG2	2:H:187:LEU:HD11	2.48	0.44
2:E:95:GLN:HA	2:E:245:ILE:O	2.18	0.44
1:D:344:VAL:HG21	1:D:349:GLU:HB2	2.00	0.44
1:D:560:MET:O	1:D:564:THR:HG23	2.18	0.44
1:C:405:LEU:HD23	1:C:405:LEU:N	2.32	0.44
2:F:176:VAL:CG2	2:F:187:LEU:HD11	2.48	0.44
1:C:416:VAL:C	1:C:418:ASN:N	2.70	0.44
1:B:60:GLY:HA3	1:B:104:TRP:NE1	2.33	0.44
1:A:136:THR:C	1:A:138:ASN:H	2.21	0.44
2:E:287:LEU:HD12	2:E:288:VAL:N	2.27	0.44
2:H:287:LEU:HD12	2:H:288:VAL:N	2.30	0.44
1:D:84:PRO:HB3	1:D:155:TYR:CE2	2.53	0.44
1:B:372:TYR:CD2	1:B:442:LEU:CD2	3.00	0.44
1:A:203:SER:O	1:A:204:TYR:CB	2.66	0.44
1:C:113:PHE:HB3	1:C:210:ASN:ND2	2.32	0.44
1:B:405:LEU:CD2	1:B:405:LEU:N	2.81	0.44
2:E:94:GLY:HA3	2:E:285:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:C	1:C:138:ASN:H	2.21	0.44
2:E:166:ALA:HB2	2:E:192:TRP:CE2	2.53	0.44
2:G:95:GLN:HA	2:G:245:ILE:O	2.18	0.44
2:H:138:TYR:CD1	2:H:138:TYR:C	2.91	0.44
2:H:269:LEU:HA	2:H:269:LEU:HD23	1.87	0.44
1:A:415:PHE:HB2	1:A:480:PHE:CD2	2.53	0.44
1:C:60:GLY:HA3	1:C:104:TRP:NE1	2.33	0.44
1:B:416:VAL:C	1:B:418:ASN:N	2.71	0.44
1:B:61:LYS:HB2	1:B:107:ILE:HG12	2.00	0.44
1:C:605:TYR:CZ	1:C:615:LYS:HB2	2.53	0.44
1:D:109:ASN:OD1	3:D:701:NAG:H2	2.16	0.44
2:H:87:TYR:CE1	2:H:287:LEU:HD13	2.53	0.44
1:D:326:SER:O	1:D:379:VAL:HG12	2.17	0.44
1:C:131:LEU:H	1:C:131:LEU:HD12	1.81	0.44
2:G:179:THR:HB	2:G:186:THR:CG2	2.48	0.44
1:A:611:LYS:O	1:A:612:PRO:C	2.55	0.44
2:H:105:ARG:HD3	2:H:241:ALA:HB2	2.00	0.44
1:D:416:VAL:C	1:D:418:ASN:N	2.70	0.44
1:D:236:GLY:O	1:D:249:TYR:HB2	2.17	0.44
1:A:156:LEU:HD12	1:A:156:LEU:C	2.38	0.44
1:A:239:SER:HB3	1:A:329:PRO:HB2	1.98	0.43
1:B:203:SER:O	1:B:204:TYR:CB	2.66	0.43
1:D:463:TRP:C	1:D:465:ASP:H	2.21	0.43
1:D:212:TYR:O	1:D:227:THR:HG21	2.17	0.43
1:C:403:ILE:HG22	1:C:405:LEU:HD22	2.00	0.43
2:E:159:ILE:HD13	2:E:199:PRO:HG3	2.00	0.43
1:A:282:ALA:O	1:A:285:SER:HB2	2.18	0.43
2:E:176:VAL:CG2	2:E:187:LEU:HD11	2.47	0.43
2:F:287:LEU:HD12	2:F:288:VAL:N	2.28	0.43
2:H:249:GLU:HB3	2:H:250:GLN:NE2	2.33	0.43
1:D:403:ILE:HG22	1:D:405:LEU:HD22	1.99	0.43
1:D:335:ILE:O	1:D:339:LYS:HG3	2.18	0.43
1:D:385:ILE:HA	1:D:386:PRO:HD2	1.81	0.43
1:C:496:HIS:O	1:C:501:SER:HB2	2.18	0.43
2:H:272:ALA:HB2	2:H:279:ILE:HD13	1.99	0.43
1:B:131:LEU:HD23	1:B:135:PHE:CE1	2.53	0.43
1:A:208:THR:HG23	1:A:208:THR:O	2.18	0.43
1:C:142:VAL:O	1:C:145:TYR:HB2	2.17	0.43
1:A:68:GLU:C	1:A:69:LEU:HD12	2.39	0.43
1:C:236:GLY:O	1:C:249:TYR:HB2	2.19	0.43
1:A:186:ILE:HD12	1:A:188:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASP:HB3	1:B:392:LEU:CD2	2.49	0.43
1:A:208:THR:C	1:A:210:ASN:N	2.70	0.43
1:C:387:ASP:HB3	1:C:392:LEU:CD2	2.48	0.43
1:B:208:THR:C	1:B:210:ASN:N	2.72	0.43
1:D:536:PRO:HB2	1:D:553:VAL:HA	2.00	0.43
2:E:111:ASP:OD2	2:E:180:ARG:NE	2.48	0.43
1:C:530:PRO:HB3	1:C:544:PHE:CD1	2.54	0.43
2:F:159:ILE:HD13	2:F:199:PRO:HG3	2.00	0.43
1:B:624:ASN:ND2	1:C:466:ARG:NH2	2.66	0.43
1:D:122:ILE:HG13	1:D:123:ASP:H	1.83	0.43
1:C:611:LYS:O	1:C:612:PRO:C	2.56	0.43
1:B:326:SER:O	1:B:379:VAL:HG12	2.18	0.43
1:B:71:ASN:OD1	1:B:72:GLU:N	2.51	0.43
1:A:387:ASP:HB3	1:A:392:LEU:CD2	2.49	0.43
1:C:536:PRO:HB2	1:C:553:VAL:HA	2.01	0.43
1:A:335:ILE:O	1:A:339:LYS:HG3	2.18	0.43
1:B:529:VAL:N	1:B:530:PRO:HD2	2.34	0.43
1:A:455:THR:O	1:A:459:MET:HG2	2.19	0.43
1:D:456:ILE:HD12	1:D:626:TRP:CH2	2.54	0.43
1:C:633:LEU:O	1:C:635:ASN:N	2.52	0.43
1:C:186:ILE:HD12	1:C:188:ASP:OD1	2.19	0.43
1:A:122:ILE:HG13	1:A:123:ASP:H	1.84	0.43
1:D:186:ILE:HD12	1:D:188:ASP:OD1	2.19	0.43
1:B:463:TRP:C	1:B:465:ASP:H	2.22	0.43
1:A:463:TRP:C	1:A:465:ASP:H	2.22	0.43
1:B:194:PRO:HG3	1:B:274:ARG:CZ	2.49	0.43
1:D:244:ALA:HB1	1:D:351:VAL:HG23	2.00	0.43
1:A:113:PHE:HB3	1:A:210:ASN:ND2	2.33	0.43
1:D:605:TYR:CZ	1:D:615:LYS:HB2	2.53	0.43
1:B:385:ILE:HA	1:B:386:PRO:HD2	1.81	0.43
1:A:240:THR:OG1	1:A:244:ALA:HB3	2.18	0.43
2:E:272:ALA:HA	2:E:279:ILE:HG21	2.01	0.43
1:B:113:PHE:HB3	1:B:210:ASN:ND2	2.33	0.43
1:A:611:LYS:N	1:A:611:LYS:HD2	2.34	0.43
1:B:565:ASN:HB3	1:B:574:GLN:O	2.19	0.43
1:A:497:SER:C	1:A:499:PHE:H	2.22	0.43
2:H:272:ALA:CB	2:H:279:ILE:HG21	2.49	0.42
2:H:192:TRP:HB3	2:H:193:PRO:HD2	1.99	0.42
2:G:94:GLY:HA3	2:G:285:VAL:HG22	2.00	0.42
1:D:407:VAL:HG21	1:D:486:VAL:HG22	2.00	0.42
1:C:282:ALA:O	1:C:285:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:234:LEU:HA	2:F:234:LEU:HD23	1.91	0.42
1:C:68:GLU:C	1:C:69:LEU:HD12	2.39	0.42
2:G:135:LEU:H	2:G:135:LEU:HG	1.55	0.42
2:F:155:GLY:C	2:F:234:LEU:HD12	2.40	0.42
2:F:261:LEU:HD12	2:F:262:TYR:N	2.34	0.42
1:D:61:LYS:HB2	1:D:107:ILE:HG12	2.00	0.42
2:E:88:ILE:HG12	2:E:257:GLN:CG	2.44	0.42
1:B:592:GLU:N	1:B:592:GLU:CD	2.71	0.42
1:B:331:LYS:HE3	1:B:332:TYR:CZ	2.54	0.42
1:D:68:GLU:C	1:D:69:LEU:HD12	2.40	0.42
1:A:605:TYR:CZ	1:A:615:LYS:HB2	2.54	0.42
1:B:236:GLY:O	1:B:249:TYR:HB2	2.19	0.42
2:G:269:LEU:HD23	2:G:269:LEU:HA	1.88	0.42
1:D:626:TRP:CE3	1:D:630:VAL:HG21	2.53	0.42
1:C:469:PRO:HA	1:C:472:ARG:NH1	2.35	0.42
1:B:428:ALA:HA	1:B:472:ARG:HD3	2.00	0.42
1:B:633:LEU:O	1:B:635:ASN:N	2.52	0.42
1:D:485:TRP:O	1:D:488:PRO:HD2	2.19	0.42
1:B:485:TRP:O	1:B:488:PRO:HD2	2.18	0.42
1:A:344:VAL:HG21	1:A:349:GLU:HB2	2.01	0.42
1:C:118:PRO:HB3	1:C:363:VAL:HG21	2.01	0.42
1:D:363:VAL:O	1:D:363:VAL:HG12	2.18	0.42
1:D:387:ASP:HB3	1:D:392:LEU:CD2	2.48	0.42
1:A:497:SER:C	1:A:499:PHE:N	2.73	0.42
1:B:426:VAL:CG2	1:B:473:ARG:HB2	2.41	0.42
1:C:326:SER:O	1:C:379:VAL:HG12	2.19	0.42
1:A:131:LEU:HD23	1:A:135:PHE:CE1	2.54	0.42
1:D:131:LEU:HD12	1:D:131:LEU:H	1.82	0.42
2:F:272:ALA:HB2	2:F:279:ILE:HD13	2.02	0.42
1:D:131:LEU:HD23	1:D:135:PHE:CE1	2.55	0.42
2:H:179:THR:HB	2:H:186:THR:CG2	2.48	0.42
1:D:565:ASN:HB3	1:D:574:GLN:O	2.20	0.42
1:A:312:ALA:HB3	1:A:403:ILE:CD1	2.50	0.42
1:C:405:LEU:O	1:C:505:PHE:HA	2.20	0.42
2:E:155:GLY:C	2:E:234:LEU:HD12	2.40	0.42
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.83	0.42
1:A:294:HIS:HB2	2:E:109:ARG:NE	2.34	0.42
1:C:203:SER:O	1:C:204:TYR:CB	2.66	0.42
1:C:536:PRO:O	1:C:553:VAL:HG22	2.20	0.42
1:B:536:PRO:HB2	1:B:553:VAL:HA	2.02	0.42
1:B:358:PRO:HD2	1:B:361:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:GLY:HA3	2:H:285:VAL:HG22	2.01	0.42
1:C:635:ASN:C	1:C:636:LEU:HG	2.40	0.42
1:D:239:SER:HB3	1:D:329:PRO:HB2	2.01	0.42
1:A:118:PRO:HB3	1:A:363:VAL:HG21	2.02	0.42
1:C:113:PHE:HB3	1:C:210:ASN:HD22	1.85	0.42
2:F:94:GLY:HA3	2:F:285:VAL:HG22	2.02	0.42
2:G:88:ILE:HG12	2:G:257:GLN:CG	2.45	0.42
2:F:87:TYR:CE1	2:F:287:LEU:HD13	2.55	0.42
1:B:540:PRO:HB3	1:B:545:PRO:O	2.20	0.42
1:B:122:ILE:HG13	1:B:123:ASP:H	1.85	0.42
1:B:132:PRO:HG2	1:B:135:PHE:HB3	2.02	0.42
1:B:387:ASP:CB	1:B:392:LEU:HD21	2.50	0.42
1:A:560:MET:O	1:A:564:THR:HG23	2.20	0.42
1:B:312:ALA:HB3	1:B:403:ILE:CD1	2.50	0.42
1:C:335:ILE:O	1:C:339:LYS:HG3	2.19	0.42
1:C:529:VAL:N	1:C:530:PRO:HD2	2.34	0.42
1:A:633:LEU:O	1:A:635:ASN:N	2.52	0.41
1:C:540:PRO:HB3	1:C:545:PRO:O	2.20	0.41
2:E:87:TYR:CE1	2:E:287:LEU:HD13	2.54	0.41
1:A:326:SER:O	1:A:379:VAL:HG12	2.19	0.41
1:C:312:ALA:HB3	1:C:403:ILE:CD1	2.50	0.41
2:F:95:GLN:HA	2:F:245:ILE:O	2.20	0.41
1:C:141:VAL:HG21	1:C:542:GLU:O	2.19	0.41
1:D:359:TYR:C	1:D:359:TYR:CD1	2.94	0.41
1:C:61:LYS:HB2	1:C:107:ILE:HG12	2.01	0.41
1:D:186:ILE:HG23	1:D:186:ILE:O	2.20	0.41
1:A:485:TRP:O	1:A:488:PRO:HD2	2.20	0.41
2:F:272:ALA:CB	2:F:279:ILE:HG21	2.50	0.41
1:D:387:ASP:CB	1:D:392:LEU:HD21	2.49	0.41
1:A:497:SER:O	1:A:499:PHE:N	2.53	0.41
2:G:176:VAL:CG2	2:G:187:LEU:HD11	2.50	0.41
1:A:194:PRO:HG3	1:A:274:ARG:CZ	2.50	0.41
1:B:438:PHE:C	1:B:438:PHE:CD2	2.93	0.41
1:D:405:LEU:O	1:D:505:PHE:HA	2.20	0.41
1:C:137:ASN:O	1:C:138:ASN:HB2	2.20	0.41
1:A:129:VAL:HG23	1:A:130:MET:N	2.34	0.41
1:D:438:PHE:C	1:D:438:PHE:CD2	2.93	0.41
2:G:272:ALA:CB	2:G:279:ILE:HG21	2.50	0.41
1:B:234:VAL:CG1	1:B:238:LEU:HD12	2.47	0.41
1:B:212:TYR:O	1:B:227:THR:HG21	2.20	0.41
1:B:403:ILE:HG22	1:B:405:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:PRO:HB3	1:B:544:PHE:CD1	2.55	0.41
1:D:60:GLY:HA3	1:D:104:TRP:NE1	2.35	0.41
2:H:111:ASP:OD2	2:H:180:ARG:NE	2.51	0.41
1:C:625:LEU:O	1:C:630:VAL:HG23	2.20	0.41
1:A:271:ASP:HA	1:A:272:PRO:HD2	1.94	0.41
1:D:157:ASN:O	1:D:226:ILE:HA	2.20	0.41
1:B:535:ILE:HB	1:B:536:PRO:HD3	2.02	0.41
1:D:208:THR:O	1:D:208:THR:HG23	2.19	0.41
1:A:61:LYS:HB2	1:A:107:ILE:HG12	2.03	0.41
1:B:467:HIS:O	1:B:469:PRO:HD3	2.21	0.41
1:C:438:PHE:C	1:C:438:PHE:CD2	2.94	0.41
2:G:137:ASP:OD1	2:G:154:VAL:C	2.59	0.41
1:A:403:ILE:HG22	1:A:405:LEU:HD22	2.03	0.41
1:B:93:HIS:O	1:B:96:GLN:HB2	2.21	0.41
1:C:456:ILE:HD12	1:C:626:TRP:CH2	2.56	0.41
2:H:137:ASP:OD1	2:H:154:VAL:C	2.59	0.41
1:D:536:PRO:O	1:D:553:VAL:HG22	2.20	0.41
1:A:93:HIS:O	1:A:96:GLN:HB2	2.21	0.41
1:C:467:HIS:O	1:C:469:PRO:HD3	2.21	0.41
1:B:186:ILE:O	1:B:186:ILE:HG23	2.21	0.41
1:A:397:GLU:OE1	2:E:235:THR:HB	2.20	0.41
1:B:605:TYR:CZ	1:B:615:LYS:HB2	2.56	0.41
1:C:122:ILE:HG13	1:C:123:ASP:H	1.86	0.41
1:B:294:HIS:HA	2:F:109:ARG:CZ	2.51	0.41
1:A:540:PRO:HB3	1:A:545:PRO:O	2.20	0.41
1:A:84:PRO:HB3	1:A:155:TYR:CE2	2.55	0.41
1:D:409:GLN:HB2	1:D:509:TYR:CD2	2.56	0.41
1:C:535:ILE:HB	1:C:536:PRO:HD3	2.03	0.41
1:B:113:PHE:HB3	1:B:210:ASN:HD22	1.86	0.41
1:A:405:LEU:O	1:A:505:PHE:HA	2.21	0.41
2:H:190:ASP:OD2	2:H:192:TRP:HZ3	2.04	0.41
1:B:212:TYR:CD2	1:B:212:TYR:N	2.89	0.41
1:D:208:THR:C	1:D:210:ASN:N	2.74	0.41
1:C:497:SER:C	1:C:499:PHE:H	2.24	0.41
1:D:498:ASN:CG	1:D:498:ASN:O	2.59	0.41
1:D:530:PRO:HB3	1:D:544:PHE:CD1	2.55	0.41
2:F:156:THR:HG22	2:F:157:ASP:N	2.36	0.41
2:G:155:GLY:C	2:G:234:LEU:HD12	2.41	0.41
2:H:155:GLY:HA3	2:H:234:LEU:CD1	2.51	0.41
1:B:52:ASP:HA	1:B:53:PRO:HD3	1.70	0.41
1:A:438:PHE:CD2	1:A:438:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PRO:HD2	1:D:361:GLU:OE2	2.21	0.41
1:A:628:GLU:C	1:A:631:PRO:HD2	2.42	0.41
1:C:271:ASP:HA	1:C:272:PRO:HD2	1.95	0.41
1:A:387:ASP:CB	1:A:392:LEU:HD21	2.51	0.41
1:D:63:ARG:NH2	1:D:107:ILE:HG21	2.36	0.41
1:A:535:ILE:HB	1:A:536:PRO:HD3	2.02	0.41
1:A:358:PRO:HD2	1:A:361:GLU:OE2	2.21	0.41
1:C:242:ASP:OD1	1:C:347:THR:HG21	2.21	0.41
1:D:632:HIS:O	1:D:635:ASN:HB3	2.21	0.40
1:C:359:TYR:CD1	1:C:360:LYS:N	2.90	0.40
1:C:409:GLN:HB2	1:C:509:TYR:CD2	2.56	0.40
1:C:560:MET:O	1:C:564:THR:HG23	2.21	0.40
1:A:331:LYS:HE3	1:A:332:TYR:CZ	2.57	0.40
2:H:155:GLY:HA3	2:H:234:LEU:HD12	2.02	0.40
1:C:610:LEU:HA	1:C:610:LEU:HD23	1.87	0.40
1:D:325:VAL:HG12	1:D:326:SER:N	2.35	0.40
1:B:405:LEU:HD23	1:B:405:LEU:H	1.85	0.40
1:D:113:PHE:HB3	1:D:210:ASN:HD22	1.86	0.40
1:C:497:SER:C	1:C:499:PHE:N	2.74	0.40
1:D:115:PRO:HB2	1:D:150:SER:HB3	2.04	0.40
1:C:628:GLU:C	1:C:631:PRO:HD2	2.41	0.40
1:D:244:ALA:CB	1:D:347:THR:HB	2.52	0.40
1:C:157:ASN:O	1:C:226:ILE:HA	2.21	0.40
1:C:455:THR:O	1:C:459:MET:HG2	2.22	0.40
2:F:118:SER:OG	2:F:257:GLN:HB2	2.22	0.40
1:C:87:ALA:HA	1:C:88:PRO:HD3	1.97	0.40
1:C:331:LYS:HE3	1:C:332:TYR:CZ	2.55	0.40
2:E:238:ASN:O	2:E:239:SER:C	2.60	0.40
2:F:168:ILE:HD12	2:F:169:ASN:N	2.37	0.40
1:D:396:GLY:O	2:H:238:ASN:ND2	2.50	0.40
1:C:286:CYS:O	1:C:287:VAL:C	2.60	0.40
1:A:467:HIS:O	1:A:469:PRO:HD3	2.22	0.40
2:H:232:ARG:HG2	2:H:232:ARG:HH11	1.86	0.40
1:B:497:SER:C	1:B:499:PHE:N	2.75	0.40
2:E:261:LEU:HD12	2:E:262:TYR:N	2.35	0.40
1:A:186:ILE:O	1:A:186:ILE:HG23	2.22	0.40
1:C:71:ASN:OD1	1:C:72:GLU:N	2.55	0.40
1:A:359:TYR:CD1	1:A:359:TYR:C	2.95	0.40
1:B:359:TYR:CD1	1:B:359:TYR:C	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:TRP:NE1	2:E:192:TRP:NE1[2_556]	1.74	0.46

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	525/574 (92%)	441 (84%)	62 (12%)	22 (4%)	3	32
1	B	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
1	C	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
1	D	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
2	E	175/243 (72%)	143 (82%)	23 (13%)	9 (5%)	2	26
2	F	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	2	23
2	G	175/243 (72%)	142 (81%)	23 (13%)	10 (6%)	2	23
2	H	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	2	23
All	All	2800/3268 (86%)	2335 (83%)	341 (12%)	124 (4%)	3	30

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	A	124	GLY
1	A	138	ASN
1	A	343	ASN
1	A	465	ASP
1	B	106	ASP
1	B	122	ILE
1	B	124	GLY
1	B	138	ASN
1	B	343	ASN
1	B	465	ASP
1	C	106	ASP

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Mol	Chain	Res	Type
1	C	122	ILE
1	C	124	GLY
1	C	138	ASN
1	C	343	ASN
1	C	465	ASP
1	D	106	ASP
1	D	122	ILE
1	D	124	GLY
1	D	138	ASN
1	D	343	ASN
1	D	465	ASP
2	E	102	PRO
2	E	137	ASP
2	E	200	ALA
2	E	231	GLY
2	F	102	PRO
2	F	137	ASP
2	F	200	ALA
2	F	231	GLY
2	G	102	PRO
2	G	137	ASP
2	G	200	ALA
2	G	231	GLY
2	H	102	PRO
2	H	137	ASP
2	H	200	ALA
2	H	231	GLY
1	A	122	ILE
1	A	123	ASP
1	A	365	GLN
1	A	466	ARG
1	B	123	ASP
1	B	365	GLN
1	B	466	ARG
1	C	123	ASP
1	C	365	GLN
1	C	466	ARG
1	D	70	ASN
1	D	123	ASP
1	D	365	GLN
1	D	466	ARG
1	D	619	ARG

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Mol	Chain	Res	Type
2	E	199	PRO
2	F	199	PRO
2	G	199	PRO
2	H	199	PRO
1	A	70	ASN
1	A	140	ASP
1	A	154	LEU
1	A	546	CYS
1	B	70	ASN
1	B	140	ASP
1	B	154	LEU
1	B	546	CYS
1	C	70	ASN
1	C	140	ASP
1	C	154	LEU
1	C	546	CYS
1	C	619	ARG
1	D	140	ASP
1	D	154	LEU
1	D	342	CYS
1	D	546	CYS
2	E	103	ASN
2	E	239	SER
2	F	103	ASN
2	F	239	SER
2	G	103	ASN
2	G	239	SER
2	H	103	ASN
2	H	239	SER
1	A	137	ASN
1	A	342	CYS
1	A	619	ARG
1	B	137	ASN
1	B	342	CYS
1	B	619	ARG
1	B	634	HIS
1	C	137	ASN
1	C	342	CYS
1	C	634	HIS
1	A	144	SER
1	A	421	ASP
1	A	498	ASN

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Mol	Chain	Res	Type
1	A	634	HIS
1	C	144	SER
1	C	421	ASP
1	D	137	ASN
1	D	144	SER
1	D	421	ASP
1	D	634	HIS
2	E	132	SER
2	F	132	SER
2	G	132	SER
2	H	132	SER
1	B	144	SER
1	B	421	ASP
1	D	341	GLY
2	E	260	GLY
2	F	260	GLY
2	H	124	ALA
1	A	341	GLY
1	B	127	PRO
1	B	341	GLY
1	C	341	GLY
1	D	127	PRO
2	G	260	GLY
2	H	260	GLY
1	C	127	PRO
2	G	93	GLY
1	A	127	PRO
2	F	93	GLY

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	455/494 (92%)	435 (96%)	20 (4%)	35	73
1	B	455/494 (92%)	435 (96%)	20 (4%)	35	73
1	C	455/494 (92%)	436 (96%)	19 (4%)	36	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	455/494 (92%)	436 (96%)	19 (4%)	36	74
2	E	143/193 (74%)	131 (92%)	12 (8%)	14	50
2	F	143/193 (74%)	132 (92%)	11 (8%)	16	54
2	G	143/193 (74%)	132 (92%)	11 (8%)	16	54
2	H	143/193 (74%)	132 (92%)	11 (8%)	16	54
All	All	2392/2748 (87%)	2269 (95%)	123 (5%)	29	69

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	125	ARG
1	A	126	LEU
1	A	206	GLU
1	A	278	PHE
1	A	288	ASN
1	A	297	GLU
1	A	323	TRP
1	A	359	TYR
1	A	379	VAL
1	A	405	LEU
1	A	438	PHE
1	A	451	VAL
1	A	466	ARG
1	A	494	ASP
1	A	555	LEU
1	A	592	GLU
1	A	593	VAL
1	A	597	ARG
1	A	624	ASN
1	B	65	ILE
1	B	125	ARG
1	B	126	LEU
1	B	206	GLU
1	B	278	PHE
1	B	288	ASN
1	B	297	GLU
1	B	323	TRP
1	B	379	VAL
1	B	405	LEU

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Mol	Chain	Res	Type
1	B	438	PHE
1	B	451	VAL
1	B	466	ARG
1	B	494	ASP
1	B	555	LEU
1	B	592	GLU
1	B	593	VAL
1	B	597	ARG
1	B	612	PRO
1	B	624	ASN
1	C	65	ILE
1	C	125	ARG
1	C	126	LEU
1	C	206	GLU
1	C	278	PHE
1	C	288	ASN
1	C	297	GLU
1	C	323	TRP
1	C	379	VAL
1	C	405	LEU
1	C	438	PHE
1	C	451	VAL
1	C	466	ARG
1	C	494	ASP
1	C	555	LEU
1	C	592	GLU
1	C	593	VAL
1	C	597	ARG
1	C	624	ASN
1	D	65	ILE
1	D	125	ARG
1	D	126	LEU
1	D	206	GLU
1	D	278	PHE
1	D	288	ASN
1	D	297	GLU
1	D	323	TRP
1	D	359	TYR
1	D	379	VAL
1	D	405	LEU
1	D	438	PHE
1	D	451	VAL

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Mol	Chain	Res	Type
1	D	466	ARG
1	D	494	ASP
1	D	555	LEU
1	D	592	GLU
1	D	593	VAL
1	D	624	ASN
2	E	100	TRP
2	E	102	PRO
2	E	106	PRO
2	E	129	VAL
2	E	157	ASP
2	E	173	TYR
2	E	179	THR
2	E	181	SER
2	E	186	THR
2	E	188	GLN
2	E	237	PHE
2	E	284	ASN
2	F	100	TRP
2	F	102	PRO
2	F	129	VAL
2	F	157	ASP
2	F	173	TYR
2	F	179	THR
2	F	181	SER
2	F	186	THR
2	F	188	GLN
2	F	237	PHE
2	F	284	ASN
2	G	100	TRP
2	G	102	PRO
2	G	129	VAL
2	G	157	ASP
2	G	173	TYR
2	G	179	THR
2	G	181	SER
2	G	186	THR
2	G	188	GLN
2	G	237	PHE
2	G	284	ASN
2	H	100	TRP
2	H	102	PRO

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Mol	Chain	Res	Type
2	H	129	VAL
2	H	157	ASP
2	H	173	TYR
2	H	179	THR
2	H	181	SER
2	H	186	THR
2	H	188	GLN
2	H	237	PHE
2	H	284	ASN

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

Mol	Chain	Res	Type
1	A	624	ASN
1	B	437	ASN
1	B	624	ASN
1	C	120	ASN
1	C	437	ASN
1	D	120	ASN
1	D	437	ASN
1	D	624	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 ⓘ

6 carbohydrates 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	$\# Z > 2$
4	NAG	E	306	2,4	14,14,15	1.19	1 (7%)	15,19,21	0.83	0
4	NAG	E	307	4	14,14,15	0.91	1 (7%)	15,19,21	0.73	0
4	NAG	F	306	2,4	14,14,15	1.22	1 (7%)	15,19,21	0.93	1 (6%)
4	NAG	F	307	4	14,14,15	0.97	1 (7%)	15,19,21	0.70	0
4	NAG	G	306	2,4	14,14,15	1.18	1 (7%)	15,19,21	0.92	0
4	NAG	G	307	4	14,14,15	1.04	1 (7%)	15,19,21	0.67	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	E	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	E	307	4	-	0/6/23/26	0/1/1/1
4	NAG	F	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	307	4	-	0/6/23/26	0/1/1/1
4	NAG	G	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	G	307	4	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	307	NAG	C1-C2	2.77	1.56	1.52
4	G	306	NAG	C1-C2	3.08	1.56	1.52
4	F	307	NAG	C1-C2	3.15	1.56	1.52
4	E	306	NAG	C1-C2	3.28	1.57	1.52
4	G	307	NAG	C1-C2	3.32	1.57	1.52
4	F	306	NAG	C1-C2	3.58	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	306	NAG	O7-C7-C8	-2.02	118.36	122.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	306	NAG	O7-C7-N2-C2
4	E	306	NAG	O7-C7-N2-C2
4	F	306	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	306	NAG	7	0
4	E	307	NAG	4	0
4	F	306	NAG	7	0
4	F	307	NAG	4	0
4	G	306	NAG	7	0
4	G	307	NAG	4	0

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	701	1	14,14,15	1.00	1 (7%)	15,19,21	0.60	0
3	NAG	A	702	1	14,14,15	1.01	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	A	703	1	14,14,15	0.77	0	15,19,21	0.73	0
3	NAG	B	701	1	14,14,15	0.96	1 (7%)	15,19,21	0.62	0
3	NAG	B	702	1	14,14,15	0.88	0	15,19,21	0.93	1 (6%)
3	NAG	B	703	1	14,14,15	0.69	0	15,19,21	0.72	0
3	NAG	C	701	1	14,14,15	0.92	1 (7%)	15,19,21	0.63	0
3	NAG	C	702	1	14,14,15	0.86	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	C	703	1	14,14,15	0.75	0	15,19,21	0.75	0
3	NAG	D	701	1	14,14,15	0.72	0	15,19,21	0.52	0
3	NAG	D	702	1	14,14,15	0.76	1 (7%)	15,19,21	0.90	1 (6%)
3	NAG	D	703	1	14,14,15	0.65	0	15,19,21	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	1/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1	-	0/6/23/26	0/1/1/1
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1
3	NAG	C	703	1	-	0/6/23/26	0/1/1/1
3	NAG	D	701	1	-	1/6/23/26	0/1/1/1
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	NAG	C1-C2	2.08	1.55	1.52
3	C	702	NAG	C1-C2	2.21	1.55	1.52
3	A	702	NAG	C1-C2	2.33	1.55	1.52
3	C	701	NAG	C1-C2	2.74	1.56	1.52
3	B	701	NAG	C1-C2	2.81	1.56	1.52
3	A	701	NAG	C1-C2	2.95	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAG	C2-N2-C7	-2.56	119.75	123.04
3	C	702	NAG	C2-N2-C7	-2.55	119.77	123.04
3	D	702	NAG	C2-N2-C7	-2.38	119.98	123.04
3	A	702	NAG	C2-N2-C7	-2.37	119.99	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NAG	O7-C7-N2-C2
3	D	701	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	NAG	1	0
3	A	702	NAG	1	0
3	A	703	NAG	1	0
3	B	701	NAG	1	0
3	B	702	NAG	1	0
3	B	703	NAG	1	0
3	C	701	NAG	1	0
3	C	702	NAG	1	0
3	C	703	NAG	1	0
3	D	701	NAG	1	0
3	D	702	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	533/574 (92%)	-0.22	2 (0%) 93 90	63, 100, 139, 162	0
1	B	533/574 (92%)	-0.24	2 (0%) 93 90	61, 96, 131, 178	0
1	C	533/574 (92%)	-0.09	6 (1%) 82 73	72, 115, 153, 180	0
1	D	533/574 (92%)	0.58	56 (10%) 8 8	75, 188, 282, 506	0
2	E	177/243 (72%)	-0.14	1 (0%) 90 85	82, 120, 139, 154	0
2	F	177/243 (72%)	-0.39	0 100 100	77, 95, 110, 122	0
2	G	177/243 (72%)	-0.11	2 (1%) 82 73	78, 105, 130, 143	0
2	H	177/243 (72%)	2.21	85 (48%) 0 0	146, 268, 426, 538	0
All	All	2840/3268 (86%)	0.10	154 (5%) 29 23	61, 112, 262, 538	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	260	GLY	11.6
2	H	263	TYR	8.2
2	H	164	SER	7.7
1	D	80	PHE	6.7
2	H	127	VAL	6.7
1	D	79	GLN	6.7
2	H	126	LEU	6.6
2	H	285	VAL	6.3
1	D	387	ASP	5.9
2	H	269	LEU	5.8
2	H	259	SER	5.8
2	H	139	LEU	5.8
1	D	214	GLY	5.7
2	H	85	THR	5.7
2	H	149	GLY	5.5
2	H	279	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
2	H	261	LEU	5.0
2	H	250	GLN	5.0
2	H	196	GLU	4.9
2	H	288	VAL	4.9
2	H	254	PHE	4.8
2	H	129	VAL	4.8
2	H	264	ASN	4.7
1	D	272	PRO	4.7
2	H	141	LEU	4.7
2	H	160	ALA	4.6
1	D	201	GLY	4.6
1	D	398	PHE	4.4
2	H	232	ARG	4.4
1	D	53	PRO	4.3
1	D	279	GLY	4.3
2	H	276	ASP	4.3
2	H	249	GLU	4.3
2	H	268	VAL	4.1
1	D	113	PHE	4.1
2	H	245	ILE	4.1
1	D	270	GLY	4.0
1	D	158	ILE	3.9
1	D	402	ASP	3.8
2	H	148	ILE	3.8
2	H	111	ASP	3.7
2	H	262	TYR	3.7
1	D	69	LEU	3.7
2	H	108	THR	3.7
2	H	193	PRO	3.6
2	H	114	ALA	3.6
2	H	243	ILE	3.6
1	D	496	HIS	3.6
2	H	165	ASN	3.6
2	H	270	ASN	3.6
1	D	268	PHE	3.6
2	H	163	GLU	3.5
1	D	267	PHE	3.4
2	H	238	ASN	3.4
1	D	595	TRP	3.4
2	H	115	ILE	3.3
2	H	194	VAL	3.3
1	D	81	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	166	ALA	3.3
2	H	96	ILE	3.3
1	D	139	LEU	3.3
2	H	140	GLU	3.2
2	H	122	LYS	3.2
1	D	65	ILE	3.1
2	H	176	VAL	3.1
2	H	110	ALA	3.0
1	D	404	MET	3.0
2	H	150	VAL	3.0
2	H	98	TYR	3.0
1	D	213	ASP	3.0
1	D	594	ALA	3.0
2	H	121	GLN	3.0
2	H	266	LEU	3.0
2	H	131	SER	3.0
2	G	94	GLY	2.9
1	D	271	ASP	2.9
2	H	177	ARG	2.9
2	H	95	GLN	2.9
2	H	86	THR	2.9
2	H	183	GLY	2.9
1	D	248	ASN	2.9
1	A	592	GLU	2.9
2	H	283	GLY	2.9
1	D	247	GLY	2.8
1	D	66	LYS	2.8
2	H	198	TYR	2.8
1	B	188	ASP	2.8
1	D	262	SER	2.8
1	D	157	ASN	2.7
2	H	89	PHE	2.7
2	G	285	VAL	2.7
1	D	365	GLN	2.7
1	D	64	GLY	2.7
1	C	188	ASP	2.7
1	D	68	GLU	2.7
1	D	219	SER	2.7
2	H	286	ARG	2.7
1	D	196	MET	2.7
1	D	256	GLN	2.7
1	C	187	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	130	ASP	2.7
2	H	88	ILE	2.7
1	C	189	SER	2.7
1	B	187	ARG	2.7
1	D	138	ASN	2.6
1	D	537	MET	2.6
1	C	201	GLY	2.6
1	D	95	PHE	2.6
2	H	195	ILE	2.6
2	E	83	ALA	2.6
1	D	244	ALA	2.6
2	H	159	ILE	2.6
2	H	235	THR	2.6
2	H	181	SER	2.6
2	H	142	HIS	2.6
2	H	237	PHE	2.6
1	D	284	GLY	2.5
1	D	67	LYS	2.5
2	H	182	GLY	2.5
1	C	107	ILE	2.5
2	H	151	LYS	2.5
2	H	192	TRP	2.4
1	D	187	ARG	2.4
2	H	287	LEU	2.4
1	D	112	GLN	2.4
2	H	116	GLY	2.4
1	D	240	THR	2.4
2	H	278	ASN	2.4
1	A	424	ASP	2.4
2	H	244	ILE	2.4
1	D	207	GLY	2.3
1	D	265	ILE	2.3
1	D	215	SER	2.3
2	H	239	SER	2.3
2	H	200	ALA	2.3
1	D	425	GLY	2.3
1	D	596	THR	2.2
1	D	200	HIS	2.2
2	H	258	LEU	2.2
2	H	93	GLY	2.2
2	H	133	SER	2.2
2	H	197	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	568	LYS	2.2
2	H	94	GLY	2.2
2	H	199	PRO	2.2
1	D	283	GLY	2.1
2	H	277	ALA	2.1
1	C	61	LYS	2.1
1	D	280	SER	2.1
2	H	162	GLU	2.1
2	H	152	PHE	2.0
1	D	281	GLY	2.0
2	H	92	GLY	2.0
1	D	316	SER	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	F	307	14/15	0.91	0.24	-	172,174,177,178	0
4	NAG	E	307	14/15	0.86	0.17	-	146,150,151,152	0
4	NAG	G	307	14/15	0.82	0.31	-	154,158,159,159	0
4	NAG	F	306	14/15	0.69	0.23	-	122,130,133,141	0
4	NAG	E	306	14/15	0.68	0.20	-	146,152,154,157	0
4	NAG	G	306	14/15	0.69	0.28	-	127,133,136,142	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	D	702	14/15	0.37	0.81	3.39	205,205,205,205	0
5	CA	E	401	1/1	0.97	0.23	0.37	89,89,89,89	0
5	CA	F	401	1/1	0.95	0.20	-0.11	76,76,76,76	0
5	CA	G	401	1/1	0.99	0.16	-0.45	79,79,79,79	0
3	NAG	B	702	14/15	0.59	0.28	-	136,138,139,140	0
5	CA	E	402	1/1	0.90	0.31	-	96,96,96,96	0
5	CA	G	402	1/1	0.68	0.28	-	111,111,111,111	0
3	NAG	A	701	14/15	0.68	0.29	-	152,155,156,157	0
3	NAG	D	701	14/15	0.39	0.45	-	219,219,219,219	0
3	NAG	B	701	14/15	0.45	0.40	-	184,187,191,192	0
3	NAG	C	701	14/15	0.46	0.25	-	216,218,219,219	0
3	NAG	B	703	14/15	0.56	0.38	-	236,240,241,242	0
3	NAG	A	702	14/15	0.71	0.25	-	145,147,148,148	0
3	NAG	A	703	14/15	0.50	0.36	-	218,222,225,225	0
3	NAG	C	702	14/15	0.73	0.51	-	186,187,189,189	0
5	CA	F	402	1/1	0.86	0.27	-	96,96,96,96	0
3	NAG	D	703	14/15	0.31	0.45	-	251,251,251,251	0
3	NAG	C	703	14/15	-0.01	0.84	-	218,222,222,222	0

6.5 Other polymers [i](#)

There are no such residues in this entry.