



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:36 AM UTC

PDB ID : 3VUO / pdb_00003vuo
Title : Crystal structure of nontoxic nonhemagglutinin subcomponent (NTNHA) from clostridium botulinum serotype D strain 4947
Authors : Sagane, Y.; Miyashita, S.-I.; Miyata, K.; Matsumoto, T.; Inui, K.; Hayashi, S.; Suzuki, T.; Hasegawa, K.; Yajima, S.; Yamano, A.; Niwa, K.; Watanabe, T.
Deposited on : 2012-07-03
Resolution : 3.90 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
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

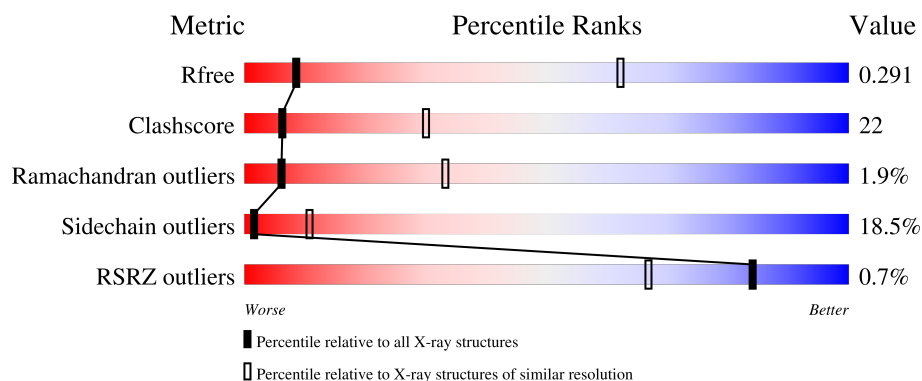
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	1196	50% 39% 7% ...

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8942 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.

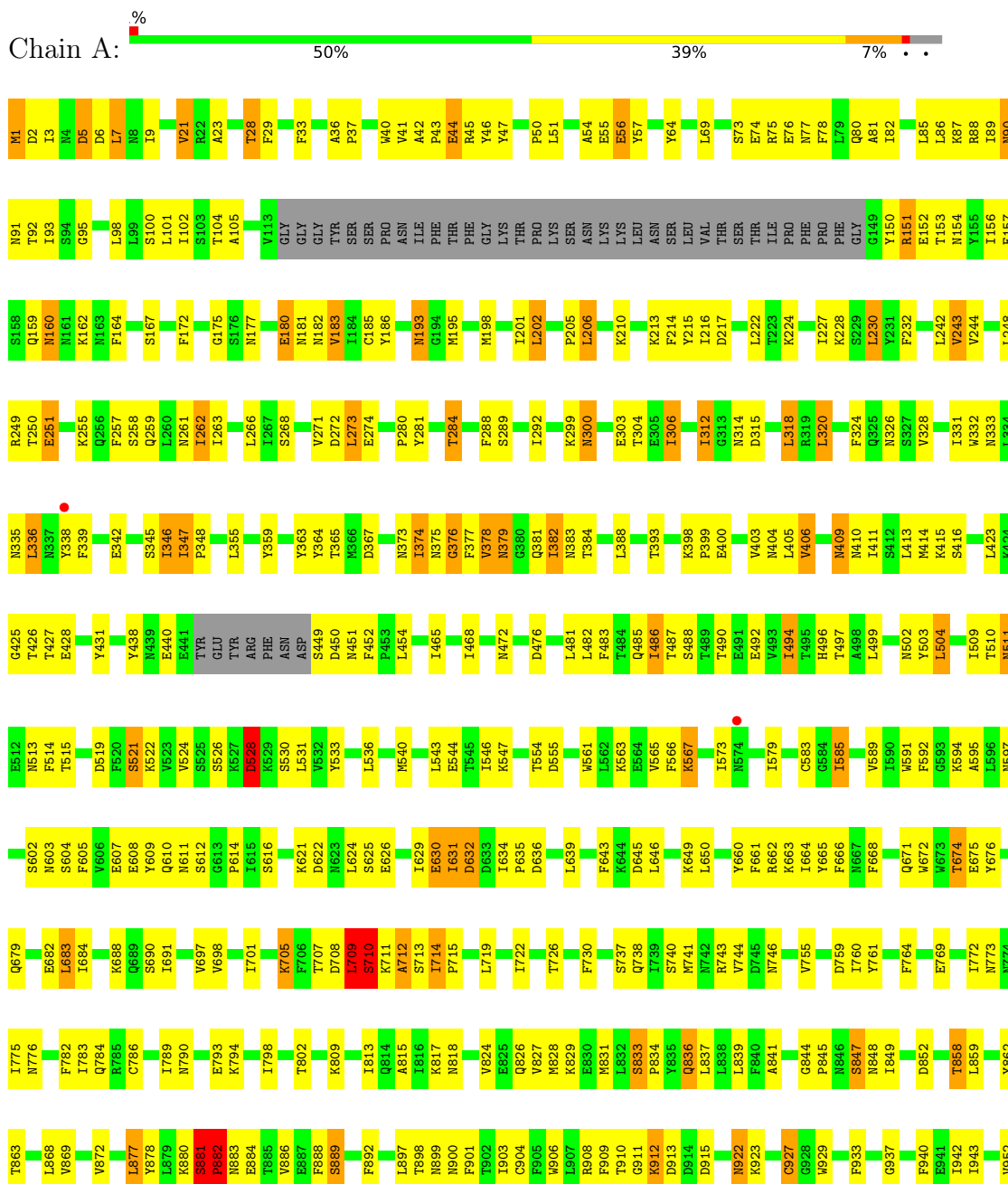
- Molecule 1 is a protein called NTNHA.

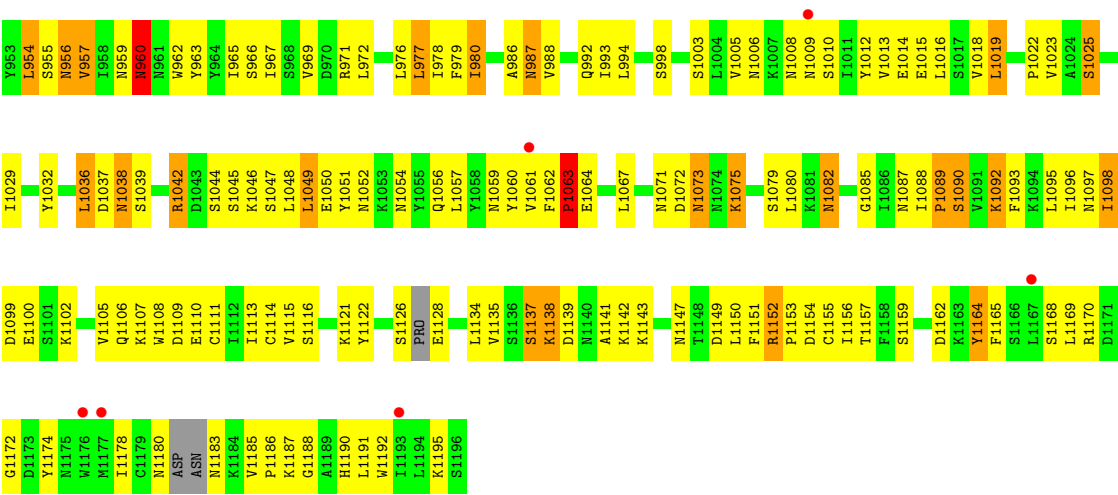
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1151	8942	5783	1418	1716	25	0	0	0

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: NTNHA





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.85Å 147.85Å 229.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.90 20.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-3.90) 95.0 (20.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.309 (Not available) , 0.291	Depositor DCC
R_{free} test set	1308 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 128.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8942	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

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	0.80	3/9106 (0.0%)	1.24	74/12287 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	SER	N-CA	-10.66	1.32	1.46
1	A	482	LEU	CA-C	5.17	1.58	1.52
1	A	691	ILE	CA-CB	5.13	1.60	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	ILE	CA-C-N	11.98	132.72	120.38
1	A	714	ILE	C-N-CA	11.98	132.72	120.38
1	A	712	ALA	N-CA-C	8.42	120.90	108.60
1	A	1036	LEU	N-CA-C	8.28	122.67	112.23
1	A	509	ILE	N-CA-C	8.15	120.32	108.58
1	A	376	GLY	N-CA-C	-8.10	102.13	111.85
1	A	922	ASN	N-CA-C	-7.60	99.13	109.54
1	A	338	TYR	CA-CB-CG	7.59	127.56	113.90
1	A	881	SER	CA-C-N	-7.38	110.61	119.84
1	A	881	SER	C-N-CA	-7.38	110.61	119.84
1	A	423	LEU	N-CA-C	7.38	120.09	110.43
1	A	284	THR	N-CA-C	7.25	117.81	108.24
1	A	573	ILE	N-CA-C	7.19	117.96	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLU	N-CA-C	-7.13	104.19	113.17
1	A	630	GLU	N-CA-C	7.10	120.50	109.07
1	A	1185	VAL	CA-C-N	6.97	126.94	119.76
1	A	1185	VAL	C-N-CA	6.97	126.94	119.76
1	A	1090	SER	N-CA-C	6.90	120.38	110.24
1	A	363	TYR	N-CA-C	6.81	119.62	108.52
1	A	338	TYR	CB-CA-C	6.61	122.86	110.63
1	A	1088	ILE	CA-C-N	6.59	128.08	119.84
1	A	1088	ILE	C-N-CA	6.59	128.08	119.84
1	A	42	ALA	CA-C-N	6.54	128.01	119.84
1	A	42	ALA	C-N-CA	6.54	128.01	119.84
1	A	398	LYS	CA-C-N	6.48	126.46	119.78
1	A	398	LYS	C-N-CA	6.48	126.46	119.78
1	A	1062	PHE	CA-C-N	6.33	127.76	119.84
1	A	1062	PHE	C-N-CA	6.33	127.76	119.84
1	A	160	ASN	N-CA-C	-6.33	105.59	113.38
1	A	272	ASP	N-CA-C	6.06	118.66	111.33
1	A	300	ASN	N-CA-C	6.01	117.91	111.36
1	A	1006	ASN	N-CA-C	5.97	119.64	111.39
1	A	36	ALA	CA-C-N	5.95	127.28	119.84
1	A	36	ALA	C-N-CA	5.95	127.28	119.84
1	A	1152	ARG	CA-C-N	5.94	125.64	119.05
1	A	1152	ARG	C-N-CA	5.94	125.64	119.05
1	A	514	PHE	N-CA-C	5.92	117.84	108.79
1	A	336	LEU	N-CA-C	5.89	119.93	112.87
1	A	1075	LYS	N-CA-C	5.79	115.48	107.73
1	A	193	ASN	N-CA-C	5.75	120.29	113.16
1	A	714	ILE	N-CA-C	5.75	114.59	108.95
1	A	710	SER	CA-C-O	5.71	128.67	120.51
1	A	709	LEU	CA-C-O	5.67	128.62	120.51
1	A	836	GLN	N-CA-C	-5.64	106.06	113.17
1	A	848	ASN	N-CA-C	5.59	118.92	107.69
1	A	528	ASP	N-CA-C	5.53	117.16	111.03
1	A	367	ASP	N-CA-C	5.50	117.60	108.20
1	A	328	VAL	CB-CA-C	-5.45	104.91	111.88
1	A	482	LEU	N-CA-C	5.42	117.25	108.26
1	A	710	SER	O-C-N	5.40	129.78	122.59
1	A	833	SER	CA-C-N	5.38	125.09	119.82
1	A	833	SER	C-N-CA	5.38	125.09	119.82
1	A	709	LEU	CA-C-N	-5.33	111.36	121.54
1	A	709	LEU	C-N-CA	-5.33	111.36	121.54
1	A	306	ILE	N-CA-C	5.29	115.51	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	ILE	N-CA-C	5.26	120.29	109.34
1	A	943	ILE	N-CA-C	5.26	116.23	108.45
1	A	452	PHE	CA-C-N	-5.25	113.28	119.84
1	A	452	PHE	C-N-CA	-5.25	113.28	119.84
1	A	722	ILE	CB-CA-C	-5.25	105.16	112.04
1	A	901	PHE	N-CA-C	5.23	116.47	108.52
1	A	743	ARG	N-CA-C	-5.23	105.58	111.28
1	A	335	ASN	N-CA-C	5.21	115.23	107.88
1	A	913	ASP	N-CA-C	5.20	121.89	110.80
1	A	1042	ARG	N-CA-C	5.20	117.31	109.41
1	A	1138	LYS	N-CA-C	5.19	116.62	111.07
1	A	746	ASN	N-CA-C	-5.06	105.65	111.07
1	A	382	ILE	CB-CA-C	-5.04	105.86	111.80
1	A	956	ASN	CA-C-N	-5.04	115.67	121.71
1	A	956	ASN	C-N-CA	-5.04	115.67	121.71
1	A	1023	VAL	N-CA-C	5.04	116.61	108.85
1	A	1092	LYS	N-CA-C	5.03	116.72	108.52
1	A	486	ILE	N-CA-C	5.02	115.41	108.23
1	A	632	ASP	N-CA-C	5.01	116.23	109.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ASP	Peptide
1	A	709	LEU	Peptide
1	A	960	ASN	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	8942	0	8241	383	0
All	All	8942	0	8241	383	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (383) 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:A:710:SER:HA	1:A:711:LYS:C	1.31	1.31
1:A:426:THR:HB	1:A:427:THR:CA	1.60	1.23
1:A:273:LEU:CD1	1:A:273:LEU:H	1.52	1.21
1:A:710:SER:CA	1:A:711:LYS:C	2.17	1.17
1:A:426:THR:CB	1:A:427:THR:HA	1.76	1.16
1:A:1100:GLU:CD	1:A:1100:GLU:H	1.53	1.15
1:A:710:SER:HB2	1:A:712:ALA:N	1.64	1.12
1:A:273:LEU:H	1:A:273:LEU:HD12	1.20	1.05
1:A:528:ASP:HB2	1:A:530:SER:H	1.24	1.02
1:A:257:PHE:H	1:A:426:THR:HG23	1.23	1.01
1:A:710:SER:HA	1:A:711:LYS:O	1.58	1.01
1:A:102:ILE:HG13	1:A:230:LEU:HD11	1.45	0.99
1:A:450:ASP:OD1	1:A:451:ASN:N	1.99	0.94
1:A:273:LEU:H	1:A:273:LEU:HD13	1.33	0.93
1:A:1126:SER:C	1:A:1128:GLU:N	2.29	0.91
1:A:261:ASN:OD1	1:A:263:ILE:HG22	1.72	0.90
1:A:273:LEU:HD13	1:A:273:LEU:N	1.85	0.89
1:A:273:LEU:CD1	1:A:273:LEU:N	2.25	0.88
1:A:438:TYR:HB2	1:A:630:GLU:HG2	1.56	0.87
1:A:1100:GLU:CD	1:A:1100:GLU:N	2.34	0.85
1:A:1056:GLN:HE22	1:A:1090:SER:CB	1.91	0.84
1:A:710:SER:CB	1:A:711:LYS:C	2.52	0.83
1:A:1107:LYS:HE3	1:A:1147:ASN:CG	2.03	0.83
1:A:528:ASP:HB2	1:A:530:SER:N	1.94	0.82
1:A:708:ASP:O	1:A:710:SER:C	2.23	0.82
1:A:281:TYR:O	1:A:281:TYR:CD1	2.33	0.81
1:A:710:SER:CB	1:A:711:LYS:HA	2.09	0.81
1:A:255:LYS:O	1:A:428:GLU:CD	2.24	0.80
1:A:954:LEU:HD13	1:A:980:ILE:HD11	1.61	0.80
1:A:710:SER:HB2	1:A:711:LYS:C	2.07	0.80
1:A:426:THR:CB	1:A:427:THR:CA	2.47	0.80
1:A:449:SER:O	1:A:450:ASP:HB3	1.81	0.79
1:A:880:LYS:CD	1:A:882:PRO:HB2	2.13	0.79
1:A:150:TYR:CE2	1:A:312:ILE:HD11	2.18	0.79
1:A:1057:LEU:HD11	1:A:1192:TRP:HB3	1.65	0.79
1:A:639:LEU:HD12	1:A:782:PHE:HE1	1.47	0.78
1:A:29:PHE:HB3	1:A:159:GLN:HE22	1.49	0.78
1:A:563:LYS:HE3	1:A:567:LYS:HE2	1.67	0.77
1:A:281:TYR:OH	1:A:440:GLU:C	2.28	0.77
1:A:426:THR:HB	1:A:427:THR:HA	0.79	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG12	1:A:157:GLU:O	1.84	0.76
1:A:714:ILE:HG22	1:A:719:LEU:HD22	1.66	0.76
1:A:710:SER:N	1:A:712:ALA:HB2	2.01	0.75
1:A:710:SER:CB	1:A:711:LYS:CA	2.63	0.74
1:A:862:TYR:HB3	1:A:886:VAL:HG23	1.70	0.74
1:A:102:ILE:HG13	1:A:230:LEU:CD1	2.17	0.73
1:A:345:SER:HA	1:A:381:GLN:OE1	1.89	0.72
1:A:1172:GLY:H	1:A:1174:TYR:H	1.36	0.72
1:A:708:ASP:C	1:A:710:SER:O	2.32	0.72
1:A:900:ASN:HB3	1:A:1022:PRO:HD3	1.70	0.72
1:A:1180:ASN:C	1:A:1183:ASN:N	2.47	0.72
1:A:29:PHE:HB3	1:A:159:GLN:NE2	2.06	0.71
1:A:85:LEU:O	1:A:89:ILE:HG13	1.90	0.71
1:A:181:ASN:O	1:A:182:ASN:HB2	1.91	0.70
1:A:299:LYS:O	1:A:303:GLU:HG2	1.92	0.70
1:A:661:PHE:HA	1:A:664:ILE:HD12	1.73	0.70
1:A:273:LEU:HD12	1:A:273:LEU:N	1.99	0.70
1:A:43:PRO:O	1:A:75:ARG:HG2	1.92	0.70
1:A:150:TYR:HE2	1:A:312:ILE:HD11	1.56	0.70
1:A:33:PHE:CE2	1:A:43:PRO:HG3	2.27	0.70
1:A:56:GLU:O	1:A:487:THR:HG22	1.91	0.70
1:A:1098:ILE:HG12	1:A:1143:LYS:HE3	1.72	0.70
1:A:1152:ARG:HB3	1:A:1155:CYS:SG	2.31	0.70
1:A:29:PHE:CB	1:A:159:GLN:HE22	2.05	0.69
1:A:29:PHE:CB	1:A:159:GLN:NE2	2.55	0.69
1:A:1060:TYR:HB2	1:A:1191:LEU:HB2	1.74	0.69
1:A:1082:ASN:HB2	1:A:1170:ARG:CZ	2.23	0.69
1:A:177:ASN:O	1:A:180:GLU:HB3	1.93	0.68
1:A:869:VAL:HG23	1:A:878:TYR:HB2	1.75	0.68
1:A:714:ILE:CG2	1:A:719:LEU:HD22	2.23	0.68
1:A:908:ARG:NH1	1:A:960:ASN:O	2.25	0.68
1:A:450:ASP:OD1	1:A:451:ASN:CA	2.41	0.68
1:A:909:PHE:CD2	1:A:933:PHE:CE1	2.81	0.68
1:A:1106:GLN:O	1:A:1109:ASP:HB2	1.94	0.68
1:A:1121:LYS:HB3	1:A:1134:LEU:HB3	1.74	0.68
1:A:1107:LYS:HG3	1:A:1147:ASN:HA	1.76	0.67
1:A:561:TRP:CE2	1:A:705:LYS:HD2	2.29	0.67
1:A:314:ASN:HB3	1:A:318:LEU:HD12	1.77	0.67
1:A:426:THR:OG1	1:A:427:THR:HB	1.94	0.66
1:A:300:ASN:O	1:A:304:THR:HG23	1.96	0.66
1:A:639:LEU:HD12	1:A:782:PHE:CE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:O	1:A:379:ASN:HB2	1.96	0.65
1:A:710:SER:OG	1:A:711:LYS:HA	1.96	0.65
1:A:836:GLN:HG3	1:A:892:PHE:CD2	2.31	0.65
1:A:23:ALA:HB3	1:A:28:THR:HG22	1.80	0.64
1:A:399:PRO:O	1:A:490:THR:HG23	1.97	0.64
1:A:426:THR:HB	1:A:428:GLU:HA	1.80	0.64
1:A:710:SER:CB	1:A:712:ALA:N	2.50	0.64
1:A:1159:SER:HB2	1:A:1164:TYR:HA	1.79	0.64
1:A:602:SER:CB	1:A:608:GLU:OE1	2.46	0.64
1:A:674:THR:HG22	1:A:675:GLU:HG3	1.79	0.63
1:A:1168:SER:HA	1:A:1178:ILE:HD13	1.80	0.63
1:A:834:PRO:O	1:A:1019:LEU:HA	1.99	0.62
1:A:373:ASN:HB2	1:A:378:VAL:HG23	1.82	0.62
1:A:609:TYR:HE1	1:A:614:PRO:HA	1.65	0.62
1:A:634:ILE:HG23	1:A:635:PRO:HD2	1.80	0.62
1:A:243:VAL:CG1	1:A:259:GLN:HB2	2.30	0.62
1:A:1063:PRO:CG	1:A:1064:GLU:H	2.13	0.61
1:A:679:GLN:O	1:A:682:GLU:HB2	2.01	0.61
1:A:160:ASN:HD22	1:A:162:LYS:CE	2.13	0.61
1:A:789:ILE:HD12	1:A:794:LYS:HG2	1.83	0.60
1:A:609:TYR:CE1	1:A:614:PRO:HA	2.37	0.60
1:A:710:SER:H	1:A:712:ALA:HB2	1.67	0.59
1:A:940:PHE:CD1	1:A:967:ILE:HD13	2.36	0.59
1:A:612:SER:HB3	1:A:616:SER:HB3	1.84	0.59
1:A:738:GLN:NE2	1:A:738:GLN:HA	2.17	0.59
1:A:214:PHE:HB3	1:A:382:ILE:HD13	1.84	0.59
1:A:1063:PRO:CG	1:A:1064:GLU:N	2.65	0.59
1:A:249:ARG:NE	1:A:258:SER:OG	2.35	0.59
1:A:521:SER:HA	1:A:524:VAL:HG22	1.85	0.58
1:A:1122:TYR:HB3	1:A:1141:ALA:HB2	1.85	0.58
1:A:636:ASP:HA	1:A:639:LEU:HD13	1.85	0.58
1:A:281:TYR:HH	1:A:440:GLU:C	2.12	0.58
1:A:869:VAL:CG2	1:A:878:TYR:HB2	2.32	0.58
1:A:41:VAL:HG12	1:A:43:PRO:HD3	1.86	0.58
1:A:1073:ASN:O	1:A:1075:LYS:CD	2.52	0.58
1:A:1168:SER:HB3	1:A:1178:ILE:HG23	1.86	0.58
1:A:1054:ASN:HA	1:A:1093:PHE:O	2.03	0.58
1:A:242:LEU:HG	1:A:262:ILE:HG21	1.86	0.57
1:A:242:LEU:HG	1:A:262:ILE:CG2	2.34	0.57
1:A:612:SER:HB3	1:A:616:SER:CB	2.34	0.57
1:A:406:VAL:HG11	1:A:494:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:THR:HA	1:A:889:SER:O	2.03	0.57
1:A:281:TYR:O	1:A:281:TYR:CG	2.57	0.57
1:A:281:TYR:CD2	1:A:281:TYR:N	2.73	0.57
1:A:281:TYR:OH	1:A:440:GLU:CA	2.53	0.57
1:A:912:LYS:HG3	1:A:1009:ASN:ND2	2.20	0.57
1:A:347:ILE:O	1:A:824:VAL:HG21	2.04	0.56
1:A:971:ARG:NH2	1:A:994:LEU:O	2.38	0.56
1:A:23:ALA:HB1	1:A:47:TYR:CE2	2.41	0.56
1:A:900:ASN:CB	1:A:1022:PRO:HD3	2.35	0.56
1:A:21:VAL:HG11	1:A:156:ILE:CB	2.36	0.56
1:A:100:SER:O	1:A:104:THR:HG22	2.06	0.56
1:A:1157:THR:HG22	1:A:1190:HIS:O	2.06	0.56
1:A:450:ASP:OD1	1:A:451:ASN:HA	2.05	0.56
1:A:903:ILE:HD13	1:A:929:TRP:CH2	2.41	0.55
1:A:912:LYS:HG3	1:A:1009:ASN:HD22	1.70	0.55
1:A:872:VAL:HG21	1:A:906:TRP:CE3	2.41	0.55
1:A:1038:ASN:HD21	1:A:1042:ARG:HH22	1.55	0.55
1:A:1098:ILE:HD11	1:A:1110:GLU:HB2	1.89	0.55
1:A:373:ASN:C	1:A:375:ASN:H	2.14	0.55
1:A:1051:TYR:CE1	1:A:1097:ASN:HB2	2.41	0.55
1:A:1159:SER:CB	1:A:1164:TYR:HA	2.37	0.55
1:A:450:ASP:OD1	1:A:450:ASP:C	2.49	0.55
1:A:688:LYS:HE2	1:A:741:MET:HE3	1.88	0.55
1:A:314:ASN:O	1:A:318:LEU:HB2	2.08	0.54
1:A:533:TYR:OH	1:A:594:LYS:O	2.25	0.54
1:A:897:LEU:HG	1:A:898:THR:HG23	1.90	0.54
1:A:977:LEU:HD12	1:A:987:ASN:HB2	1.90	0.54
1:A:6:ASP:HB3	1:A:7:LEU:HD13	1.89	0.54
1:A:281:TYR:OH	1:A:440:GLU:HA	2.07	0.54
1:A:709:LEU:O	1:A:710:SER:HB3	2.08	0.54
1:A:33:PHE:HE2	1:A:43:PRO:HG3	1.73	0.54
1:A:216:ILE:HG22	1:A:217:ASP:N	2.23	0.54
1:A:243:VAL:HG13	1:A:259:GLN:HB2	1.89	0.54
1:A:1049:LEU:HD23	1:A:1105:VAL:HG21	1.90	0.53
1:A:789:ILE:CD1	1:A:794:LYS:HG2	2.38	0.53
1:A:29:PHE:HB2	1:A:159:GLN:NE2	2.23	0.53
1:A:346:ILE:HD11	1:A:831:MET:HG3	1.91	0.53
1:A:839:LEU:HD13	1:A:888:PHE:HE1	1.73	0.53
1:A:102:ILE:CG1	1:A:230:LEU:CD1	2.86	0.53
1:A:262:ILE:O	1:A:266:LEU:HG	2.08	0.53
1:A:708:ASP:C	1:A:710:SER:C	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD3	1:A:69:LEU:HB2	1.89	0.53
1:A:160:ASN:HD22	1:A:162:LYS:HE2	1.74	0.53
1:A:841:ALA:HA	1:A:849:ILE:O	2.09	0.53
1:A:76:GLU:CD	1:A:80:GLN:HE21	2.17	0.52
1:A:955:SER:O	1:A:956:ASN:HB2	2.10	0.52
1:A:1025:SER:O	1:A:1029:ILE:HD12	2.09	0.52
1:A:183:VAL:HG21	1:A:228:LYS:HB3	1.92	0.52
1:A:710:SER:CB	1:A:712:ALA:CB	2.87	0.52
1:A:769:GLU:HA	1:A:772:ILE:CG1	2.40	0.52
1:A:737:SER:O	1:A:741:MET:HG3	2.10	0.52
1:A:908:ARG:HD3	1:A:962:TRP:CD1	2.45	0.52
1:A:789:ILE:HB	1:A:793:GLU:CB	2.40	0.52
1:A:1061:VAL:HG23	1:A:1188:GLY:O	2.10	0.52
1:A:214:PHE:CB	1:A:382:ILE:HD13	2.39	0.51
1:A:1178:ILE:HD12	1:A:1180:ASN:HB3	1.92	0.51
1:A:976:LEU:O	1:A:987:ASN:HA	2.10	0.51
1:A:376:GLY:O	1:A:377:PHE:C	2.52	0.51
1:A:784:GLN:HE21	1:A:798:ILE:HD11	1.75	0.51
1:A:271:VAL:O	1:A:274:GLU:HB2	2.10	0.51
1:A:431:TYR:CE1	1:A:671:GLN:HG2	2.46	0.51
1:A:815:ALA:HA	1:A:818:ASN:HB2	1.93	0.51
1:A:44:GLU:HG3	1:A:75:ARG:HE	1.76	0.51
1:A:92:THR:HG23	1:A:342:GLU:OE2	2.10	0.51
1:A:536:LEU:O	1:A:540:MET:HG3	2.11	0.51
1:A:1172:GLY:H	1:A:1174:TYR:N	2.08	0.50
1:A:33:PHE:HE2	1:A:43:PRO:CG	2.24	0.50
1:A:214:PHE:HB3	1:A:382:ILE:CD1	2.41	0.50
1:A:813:ILE:O	1:A:817:LYS:HG3	2.11	0.50
1:A:406:VAL:HA	1:A:411:ILE:O	2.11	0.50
1:A:544:GLU:O	1:A:547:LYS:HB2	2.11	0.50
1:A:772:ILE:HA	1:A:775:ILE:HD12	1.93	0.50
1:A:952:VAL:HG11	1:A:978:ILE:CD1	2.40	0.50
1:A:76:GLU:O	1:A:77:ASN:C	2.55	0.50
1:A:404:ASN:CG	1:A:415:LYS:HD3	2.37	0.50
1:A:1168:SER:HA	1:A:1178:ILE:CD1	2.41	0.50
1:A:54:ALA:HB3	1:A:57:TYR:HD2	1.75	0.50
1:A:511:ASN:HB3	1:A:513:ASN:O	2.11	0.50
1:A:740:SER:O	1:A:744:VAL:HG13	2.12	0.50
1:A:1014:GLU:HG2	1:A:1015:GLU:N	2.26	0.50
1:A:1092:LYS:HG3	1:A:1116:SER:HB2	1.93	0.50
1:A:315:ASP:HB2	1:A:468:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:MET:O	1:A:829:LYS:C	2.55	0.49
1:A:1168:SER:HB3	1:A:1178:ILE:CG2	2.42	0.49
1:A:64:TYR:CE1	1:A:177:ASN:HB2	2.47	0.49
1:A:683:LEU:O	1:A:684:ILE:C	2.56	0.49
1:A:708:ASP:O	1:A:710:SER:CA	2.60	0.49
1:A:216:ILE:HD11	1:A:348:PRO:HD3	1.95	0.49
1:A:288:PHE:HA	1:A:332:TRP:CH2	2.47	0.49
1:A:1060:TYR:CB	1:A:1191:LEU:HB2	2.41	0.49
1:A:1102:LYS:NZ	1:A:1109:ASP:OD2	2.38	0.49
1:A:98:LEU:HA	1:A:454:LEU:HD13	1.95	0.49
1:A:318:LEU:HD13	1:A:465:ILE:HG23	1.94	0.49
1:A:383:ASN:O	1:A:384:THR:C	2.56	0.49
1:A:592:PHE:HB3	1:A:605:PHE:CE2	2.48	0.49
1:A:320:LEU:O	1:A:324:PHE:HD2	1.96	0.48
1:A:826:GLN:O	1:A:829:LYS:HB2	2.13	0.48
1:A:1044:SER:HA	1:A:1154:ASP:HB2	1.95	0.48
1:A:786:CYS:HB3	1:A:789:ILE:HG13	1.93	0.48
1:A:160:ASN:O	1:A:162:LYS:HD3	2.13	0.48
1:A:373:ASN:C	1:A:375:ASN:N	2.72	0.48
1:A:813:ILE:HG22	1:A:817:LYS:HE2	1.96	0.48
1:A:579:ILE:O	1:A:585:ILE:HG12	2.13	0.48
1:A:705:LYS:O	1:A:708:ASP:HB3	2.13	0.48
1:A:709:LEU:O	1:A:710:SER:CB	2.60	0.48
1:A:46:TYR:HB2	1:A:202:LEU:HG	1.96	0.48
1:A:646:LEU:HD21	1:A:786:CYS:SG	2.54	0.48
1:A:55:GLU:C	1:A:57:TYR:H	2.22	0.48
1:A:101:LEU:O	1:A:105:ALA:HB2	2.14	0.48
1:A:708:ASP:O	1:A:710:SER:N	2.46	0.48
1:A:1180:ASN:C	1:A:1183:ASN:HA	2.39	0.48
1:A:215:TYR:O	1:A:381:GLN:HG2	2.13	0.47
1:A:880:LYS:CD	1:A:882:PRO:N	2.77	0.47
1:A:306:ILE:HA	1:A:312:ILE:HD12	1.96	0.47
1:A:449:SER:O	1:A:450:ASP:CB	2.57	0.47
1:A:40:TRP:CD1	1:A:167:SER:HB2	2.49	0.47
1:A:528:ASP:OD1	1:A:528:ASP:N	2.47	0.47
1:A:1180:ASN:C	1:A:1183:ASN:CA	2.88	0.47
1:A:499:LEU:O	1:A:502:ASN:HB2	2.15	0.47
1:A:880:LYS:CD	1:A:882:PRO:CB	2.87	0.47
1:A:957:VAL:CG1	1:A:963:TYR:CD2	2.98	0.47
1:A:224:LYS:HB2	1:A:336:LEU:HD11	1.96	0.47
1:A:503:TYR:CE1	1:A:597:ASN:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:ILE:HD12	1:A:1098:ILE:H	1.78	0.47
1:A:503:TYR:CD1	1:A:597:ASN:HB2	2.50	0.47
1:A:769:GLU:HA	1:A:772:ILE:HG12	1.97	0.47
1:A:962:TRP:CH2	1:A:1012:TYR:HB3	2.50	0.47
1:A:965:ILE:HG13	1:A:980:ILE:HD13	1.97	0.47
1:A:923:LYS:HA	1:A:927:CYS:O	2.15	0.46
1:A:977:LEU:HB3	1:A:979:PHE:CE2	2.50	0.46
1:A:215:TYR:CE2	1:A:384:THR:O	2.68	0.46
1:A:216:ILE:HG22	1:A:217:ASP:H	1.80	0.46
1:A:409:ASN:OD1	1:A:409:ASN:N	2.46	0.46
1:A:426:THR:HB	1:A:427:THR:CB	2.37	0.46
1:A:55:GLU:C	1:A:57:TYR:N	2.73	0.46
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.66	0.46
1:A:1095:LEU:C	1:A:1096:ILE:HG13	2.40	0.46
1:A:280:PRO:HD2	1:A:666:PHE:HE2	1.81	0.46
1:A:1079:SER:OG	1:A:1080:LEU:N	2.48	0.46
1:A:714:ILE:HB	1:A:719:LEU:HD21	1.98	0.46
1:A:426:THR:HG1	1:A:427:THR:HB	1.82	0.45
1:A:306:ILE:HG23	1:A:312:ILE:HD13	1.99	0.45
1:A:607:GLU:O	1:A:610:GLN:HB3	2.16	0.45
1:A:162:LYS:HE2	1:A:162:LYS:HB2	1.61	0.45
1:A:378:VAL:O	1:A:379:ASN:CB	2.63	0.45
1:A:579:ILE:HD11	1:A:609:TYR:CD2	2.51	0.45
1:A:710:SER:CB	1:A:712:ALA:HB3	2.46	0.45
1:A:33:PHE:CE2	1:A:43:PRO:CG	2.98	0.45
1:A:364:TYR:CE1	1:A:388:LEU:HG	2.52	0.45
1:A:612:SER:CB	1:A:616:SER:CB	2.95	0.45
1:A:790:ASN:O	1:A:794:LYS:HG3	2.17	0.45
1:A:604:SER:OG	1:A:607:GLU:HG2	2.17	0.45
1:A:1092:LYS:O	1:A:1115:VAL:HA	2.16	0.45
1:A:852:ASP:OD1	1:A:858:THR:HB	2.17	0.45
1:A:937:GLY:HA3	1:A:954:LEU:O	2.17	0.45
1:A:543:LEU:HD23	1:A:546:ILE:HD11	1.99	0.45
1:A:922:ASN:CG	1:A:998:SER:OG	2.60	0.45
1:A:726:THR:HG22	1:A:730:PHE:CD1	2.52	0.44
1:A:790:ASN:H	1:A:790:ASN:ND2	2.15	0.44
1:A:839:LEU:HD22	1:A:1016:LEU:HB3	1.99	0.44
1:A:872:VAL:N	1:A:1014:GLU:OE2	2.48	0.44
1:A:78:PHE:CD2	1:A:78:PHE:C	2.94	0.44
1:A:403:VAL:N	1:A:416:SER:O	2.45	0.44
1:A:1032:TYR:O	1:A:1036:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:ASN:CG	1:A:1099:ASP:H	2.25	0.44
1:A:755:VAL:O	1:A:759:ASP:HB2	2.17	0.44
1:A:151:ARG:HA	1:A:472:ASN:O	2.18	0.44
1:A:957:VAL:HG13	1:A:963:TYR:CD2	2.52	0.44
1:A:40:TRP:HD1	1:A:167:SER:HB2	1.83	0.44
1:A:217:ASP:HA	1:A:377:PHE:HE2	1.82	0.44
1:A:831:MET:H	1:A:831:MET:HG2	1.70	0.44
1:A:1:MET:C	1:A:3:ILE:H	2.26	0.44
1:A:405:LEU:O	1:A:413:LEU:HB2	2.18	0.44
1:A:710:SER:HB3	1:A:712:ALA:HB3	2.00	0.44
1:A:839:LEU:HD13	1:A:888:PHE:CE1	2.52	0.44
1:A:5:ASP:CG	1:A:87:LYS:HE3	2.43	0.44
1:A:427:THR:HA	1:A:428:GLU:HA	1.52	0.44
1:A:1149:ASP:HB3	1:A:1152:ARG:HB2	1.99	0.44
1:A:561:TRP:CZ2	1:A:705:LYS:HD2	2.53	0.43
1:A:625:SER:O	1:A:626:GLU:C	2.61	0.43
1:A:1038:ASN:HD21	1:A:1042:ARG:NH2	2.16	0.43
1:A:589:VAL:HG11	1:A:591:TRP:CE2	2.54	0.43
1:A:660:TYR:O	1:A:663:LYS:HB2	2.18	0.43
1:A:698:VAL:O	1:A:701:ILE:HB	2.17	0.43
1:A:710:SER:HB2	1:A:712:ALA:H	1.71	0.43
1:A:859:LEU:HB2	1:A:889:SER:HB3	1.99	0.43
1:A:7:LEU:HD13	1:A:7:LEU:N	2.33	0.43
1:A:186:TYR:HB2	1:A:198:MET:O	2.19	0.43
1:A:227:ILE:HD11	1:A:339:PHE:CE2	2.54	0.43
1:A:406:VAL:CG1	1:A:494:ILE:HD12	2.48	0.43
1:A:74:GLU:O	1:A:75:ARG:C	2.61	0.43
1:A:81:ALA:HB1	1:A:205:PRO:HB2	2.01	0.43
1:A:579:ILE:HD11	1:A:609:TYR:HD2	1.84	0.43
1:A:672:TRP:O	1:A:676:TYR:HB2	2.18	0.43
1:A:769:GLU:O	1:A:773:ASN:HB2	2.19	0.43
1:A:868:LEU:CD2	1:A:877:LEU:HD12	2.48	0.43
1:A:186:TYR:CD1	1:A:198:MET:HE2	2.54	0.43
1:A:213:LYS:H	1:A:213:LYS:CD	2.31	0.43
1:A:90:ASN:C	1:A:92:THR:H	2.27	0.43
1:A:426:THR:CB	1:A:427:THR:HB	2.48	0.43
1:A:837:LEU:HD23	1:A:1018:VAL:HG23	2.00	0.43
1:A:940:PHE:CE1	1:A:967:ILE:HG21	2.54	0.43
1:A:232:PHE:CD1	1:A:232:PHE:N	2.86	0.43
1:A:672:TRP:HA	1:A:676:TYR:HD2	1.83	0.43
1:A:78:PHE:HB2	1:A:206:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:TYR:CD1	1:A:1138:LYS:HA	2.54	0.42
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.71	0.42
1:A:9:ILE:H	1:A:76:GLU:CD	2.28	0.42
1:A:519:ASP:CG	1:A:522:LYS:HB2	2.44	0.42
1:A:624:LEU:HA	1:A:624:LEU:HD12	1.66	0.42
1:A:877:LEU:N	1:A:1013:VAL:O	2.52	0.42
1:A:503:TYR:HB3	1:A:595:ALA:O	2.19	0.42
1:A:911:GLY:C	1:A:912:LYS:HG2	2.42	0.42
1:A:1085:GLY:C	1:A:1087:ASN:H	2.27	0.42
1:A:92:THR:CG2	1:A:342:GLU:OE2	2.67	0.42
1:A:665:TYR:O	1:A:668:PHE:HB2	2.19	0.42
1:A:709:LEU:HA	1:A:709:LEU:HD12	1.48	0.42
1:A:1051:TYR:HB3	1:A:1052:ASN:HD22	1.84	0.42
1:A:438:TYR:HB2	1:A:630:GLU:CG	2.39	0.42
1:A:709:LEU:N	1:A:710:SER:O	2.53	0.42
1:A:82:ILE:HG22	1:A:86:LEU:HD12	2.01	0.42
1:A:167:SER:OG	1:A:198:MET:SD	2.78	0.42
1:A:157:GLU:CG	1:A:164:PHE:HE1	2.32	0.42
1:A:92:THR:HG22	1:A:95:GLY:H	1.85	0.41
1:A:193:ASN:OD1	1:A:195:MET:CG	2.68	0.41
1:A:566:PHE:CD2	1:A:566:PHE:C	2.98	0.41
1:A:1128:GLU:OE1	1:A:1128:GLU:HA	2.20	0.41
1:A:195:MET:HE3	1:A:195:MET:HB3	1.88	0.41
1:A:504:LEU:HD13	1:A:504:LEU:HA	1.80	0.41
1:A:1038:ASN:O	1:A:1039:SER:CB	2.68	0.41
1:A:232:PHE:N	1:A:232:PHE:HD1	2.18	0.41
1:A:426:THR:CB	1:A:427:THR:CB	2.97	0.41
1:A:962:TRP:HB2	1:A:1046:LYS:HB2	2.03	0.41
1:A:262:ILE:HG23	1:A:263:ILE:N	2.35	0.41
1:A:1044:SER:OG	1:A:1195:LYS:HB2	2.21	0.41
1:A:877:LEU:HD12	1:A:877:LEU:HA	1.79	0.41
1:A:909:PHE:CD2	1:A:933:PHE:HE1	2.35	0.41
1:A:1098:ILE:H	1:A:1098:ILE:CD1	2.31	0.41
1:A:172:PHE:N	1:A:201:ILE:O	2.32	0.41
1:A:760:ILE:N	1:A:760:ILE:HD12	2.36	0.41
1:A:908:ARG:NH1	1:A:1045:SER:HB3	2.36	0.41
1:A:1135:VAL:HG23	1:A:1137:SER:H	1.85	0.41
1:A:522:LYS:O	1:A:531:LEU:HD12	2.21	0.41
1:A:555:ASP:OD1	1:A:555:ASP:N	2.53	0.41
1:A:965:ILE:N	1:A:965:ILE:HD12	2.36	0.40
1:A:1059:ASN:OD1	1:A:1061:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:HB3	1:A:154:ASN:OD1	2.21	0.40
1:A:425:GLY:O	1:A:426:THR:C	2.64	0.40
1:A:526:SER:C	1:A:528:ASP:H	2.30	0.40
1:A:794:LYS:O	1:A:798:ILE:HD12	2.21	0.40
1:A:710:SER:HB2	1:A:712:ALA:CB	2.50	0.40
1:A:761:TYR:O	1:A:764:PHE:HB3	2.21	0.40
1:A:899:ASN:O	1:A:971:ARG:HG3	2.21	0.40
1:A:374:ILE:H	1:A:374:ILE:HG13	1.70	0.40
1:A:881:SER:O	1:A:1008:ASN:N	2.54	0.40
1:A:214:PHE:CE1	1:A:346:ILE:HD13	2.56	0.40
1:A:776:ASN:OD1	1:A:802:THR:HG22	2.22	0.40
1:A:783:ILE:O	1:A:786:CYS:HB2	2.22	0.40
1:A:827:VAL:O	1:A:831:MET:HG2	2.20	0.40
1:A:844:GLY:N	1:A:847:SER:O	2.54	0.40
1:A:978:ILE:HD12	1:A:986:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1051/1196 (88%)	946 (90%)	85 (8%)	20 (2%)	6	33

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	ILE
1	A	881	SER
1	A	709	LEU
1	A	710	SER
1	A	882	PRO
1	A	1162	ASP

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Mol	Chain	Res	Type
1	A	809	LYS
1	A	1089	PRO
1	A	2	ASP
1	A	56	GLU
1	A	91	ASN
1	A	379	ASN
1	A	884	GLU
1	A	845	PRO
1	A	858	THR
1	A	643	PHE
1	A	37	PRO
1	A	175	GLY
1	A	1063	PRO
1	A	262	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	820/1123 (73%)	668 (82%)	152 (18%)	1 11

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	21	VAL
1	A	28	THR
1	A	44	GLU
1	A	50	PRO
1	A	51	LEU
1	A	73	SER
1	A	88	ARG
1	A	90	ASN
1	A	93	ILE
1	A	151	ARG

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Mol	Chain	Res	Type
1	A	153	THR
1	A	180	GLU
1	A	183	VAL
1	A	185	CYS
1	A	202	LEU
1	A	206	LEU
1	A	210	LYS
1	A	222	LEU
1	A	230	LEU
1	A	243	VAL
1	A	244	VAL
1	A	248	LEU
1	A	250	THR
1	A	251	GLU
1	A	268	SER
1	A	273	LEU
1	A	284	THR
1	A	289	SER
1	A	292	ILE
1	A	312	ILE
1	A	318	LEU
1	A	320	LEU
1	A	326	ASN
1	A	331	ILE
1	A	333	ASN
1	A	346	ILE
1	A	347	ILE
1	A	355	LEU
1	A	359	TYR
1	A	365	THR
1	A	374	ILE
1	A	378	VAL
1	A	393	THR
1	A	400	GLU
1	A	406	VAL
1	A	409	ASN
1	A	410	ASN
1	A	414	MET
1	A	476	ASP
1	A	481	LEU
1	A	483	PHE
1	A	485	GLN

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Mol	Chain	Res	Type
1	A	486	ILE
1	A	488	SER
1	A	492	GLU
1	A	494	ILE
1	A	496	HIS
1	A	497	THR
1	A	504	LEU
1	A	510	THR
1	A	511	ASN
1	A	515	THR
1	A	521	SER
1	A	528	ASP
1	A	554	THR
1	A	565	VAL
1	A	567	LYS
1	A	583	CYS
1	A	585	ILE
1	A	603	ASN
1	A	611	ASN
1	A	621	LYS
1	A	622	ASP
1	A	629	ILE
1	A	632	ASP
1	A	645	ASP
1	A	649	LYS
1	A	650	LEU
1	A	662	ARG
1	A	674	THR
1	A	683	LEU
1	A	690	SER
1	A	697	VAL
1	A	705	LYS
1	A	707	THR
1	A	709	LEU
1	A	710	SER
1	A	713	SER
1	A	715	PRO
1	A	833	SER
1	A	847	SER
1	A	863	THR
1	A	877	LEU
1	A	882	PRO

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Mol	Chain	Res	Type
1	A	883	ASN
1	A	889	SER
1	A	904	CYS
1	A	910	THR
1	A	912	LYS
1	A	915	ASP
1	A	927	CYS
1	A	942	ILE
1	A	954	LEU
1	A	957	VAL
1	A	959	ASN
1	A	960	ASN
1	A	966	SER
1	A	969	VAL
1	A	972	LEU
1	A	977	LEU
1	A	980	ILE
1	A	987	ASN
1	A	988	VAL
1	A	992	GLN
1	A	993	ILE
1	A	1003	SER
1	A	1005	VAL
1	A	1010	SER
1	A	1019	LEU
1	A	1025	SER
1	A	1037	ASP
1	A	1038	ASN
1	A	1047	SER
1	A	1048	LEU
1	A	1049	LEU
1	A	1050	GLU
1	A	1063	PRO
1	A	1067	LEU
1	A	1071	ASN
1	A	1072	ASP
1	A	1073	ASN
1	A	1082	ASN
1	A	1089	PRO
1	A	1098	ILE
1	A	1108	TRP
1	A	1111	CYS

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Mol	Chain	Res	Type
1	A	1113	ILE
1	A	1114	CYS
1	A	1137	SER
1	A	1139	ASP
1	A	1142	LYS
1	A	1150	LEU
1	A	1151	PHE
1	A	1153	PRO
1	A	1156	ILE
1	A	1164	TYR
1	A	1165	PHE
1	A	1169	LEU
1	A	1186	PRO
1	A	1187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	90	ASN
1	A	212	ASN
1	A	285	ASN
1	A	375	ASN
1	A	836	GLN
1	A	925	ASN
1	A	960	ASN
1	A	975	GLN
1	A	984	ASN
1	A	1009	ASN
1	A	1052	ASN
1	A	1056	GLN
1	A	1082	ASN
1	A	1140	ASN
1	A	1183	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1151/1196 (96%)	-0.40	8 (0%)	84 67	66, 126, 251, 352	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1009	ASN	2.8
1	A	1061	VAL	2.6
1	A	1177	MET	2.4
1	A	1167	LEU	2.4
1	A	1193	ILE	2.1
1	A	1176	TRP	2.0
1	A	574	ASN	2.0
1	A	338	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.