



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:21 AM UTC

PDB ID : 3WIN / pdb_00003win
Title : Clostridium botulinum Hemagglutinin
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Deposited on : 2013-09-19
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

<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

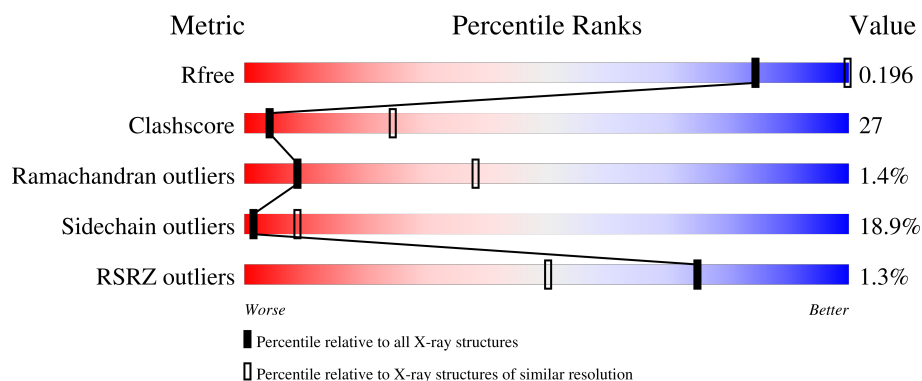
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	D	194	% 55% 24% 6% 14%
2	E	431	59% 30% 8%
3	C	168	2% 51% 27% 7% 16%
4	A	316	3% 42% 34% 13% 9%
4	B	316	% 50% 31% 9% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10522 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 HA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	167	Total	C	N	O	S	0	0	0
			1361	883	218	258	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	expression tag	UNP Q33CP8
D	-4	ALA	-	expression tag	UNP Q33CP8
D	-3	SER	-	expression tag	UNP Q33CP8
D	-2	TRP	-	expression tag	UNP Q33CP8
D	-1	SER	-	expression tag	UNP Q33CP8
D	0	HIS	-	expression tag	UNP Q33CP8
D	1	PRO	-	expression tag	UNP Q33CP8
D	2	GLN	-	expression tag	UNP Q33CP8
D	3	PHE	-	expression tag	UNP Q33CP8
D	4	GLU	-	expression tag	UNP Q33CP8
D	5	LYS	-	expression tag	UNP Q33CP8
D	6	GLY	-	expression tag	UNP Q33CP8
D	7	ALA	-	expression tag	UNP Q33CP8
D	8	LEU	-	expression tag	UNP Q33CP8
D	9	GLU	-	expression tag	UNP Q33CP8
D	10	VAL	-	expression tag	UNP Q33CP8
D	11	LEU	-	expression tag	UNP Q33CP8
D	12	PHE	-	expression tag	UNP Q33CP8
D	13	GLN	-	expression tag	UNP Q33CP8
D	14	GLY	-	expression tag	UNP Q33CP8
D	15	PRO	-	expression tag	UNP Q33CP8
D	16	GLY	-	expression tag	UNP Q33CP8
D	17	TYR	-	expression tag	UNP Q33CP8
D	18	GLN	-	expression tag	UNP Q33CP8

- Molecule 2 is a protein called HA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	419	Total	C	N	O	S	0	0	0
			3347	2113	559	671	4			

- Molecule 3 is a protein called 17 kD hemagglutinin component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	141	Total	C	N	O	S	0	0	0
			1156	746	184	221	5			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	expression tag	UNP Q45841
C	-20	GLY	-	expression tag	UNP Q45841
C	-19	SER	-	expression tag	UNP Q45841
C	-18	SER	-	expression tag	UNP Q45841
C	-17	HIS	-	expression tag	UNP Q45841
C	-16	HIS	-	expression tag	UNP Q45841
C	-15	HIS	-	expression tag	UNP Q45841
C	-14	HIS	-	expression tag	UNP Q45841
C	-13	HIS	-	expression tag	UNP Q45841
C	-12	HIS	-	expression tag	UNP Q45841
C	-11	SER	-	expression tag	UNP Q45841
C	-10	SER	-	expression tag	UNP Q45841
C	-9	GLY	-	expression tag	UNP Q45841
C	-8	LEU	-	expression tag	UNP Q45841
C	-7	VAL	-	expression tag	UNP Q45841
C	-6	PRO	-	expression tag	UNP Q45841
C	-5	ARG	-	expression tag	UNP Q45841
C	-4	GLY	-	expression tag	UNP Q45841
C	-3	SER	-	expression tag	UNP Q45841
C	-2	HIS	-	expression tag	UNP Q45841
C	-1	MET	-	expression tag	UNP Q45841
C	0	ALA	-	expression tag	UNP Q45841
C	1	SER	-	expression tag	UNP Q45841

- Molecule 4 is a protein called HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	286	Total	C	N	O	S	0	0	0
			2304	1465	390	444	5			
4	B	286	Total	C	N	O	S	0	0	0
			2304	1465	390	444	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q33CP6
A	-20	ALA	-	expression tag	UNP Q33CP6
A	-19	SER	-	expression tag	UNP Q33CP6
A	-18	TRP	-	expression tag	UNP Q33CP6
A	-17	SER	-	expression tag	UNP Q33CP6
A	-16	HIS	-	expression tag	UNP Q33CP6
A	-15	PRO	-	expression tag	UNP Q33CP6
A	-14	GLN	-	expression tag	UNP Q33CP6
A	-13	PHE	-	expression tag	UNP Q33CP6
A	-12	GLU	-	expression tag	UNP Q33CP6
A	-11	LYS	-	expression tag	UNP Q33CP6
A	-10	GLY	-	expression tag	UNP Q33CP6
A	-9	ALA	-	expression tag	UNP Q33CP6
A	-8	LEU	-	expression tag	UNP Q33CP6
A	-7	GLU	-	expression tag	UNP Q33CP6
A	-6	VAL	-	expression tag	UNP Q33CP6
A	-5	LEU	-	expression tag	UNP Q33CP6
A	-4	PHE	-	expression tag	UNP Q33CP6
A	-3	GLN	-	expression tag	UNP Q33CP6
A	-2	GLY	-	expression tag	UNP Q33CP6
A	-1	PRO	-	expression tag	UNP Q33CP6
A	0	GLY	-	expression tag	UNP Q33CP6
A	1	TYR	-	expression tag	UNP Q33CP6
A	2	PRO	-	expression tag	UNP Q33CP6
A	3	ASP	-	expression tag	UNP Q33CP6
A	4	ASP	-	expression tag	UNP Q33CP6
A	5	ASP	-	expression tag	UNP Q33CP6
A	6	ASP	-	expression tag	UNP Q33CP6
B	-21	MET	-	expression tag	UNP Q33CP6
B	-20	ALA	-	expression tag	UNP Q33CP6
B	-19	SER	-	expression tag	UNP Q33CP6
B	-18	TRP	-	expression tag	UNP Q33CP6
B	-17	SER	-	expression tag	UNP Q33CP6
B	-16	HIS	-	expression tag	UNP Q33CP6
B	-15	PRO	-	expression tag	UNP Q33CP6
B	-14	GLN	-	expression tag	UNP Q33CP6
B	-13	PHE	-	expression tag	UNP Q33CP6
B	-12	GLU	-	expression tag	UNP Q33CP6
B	-11	LYS	-	expression tag	UNP Q33CP6
B	-10	GLY	-	expression tag	UNP Q33CP6
B	-9	ALA	-	expression tag	UNP Q33CP6
B	-8	LEU	-	expression tag	UNP Q33CP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q33CP6
B	-6	VAL	-	expression tag	UNP Q33CP6
B	-5	LEU	-	expression tag	UNP Q33CP6
B	-4	PHE	-	expression tag	UNP Q33CP6
B	-3	GLN	-	expression tag	UNP Q33CP6
B	-2	GLY	-	expression tag	UNP Q33CP6
B	-1	PRO	-	expression tag	UNP Q33CP6
B	0	GLY	-	expression tag	UNP Q33CP6
B	1	TYR	-	expression tag	UNP Q33CP6
B	2	PRO	-	expression tag	UNP Q33CP6
B	3	ASP	-	expression tag	UNP Q33CP6
B	4	ASP	-	expression tag	UNP Q33CP6
B	5	ASP	-	expression tag	UNP Q33CP6
B	6	ASP	-	expression tag	UNP Q33CP6

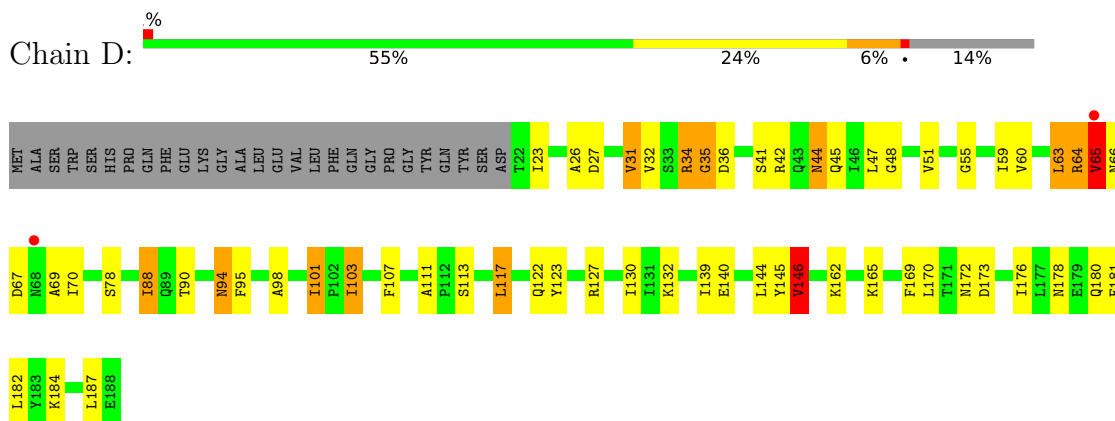
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total O 2 2	0	0
5	E	19	Total O 19 19	0	0
5	C	7	Total O 7 7	0	0
5	A	11	Total O 11 11	0	0
5	B	11	Total O 11 11	0	0

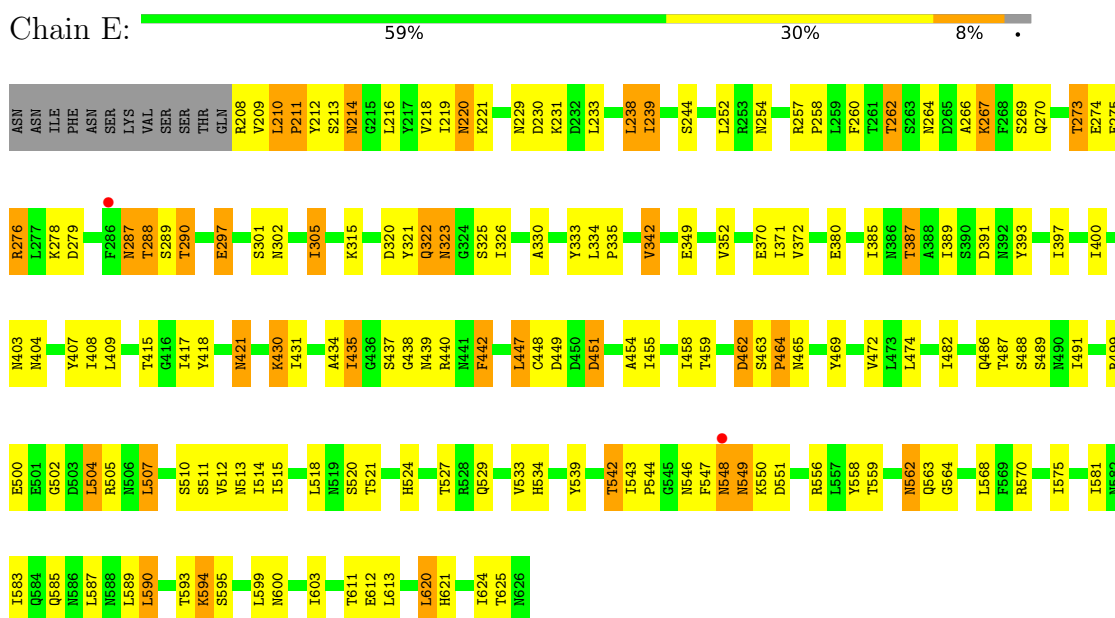
3 Residue-property plots

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: HA3

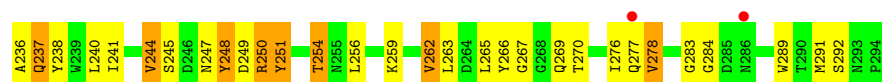


• Molecule 2: HA3



• Molecule 3: 17 kD hemagglutinin component





4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	324.73Å 324.73Å 117.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.43 – 3.50 48.43 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.43-3.50) 98.2 (48.43-3.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.200 , 0.251 0.199 , 0.196	Depositor DCC
R_{free} test set	2268 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	99.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10522	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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	D	0.77	0/1393	1.10	6/1891 (0.3%)
2	E	0.78	5/3409 (0.1%)	1.06	12/4636 (0.3%)
3	C	0.75	1/1186 (0.1%)	1.09	5/1611 (0.3%)
4	A	0.68	0/2354	1.08	10/3208 (0.3%)
4	B	0.73	0/2354	1.06	9/3208 (0.3%)
All	All	0.74	6/10696 (0.1%)	1.07	42/14554 (0.3%)

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	D	0	1
2	E	0	1
4	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	210	LEU	C-N	5.65	1.41	1.33
2	E	463	SER	C-N	5.39	1.40	1.33
2	E	464	PRO	N-CD	5.39	1.55	1.47
2	E	370	GLU	CA-C	-5.22	1.48	1.53
3	C	9	PRO	N-CD	5.11	1.54	1.47
2	E	211	PRO	N-CD	5.07	1.54	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	285	ASP	N-CA-CB	18.14	141.14	110.49
4	A	285	ASP	CB-CA-C	-9.48	91.55	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	439	ASN	N-CA-C	-8.37	97.39	110.36
4	B	43	THR	N-CA-C	-8.30	98.00	109.95
3	C	73	PHE	N-CA-C	-7.71	98.85	109.95
3	C	21	GLY	N-CA-C	-7.63	100.83	112.51
4	B	245	SER	N-CA-C	7.53	120.45	111.33
1	D	35	GLY	N-CA-C	7.03	121.67	112.25
4	A	79	ALA	CA-C-N	-6.82	113.18	120.47
4	A	79	ALA	C-N-CA	-6.82	113.18	120.47
4	B	247	ASN	N-CA-C	6.79	119.65	108.99
2	E	463	SER	CA-C-N	-6.77	112.99	119.76
2	E	463	SER	C-N-CA	-6.77	112.99	119.76
2	E	210	LEU	CA-C-N	-6.72	113.04	119.76
2	E	210	LEU	C-N-CA	-6.72	113.04	119.76
4	B	125	VAL	N-CA-C	-6.71	105.21	111.45
3	C	112	TRP	N-CA-C	-6.49	100.67	110.28
4	B	284	GLY	N-CA-C	6.27	118.48	110.20
4	B	118	LEU	N-CA-C	6.14	119.49	109.24
4	A	31	VAL	N-CA-C	6.06	113.88	107.76
4	A	286	ASN	N-CA-C	-6.04	104.26	111.69
4	A	167	LYS	N-CA-C	-6.03	99.07	108.90
2	E	594	LYS	N-CA-C	5.90	117.92	110.24
2	E	514	ILE	N-CA-C	5.85	116.36	108.17
1	D	34	ARG	N-CA-C	-5.84	100.81	109.86
1	D	48	GLY	N-CA-C	-5.79	104.06	112.17
4	A	16	VAL	N-CA-C	5.77	116.67	108.42
4	B	204	GLN	N-CA-C	5.73	119.02	110.14
3	C	124	GLN	CA-C-N	5.68	125.44	119.76
3	C	124	GLN	C-N-CA	5.68	125.44	119.76
2	E	231	LYS	N-CA-C	-5.56	105.75	112.54
4	A	83	ASN	N-CA-C	5.51	118.22	109.24
1	D	146	VAL	CA-C-N	5.48	125.66	119.90
1	D	146	VAL	C-N-CA	5.48	125.66	119.90
1	D	36	ASP	N-CA-C	-5.40	103.26	110.55
2	E	254	ASN	N-CA-C	5.25	117.00	111.28
4	B	278	VAL	N-CA-CB	-5.17	103.20	111.58
2	E	459	THR	CB-CA-C	-5.12	101.14	111.17
4	A	247	ASN	N-CA-C	-5.11	105.71	111.28
4	B	237	GLN	N-CA-C	-5.11	103.79	110.53
2	E	290	THR	N-CA-C	-5.09	107.23	113.50
2	E	214	ASN	N-CA-C	5.02	117.32	110.24

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	15	ILE	Peptide
4	B	244	VAL	Peptide
1	D	35	GLY	Peptide
2	E	438	GLY	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	D	1361	0	1338	39	0
2	E	3347	0	3274	117	0
3	C	1156	0	1113	46	0
4	A	2304	0	2240	265	0
4	B	2304	0	2241	107	0
5	A	11	0	0	1	0
5	B	11	0	0	0	0
5	C	7	0	0	0	0
5	D	2	0	0	0	0
5	E	19	0	0	2	0
All	All	10522	0	10206	566	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 27.

All (566) 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)
4:B:46:TYR:CZ	4:B:68:ILE:HD11	1.40	1.56
1:D:65:VAL:CG2	1:D:66:ASN:H	1.11	1.41
4:A:162:ILE:HD11	4:A:250:ARG:NH2	1.22	1.40
4:A:162:ILE:CD1	4:A:250:ARG:NH2	1.90	1.34
4:A:9:ASN:N	4:A:61:TYR:HH	1.36	1.21
4:B:46:TYR:CE2	4:B:68:ILE:HD11	1.77	1.20
4:B:46:TYR:CZ	4:B:68:ILE:CD1	2.24	1.20
4:A:15:ILE:CG2	4:A:147:TYR:HD1	1.55	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LEU:CB	4:A:286:ASN:HB2	1.72	1.19
4:A:265:LEU:H	4:A:286:ASN:ND2	1.41	1.18
2:E:264:ASN:OD1	2:E:267:LYS:N	1.78	1.17
4:B:46:TYR:CE2	4:B:68:ILE:CD1	2.30	1.15
1:D:65:VAL:HG22	1:D:66:ASN:H	1.02	1.14
4:A:15:ILE:HG23	4:A:147:TYR:HD1	1.07	1.10
4:A:15:ILE:HD11	4:A:66:MET:HG3	1.31	1.10
4:A:245:SER:HA	4:A:248:TYR:HD1	1.13	1.09
4:A:265:LEU:HB3	4:A:286:ASN:HB2	1.13	1.09
4:A:172:VAL:HG22	4:A:180:ASN:OD1	1.52	1.08
2:E:403:ASN:O	2:E:486:GLN:NE2	1.87	1.07
4:A:233:ASN:ND2	4:A:235:ASP:OD2	1.87	1.07
1:D:65:VAL:CG2	1:D:66:ASN:N	1.86	1.06
4:A:15:ILE:CG2	4:A:147:TYR:CD1	2.39	1.06
1:D:65:VAL:HG23	1:D:66:ASN:H	0.92	1.06
4:A:177:LEU:HD13	4:A:178:ALA:N	1.70	1.05
1:D:65:VAL:HG23	1:D:66:ASN:N	1.50	1.04
4:A:177:LEU:HD13	4:A:178:ALA:H	1.19	1.04
4:A:284:GLY:O	4:A:285:ASP:OD1	1.76	1.03
2:E:404:ASN:HA	2:E:486:GLN:NE2	1.73	1.02
4:B:68:ILE:HD13	4:B:68:ILE:H	1.22	1.02
3:C:137:SER:HA	3:C:140:MET:HE2	1.39	1.01
4:A:217:TRP:NE1	4:A:222:GLY:O	1.93	1.00
4:A:219:PHE:CZ	4:A:257:ARG:NE	2.30	1.00
4:B:232:GLN:O	4:B:233:ASN:ND2	1.94	0.99
4:A:15:ILE:HG23	4:A:147:TYR:CD1	1.97	0.99
4:A:73:LEU:HD23	4:A:87:GLN:C	1.89	0.98
4:A:277:GLN:HG2	4:A:278:VAL:H	1.26	0.98
4:A:263:LEU:C	4:A:289:TRP:HZ2	1.72	0.97
4:A:218:ILE:HD12	4:A:219:PHE:H	1.26	0.95
4:A:177:LEU:HD11	4:A:226:ARG:HE	1.32	0.95
4:A:245:SER:HA	4:A:248:TYR:CD1	2.00	0.95
1:D:94:ASN:HD22	1:D:94:ASN:C	1.73	0.93
4:A:265:LEU:CG	4:A:268:GLY:HA2	1.98	0.93
4:B:234:ASN:ND2	4:B:236:ALA:H	1.67	0.93
4:A:15:ILE:HG21	4:A:147:TYR:CD1	2.01	0.92
4:A:177:LEU:HB2	4:A:227:VAL:HG22	1.51	0.92
2:E:549:ASN:ND2	2:E:549:ASN:O	2.02	0.91
2:E:462:ASP:HB2	2:E:529:GLN:NE2	1.85	0.91
4:B:234:ASN:HD22	4:B:236:ALA:H	0.93	0.91
4:B:248:TYR:HB3	4:B:250:ARG:CD	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:VAL:HG11	2:E:613:LEU:CD2	2.00	0.91
1:D:65:VAL:HG22	1:D:66:ASN:N	1.68	0.91
2:E:209:VAL:HG13	2:E:211:PRO:HD3	1.54	0.90
3:C:5:ARG:HG3	3:C:5:ARG:HH11	1.35	0.89
4:A:219:PHE:CZ	4:A:257:ARG:CZ	2.56	0.89
4:A:162:ILE:CG2	4:A:285:ASP:O	2.21	0.88
4:A:265:LEU:H	4:A:286:ASN:HD22	1.14	0.88
2:E:549:ASN:OD1	3:C:140:MET:CE	2.20	0.88
4:A:265:LEU:HG	4:A:268:GLY:HA2	1.56	0.88
4:A:217:TRP:CZ3	4:A:219:PHE:HE1	1.92	0.88
4:A:177:LEU:HD22	4:A:226:ARG:HG2	1.53	0.88
4:A:9:ASN:N	4:A:61:TYR:OH	2.06	0.88
4:A:263:LEU:HD23	4:A:289:TRP:CZ2	2.08	0.88
3:C:5:ARG:O	3:C:6:THR:OG1	1.92	0.87
4:A:178:ALA:HA	4:A:226:ARG:HG3	1.56	0.87
4:A:162:ILE:HG22	4:A:285:ASP:O	1.73	0.87
4:A:263:LEU:O	4:A:289:TRP:HZ2	1.57	0.87
4:A:233:ASN:N	4:A:234:ASN:HA	1.89	0.86
4:A:73:LEU:CD2	4:A:87:GLN:C	2.48	0.86
4:B:248:TYR:HB3	4:B:250:ARG:HD3	1.57	0.86
4:A:173:SER:OG	4:A:175:THR:HG22	1.75	0.86
4:A:264:ASP:O	4:A:276:ILE:O	1.92	0.85
4:A:246:ASP:OD1	4:A:247:ASN:N	2.08	0.85
4:A:265:LEU:N	4:A:286:ASN:ND2	2.24	0.85
4:A:73:LEU:HD23	4:A:87:GLN:O	1.76	0.85
4:A:263:LEU:HG	4:A:289:TRP:CH2	2.11	0.85
4:B:46:TYR:CE2	4:B:68:ILE:HD13	2.11	0.85
1:D:63:LEU:C	1:D:63:LEU:HD12	2.01	0.85
4:B:46:TYR:CE1	4:B:68:ILE:CD1	2.59	0.85
2:E:404:ASN:HA	2:E:486:GLN:HE22	1.38	0.85
4:A:264:ASP:OD2	4:A:265:LEU:N	2.10	0.84
4:A:162:ILE:HD13	4:A:250:ARG:NH2	1.91	0.84
4:B:234:ASN:HD21	4:B:236:ALA:HB3	1.42	0.83
4:A:263:LEU:CG	4:A:289:TRP:CZ2	2.61	0.83
4:A:177:LEU:CD1	4:A:178:ALA:N	2.40	0.83
4:A:263:LEU:O	4:A:289:TRP:CZ2	2.30	0.83
4:B:70:ASN:O	4:B:73:LEU:HD22	1.78	0.83
4:B:46:TYR:CE1	4:B:68:ILE:HD11	2.13	0.82
1:D:63:LEU:O	1:D:64:ARG:HB2	1.80	0.82
4:A:177:LEU:CD1	4:A:178:ALA:H	1.93	0.82
2:E:568:LEU:HD23	2:E:583:ILE:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:ILE:CD1	2:E:408:ILE:CG2	2.58	0.81
2:E:549:ASN:OD1	3:C:140:MET:HE3	1.80	0.81
4:A:162:ILE:HD11	4:A:250:ARG:HH22	0.89	0.81
4:A:178:ALA:O	4:A:179:VAL:HG13	1.80	0.81
4:B:234:ASN:HD22	4:B:236:ALA:N	1.77	0.81
4:A:287:GLN:O	4:A:289:TRP:NE1	2.14	0.81
4:A:15:ILE:HG21	4:A:147:TYR:CE1	2.16	0.80
4:A:162:ILE:HG23	4:A:163:LEU:HD22	1.62	0.80
4:A:263:LEU:C	4:A:289:TRP:CZ2	2.60	0.79
4:A:277:GLN:HG2	4:A:278:VAL:N	1.96	0.79
4:A:263:LEU:CB	4:A:289:TRP:CZ2	2.66	0.79
4:A:263:LEU:HB3	4:A:289:TRP:CZ2	2.18	0.79
3:C:137:SER:HA	3:C:140:MET:CE	2.13	0.79
4:A:15:ILE:HD11	4:A:66:MET:CG	2.12	0.78
4:A:277:GLN:CG	4:A:278:VAL:H	1.96	0.78
4:A:72:ASN:O	4:A:72:ASN:ND2	2.17	0.78
4:A:245:SER:CA	4:A:248:TYR:HD1	1.97	0.77
4:A:265:LEU:N	4:A:286:ASN:HD22	1.80	0.77
4:B:46:TYR:CD2	4:B:68:ILE:HD13	2.19	0.77
4:A:265:LEU:HB3	4:A:286:ASN:CB	2.07	0.77
2:E:210:LEU:CD1	2:E:321:TYR:OH	2.32	0.77
4:A:12:ASN:OD1	4:A:54:TYR:CB	2.33	0.76
4:A:177:LEU:HD11	4:A:226:ARG:NE	1.99	0.76
4:A:177:LEU:CD1	4:A:226:ARG:HE	1.98	0.75
2:E:502:GLY:O	2:E:505:ARG:HD3	1.86	0.75
4:A:265:LEU:HB2	4:A:286:ASN:HB2	1.64	0.75
4:B:46:TYR:CD2	4:B:68:ILE:CD1	2.69	0.75
4:A:283:GLY:HA3	4:A:287:GLN:HG3	1.69	0.74
4:B:79:ALA:HB1	4:B:80:PRO:CD	2.18	0.74
4:A:162:ILE:CD1	4:A:250:ARG:HH21	1.94	0.74
4:A:263:LEU:HD23	4:A:289:TRP:CH2	2.23	0.74
4:A:32:PRO:HG3	4:A:47:LEU:HD21	1.68	0.74
4:A:219:PHE:HZ	4:A:257:ARG:NE	1.83	0.74
4:B:67:ASN:OD1	4:B:70:ASN:N	2.14	0.74
3:C:5:ARG:HG3	3:C:5:ARG:NH1	1.98	0.73
4:A:283:GLY:CA	4:A:287:GLN:HG3	2.19	0.73
4:A:9:ASN:HA	4:A:12:ASN:HB2	1.69	0.73
4:A:178:ALA:CA	4:A:226:ARG:HG3	2.18	0.73
4:A:218:ILE:HD12	4:A:219:PHE:N	2.02	0.73
4:A:263:LEU:CD2	4:A:289:TRP:CZ2	2.72	0.73
4:B:44:ARG:NH1	4:B:151:ASP:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:263:LEU:HD23	4:A:289:TRP:CE2	2.24	0.72
4:B:234:ASN:ND2	4:B:236:ALA:HB3	2.05	0.72
4:A:263:LEU:CD2	4:A:289:TRP:CH2	2.72	0.71
4:A:79:ALA:HB1	4:A:80:PRO:HD3	1.72	0.71
4:A:218:ILE:HG21	4:A:224:THR:OG1	1.89	0.71
2:E:385:ILE:HD11	2:E:408:ILE:HG21	1.71	0.71
4:A:218:ILE:HG23	4:A:221:ASP:O	1.91	0.71
4:A:217:TRP:CZ3	4:A:219:PHE:CE1	2.78	0.71
4:B:248:TYR:HB3	4:B:250:ARG:HD2	1.72	0.71
4:A:247:ASN:ND2	5:A:301:HOH:O	2.06	0.70
4:A:265:LEU:CD2	4:A:268:GLY:HA2	2.22	0.70
2:E:385:ILE:HD12	2:E:408:ILE:CG2	2.21	0.70
4:A:177:LEU:CD1	4:A:226:ARG:NE	2.55	0.70
4:A:105:ASN:ND2	4:A:107:SER:OG	2.24	0.70
4:A:217:TRP:HE1	4:A:222:GLY:C	1.98	0.69
4:A:219:PHE:CE1	4:A:257:ARG:NE	2.57	0.69
2:E:209:VAL:HG13	2:E:211:PRO:CD	2.22	0.69
4:A:263:LEU:HG	4:A:289:TRP:CZ2	2.24	0.69
4:A:219:PHE:HZ	4:A:257:ARG:HG3	1.56	0.69
4:A:263:LEU:CG	4:A:289:TRP:CH2	2.76	0.69
2:E:385:ILE:HD11	2:E:408:ILE:CG2	2.23	0.68
4:A:11:LEU:C	4:A:11:LEU:HD12	2.18	0.68
4:B:46:TYR:CE1	4:B:68:ILE:HD12	2.27	0.68
4:A:177:LEU:HD21	4:A:226:ARG:CZ	2.24	0.67
2:E:489:SER:OG	2:E:491:ILE:HG22	1.94	0.67
2:E:543:ILE:HD11	2:E:599:LEU:C	2.19	0.67
3:C:23:LEU:HD23	3:C:35:SER:N	2.09	0.66
4:A:177:LEU:CB	4:A:227:VAL:HG22	2.25	0.66
4:B:55:ASP:HB3	4:B:58:LYS:HB2	1.76	0.66
2:E:620:LEU:HD23	2:E:621:HIS:N	2.11	0.66
2:E:404:ASN:CA	2:E:486:GLN:NE2	2.57	0.66
4:A:207:ASN:OD1	4:A:208:LYS:N	2.29	0.66
4:A:194:ILE:C	4:A:194:ILE:HD13	2.20	0.66
1:D:66:ASN:HA	1:D:69:ALA:HB3	1.76	0.65
4:A:12:ASN:OD1	4:A:54:TYR:HB3	1.97	0.65
1:D:94:ASN:C	1:D:94:ASN:ND2	2.47	0.65
4:B:68:ILE:CD1	4:B:68:ILE:H	1.97	0.65
1:D:63:LEU:O	1:D:64:ARG:CB	2.44	0.65
2:E:549:ASN:OD1	3:C:140:MET:HE1	1.97	0.65
2:E:548:ASN:HB2	2:E:551:ASP:CG	2.22	0.64
4:B:234:ASN:HD21	4:B:236:ALA:CB	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LEU:HD23	4:A:268:GLY:HA2	1.79	0.64
4:A:124:THR:O	4:A:127:ARG:HD3	1.98	0.63
4:A:162:ILE:HD13	4:A:250:ARG:HH21	1.59	0.63
4:A:218:ILE:CD1	4:A:219:PHE:H	2.05	0.63
2:E:209:VAL:HG11	2:E:613:LEU:HD21	1.79	0.63
4:A:12:ASN:OD1	4:A:54:TYR:N	2.31	0.63
4:A:172:VAL:CG2	4:A:180:ASN:OD1	2.39	0.62
2:E:442:PHE:HA	2:E:448:CYS:SG	2.39	0.62
4:A:217:TRP:CG	4:A:218:ILE:H	2.17	0.62
4:A:11:LEU:O	4:A:14:LYS:HB2	1.99	0.62
4:A:180:ASN:CA	4:A:276:ILE:HD11	2.29	0.62
4:B:149:ILE:HD12	4:B:196:TYR:CE2	2.35	0.62
4:B:169:VAL:O	4:B:192:TRP:HZ3	1.82	0.62
2:E:260:PHE:CE1	2:E:273:THR:HG21	2.36	0.61
4:A:283:GLY:HA2	4:A:287:GLN:CG	2.30	0.61
4:B:232:GLN:C	4:B:233:ASN:HD22	2.03	0.61
4:A:79:ALA:CB	4:A:80:PRO:CD	2.78	0.61
2:E:403:ASN:C	2:E:486:GLN:NE2	2.59	0.60
1:D:94:ASN:HD22	1:D:95:PHE:N	1.98	0.60
2:E:209:VAL:HG11	2:E:613:LEU:HD23	1.82	0.60
3:C:5:ARG:C	3:C:6:THR:HG1	2.01	0.60
4:A:215:LEU:HD23	4:A:239:TRP:CZ2	2.37	0.60
4:A:283:GLY:N	4:A:287:GLN:OE1	2.34	0.60
2:E:431:ILE:HG23	2:E:458:ILE:HB	1.84	0.59
2:E:539:TYR:CE1	2:E:620:LEU:HD12	2.36	0.59
4:B:77:TRP:CD1	4:B:131:LEU:HD12	2.37	0.59
4:B:152:PHE:HE2	4:B:251:TYR:CE2	2.19	0.59
4:B:244:VAL:HG23	4:B:244:VAL:O	2.01	0.59
4:A:162:ILE:CD1	4:A:250:ARG:CZ	2.78	0.59
4:B:46:TYR:CD1	4:B:68:ILE:HD12	2.38	0.59
4:A:203:TYR:CD2	4:A:241:ILE:HD12	2.37	0.59
4:A:263:LEU:CB	4:A:289:TRP:HZ2	2.11	0.59
3:C:21:GLY:O	3:C:22:SER:OG	2.17	0.59
4:A:108:PHE:CG	4:A:144:ILE:HD12	2.37	0.59
4:B:79:ALA:HB1	4:B:80:PRO:HD3	1.84	0.59
4:A:180:ASN:HA	4:A:276:ILE:HD11	1.85	0.58
3:C:19:PHE:HD2	3:C:119:GLU:HA	1.68	0.58
4:B:234:ASN:ND2	4:B:236:ALA:N	2.45	0.58
3:C:21:GLY:O	3:C:22:SER:CB	2.51	0.58
4:B:66:MET:HE2	4:B:66:MET:HA	1.84	0.58
4:A:88:GLN:HE21	4:A:88:GLN:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:162:ILE:HD11	4:A:250:ARG:CZ	2.21	0.58
2:E:500:GLU:HG2	2:E:504:LEU:HB3	1.85	0.58
2:E:447:LEU:HD23	2:E:447:LEU:C	2.28	0.58
4:A:180:ASN:C	4:A:276:ILE:HD11	2.28	0.58
4:A:248:TYR:CD2	4:A:249:ASP:N	2.72	0.58
4:A:233:ASN:N	4:A:234:ASN:CA	2.66	0.57
4:B:79:ALA:CB	4:B:80:PRO:CD	2.82	0.57
4:A:162:ILE:HG21	4:A:285:ASP:HB3	1.86	0.57
4:B:58:LYS:O	4:B:59:ALA:HB3	2.04	0.57
4:A:81:THR:OG1	4:A:82:HIS:N	2.38	0.57
4:A:289:TRP:CD1	4:A:289:TRP:N	2.73	0.57
2:E:334:LEU:HD12	2:E:335:PRO:HD2	1.87	0.57
3:C:118:ASN:O	3:C:119:GLU:HB2	2.05	0.57
2:E:214:ASN:HB2	2:E:322:GLN:HA	1.86	0.56
3:C:127:LEU:HD21	4:A:118:LEU:HD21	1.87	0.56
2:E:447:LEU:HD23	2:E:447:LEU:O	2.05	0.56
4:A:78:ASN:O	4:A:79:ALA:C	2.48	0.56
1:D:31:VAL:HG22	1:D:88:ILE:HG22	1.87	0.56
4:A:223:ASN:HB3	4:A:277:GLN:HG3	1.88	0.56
4:A:265:LEU:CB	4:A:268:GLY:HA2	2.34	0.56
4:A:265:LEU:CB	4:A:286:ASN:CB	2.66	0.56
4:B:115:ASN:OD1	4:B:117:ASN:HB2	2.05	0.56
4:B:171:GLN:HE21	4:B:227:VAL:HG21	1.70	0.56
4:B:251:TYR:N	4:B:251:TYR:CD1	2.73	0.56
2:E:568:LEU:HD23	2:E:583:ILE:CG2	2.34	0.56
2:E:403:ASN:C	2:E:486:GLN:HE21	2.05	0.56
3:C:113:ASP:OD1	3:C:114:ILE:N	2.38	0.56
4:A:217:TRP:CZ2	4:A:222:GLY:HA2	2.41	0.56
4:A:219:PHE:CZ	4:A:257:ARG:HG3	2.40	0.56
4:A:177:LEU:O	4:A:178:ALA:HB3	2.06	0.56
4:A:61:TYR:CD2	4:A:99:LEU:HD22	2.41	0.56
4:A:219:PHE:CZ	4:A:257:ARG:NH1	2.74	0.55
2:E:209:VAL:CG1	2:E:613:LEU:CD2	2.82	0.55
2:E:487:THR:O	2:E:488:SER:HB3	2.05	0.55
4:A:16:VAL:HG11	4:A:144:ILE:HG23	1.88	0.55
2:E:219:ILE:HG12	2:E:372:VAL:HG12	1.88	0.55
4:A:177:LEU:H	4:A:177:LEU:HD12	1.71	0.55
2:E:434:ALA:HB3	2:E:437:SER:OG	2.06	0.55
4:A:73:LEU:CD2	4:A:87:GLN:CA	2.84	0.55
4:A:79:ALA:CB	4:A:80:PRO:HD3	2.37	0.55
4:A:162:ILE:CG2	4:A:285:ASP:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:ILE:CD1	2:E:408:ILE:HG21	2.33	0.55
4:A:238:TYR:C	4:A:239:TRP:CD1	2.85	0.55
3:C:19:PHE:CD2	3:C:119:GLU:HA	2.42	0.55
4:A:237:GLN:C	4:A:238:TYR:CD1	2.86	0.54
2:E:549:ASN:HD22	2:E:549:ASN:C	2.08	0.54
4:A:81:THR:HG23	4:A:83:ASN:H	1.72	0.54
2:E:209:VAL:HG11	2:E:613:LEU:CG	2.38	0.54
4:A:31:VAL:HG23	4:A:31:VAL:O	2.06	0.54
4:A:217:TRP:HZ3	4:A:219:PHE:HE1	1.50	0.54
4:A:246:ASP:N	4:A:248:TYR:CD1	2.73	0.54
2:E:518:LEU:HD22	2:E:524:HIS:CD2	2.42	0.54
4:B:34:ASN:OD1	4:B:34:ASN:C	2.51	0.54
4:A:28:PHE:CZ	4:A:129:LEU:HD11	2.43	0.54
3:C:7:PHE:C	3:C:7:PHE:CD1	2.85	0.54
3:C:99:MET:HE2	3:C:143:LEU:HD11	1.88	0.54
4:B:248:TYR:HD1	4:B:250:ARG:CZ	2.21	0.54
4:A:159:ILE:HB	4:A:169:VAL:CG1	2.38	0.54
4:A:219:PHE:O	4:A:220:SER:HB2	2.08	0.54
2:E:518:LEU:HD13	2:E:624:ILE:HD11	1.89	0.53
4:A:43:THR:HG23	4:A:48:GLU:HB2	1.90	0.53
4:A:178:ALA:O	4:A:179:VAL:CG1	2.54	0.53
4:A:283:GLY:CA	4:A:287:GLN:CG	2.85	0.53
2:E:385:ILE:HG22	2:E:387:THR:O	2.08	0.53
4:A:265:LEU:HB3	4:A:268:GLY:HA2	1.91	0.53
4:B:29:TYR:CZ	4:B:47:LEU:HD13	2.43	0.53
2:E:430:LYS:HE2	2:E:462:ASP:OD1	2.07	0.53
4:A:34:ASN:OD1	4:A:35:GLY:N	2.40	0.53
4:A:115:ASN:C	4:A:115:ASN:OD1	2.52	0.53
4:A:246:ASP:CG	4:A:247:ASN:H	2.10	0.53
1:D:117:LEU:HD12	1:D:117:LEU:C	2.34	0.53
3:C:23:LEU:HD23	3:C:34:PHE:C	2.34	0.53
4:B:46:TYR:OH	4:B:68:ILE:HD11	2.00	0.53
4:B:73:LEU:HD23	4:B:73:LEU:O	2.08	0.53
4:A:218:ILE:HG22	4:A:224:THR:O	2.09	0.53
4:A:283:GLY:HA2	4:A:287:GLN:HG3	1.90	0.53
4:B:72:ASN:OD1	4:B:89:ASP:HB3	2.08	0.53
4:B:267:GLY:O	4:B:269:GLN:N	2.42	0.53
4:A:237:GLN:O	4:A:238:TYR:HD1	1.92	0.53
2:E:209:VAL:O	2:E:210:LEU:HD12	2.08	0.53
3:C:15:ILE:HG12	3:C:143:LEU:HD22	1.89	0.53
4:A:178:ALA:HA	4:A:226:ARG:CG	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:230:SER:O	4:B:231:ALA:HB3	2.08	0.53
2:E:210:LEU:HD13	2:E:321:TYR:OH	2.08	0.52
4:B:119:VAL:HG13	4:B:134:LEU:HD11	1.90	0.52
4:A:172:VAL:HG23	4:A:177:LEU:O	2.10	0.52
3:C:99:MET:CE	3:C:143:LEU:HD11	2.40	0.52
4:A:237:GLN:C	4:A:238:TYR:HD1	2.17	0.52
1:D:63:LEU:HD12	1:D:64:ARG:N	2.24	0.52
1:D:78:SER:OG	1:D:140:GLU:OE2	2.27	0.52
4:A:12:ASN:OD1	4:A:54:TYR:HB2	2.10	0.52
4:B:108:PHE:CD1	4:B:144:ILE:HD12	2.45	0.52
4:B:116:PRO:O	4:B:118:LEU:N	2.42	0.52
4:A:61:TYR:OH	4:B:103:ILE:HG22	2.09	0.52
4:A:177:LEU:HD12	4:A:177:LEU:N	2.24	0.52
4:A:73:LEU:HD22	4:A:87:GLN:N	2.25	0.51
3:C:121:ILE:HD13	3:C:121:ILE:H	1.75	0.51
4:B:152:PHE:CZ	4:B:291:MET:HE2	2.45	0.51
2:E:209:VAL:C	2:E:210:LEU:HG	2.36	0.51
4:B:234:ASN:ND2	4:B:236:ALA:CB	2.70	0.51
2:E:269:SER:O	2:E:273:THR:HG22	2.11	0.51
4:A:233:ASN:H	4:A:234:ASN:HA	1.72	0.51
2:E:549:ASN:CG	3:C:140:MET:HE3	2.34	0.51
4:A:210:LEU:HD22	4:A:210:LEU:O	2.10	0.51
2:E:559:THR:HG22	2:E:589:LEU:HB3	1.92	0.50
2:E:507:LEU:O	2:E:510:SER:HB3	2.11	0.50
3:C:93:ALA:O	3:C:94:VAL:C	2.53	0.50
4:B:116:PRO:O	4:B:117:ASN:C	2.54	0.50
3:C:110:TYR:HB3	3:C:128:LEU:HG	1.92	0.50
4:A:84:ILE:HD11	4:A:131:LEU:HD13	1.94	0.50
4:A:88:GLN:HA	4:A:88:GLN:NE2	2.26	0.50
2:E:404:ASN:CA	2:E:486:GLN:HE22	2.18	0.50
4:B:68:ILE:HD13	4:B:68:ILE:N	2.07	0.50
4:B:263:LEU:HD23	4:B:289:TRP:CE2	2.46	0.50
2:E:209:VAL:HG11	2:E:613:LEU:HG	1.94	0.50
2:E:469:TYR:CZ	2:E:512:VAL:HG11	2.47	0.49
4:B:241:ILE:HG22	4:B:251:TYR:HD2	1.75	0.49
2:E:239:ILE:HB	2:E:305:ILE:HG22	1.94	0.49
4:A:78:ASN:O	4:A:81:THR:HG22	2.12	0.49
4:B:15:ILE:HD11	4:B:66:MET:SD	2.52	0.49
2:E:260:PHE:CZ	2:E:262:THR:CG2	2.95	0.49
2:E:209:VAL:CG1	2:E:211:PRO:HD3	2.36	0.49
4:B:225:VAL:HG13	4:B:277:GLN:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:162:ILE:CG2	4:A:163:LEU:HD22	2.37	0.49
4:A:177:LEU:HD21	4:A:226:ARG:NH1	2.28	0.49
1:D:144:LEU:HD11	1:D:146:VAL:HG12	1.93	0.49
4:A:125:VAL:HG13	4:A:126:ALA:N	2.28	0.49
2:E:421:ASN:C	2:E:421:ASN:HD22	2.21	0.49
2:E:558:TYR:CD1	5:E:701:HOH:O	2.55	0.49
4:A:11:LEU:HD11	4:A:52:ILE:HG21	1.94	0.49
4:A:88:GLN:HE21	4:A:88:GLN:CA	2.24	0.49
3:C:24:TYR:CD1	3:C:24:TYR:N	2.81	0.48
4:A:233:ASN:HD22	4:A:235:ASP:H	1.61	0.48
3:C:13:TYR:CD2	3:C:47:VAL:CG1	2.95	0.48
4:A:233:ASN:ND2	4:A:233:ASN:H	2.11	0.48
3:C:23:LEU:CD2	3:C:34:PHE:C	2.87	0.48
4:B:23:ASN:CG	4:B:26:LEU:HD13	2.39	0.48
4:B:111:ALA:HB2	4:B:119:VAL:HG12	1.95	0.48
4:B:234:ASN:O	4:B:235:ASP:HB2	2.12	0.48
1:D:66:ASN:HA	1:D:69:ALA:CB	2.41	0.48
2:E:287:ASN:N	2:E:287:ASN:HD22	2.11	0.48
4:A:284:GLY:O	4:A:285:ASP:CG	2.53	0.48
2:E:320:ASP:OD1	2:E:322:GLN:NE2	2.47	0.48
4:A:62:LYS:NZ	4:A:91:ASN:OD1	2.47	0.48
4:A:223:ASN:O	4:A:277:GLN:HA	2.13	0.48
4:B:76:THR:HG23	4:B:95:GLN:HG2	1.94	0.48
4:A:175:THR:HG23	4:A:176:ASN:N	2.28	0.48
4:A:217:TRP:HZ2	4:A:222:GLY:HA2	1.79	0.48
4:B:135:ASN:C	4:B:135:ASN:HD22	2.21	0.48
2:E:548:ASN:CB	2:E:551:ASP:CG	2.87	0.48
4:B:152:PHE:CE2	4:B:251:TYR:CE2	3.02	0.48
4:B:46:TYR:CD1	4:B:68:ILE:CD1	2.95	0.47
2:E:431:ILE:HG21	2:E:472:VAL:HG11	1.96	0.47
2:E:558:TYR:CG	5:E:701:HOH:O	2.68	0.47
4:B:111:ALA:CB	4:B:119:VAL:HG12	2.45	0.47
2:E:543:ILE:HD11	2:E:599:LEU:O	2.14	0.47
4:A:77:TRP:HA	4:A:84:ILE:HD12	1.96	0.47
4:A:135:ASN:O	4:A:140:ILE:HD11	2.15	0.47
4:A:237:GLN:O	4:A:238:TYR:HB2	2.14	0.47
4:B:225:VAL:CG1	4:B:277:GLN:HA	2.45	0.47
2:E:409:LEU:HD23	2:E:447:LEU:HD11	1.96	0.47
4:A:11:LEU:C	4:A:11:LEU:CD1	2.86	0.47
4:A:124:THR:O	4:A:127:ARG:CD	2.62	0.47
4:A:265:LEU:HG	4:A:268:GLY:CA	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:180:ASN:C	4:B:276:ILE:HD13	2.39	0.47
4:B:234:ASN:ND2	4:B:234:ASN:C	2.73	0.47
1:D:47:LEU:HD21	1:D:123:TYR:CZ	2.49	0.47
4:A:286:ASN:ND2	4:A:286:ASN:C	2.73	0.47
2:E:214:ASN:HB3	2:E:323:ASN:H	1.79	0.47
3:C:23:LEU:C	3:C:24:TYR:CD1	2.92	0.47
4:B:29:TYR:OH	4:B:47:LEU:HD13	2.15	0.47
4:A:12:ASN:C	4:A:12:ASN:ND2	2.73	0.47
4:A:262:VAL:HG11	4:A:281:SER:HA	1.97	0.47
4:A:218:ILE:CD1	4:A:219:PHE:N	2.72	0.47
4:A:231:ALA:O	4:A:234:ASN:HB2	2.15	0.47
1:D:44:ASN:O	1:D:45:GLN:HB2	2.14	0.47
2:E:276:ARG:NH1	2:E:279:ASP:OD2	2.48	0.47
3:C:23:LEU:HD23	3:C:35:SER:CA	2.45	0.47
4:A:223:ASN:CG	4:A:277:GLN:HE21	2.23	0.47
4:B:98:LEU:N	4:B:98:LEU:HD12	2.30	0.46
1:D:44:ASN:OD1	1:D:44:ASN:N	2.47	0.46
2:E:211:PRO:HD3	2:E:613:LEU:HD21	1.98	0.46
2:E:258:PRO:HB3	2:E:335:PRO:HD3	1.96	0.46
4:A:277:GLN:CG	4:A:278:VAL:N	2.62	0.46
4:A:44:ARG:CZ	4:A:155:PHE:CD1	2.99	0.46
4:A:167:LYS:HA	4:A:182:TYR:O	2.15	0.46
2:E:397:ILE:O	2:E:397:ILE:HD12	2.16	0.46
3:C:5:ARG:HH11	3:C:5:ARG:CG	2.14	0.46
4:A:200:LYS:O	4:A:201:ALA:HB3	2.14	0.46
1:D:42:ARG:HG2	1:D:169:PHE:CZ	2.51	0.46
1:D:44:ASN:HA	1:D:122:GLN:HG3	1.97	0.46
4:B:241:ILE:HG22	4:B:251:TYR:CD2	2.50	0.46
4:B:188:LEU:HB2	4:B:209:ILE:HG23	1.98	0.46
1:D:176:ILE:HD12	2:E:238:LEU:HD12	1.98	0.46
4:B:216:THR:HG23	4:B:237:GLN:HG3	1.97	0.46
4:B:237:GLN:O	4:B:238:TYR:HB2	2.16	0.46
3:C:92:ILE:HD11	3:C:140:MET:HG3	1.97	0.46
4:A:14:LYS:O	4:A:51:ARG:HA	2.16	0.46
1:D:67:ASP:C	1:D:69:ALA:N	2.73	0.46
4:A:217:TRP:CD1	4:A:218:ILE:H	2.32	0.46
4:B:265:LEU:O	4:B:266:TYR:HB3	2.16	0.46
4:A:265:LEU:HB2	4:A:286:ASN:CB	2.39	0.45
2:E:210:LEU:HD12	2:E:210:LEU:O	2.16	0.45
4:B:79:ALA:HB1	4:B:80:PRO:HD2	1.97	0.45
4:B:61:TYR:CD1	4:B:99:LEU:HD12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:233:ASN:ND2	4:B:233:ASN:C	2.73	0.45
4:A:12:ASN:HD22	4:A:13:ASP:HB2	1.80	0.45
4:A:174:MET:HB2	4:A:209:ILE:HG12	1.98	0.45
4:A:217:TRP:CG	4:A:218:ILE:N	2.82	0.45
2:E:219:ILE:HG22	2:E:220:ASN:N	2.31	0.45
2:E:548:ASN:O	2:E:549:ASN:HB3	2.17	0.45
4:B:28:PHE:CZ	4:B:129:LEU:HD11	2.52	0.45
4:B:176:ASN:OD1	4:B:176:ASN:C	2.60	0.45
1:D:55:GLY:HA2	1:D:111:ALA:O	2.17	0.45
1:D:98:ALA:O	1:D:101:ILE:HD13	2.16	0.45
2:E:542:THR:HB	2:E:603:ILE:HG12	1.98	0.45
4:A:31:VAL:O	4:A:31:VAL:CG2	2.65	0.45
2:E:270:GLN:HA	2:E:273:THR:CG2	2.47	0.45
2:E:385:ILE:HD12	2:E:408:ILE:HG23	1.98	0.45
2:E:533:VAL:O	2:E:534:HIS:HB2	2.15	0.45
4:A:109:ILE:HG23	4:A:119:VAL:HG11	1.99	0.45
4:A:192:TRP:HZ3	4:A:207:ASN:ND2	2.14	0.45
2:E:297:GLU:HG3	2:E:342:VAL:HG11	1.99	0.45
2:E:547:PHE:O	2:E:547:PHE:CD1	2.70	0.45
4:A:28:PHE:CE1	4:A:129:LEU:HD11	2.52	0.44
2:E:435:ILE:HG12	2:E:454:ALA:O	2.17	0.44
4:A:247:ASN:O	4:A:248:TYR:CD2	2.70	0.44
4:A:283:GLY:HA2	4:A:287:GLN:CD	2.43	0.44
2:E:211:PRO:O	2:E:212:TYR:CD2	2.70	0.44
2:E:449:ASP:C	2:E:451:ASP:H	2.26	0.44
4:A:231:ALA:O	4:A:234:ASN:N	2.50	0.44
4:A:266:TYR:O	4:A:266:TYR:CD2	2.70	0.44
1:D:127:ARG:HD2	1:D:145:TYR:CE1	2.53	0.44
2:E:563:GLN:OE1	2:E:564:GLY:N	2.50	0.44
4:A:12:ASN:C	4:A:12:ASN:HD22	2.24	0.44
4:A:102:ASP:O	4:A:104:GLY:N	2.48	0.44
4:A:209:ILE:HG23	4:A:210:LEU:HD12	1.98	0.44
4:B:240:LEU:N	4:B:240:LEU:HD22	2.31	0.44
2:E:209:VAL:CG1	2:E:613:LEU:HD21	2.46	0.44
4:A:237:GLN:O	4:A:238:TYR:CD1	2.70	0.44
4:A:276:ILE:N	4:A:276:ILE:HD13	2.33	0.44
4:A:287:GLN:O	4:A:289:TRP:CD1	2.70	0.44
2:E:543:ILE:HB	2:E:544:PRO:HD2	2.00	0.44
4:A:53:ILE:HB	4:A:62:LYS:HG3	1.99	0.44
4:A:283:GLY:HA3	4:A:284:GLY:HA2	1.69	0.44
1:D:64:ARG:O	1:D:64:ARG:HG2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:246:ASP:O	4:A:248:TYR:CD1	2.70	0.44
4:B:58:LYS:O	4:B:59:ALA:CB	2.66	0.44
2:E:464:PRO:C	2:E:465:ASN:CG	2.85	0.43
4:A:145:GLU:CD	4:A:149:ILE:HD11	2.43	0.43
2:E:562:ASN:HB3	2:E:612:GLU:O	2.18	0.43
4:A:215:LEU:CD2	4:A:239:TRP:CZ2	3.01	0.43
4:A:44:ARG:NH1	4:A:155:PHE:CD1	2.86	0.43
4:A:73:LEU:CD2	4:A:87:GLN:N	2.81	0.43
4:A:211:SER:O	4:A:212:ASN:ND2	2.48	0.43
4:A:11:LEU:HD12	4:A:11:LEU:O	2.19	0.43
4:A:145:GLU:OE1	4:A:149:ILE:HD11	2.18	0.43
4:A:219:PHE:HZ	4:A:257:ARG:CG	2.26	0.43
4:A:246:ASP:O	4:A:248:TYR:CG	2.72	0.43
4:B:77:TRP:CD1	4:B:77:TRP:C	2.97	0.43
1:D:63:LEU:CD1	1:D:103:ILE:O	2.66	0.43
2:E:385:ILE:HD12	2:E:408:ILE:HG22	1.98	0.43
2:E:389:ILE:HD12	2:E:393:TYR:HB3	2.01	0.43
4:A:177:LEU:CD1	4:A:177:LEU:C	2.86	0.43
2:E:322:GLN:HE21	2:E:322:GLN:CA	2.31	0.43
2:E:418:TYR:CD2	2:E:499:ARG:HA	2.54	0.43
3:C:124:GLN:HE22	4:A:115:ASN:HB2	1.84	0.43
1:D:172:ASN:O	1:D:173:ASP:C	2.62	0.42
3:C:16:LYS:HD3	3:C:23:LEU:O	2.19	0.42
4:A:266:TYR:O	4:A:266:TYR:CG	2.70	0.42
4:B:233:ASN:HD22	4:B:233:ASN:C	2.27	0.42
4:B:249:ASP:O	4:B:251:TYR:HE1	2.02	0.42
2:E:418:TYR:CD1	2:E:474:LEU:HD12	2.54	0.42
2:E:543:ILE:HG13	2:E:600:ASN:HA	2.01	0.42
4:B:46:TYR:CG	4:B:68:ILE:CD1	3.02	0.42
4:B:185:ASN:C	4:B:187:ASP:H	2.26	0.42
2:E:260:PHE:HE1	2:E:330:ALA:HB1	1.84	0.42
4:A:76:THR:HG23	4:A:95:GLN:HG2	2.00	0.42
4:A:84:ILE:HD11	4:A:131:LEU:CD1	2.50	0.42
4:A:123:ASP:OD1	4:A:125:VAL:HG12	2.19	0.42
2:E:590:LEU:HD13	2:E:590:LEU:C	2.44	0.42
3:C:121:ILE:H	3:C:121:ILE:CD1	2.32	0.42
4:A:177:LEU:HD13	4:A:226:ARG:NE	2.34	0.42
4:A:177:LEU:HD23	4:A:227:VAL:O	2.18	0.42
4:A:218:ILE:CG1	4:A:219:PHE:N	2.81	0.42
4:A:246:ASP:N	4:A:248:TYR:HD1	2.15	0.42
1:D:26:ALA:O	1:D:27:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:LEU:HD13	3:C:76:ILE:HG22	2.01	0.42
4:B:26:LEU:HD12	4:B:26:LEU:N	2.34	0.42
2:E:220:ASN:C	2:E:220:ASN:HD22	2.28	0.42
3:C:94:VAL:O	3:C:96:THR:HG23	2.20	0.42
4:B:20:CYS:SG	4:B:39:LEU:HD22	2.60	0.42
2:E:264:ASN:OD1	2:E:266:ALA:N	2.53	0.42
2:E:562:ASN:C	2:E:590:LEU:HD23	2.44	0.42
4:A:192:TRP:CZ3	4:A:207:ASN:CG	2.98	0.42
4:B:154:ASN:HA	4:B:194:ILE:O	2.19	0.42
4:B:203:TYR:O	4:B:238:TYR:HA	2.20	0.42
2:E:620:LEU:HD23	2:E:620:LEU:C	2.44	0.42
2:E:543:ILE:HD13	2:E:543:ILE:HG21	1.87	0.42
4:A:223:ASN:ND2	4:A:277:GLN:NE2	2.67	0.42
4:B:169:VAL:O	4:B:192:TRP:CZ3	2.69	0.42
1:D:47:LEU:HD21	1:D:123:TYR:CE2	2.55	0.42
3:C:54:ARG:NH2	3:C:54:ARG:HB3	2.35	0.42
4:A:204:GLN:NE2	4:A:238:TYR:CZ	2.88	0.42
4:B:244:VAL:O	4:B:244:VAL:CG2	2.68	0.42
1:D:59:ILE:HA	1:D:107:PHE:O	2.20	0.41
4:A:73:LEU:HD23	4:A:73:LEU:HA	1.84	0.41
4:A:177:LEU:CD2	4:A:227:VAL:O	2.68	0.41
1:D:32:VAL:HG11	1:D:181:PHE:CE1	2.56	0.41
1:D:34:ARG:HA	1:D:180:GLN:O	2.19	0.41
2:E:274:GLU:O	2:E:275:GLU:C	2.63	0.41
3:C:5:ARG:O	3:C:7:PHE:N	2.45	0.41
4:B:28:PHE:CE1	4:B:129:LEU:HD11	2.56	0.41
4:A:74:VAL:O	4:A:76:THR:OG1	2.39	0.41
4:B:149:ILE:HD12	4:B:196:TYR:CZ	2.55	0.41
1:D:178:ASN:OD1	1:D:178:ASN:N	2.53	0.41
2:E:315:LYS:HE3	2:E:333:TYR:OH	2.21	0.41
2:E:539:TYR:CD1	2:E:620:LEU:HD12	2.56	0.41
4:A:207:ASN:ND2	4:A:209:ILE:HG22	2.36	0.41
4:A:230:SER:HA	4:A:237:GLN:NE2	2.35	0.41
2:E:209:VAL:CG1	2:E:613:LEU:HD23	2.49	0.41
2:E:257:ARG:HE	2:E:257:ARG:HB2	1.71	0.41
2:E:407:TYR:HA	2:E:482:ILE:O	2.21	0.41
4:B:149:ILE:O	4:B:153:LYS:HB2	2.21	0.41
4:B:188:LEU:CB	4:B:209:ILE:HG23	2.51	0.41
2:E:559:THR:HG23	2:E:590:LEU:HA	2.02	0.41
3:C:66:LYS:HB3	3:C:78:LEU:HD22	2.02	0.41
4:B:249:ASP:O	4:B:251:TYR:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LEU:HD23	4:A:268:GLY:CA	2.49	0.41
2:E:417:ILE:HG13	2:E:505:ARG:HG2	2.03	0.41
3:C:6:THR:OG1	3:C:7:PHE:N	2.54	0.41
3:C:44:LYS:HB2	3:C:61:VAL:HG11	2.03	0.41
3:C:55:CYS:SG	3:C:86:TYR:HB3	2.61	0.41
4:A:73:LEU:HD21	4:A:87:GLN:C	2.43	0.41
4:A:174:MET:HB2	4:A:209:ILE:CG1	2.51	0.41
4:A:263:LEU:HD23	4:A:289:TRP:CZ3	2.55	0.41
4:B:108:PHE:CG	4:B:144:ILE:HD12	2.56	0.41
1:D:63:LEU:HD13	1:D:63:LEU:HA	1.46	0.41
2:E:229:ASN:O	2:E:230:ASP:C	2.64	0.41
3:C:7:PHE:CD1	3:C:7:PHE:O	2.74	0.41
4:A:172:VAL:HG22	4:A:180:ASN:CG	2.38	0.41
4:A:175:THR:CG2	4:A:176:ASN:N	2.84	0.41
4:A:248:TYR:HD2	4:A:249:ASP:N	2.18	0.40
4:B:41:GLN:O	4:B:48:GLU:OE1	2.39	0.40
4:B:254:THR:HG22	4:B:262:VAL:HG12	2.03	0.40
4:A:31:VAL:CG2	4:A:36:ASN:HB2	2.50	0.40
4:A:162:ILE:HG21	4:A:285:ASP:O	2.12	0.40
4:A:221:ASP:OD1	4:A:224:THR:HG23	2.20	0.40
3:C:92:ILE:HD11	3:C:140:MET:CG	2.50	0.40
4:A:266:TYR:HD1	4:A:277:GLN:OE1	2.05	0.40
2:E:539:TYR:CZ	2:E:620:LEU:HD12	2.57	0.40
4:A:31:VAL:HG22	4:A:36:ASN:HB2	2.02	0.40
4:B:103:ILE:HD13	4:B:103:ILE:HA	1.87	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	D	165/194 (85%)	144 (87%)	19 (12%)	2 (1%)	10 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	417/431 (97%)	392 (94%)	22 (5%)	3 (1%)	18	51
3	C	139/168 (83%)	120 (86%)	18 (13%)	1 (1%)	18	51
4	A	284/316 (90%)	249 (88%)	28 (10%)	7 (2%)	4	28
4	B	284/316 (90%)	250 (88%)	29 (10%)	5 (2%)	6	34
All	All	1289/1425 (90%)	1155 (90%)	116 (9%)	18 (1%)	9	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	ARG
1	D	65	VAL
4	A	79	ALA
4	A	246	ASP
2	E	288	THR
4	A	285	ASP
4	B	46	TYR
4	B	79	ALA
4	B	117	ASN
2	E	451	ASP
4	B	283	GLY
2	E	440	ARG
3	C	29	SER
4	A	238	TYR
4	B	186	ASN
4	A	34	ASN
4	A	104	GLY
4	A	179	VAL

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	D	150/172 (87%)	124 (83%)	26 (17%)	2	11
2	E	380/392 (97%)	309 (81%)	71 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/154 (86%)	111 (84%)	21 (16%)	2	14
4	A	257/283 (91%)	202 (79%)	55 (21%)	1	6
4	B	257/283 (91%)	208 (81%)	49 (19%)	1	8
All	All	1176/1284 (92%)	954 (81%)	222 (19%)	1	9

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	ILE
1	D	31	VAL
1	D	41	SER
1	D	44	ASN
1	D	51	VAL
1	D	60	VAL
1	D	63	LEU
1	D	65	VAL
1	D	70	ILE
1	D	88	ILE
1	D	90	THR
1	D	94	ASN
1	D	101	ILE
1	D	103	ILE
1	D	113	SER
1	D	117	LEU
1	D	130	ILE
1	D	132	LYS
1	D	139	ILE
1	D	146	VAL
1	D	162	LYS
1	D	165	LYS
1	D	170	LEU
1	D	182	LEU
1	D	184	LYS
1	D	187	LEU
2	E	208	ARG
2	E	213	SER
2	E	216	LEU
2	E	218	VAL
2	E	220	ASN
2	E	221	LYS
2	E	233	LEU

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Mol	Chain	Res	Type
2	E	238	LEU
2	E	239	ILE
2	E	244	SER
2	E	252	LEU
2	E	262	THR
2	E	267	LYS
2	E	273	THR
2	E	276	ARG
2	E	278	LYS
2	E	287	ASN
2	E	288	THR
2	E	289	SER
2	E	290	THR
2	E	297	GLU
2	E	301	SER
2	E	302	ASN
2	E	305	ILE
2	E	322	GLN
2	E	323	ASN
2	E	325	SER
2	E	326	ILE
2	E	342	VAL
2	E	349	GLU
2	E	352	VAL
2	E	371	ILE
2	E	380	GLU
2	E	387	THR
2	E	391	ASP
2	E	400	ILE
2	E	415	THR
2	E	421	ASN
2	E	430	LYS
2	E	435	ILE
2	E	442	PHE
2	E	447	LEU
2	E	455	ILE
2	E	462	ASP
2	E	504	LEU
2	E	507	LEU
2	E	511	SER
2	E	513	ASN
2	E	515	ILE

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Mol	Chain	Res	Type
2	E	520	SER
2	E	521	THR
2	E	527	THR
2	E	542	THR
2	E	546	ASN
2	E	548	ASN
2	E	549	ASN
2	E	550	LYS
2	E	556	ARG
2	E	562	ASN
2	E	570	ARG
2	E	575	ILE
2	E	581	ILE
2	E	585	GLN
2	E	587	LEU
2	E	590	LEU
2	E	593	THR
2	E	594	LYS
2	E	595	SER
2	E	611	THR
2	E	620	LEU
2	E	625	THR
3	C	8	LEU
3	C	12	ASN
3	C	16	LYS
3	C	20	SER
3	C	23	LEU
3	C	24	TYR
3	C	29	SER
3	C	32	LEU
3	C	37	GLU
3	C	47	VAL
3	C	50	MET
3	C	52	GLU
3	C	79	ASP
3	C	80	SER
3	C	96	THR
3	C	107	GLU
3	C	121	ILE
3	C	134	ILE
3	C	139	GLN
3	C	140	MET

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Mol	Chain	Res	Type
3	C	142	LYS
4	A	12	ASN
4	A	13	ASP
4	A	14	LYS
4	A	16	VAL
4	A	24	THR
4	A	30	GLN
4	A	43	THR
4	A	52	ILE
4	A	56	SER
4	A	63	ILE
4	A	71	THR
4	A	74	VAL
4	A	84	ILE
4	A	88	GLN
4	A	90	SER
4	A	94	ASN
4	A	99	LEU
4	A	105	ASN
4	A	120	LEU
4	A	127	ARG
4	A	131	LEU
4	A	135	ASN
4	A	138	SER
4	A	143	ILE
4	A	147	TYR
4	A	149	ILE
4	A	156	THR
4	A	170	GLN
4	A	171	GLN
4	A	177	LEU
4	A	180	ASN
4	A	186	ASN
4	A	194	ILE
4	A	195	ILE
4	A	210	LEU
4	A	212	ASN
4	A	216	THR
4	A	218	ILE
4	A	220	SER
4	A	221	ASP
4	A	226	ARG

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Mol	Chain	Res	Type
4	A	229	SER
4	A	233	ASN
4	A	237	GLN
4	A	240	LEU
4	A	245	SER
4	A	248	TYR
4	A	249	ASP
4	A	276	ILE
4	A	285	ASP
4	A	286	ASN
4	A	287	GLN
4	A	289	TRP
4	A	290	THR
4	A	292	SER
4	B	13	ASP
4	B	14	LYS
4	B	15	ILE
4	B	16	VAL
4	B	24	THR
4	B	26	LEU
4	B	34	ASN
4	B	36	ASN
4	B	41	GLN
4	B	66	MET
4	B	67	ASN
4	B	68	ILE
4	B	71	THR
4	B	82	HIS
4	B	84	ILE
4	B	87	GLN
4	B	94	ASN
4	B	103	ILE
4	B	107	SER
4	B	109	ILE
4	B	116	PRO
4	B	124	THR
4	B	135	ASN
4	B	145	GLU
4	B	158	ARG
4	B	172	VAL
4	B	190	GLN
4	B	199	GLU

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Mol	Chain	Res	Type
4	B	204	GLN
4	B	209	ILE
4	B	218	ILE
4	B	219	PHE
4	B	220	SER
4	B	225	VAL
4	B	228	SER
4	B	229	SER
4	B	233	ASN
4	B	234	ASN
4	B	235	ASP
4	B	248	TYR
4	B	250	ARG
4	B	251	TYR
4	B	254	THR
4	B	256	LEU
4	B	259	LYS
4	B	262	VAL
4	B	270	THR
4	B	278	VAL
4	B	292	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	86	ASN
1	D	89	GLN
1	D	94	ASN
1	D	136	HIS
2	E	220	ASN
2	E	287	ASN
2	E	322	GLN
2	E	364	GLN
2	E	396	ASN
2	E	402	ASN
2	E	403	ASN
2	E	413	ASN
2	E	425	ASN
2	E	494	GLN
2	E	517	ASN
2	E	524	HIS
2	E	529	GLN

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Mol	Chain	Res	Type
2	E	554	ASN
2	E	582	ASN
3	C	60	ASN
3	C	138	ASN
3	C	139	GLN
4	A	36	ASN
4	A	45	ASN
4	A	82	HIS
4	A	88	GLN
4	A	105	ASN
4	A	117	ASN
4	A	135	ASN
4	A	136	ASN
4	A	185	ASN
4	A	204	GLN
4	A	223	ASN
4	A	233	ASN
4	A	242	ASN
4	A	269	GLN
4	A	277	GLN
4	B	30	GLN
4	B	36	ASN
4	B	91	ASN
4	B	135	ASN
4	B	170	GLN
4	B	171	GLN
4	B	233	ASN
4	B	234	ASN
4	B	242	ASN
4	B	286	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 [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

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	D	167/194 (86%)	-0.23	2 (1%) 76 52	71, 100, 146, 182	0
2	E	419/431 (97%)	-0.22	2 (0%) 87 68	55, 100, 138, 186	0
3	C	141/168 (83%)	-0.08	3 (2%) 63 38	73, 99, 146, 180	0
4	A	286/316 (90%)	0.11	8 (2%) 55 32	81, 129, 200, 221	0
4	B	286/316 (90%)	-0.08	2 (0%) 84 63	80, 111, 166, 203	0
All	All	1299/1425 (91%)	-0.10	17 (1%) 75 50	55, 106, 175, 221	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	277	GLN	4.5
4	A	191	LYS	3.3
2	E	286	PHE	3.1
1	D	68	ASN	3.0
3	C	106	ASN	2.9
3	C	117	THR	2.9
4	A	246	ASP	2.7
4	A	247	ASN	2.6
2	E	548	ASN	2.4
4	A	164	ALA	2.3
4	A	174	MET	2.3
3	C	105	VAL	2.2
4	A	161	PRO	2.2
4	A	289	TRP	2.1
4	A	248	TYR	2.1
1	D	65	VAL	2.1
4	B	286	ASN	2.1

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.