Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:13 PM GMT

PDB ID	:	3WIN
Title	:	Clostridium botulinum Hemagglutinin
Authors	:	Amatsu, S.; Sugawara, Y.; Matsumura, T.; Fujinaga, Y.; Kitadokoro, K.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

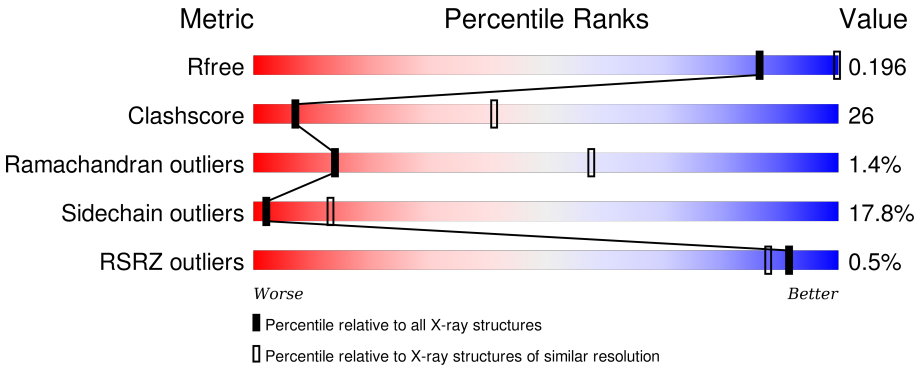
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	60% 21% 6% 14%
2	E	431	62% 29% 6% .
3	C	168	54% 26% . 16%
4	A	316	% 41% 37% 13% 9%
4	B	316	2% 53% 29% 8% 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.

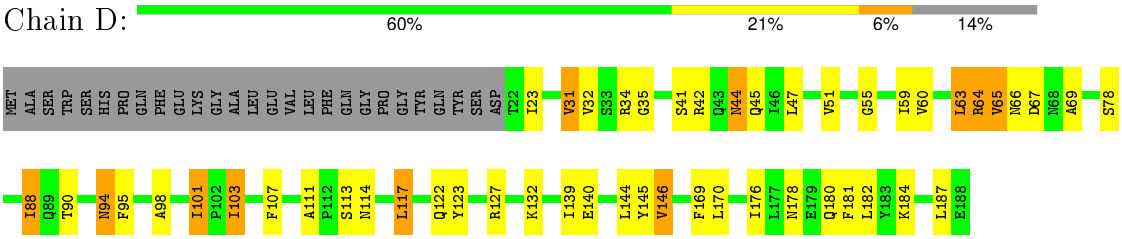
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total O 2 2	0	0
5	E	19	Total O 19 19	0	0
5	C	7	Total O 7 7	0	0
5	A	11	Total O 11 11	0	0
5	B	11	Total O 11 11	0	0

3 Residue-property plots (i)

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.

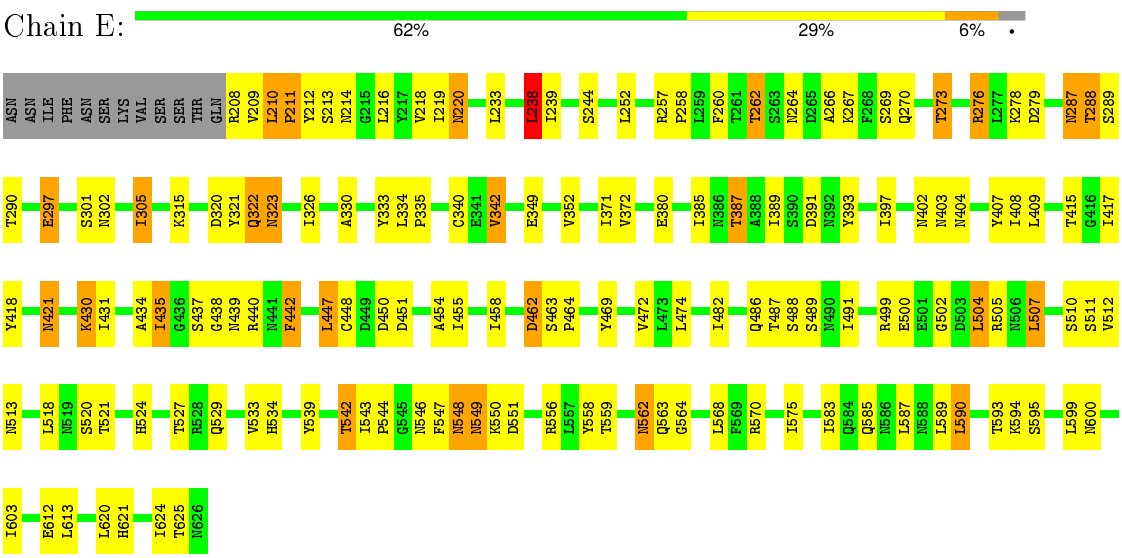
- Molecule 1: HA3

Chain D:



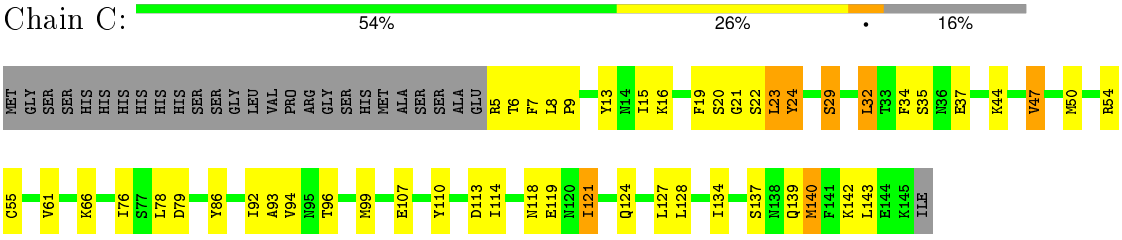
- Molecule 2: HA3

Chain E:



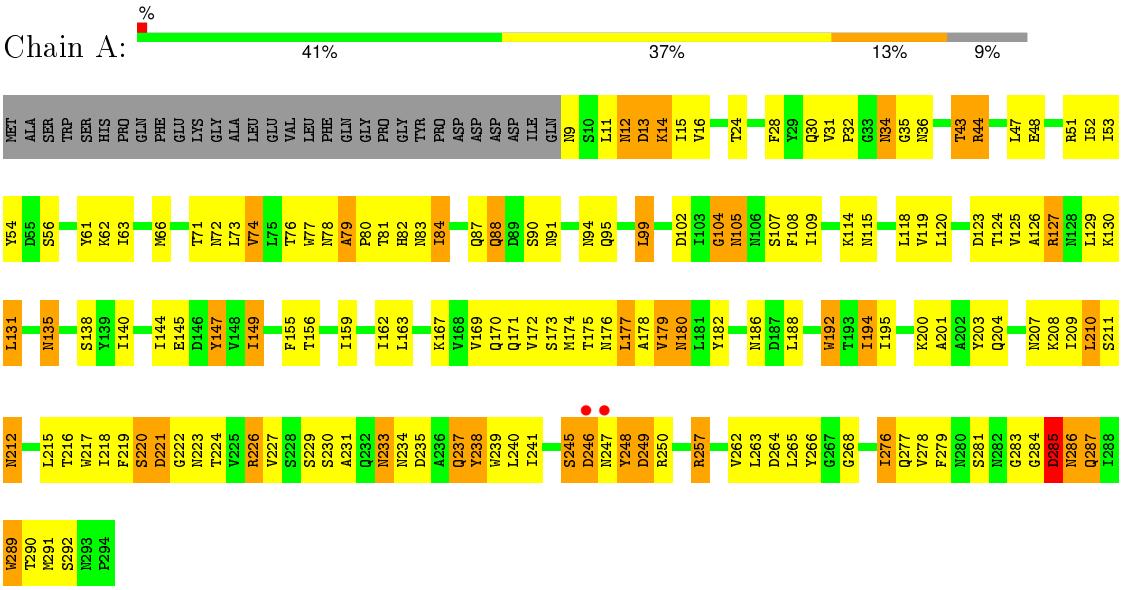
- Molecule 3: 17 kD hemagglutinin component

Chain C:



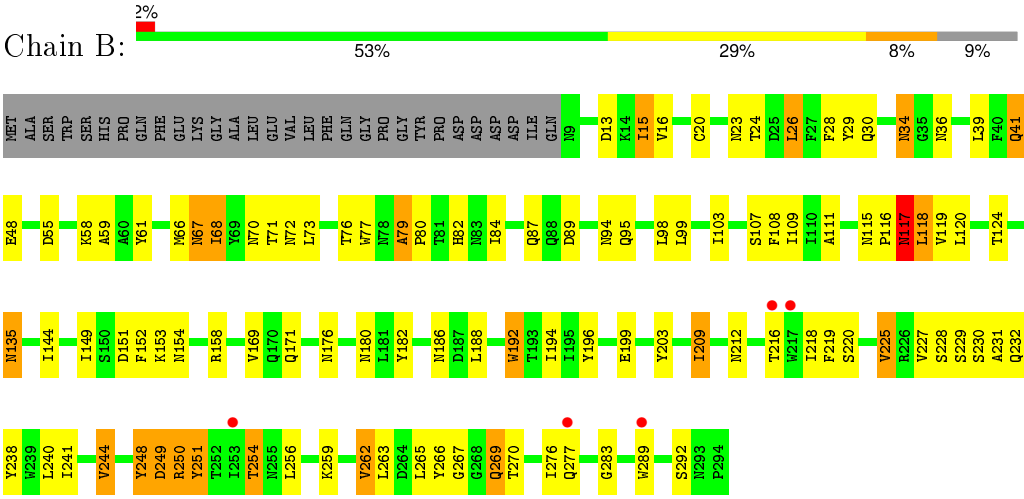
- Molecule 4: HA1

Chain A:



- Molecule 4: HA1

Chain B:



4 Data and refinement statistics (i)

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 49.16 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.43-3.50) 98.3 (49.16-3.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.24%)	DCC
Wilson B-factor (Å^2)	99.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 45592 reflections	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.58	0/1393	0.81	0/1891
2	E	0.57	2/3409 (0.1%)	0.81	4/4636 (0.1%)
3	C	0.58	1/1186 (0.1%)	0.78	0/1611
4	A	0.49	0/2354	0.80	2/3208 (0.1%)
4	B	0.53	0/2354	0.79	0/3208
All	All	0.55	3/10696 (0.0%)	0.80	6/14554 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	464	PRO	N-CD	5.32	1.55	1.47
3	C	9	PRO	N-CD	5.04	1.54	1.47
2	E	211	PRO	N-CD	5.00	1.54	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	285	ASP	N-CA-CB	16.97	141.14	110.60
4	A	285	ASP	CB-CA-C	-9.43	91.55	110.40
2	E	238	LEU	CA-CB-CG	7.30	132.09	115.30
2	E	210	LEU	C-N-CD	5.74	140.45	128.40
2	E	463	SER	C-N-CD	5.65	140.26	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	439	ASN	N-CA-C	-5.04	97.39	111.00

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 (i)

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	37	0
2	E	3347	0	3274	107	0
3	C	1156	0	1113	47	0
4	A	2304	0	2240	256	0
4	B	2304	0	2241	102	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	542	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 26.

All (542) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:265:LEU:CB	4:A:286:ASN:HB2	1.72	1.19
4:A:15:ILE:CG2	4:A:147:TYR:HD1	1.55	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
3:C:137:SER:HA	3:C:140:MET:HE2	1.33	1.10
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:H	4:B:68:ILE:HD13	1.22	1.02
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:277:GLN:HG2	4:A:278:VAL:H	1.26	0.98
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
4:A:73:LEU:HD23	4:A:87:GLN:C	1.89	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:263:LEU:C	4:A:289:TRP:HZ2	1.72	0.93
4:A:15:ILE:HG21	4:A:147:TYR:CD1	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:177:LEU:HB2	4:A:227:VAL:HG22	1.51	0.92
2:E:549:ASN:O	2:E:549:ASN:ND2	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
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
1:D:94:ASN:C	1:D:94:ASN:HD22	1.73	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
4:A:178:ALA:HA	4:A:226:ARG:HG3	1.56	0.87
3:C:5:ARG:O	3:C:6:THR:OG1	1.92	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: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:265:LEU:N	4:A:286:ASN:ND2	2.24	0.85
4:A:246:ASP:OD1	4:A:247:ASN:N	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:46:TYR:CE1	4:B:68:ILE:HD11	2.13	0.82
4:A:177:LEU:CD1	4:A:178:ALA:H	1.93	0.82
1:D:63:LEU:O	1:D:64:ARG:HB2	1.80	0.82
2:E:568:LEU:HD23	2:E:583:ILE:HG21	1.61	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
2:E:385:ILE:CD1	2:E:408:ILE:CG2	2.58	0.81
4:A:73:LEU:CD2	4:A:87:GLN:C	2.48	0.81
2:E:549:ASN:OD1	3:C:140:MET:HE1	1.81	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:277:GLN:HG2	4:A:278:VAL:N	1.96	0.79
1:D:63:LEU:C	1:D:63:LEU:HD12	2.01	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
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:B:46:TYR:CD2	4:B:68:ILE:HD13	2.19	0.77
4:A:265:LEU:N	4:A:286:ASN:HD22	1.80	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
3:C:137:SER:HA	3:C:140:MET:CE	2.13	0.75
4:B:46:TYR:CD2	4:B:68:ILE:CD1	2.69	0.75
4:A:263:LEU:C	4:A:289:TRP:CZ2	2.60	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:219:PHE:HZ	4:A:257:ARG:NE	1.83	0.74
4:A:32:PRO:HG3	4:A:47:LEU:HD21	1.68	0.74
4:B:67:ASN:OD1	4:B:70:ASN:N	2.14	0.74
4:A:283:GLY:CA	4:A:287:GLN:HG3	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ARG:NH1	3:C:5:ARG:HG3	1.98	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:263:LEU:CD2	4:A:289:TRP:CZ2	2.72	0.73
4:A:218:ILE:HD12	4:A:219:PHE:N	2.02	0.73
4:B:44:ARG:NH1	4:B:151:ASP:O	2.21	0.72
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:218:ILE:HG21	4:A:224:THR:OG1	1.89	0.71
4:A:79:ALA:HB1	4:A:80:PRO:HD3	1.72	0.71
4:A:218:ILE:HG23	4:A:221:ASP:O	1.91	0.71
2:E:385:ILE:HD11	2:E:408:ILE:HG21	1.71	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:265:LEU:CD2	4:A:268:GLY:HA2	2.22	0.70
4:A:247:ASN:ND2	5:A:301:HOH:O	2.06	0.70
4:A:177:LEU:CD1	4:A:226:ARG:NE	2.55	0.70
2:E:385:ILE:HD12	2:E:408:ILE:CG2	2.21	0.70
4:A:105:ASN:ND2	4:A:107:SER:OG	2.24	0.70
4:A:219:PHE:CE1	4:A:257:ARG:NE	2.57	0.69
4:A:263:LEU:HG	4:A:289:TRP:CZ2	2.24	0.69
2:E:209:VAL:HG13	2:E:211:PRO:CD	2.22	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: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
1:D:94:ASN:C	1:D:94:ASN:ND2	2.47	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
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
2:E:549:ASN:OD1	3:C:140:MET:HE3	1.96	0.65
4:B:68:ILE:H	4:B:68:ILE:CD1	1.97	0.65
1:D:63:LEU:O	1:D:64:ARG:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:217:TRP:HE1	4:A:222:GLY:C	1.98	0.65
4:B:234:ASN:HD21	4:B:236:ALA:CB	2.09	0.64
4:A:265:LEU:HD23	4:A:268:GLY:HA2	1.79	0.64
4:A:11:LEU:HD12	4:A:11:LEU:C	2.18	0.63
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
4:A:12:ASN:OD1	4:A:54:TYR:N	2.31	0.63
2:E:209:VAL:HG11	2:E:613:LEU:HD21	1.79	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
2:E:543:ILE:HD11	2:E:599:LEU:C	2.19	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
3:C:21:GLY:O	3:C:22:SER:OG	2.17	0.62
4:B:149:ILE:HD12	4:B:196:TYR:CE2	2.35	0.62
4:A:263:LEU:CB	4:A:289:TRP:HZ2	2.11	0.62
4:B:169:VAL:O	4:B:192:TRP:HZ3	1.82	0.62
4:A:194:ILE:HD13	4:A:194:ILE:C	2.20	0.61
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:A:79:ALA:CB	4:A:80:PRO:CD	2.78	0.61
2:E:209:VAL:HG11	2:E:613:LEU:HD23	1.82	0.60
1:D:94:ASN:HD22	1:D:95:PHE:N	1.98	0.60
4:A:215:LEU:HD23	4:A:239:TRP:CZ2	2.37	0.60
2:E:548:ASN:HB2	2:E:551:ASP:CG	2.22	0.60
4:A:283:GLY:N	4:A:287:GLN:OE1	2.34	0.60
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
2:E:431:ILE:HG23	2:E:458:ILE:HB	1.84	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:B:79:ALA:HB1	4:B:80:PRO:HD3	1.84	0.59
4:A:108:PHE:CG	4:A:144:ILE:HD12	2.37	0.59
4:A:180:ASN:HA	4:A:276:ILE:HD11	1.85	0.58
4:B:234:ASN:ND2	4:B:236:ALA:N	2.45	0.58
3:C:19:PHE:HD2	3:C:119:GLU:HA	1.68	0.58
3:C:21:GLY:O	3:C:22:SER:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:58:LYS:O	4:B:59:ALA:HB3	2.04	0.58
4:A:162:ILE:HD11	4:A:250:ARG:CZ	2.21	0.58
4:A:88:GLN:HA	4:A:88:GLN:HE21	1.68	0.58
2:E:500:GLU:HG2	2:E:504:LEU:HB3	1.85	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: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
3:C:118:ASN:O	3:C:119:GLU:HB2	2.05	0.57
2:E:334:LEU:HD12	2:E:335:PRO:HD2	1.87	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:O	2:E:447:LEU:HD23	2.05	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:232:GLN:C	4:B:233:ASN:HD22	2.03	0.56
4:A:223:ASN:HB3	4:A:277:GLN:HG3	1.88	0.56
4:B:251:TYR:CD1	4:B:251:TYR:N	2.73	0.56
4:B:171:GLN:HE21	4:B:227:VAL:HG21	1.70	0.56
1:D:31:VAL:HG22	1:D:88:ILE:HG22	1.87	0.56
4:B:115:ASN:OD1	4:B:117:ASN:HB2	2.05	0.56
2:E:568:LEU:HD23	2:E:583:ILE:CG2	2.34	0.56
3:C:137:SER:CA	3:C:140:MET:HE2	2.22	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
3:C:113:ASP:OD1	3:C:114:ILE:N	2.38	0.56
4:A:177:LEU:O	4:A:178:ALA:HB3	2.06	0.56
2:E:403:ASN:C	2:E:486:GLN:NE2	2.59	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
4:A:16:VAL:HG11	4:A:144:ILE:HG23	1.88	0.55
2:E:487:THR:O	2:E:488:SER:HB3	2.05	0.55
4:A:177:LEU:HD12	4:A:177:LEU:H	1.71	0.55
2:E:219:ILE:HG12	2:E:372:VAL:HG12	1.88	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
2:E:434:ALA:HB3	2:E:437:SER:OG	2.06	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
3:C:19:PHE:CD2	3:C:119:GLU:HA	2.42	0.55
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:O	4:A:31:VAL:HG23	2.06	0.54
4:A:246:ASP:N	4:A:248:TYR:CD1	2.73	0.54
4:A:217:TRP:HZ3	4:A:219:PHE:HE1	1.50	0.54
2:E:518:LEU:HD22	2:E:524:HIS:CD2	2.42	0.54
4:A:28:PHE:CZ	4:A:129:LEU:HD11	2.43	0.54
4:B:248:TYR:HD1	4:B:250:ARG:CZ	2.21	0.54
4:A:219:PHE:O	4:A:220:SER:HB2	2.08	0.54
4:A:159:ILE:HB	4:A:169:VAL:CG1	2.38	0.54
4:A:180:ASN:C	4:A:276:ILE:HD11	2.28	0.53
2:E:518:LEU:HD13	2:E:624:ILE:HD11	1.89	0.53
4:A:283:GLY:CA	4:A:287:GLN:CG	2.85	0.53
4:A:178:ALA:O	4:A:179:VAL:CG1	2.54	0.53
4:A:43:THR:HG23	4:A:48:GLU:HB2	1.90	0.53
4:A:265:LEU:HB3	4:A:268:GLY:HA2	1.91	0.53
2:E:385:ILE:HG22	2:E:387:THR:O	2.08	0.53
2:E:447:LEU:C	2:E:447:LEU:HD23	2.28	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:B:46:TYR:OH	4:B:68:ILE:HD11	2.00	0.53
4:B:73:LEU:O	4:B:73:LEU:HD23	2.08	0.53
4:A:283:GLY:HA2	4:A:287:GLN:HG3	1.90	0.53
4:A:218:ILE:HG22	4:A:224:THR:O	2.09	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
4:A:178:ALA:HA	4:A:226:ARG:CG	2.34	0.53
2:E:209:VAL:O	2:E:210:LEU:HD12	2.08	0.53
3:C:5:ARG:C	3:C:6:THR:HG1	2.04	0.53
3:C:15:ILE:HG12	3:C:143:LEU:HD22	1.89	0.53
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
1:D:63:LEU:HD12	1:D:64:ARG:N	2.24	0.52
4:A:12:ASN:OD1	4:A:54:TYR:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:PRO:O	4:B:118:LEU:N	2.42	0.52
1:D:78:SER:OG	1:D:140:GLU:OE2	2.27	0.52
4:B:108:PHE:CD1	4:B:144:ILE:HD12	2.45	0.52
4:A:61:TYR:OH	4:B:103:ILE:HG22	2.09	0.52
4:A:78:ASN:O	4:A:79:ALA:C	2.48	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: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
4:A:210:LEU:O	4:A:210:LEU:HD22	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
4:A:88:GLN:HA	4:A:88:GLN:NE2	2.26	0.50
4:A:84:ILE:HD11	4:A:131:LEU:HD13	1.94	0.50
3:C:110:TYR:HB3	3:C:128:LEU:HG	1.92	0.50
4:B:68:ILE:HD13	4:B:68:ILE:N	2.07	0.50
2:E:404:ASN:CA	2:E:486:GLN:HE22	2.18	0.50
4:A:238:TYR:C	4:A:239:TRP:CD1	2.85	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:549:ASN:C	2:E:549:ASN:HD22	2.08	0.49
4:B:241:ILE:HG22	4:B:251:TYR:HD2	1.75	0.49
2:E:469:TYR:CZ	2:E:512:VAL:HG11	2.47	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
4:B:34:ASN:OD1	4:B:34:ASN:C	2.51	0.49
2:E:209:VAL:CG1	2:E:211:PRO:HD3	2.36	0.49
3:C:7:PHE:CD1	3:C:7:PHE:C	2.85	0.49
4:B:225:VAL:HG13	4:B:277:GLN:HA	1.94	0.49
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
4:A:11:LEU:HD11	4:A:52:ILE:HG21	1.94	0.49
4:A:237:GLN:C	4:A:238:TYR:CD1	2.86	0.49
4:A:88:GLN:CA	4:A:88:GLN:HE21	2.24	0.49
2:E:558:TYR:CD1	5:E:701:HOH:O	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:TYR:N	3:C:24:TYR:CD1	2.81	0.48
4:A:233:ASN:HD22	4:A:235:ASP:H	1.61	0.48
4:A:233:ASN:H	4:A:233:ASN:ND2	2.11	0.48
3:C:13:TYR:CD2	3:C:47:VAL:CG1	2.95	0.48
4:A:246:ASP:CG	4:A:247:ASN:H	2.10	0.48
4:B:234:ASN:O	4:B:235:ASP:HB2	2.12	0.48
4:B:111:ALA:HB2	4:B:119:VAL:HG12	1.95	0.48
4:A:115:ASN:C	4:A:115:ASN:OD1	2.52	0.48
1:D:66:ASN:HA	1:D:69:ALA:CB	2.41	0.48
3:C:23:LEU:HD23	3:C:34:PHE:C	2.34	0.48
2:E:287:ASN:HD22	2:E:287:ASN:N	2.11	0.48
1:D:117:LEU:C	1:D:117:LEU:HD12	2.34	0.48
4:A:223:ASN:O	4:A:277:GLN:HA	2.13	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:B:76:THR:HG23	4:B:95:GLN:HG2	1.94	0.48
4:A:217:TRP:HZ2	4:A:222:GLY:HA2	1.79	0.48
4:A:175:THR:HG23	4:A:176:ASN:N	2.28	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
4:A:237:GLN:C	4:A:238:TYR:HD1	2.17	0.47
2:E:431:ILE:HG21	2:E:472:VAL:HG11	1.96	0.47
4:B:111:ALA:CB	4:B:119:VAL:HG12	2.45	0.47
2:E:558:TYR:CG	5:E:701:HOH:O	2.68	0.47
2:E:543:ILE:HD11	2:E:599:LEU:O	2.14	0.47
4:A:237:GLN:O	4:A:238:TYR:HB2	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:B:225:VAL:CG1	4:B:277:GLN:HA	2.45	0.47
4:A:265:LEU:HG	4:A:268:GLY:CA	2.35	0.47
4:A:124:THR:O	4:A:127:ARG:CD	2.62	0.47
2:E:409:LEU:HD23	2:E:447:LEU:HD11	1.96	0.47
1:D:47:LEU:HD21	1:D:123:TYR:CZ	2.49	0.47
2:E:214:ASN:HB3	2:E:323:ASN:H	1.79	0.47
4:B:29:TYR:OH	4:B:47:LEU:HD13	2.15	0.47
1:D:44:ASN:O	1:D:45:GLN:HB2	2.14	0.47
4:A:262:VAL:HG11	4:A:281:SER:HA	1.97	0.47
4:A:231:ALA:O	4:A:234:ASN:HB2	2.15	0.47
4:A:218:ILE:CD1	4:A:219:PHE:N	2.72	0.47
3:C:23:LEU:HD23	3:C:35:SER:CA	2.45	0.47
2:E:276:ARG:NH1	2:E:279:ASP:OD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:VAL:C	2:E:210:LEU:HG	2.36	0.46
4:B:98:LEU:N	4:B:98:LEU:HD12	2.30	0.46
4:A:277:GLN:CG	4:A:278:VAL:N	2.62	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
1:D:44:ASN:N	1:D:44:ASN:OD1	2.47	0.46
2:E:533:VAL:O	2:E:534:HIS:HB2	2.15	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
3:C:5:ARG:CG	3:C:5:ARG:HH11	2.14	0.46
4:A:200:LYS:O	4:A:201:ALA:HB3	2.14	0.46
2:E:397:ILE:O	2:E:397:ILE:HD12	2.16	0.46
4:B:241:ILE:HG22	4:B:251:TYR:CD2	2.50	0.46
1:D:44:ASN:HA	1:D:122:GLN:HG3	1.97	0.46
1:D:42:ARG:HG2	1:D:169:PHE:CZ	2.51	0.46
1:D:64:ARG:O	1:D:64:ARG:HG2	2.15	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
4:B:265:LEU:O	4:B:266:TYR:HB3	2.16	0.46
4:B:116:PRO:O	4:B:117:ASN:C	2.54	0.46
3:C:93:ALA:O	3:C:94:VAL:C	2.53	0.46
4:A:265:LEU:HB2	4:A:286:ASN:CB	2.39	0.45
2:E:219:ILE:HG22	2:E:220:ASN:N	2.31	0.45
2:E:210:LEU:O	2:E:210:LEU:HD12	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
4:A:12:ASN:HD22	4:A:13:ASP:HB2	1.80	0.45
4:A:217:TRP:CG	4:A:218:ILE:N	2.82	0.45
4:A:174:MET:HB2	4:A:209:ILE:HG12	1.98	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
1:D:98:ALA:O	1:D:101:ILE:HD13	2.16	0.45
1:D:55:GLY:HA2	1:D:111:ALA:O	2.17	0.45
4:A:31:VAL:CG2	4:A:31:VAL:O	2.65	0.45
2:E:542:THR:HB	2:E:603:ILE:HG12	1.98	0.45
2:E:385:ILE:HD12	2:E:408:ILE:HG23	1.98	0.45
2:E:270:GLN:HA	2:E:273:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:TRP:HZ3	4:A:207:ASN:ND2	2.14	0.45
4:A:109:ILE:HG23	4:A:119:VAL:HG11	1.99	0.45
2:E:297:GLU:HG3	2:E:342:VAL:HG11	1.99	0.45
2:E:547:PHE:CD1	2:E:547:PHE:O	2.70	0.45
4:A:28:PHE:CE1	4:A:129:LEU:HD11	2.52	0.44
4:A:247:ASN:O	4:A:248:TYR:CD2	2.70	0.44
2:E:435:ILE:HG12	2:E:454:ALA:O	2.17	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
2:E:211:PRO:O	2:E:212:TYR:CD2	2.70	0.44
4:A:102:ASP:O	4:A:104:GLY:N	2.48	0.44
2:E:563:GLN:OE1	2:E:564:GLY:N	2.50	0.44
1:D:127:ARG:HD2	1:D:145:TYR:CE1	2.53	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:421:ASN:C	2:E:421:ASN:HD22	2.21	0.44
4:A:287:GLN:O	4:A:289:TRP:CD1	2.70	0.44
4:A:276:ILE:N	4:A:276:ILE:HD13	2.33	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:283:GLY:HA3	4:A:284:GLY:HA2	1.69	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: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
3:C:99:MET:HE2	3:C:143:LEU:HD11	1.98	0.43
4:B:23:ASN:CG	4:B:26:LEU:HD13	2.39	0.43
3:C:23:LEU:CD2	3:C:34:PHE:C	2.87	0.43
4:A:284:GLY:O	4:A:285:ASP:CG	2.53	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:73:LEU:CD2	4:A:87:GLN:N	2.81	0.43
4:A:44:ARG:NH1	4:A:155:PHE:CD1	2.86	0.43
4:A:211:SER:O	4:A:212:ASN:ND2	2.48	0.43
4:A:246:ASP:O	4:A:248:TYR:CG	2.72	0.43
4:A:219:PHE:HZ	4:A:257:ARG:CG	2.26	0.43
4:A:11:LEU:CD1	4:A:11:LEU:C	2.86	0.43
4:A:11:LEU:O	4:A:11:LEU:HD12	2.19	0.43
4:A:145:GLU:OE1	4:A:149:ILE:HD11	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:548:ASN:CB	2:E:551:ASP:CG	2.87	0.43
2:E:389:ILE:HD12	2:E:393:TYR:HB3	2.01	0.43
2:E:322:GLN:CA	2:E:322:GLN:HE21	2.31	0.43
3:C:124:GLN:HE22	4:A:115:ASN:HB2	1.84	0.43
2:E:418:TYR:CD2	2:E:499:ARG:HA	2.54	0.43
4:B:135:ASN:C	4:B:135:ASN:HD22	2.21	0.43
4:A:266:TYR:O	4:A:266:TYR:CG	2.70	0.42
3:C:16:LYS:HD3	3:C:23:LEU:O	2.19	0.42
4:B:249:ASP:O	4:B:251:TYR:HE1	2.02	0.42
4:B:180:ASN:C	4:B:276:ILE:HD13	2.39	0.42
4:B:46:TYR:CG	4:B:68:ILE:CD1	3.02	0.42
4:B:234:ASN:C	4:B:234:ASN:ND2	2.73	0.42
2:E:543:ILE:HG13	2:E:600:ASN:HA	2.01	0.42
2:E:418:TYR:CD1	2:E:474:LEU:HD12	2.54	0.42
4:A:286:ASN:ND2	4:A:286:ASN:C	2.73	0.42
2:E:260:PHE:HE1	2:E:330:ALA:HB1	1.84	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
4:A:76:THR:HG23	4:A:95:GLN:HG2	2.00	0.42
4:A:177:LEU:HD23	4:A:227:VAL:O	2.18	0.42
4:A:177:LEU:HD13	4:A:226:ARG:NE	2.34	0.42
4:A:246:ASP:N	4:A:248:TYR:HD1	2.15	0.42
4:A:218:ILE:CG1	4:A:219:PHE:N	2.81	0.42
3:C:121:ILE:CD1	3:C:121:ILE:H	2.32	0.42
3:C:23:LEU:C	3:C:24:TYR:CD1	2.92	0.42
4:B:26:LEU:N	4:B:26:LEU:HD12	2.34	0.42
3:C:32:LEU:HD13	3:C:76:ILE:HG22	2.01	0.42
4:A:12:ASN:C	4:A:12:ASN:ND2	2.73	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
4:B:203:TYR:O	4:B:238:TYR:HA	2.20	0.42
4:B:154:ASN:HA	4:B:194:ILE:O	2.19	0.42
4:A:223:ASN:CG	4:A:277:GLN:HE21	2.23	0.42
4:A:223:ASN:ND2	4:A:277:GLN:NE2	2.67	0.42
2:E:543:ILE:HG21	2:E:543:ILE:HD13	1.87	0.42
4:B:169:VAL:O	4:B:192:TRP:CZ3	2.69	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:47:LEU:HD21	1:D:123:TYR:CE2	2.55	0.42
3:C:54:ARG:HB3	3:C:54:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:177:LEU:CD2	4:A:227:VAL:O	2.68	0.41
4:A:73:LEU:HD23	4:A:73:LEU:HA	1.84	0.41
1:D:59:ILE:HA	1:D:107:PHE:O	2.20	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
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
4:B:149:ILE:HD12	4:B:196:TYR:CZ	2.55	0.41
4:A:74:VAL:O	4:A:76:THR:OG1	2.39	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:315:LYS:HE3	2:E:333:TYR:OH	2.21	0.41
1:D:178:ASN:OD1	1:D:178:ASN:N	2.53	0.41
2:E:209:VAL:CG1	2:E:613:LEU:HD23	2.49	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:407:TYR:HA	2:E:482:ILE:O	2.21	0.41
2:E:257:ARG:HE	2:E:257:ARG:HB2	1.71	0.41
1:D:67:ASP:C	1:D:69:ALA:N	2.73	0.41
4:B:249:ASP:O	4:B:251:TYR:CE1	2.74	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:A:265:LEU:HD23	4:A:268:GLY:CA	2.49	0.41
3:C:99:MET:HE1	3:C:143:LEU:HD11	2.01	0.41
4:A:263:LEU:HD23	4:A:289:TRP:CZ3	2.55	0.41
3:C:6:THR:OG1	3:C:7:PHE:N	2.54	0.41
2:E:417:ILE:HG13	2:E:505:ARG:HG2	2.03	0.41
4:A:174:MET:HB2	4:A:209:ILE:CG1	2.51	0.41
4:B:108:PHE:CG	4:B:144:ILE:HD12	2.56	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:B:233:ASN:ND2	4:B:233:ASN:C	2.73	0.41
3:C:7:PHE:O	3:C:7:PHE:CD1	2.74	0.41
4:A:175:THR:CG2	4:A:176:ASN:N	2.84	0.41
1:D:63:LEU:HA	1:D:63:LEU:HD13	1.46	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:176:ASN:C	4:B:176:ASN:OD1	2.60	0.40
4:B:254:THR:HG22	4:B:262:VAL:HG12	2.03	0.40
4:A:162:ILE:HG21	4:A:285:ASP:O	2.12	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:ASP:OD1	4:A:224:THR:HG23	2.20	0.40
4:A:31:VAL:CG2	4:A:36:ASN:HB2	2.50	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
4:B:103:ILE:HD13	4:B:103:ILE:HA	1.87	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	165/194 (85%)	144 (87%)	19 (12%)	2 (1%)	16 61
2	E	417/431 (97%)	392 (94%)	22 (5%)	3 (1%)	26 72
3	C	139/168 (83%)	120 (86%)	18 (13%)	1 (1%)	26 72
4	A	284/316 (90%)	249 (88%)	28 (10%)	7 (2%)	7 46
4	B	284/316 (90%)	250 (88%)	29 (10%)	5 (2%)	11 53
All	All	1289/1425 (90%)	1155 (90%)	116 (9%)	18 (1%)	14 58

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

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Mol	Chain	Res	Type
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 (i)

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%)	128 (85%)	22 (15%)	4 22
2	E	380/392 (97%)	315 (83%)	65 (17%)	2 15
3	C	132/154 (86%)	116 (88%)	16 (12%)	6 30
4	A	257/283 (91%)	199 (77%)	58 (23%)	1 6
4	B	257/283 (91%)	209 (81%)	48 (19%)	2 11
All	All	1176/1284 (92%)	967 (82%)	209 (18%)	2 13

All (209) 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	88	ILE

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Mol	Chain	Res	Type
1	D	90	THR
1	D	94	ASN
1	D	101	ILE
1	D	103	ILE
1	D	113	SER
1	D	114	ASN
1	D	117	LEU
1	D	132	LYS
1	D	139	ILE
1	D	146	VAL
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	233	LEU
2	E	238	LEU
2	E	244	SER
2	E	252	LEU
2	E	262	THR
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	326	ILE
2	E	340	CYS
2	E	342	VAL
2	E	349	GLU
2	E	352	VAL

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Mol	Chain	Res	Type
2	E	371	ILE
2	E	380	GLU
2	E	387	THR
2	E	391	ASP
2	E	402	ASN
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	450	ASP
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	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	585	GLN
2	E	587	LEU
2	E	590	LEU
2	E	593	THR
2	E	594	LYS
2	E	595	SER
2	E	625	THR
3	C	8	LEU
3	C	20	SER
3	C	23	LEU
3	C	24	TYR
3	C	29	SER

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Mol	Chain	Res	Type
3	C	32	LEU
3	C	37	GLU
3	C	47	VAL
3	C	50	MET
3	C	79	ASP
3	C	107	GLU
3	C	121	ILE
3	C	134	ILE
3	C	139	GLN
3	C	140	MET
3	C	142	LYS
4	A	12	ASN
4	A	13	ASP
4	A	14	LYS
4	A	24	THR
4	A	30	GLN
4	A	43	THR
4	A	44	ARG
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	114	LYS
4	A	120	LEU
4	A	127	ARG
4	A	130	LYS
4	A	131	LEU
4	A	135	ASN
4	A	138	SER
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

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Mol	Chain	Res	Type
4	A	186	ASN
4	A	188	LEU
4	A	192	TRP
4	A	194	ILE
4	A	195	ILE
4	A	210	LEU
4	A	212	ASN
4	A	216	THR
4	A	220	SER
4	A	221	ASP
4	A	226	ARG
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	257	ARG
4	A	276	ILE
4	A	279	PHE
4	A	286	ASN
4	A	287	GLN
4	A	289	TRP
4	A	290	THR
4	A	291	MET
4	A	292	SER
4	B	13	ASP
4	B	16	VAL
4	B	24	THR
4	B	26	LEU
4	B	30	GLN
4	B	34	ASN
4	B	36	ASN
4	B	41	GLN
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

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Mol	Chain	Res	Type
4	B	107	SER
4	B	109	ILE
4	B	117	ASN
4	B	118	LEU
4	B	120	LEU
4	B	124	THR
4	B	135	ASN
4	B	158	ARG
4	B	182	TYR
4	B	192	TRP
4	B	199	GLU
4	B	209	ILE
4	B	212	ASN
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	249	ASP
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	269	GLN
4	B	270	THR
4	B	292	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) 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

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Mol	Chain	Res	Type
2	E	270	GLN
2	E	287	ASN
2	E	322	GLN
2	E	328	ASN
2	E	396	ASN
2	E	402	ASN
2	E	403	ASN
2	E	421	ASN
2	E	494	GLN
2	E	517	ASN
2	E	524	HIS
2	E	554	ASN
3	C	60	ASN
4	A	82	HIS
4	A	88	GLN
4	A	105	ASN
4	A	135	ASN
4	A	185	ASN
4	A	204	GLN
4	A	233	ASN
4	A	242	ASN
4	A	269	GLN
4	A	277	GLN
4	B	78	ASN
4	B	91	ASN
4	B	117	ASN
4	B	135	ASN
4	B	170	GLN
4	B	171	GLN
4	B	189	ASN
4	B	233	ASN
4	B	234	ASN
4	B	237	GLN
4	B	242	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.32	0	100	100	71, 100, 146, 182	0
2	E	419/431 (97%)	-0.50	0	100	100	55, 100, 138, 186	0
3	C	141/168 (83%)	-0.38	0	100	100	73, 99, 146, 180	0
4	A	286/316 (90%)	-0.21	2 (0%)	89	82	81, 129, 200, 221	0
4	B	286/316 (90%)	-0.09	5 (1%)	73	64	80, 111, 166, 203	0
All	All	1299/1425 (91%)	-0.31	7 (0%)	91	88	55, 106, 175, 221	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	217	TRP	3.0
4	B	253	ILE	2.5
4	A	246	ASP	2.4
4	B	277	GLN	2.3
4	B	289	TRP	2.1
4	A	247	ASN	2.0
4	B	216	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.