Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 10:31 PM EDT

PDB ID	:	2WRD
Title	:	structure of H2 japan hemagglutinin
Authors	:	Liu, J.; Stevens, D.J.; Haire, L.F.; Walker, P.A.; Coombs, P.J.; Russell, R.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2009-09-01
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

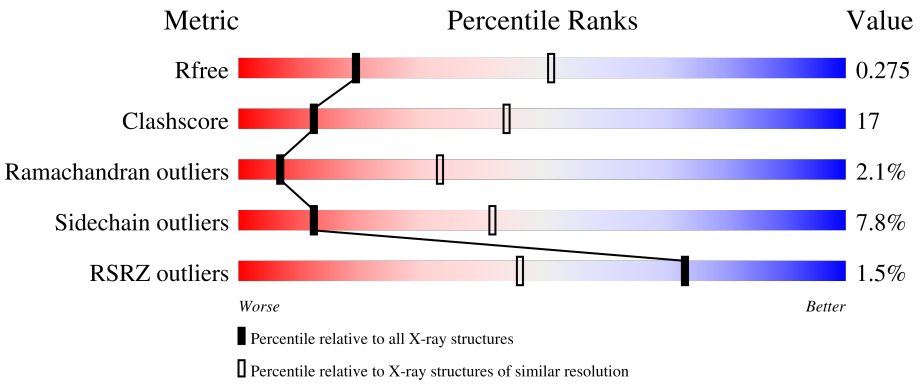
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	62% 28% • 7%
1	B	505	% 61% 32% • • •
1	C	505	3% 62% 29% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11367 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3724	2347	637	716	24	0	0	0
1	B	486	3843	2418	660	741	24	0	0	0
1	C	481	3800	2393	654	729	24	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

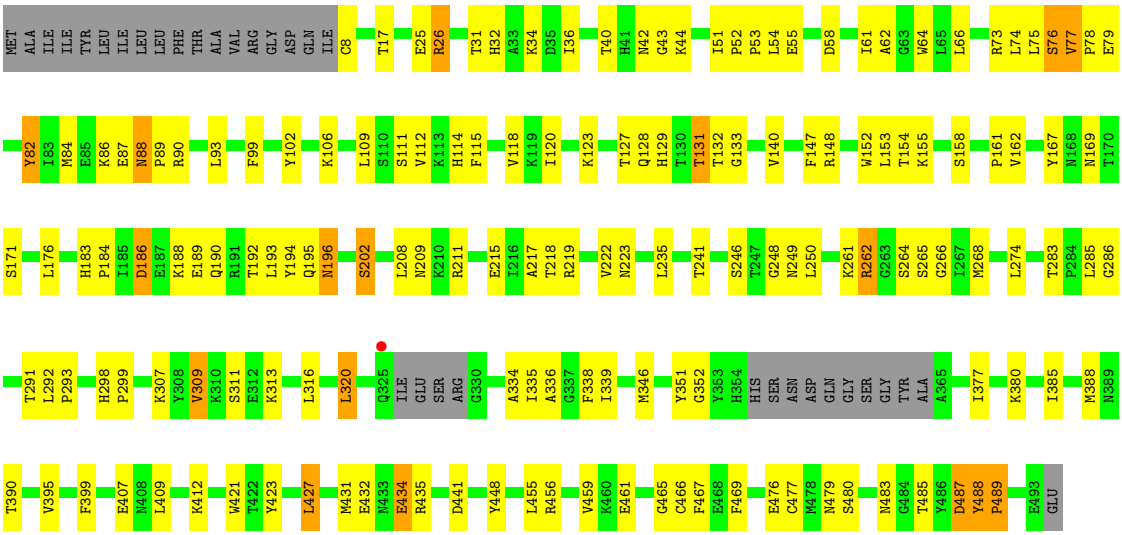
Chain	Residue	Modelled	Actual	Comment	Reference
A	107	HIS	TYR	conflict	UNP Q67085
A	159	ASN	ASP	conflict	UNP Q67085
A	185	ILE	ASN	conflict	UNP Q67085
A	188	LYS	THR	conflict	UNP Q67085
A	307	LYS	ARG	conflict	UNP Q67085
B	107	HIS	TYR	conflict	UNP Q67085
B	159	ASN	ASP	conflict	UNP Q67085
B	185	ILE	ASN	conflict	UNP Q67085
B	188	LYS	THR	conflict	UNP Q67085
B	307	LYS	ARG	conflict	UNP Q67085
C	107	HIS	TYR	conflict	UNP Q67085
C	159	ASN	ASP	conflict	UNP Q67085
C	185	ILE	ASN	conflict	UNP Q67085
C	188	LYS	THR	conflict	UNP Q67085
C	307	LYS	ARG	conflict	UNP Q67085

3 Residue-property plots (i)

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.

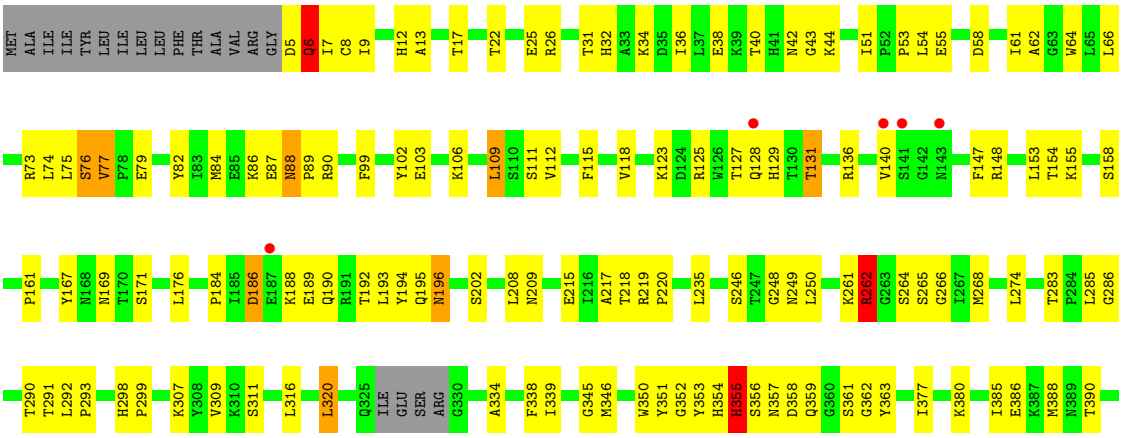
• Molecule 1: HEMAGGLUTININ

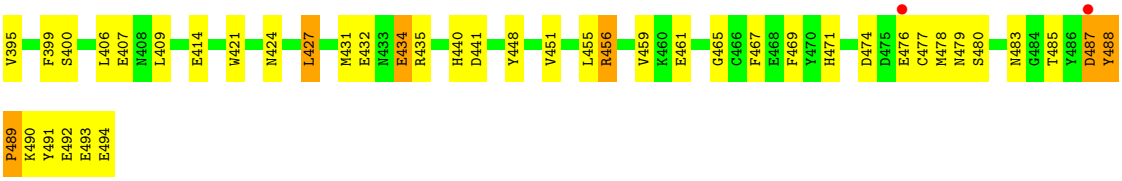
Chain A:



• Molecule 1: HEMAGGLUTININ

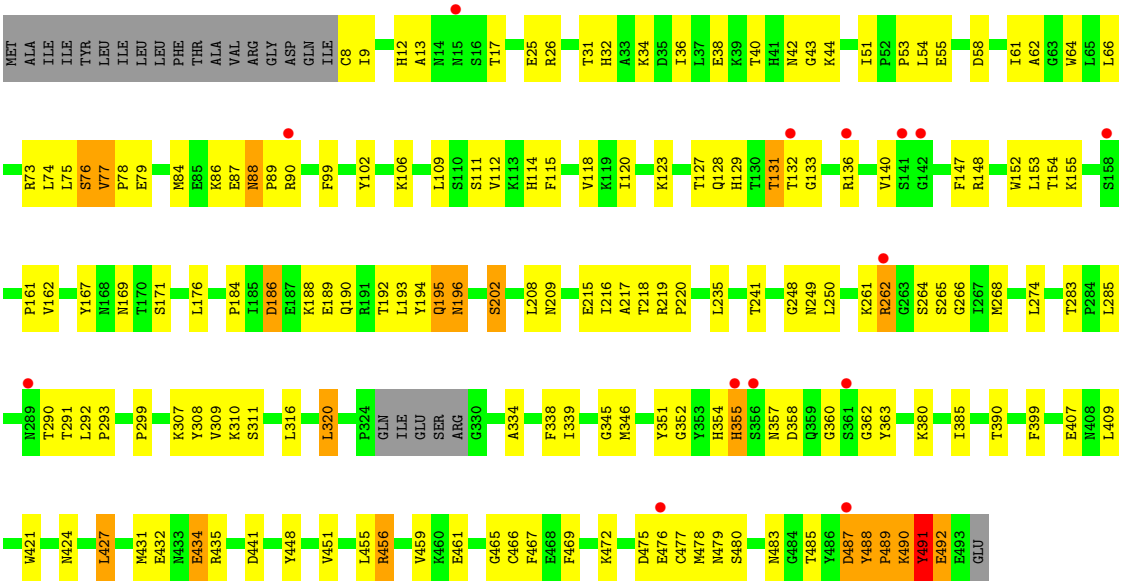
Chain B:





- Molecule 1: HEMAGGLUTININ

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.15Å 118.36Å 221.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 3.00 19.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.89-3.00) 80.4 (19.94-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.277 , 0.333 0.275 , 0.275	Depositor DCC
R_{free} test set	1658 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11367	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/3807	0.66	0/5149
1	B	0.56	0/3930	0.67	1/5315 (0.0%)
1	C	0.48	0/3887	0.63	0/5257
All	All	0.52	0/11624	0.66	1/15721 (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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	491	TYR	Peptide
1	C	490	LYS	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	A	3724	0	3599	112	0
1	B	3843	0	3709	155	0
1	C	3800	0	3674	129	0
All	All	11367	0	10982	377	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 17.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASP:HA	1:A:488:TYR:HB2	1.37	1.05
1:C:487:ASP:HA	1:C:488:TYR:HB2	1.37	1.04
1:B:487:ASP:HA	1:B:488:TYR:HB2	1.40	1.02
1:A:488:TYR:H	1:A:489:PRO:HD3	1.25	0.97
1:B:488:TYR:H	1:B:489:PRO:HD3	1.31	0.95
1:C:488:TYR:H	1:C:489:PRO:HD3	1.31	0.93
1:B:9:ILE:HD11	1:B:451:VAL:HG21	1.49	0.93
1:A:488:TYR:N	1:A:489:PRO:HD3	1.87	0.90
1:A:487:ASP:HA	1:A:488:TYR:CB	2.04	0.88
1:B:261:LYS:HA	1:B:262:ARG:HB2	1.54	0.88
1:C:196:ASN:N	1:C:196:ASN:HD22	1.70	0.88
1:C:488:TYR:N	1:C:489:PRO:HD3	1.90	0.86
1:B:487:ASP:HA	1:B:488:TYR:CB	2.05	0.85
1:A:196:ASN:N	1:A:196:ASN:HD22	1.75	0.84
1:C:261:LYS:HA	1:C:262:ARG:HB2	1.58	0.84
1:C:487:ASP:HA	1:C:488:TYR:CB	2.06	0.84
1:B:488:TYR:N	1:B:489:PRO:HD3	1.88	0.84
1:A:127:THR:O	1:A:128:GLN:HB2	1.77	0.84
1:A:488:TYR:H	1:A:489:PRO:CD	1.91	0.82
1:B:196:ASN:N	1:B:196:ASN:HD22	1.76	0.81
1:C:489:PRO:HD2	1:C:490:LYS:HE2	1.62	0.81
1:B:112:VAL:HG11	1:B:115:PHE:HB2	1.64	0.80
1:C:112:VAL:HG11	1:C:115:PHE:HB2	1.63	0.79
1:B:127:THR:O	1:B:128:GLN:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:LYS:HA	1:C:491:TYR:HB3	1.62	0.79
1:C:261:LYS:HB2	1:C:262:ARG:HB3	1.66	0.78
1:B:355:HIS:O	1:B:355:HIS:CG	2.37	0.78
1:B:488:TYR:H	1:B:489:PRO:CD	1.98	0.77
1:C:127:THR:O	1:C:128:GLN:HB2	1.83	0.77
1:A:307:LYS:HG2	1:A:421:TRP:CE2	2.20	0.77
1:A:53:PRO:HG2	1:A:84:MET:HE3	1.67	0.77
1:B:307:LYS:HG2	1:B:421:TRP:CE2	2.20	0.76
1:C:488:TYR:H	1:C:489:PRO:CD	1.97	0.76
1:C:77:VAL:HG23	1:C:79:GLU:H	1.52	0.75
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.68	0.74
1:B:483:ASN:HB3	1:B:485:THR:OG1	1.87	0.74
1:B:493:GLU:H	1:B:494:GLU:HA	1.53	0.73
1:C:53:PRO:HG2	1:C:84:MET:HE3	1.70	0.73
1:A:483:ASN:HB3	1:A:485:THR:OG1	1.89	0.73
1:B:53:PRO:HG2	1:B:84:MET:CE	2.19	0.73
1:B:77:VAL:HG23	1:B:79:GLU:H	1.51	0.73
1:B:53:PRO:HG2	1:B:84:MET:HE3	1.70	0.73
1:A:31:THR:HG23	1:A:320:LEU:O	1.89	0.72
1:B:8:CYS:O	1:B:353:TYR:HA	1.88	0.72
1:B:261:LYS:HA	1:B:262:ARG:CB	2.20	0.72
1:B:58:ASP:HB3	1:B:86:LYS:HD2	1.69	0.72
1:B:261:LYS:HB2	1:B:262:ARG:HB3	1.72	0.72
1:A:53:PRO:HG2	1:A:84:MET:CE	2.20	0.72
1:C:58:ASP:HB3	1:C:86:LYS:HD2	1.72	0.71
1:C:483:ASN:HB3	1:C:485:THR:OG1	1.90	0.71
1:A:435:ARG:HH21	1:C:434:GLU:CD	1.94	0.71
1:A:58:ASP:HB3	1:A:86:LYS:HD2	1.72	0.71
1:C:196:ASN:N	1:C:196:ASN:ND2	2.38	0.70
1:B:493:GLU:H	1:B:494:GLU:HG3	1.57	0.70
1:A:202:SER:OG	1:C:217:ALA:HB2	1.91	0.70
1:A:261:LYS:HA	1:A:262:ARG:CB	2.22	0.70
1:B:155:LYS:HE3	1:B:192:THR:O	1.91	0.70
1:B:359:GLN:HE22	1:B:474:ASP:HB2	1.57	0.69
1:B:111:SER:HB2	1:B:265:SER:HB3	1.74	0.69
1:A:53:PRO:HD2	1:A:274:LEU:HD22	1.75	0.69
1:A:129:HIS:HE1	1:A:161:PRO:O	1.75	0.68
1:C:261:LYS:HA	1:C:262:ARG:CB	2.22	0.68
1:B:53:PRO:HD2	1:B:274:LEU:HD22	1.75	0.68
1:B:455:LEU:HD13	1:B:459:VAL:HG11	1.73	0.68
1:B:493:GLU:N	1:B:494:GLU:HG3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PRO:HD2	1:C:274:LEU:HD22	1.76	0.68
1:A:77:VAL:HG23	1:A:79:GLU:H	1.59	0.68
1:C:129:HIS:HE1	1:C:161:PRO:O	1.76	0.68
1:B:359:GLN:NE2	1:B:474:ASP:HB2	2.08	0.67
1:C:293:PRO:HG3	1:C:385:ILE:HA	1.75	0.67
1:B:459:VAL:HG12	1:B:469:PHE:HA	1.77	0.67
1:B:471:HIS:CG	1:B:490:LYS:HG2	2.29	0.67
1:C:489:PRO:O	1:C:490:LYS:HD3	1.95	0.67
1:A:380:LYS:HE2	1:A:432:GLU:OE2	1.95	0.66
1:B:196:ASN:N	1:B:196:ASN:ND2	2.43	0.66
1:A:196:ASN:N	1:A:196:ASN:ND2	2.43	0.66
1:C:53:PRO:HG2	1:C:84:MET:CE	2.26	0.65
1:B:129:HIS:HE1	1:B:161:PRO:O	1.80	0.65
1:A:346:MET:SD	1:A:352:GLY:HA3	2.37	0.65
1:A:167:TYR:CE2	1:A:169:ASN:HA	2.32	0.65
1:C:431:MET:O	1:C:435:ARG:HG2	1.96	0.65
1:A:265:SER:OG	1:A:266:GLY:N	2.31	0.64
1:A:455:LEU:HD13	1:A:459:VAL:HG11	1.80	0.64
1:A:140:VAL:HG21	1:A:148:ARG:HH22	1.62	0.63
1:C:140:VAL:HG21	1:C:148:ARG:HH22	1.63	0.63
1:C:491:TYR:C	1:C:491:TYR:CD2	2.71	0.63
1:C:87:GLU:O	1:C:88:ASN:HB2	1.98	0.63
1:A:293:PRO:HG3	1:A:385:ILE:HA	1.80	0.63
1:B:61:ILE:HD12	1:B:106:LYS:HD2	1.81	0.63
1:B:87:GLU:O	1:B:88:ASN:HB2	1.99	0.62
1:C:186:ASP:HB3	1:C:189:GLU:H	1.64	0.62
1:C:51:ILE:HD12	1:C:262:ARG:HH22	1.64	0.62
1:C:459:VAL:HG12	1:C:469:PHE:HA	1.80	0.62
1:C:167:TYR:CE2	1:C:169:ASN:HA	2.34	0.62
1:B:380:LYS:HE2	1:B:432:GLU:OE2	2.00	0.61
1:C:155:LYS:HE3	1:C:192:THR:O	1.99	0.61
1:C:309:VAL:HG12	1:C:311:SER:H	1.65	0.61
1:B:261:LYS:CA	1:B:262:ARG:CB	2.78	0.61
1:B:431:MET:O	1:B:435:ARG:HG2	2.00	0.61
1:A:488:TYR:N	1:A:489:PRO:CD	2.59	0.61
1:C:354:HIS:O	1:C:355:HIS:O	2.19	0.61
1:C:111:SER:HB2	1:C:265:SER:HB3	1.82	0.60
1:C:261:LYS:CA	1:C:262:ARG:CB	2.79	0.60
1:C:307:LYS:HG2	1:C:421:TRP:CE2	2.36	0.60
1:A:459:VAL:HG12	1:A:469:PHE:HA	1.83	0.60
1:C:448:TYR:CE1	1:C:465:GLY:HA2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:GLU:CD	1:C:435:ARG:HH21	2.04	0.60
1:C:265:SER:OG	1:C:266:GLY:N	2.35	0.60
1:C:455:LEU:HD13	1:C:459:VAL:HG11	1.83	0.60
1:B:186:ASP:HB3	1:B:189:GLU:H	1.67	0.59
1:B:493:GLU:N	1:B:494:GLU:HA	2.10	0.59
1:A:309:VAL:HG12	1:A:311:SER:H	1.67	0.59
1:B:5:ASP:O	1:B:6:GLN:HB3	2.00	0.59
1:A:261:LYS:CA	1:A:262:ARG:CB	2.80	0.59
1:C:196:ASN:ND2	1:C:196:ASN:H	1.99	0.59
1:B:485:THR:HG22	1:B:485:THR:O	2.03	0.59
1:A:87:GLU:O	1:A:88:ASN:HB2	2.02	0.59
1:B:140:VAL:HG21	1:B:148:ARG:HH22	1.66	0.59
1:A:111:SER:HB2	1:A:265:SER:HB3	1.85	0.59
1:C:490:LYS:HA	1:C:491:TYR:CB	2.32	0.58
1:A:186:ASP:HB3	1:A:189:GLU:H	1.67	0.58
1:B:488:TYR:N	1:B:489:PRO:CD	2.61	0.58
1:B:31:THR:HG23	1:B:320:LEU:O	2.04	0.58
1:B:448:TYR:CE1	1:B:465:GLY:HA2	2.38	0.58
1:B:7:ILE:HG23	1:B:8:CYS:N	2.18	0.58
1:A:62:ALA:O	1:A:66:LEU:HB2	2.04	0.57
1:C:154:THR:HG21	1:C:193:LEU:HD22	1.85	0.57
1:B:7:ILE:HA	1:B:355:HIS:HA	1.87	0.57
1:C:380:LYS:HE2	1:C:432:GLU:OE2	2.04	0.57
1:C:184:PRO:HG2	1:C:190:GLN:HE21	1.70	0.57
1:C:485:THR:HG22	1:C:485:THR:O	2.04	0.57
1:A:485:THR:O	1:A:485:THR:HG22	2.05	0.56
1:C:487:ASP:OD1	1:C:487:ASP:C	2.43	0.56
1:A:211:ARG:HH12	1:C:216:ILE:HB	1.69	0.56
1:B:265:SER:OG	1:B:266:GLY:N	2.37	0.56
1:B:293:PRO:HG3	1:B:385:ILE:HA	1.87	0.56
1:B:355:HIS:O	1:B:355:HIS:ND1	2.38	0.56
1:B:471:HIS:CE1	1:B:490:LYS:HE2	2.41	0.56
1:B:55:GLU:HB2	1:B:75:LEU:HD12	1.89	0.55
1:C:345:GLY:HA3	1:C:363:TYR:CE1	2.42	0.55
1:B:112:VAL:C	1:B:262:ARG:HD3	2.27	0.55
1:B:354:HIS:O	1:B:355:HIS:C	2.44	0.55
1:C:31:THR:HG23	1:C:320:LEU:O	2.07	0.55
1:A:448:TYR:CE1	1:A:465:GLY:HA2	2.41	0.55
1:C:9:ILE:HD11	1:C:451:VAL:HG21	1.89	0.55
1:C:55:GLU:HB2	1:C:75:LEU:HD12	1.88	0.55
1:A:154:THR:HG21	1:A:193:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLY:C	1:A:249:ASN:HD22	2.10	0.55
1:B:355:HIS:HB2	1:B:478:MET:SD	2.47	0.55
1:A:431:MET:O	1:A:435:ARG:HG2	2.08	0.54
1:B:487:ASP:C	1:B:487:ASP:OD1	2.44	0.54
1:B:186:ASP:C	1:B:188:LYS:H	2.11	0.54
1:C:476:GLU:OE2	1:C:476:GLU:HA	2.07	0.54
1:A:476:GLU:OE2	1:A:476:GLU:HA	2.07	0.54
1:B:6:GLN:O	1:B:6:GLN:HG3	2.06	0.54
1:B:184:PRO:HG2	1:B:190:GLN:HE21	1.73	0.54
1:A:196:ASN:ND2	1:A:196:ASN:H	2.05	0.54
1:A:217:ALA:O	1:A:219:ARG:HG3	2.08	0.54
1:B:471:HIS:CD2	1:B:490:LYS:HG2	2.43	0.53
1:A:42:ASN:O	1:A:44:LYS:HG3	2.09	0.53
1:C:194:TYR:O	1:C:196:ASN:N	2.39	0.53
1:B:346:MET:SD	1:B:352:GLY:HA3	2.49	0.53
1:B:309:VAL:HG12	1:B:311:SER:H	1.73	0.53
1:C:491:TYR:CE2	1:C:492:GLU:CB	2.92	0.53
1:B:320:LEU:HB3	1:B:440:HIS:CG	2.43	0.52
1:C:217:ALA:O	1:C:219:ARG:HG3	2.08	0.52
1:A:487:ASP:OD1	1:A:487:ASP:C	2.47	0.52
1:B:217:ALA:HB2	1:C:202:SER:OG	2.09	0.52
1:B:355:HIS:CE1	1:B:361:SER:O	2.62	0.52
1:A:36:ILE:HA	1:A:292:LEU:HD22	1.91	0.52
1:A:54:LEU:HD12	1:A:55:GLU:N	2.24	0.52
1:A:434:GLU:CD	1:B:435:ARG:HH21	2.13	0.52
1:C:346:MET:SD	1:C:352:GLY:HA3	2.49	0.52
1:B:42:ASN:O	1:B:44:LYS:HG3	2.09	0.52
1:B:345:GLY:HA3	1:B:363:TYR:CE1	2.45	0.52
1:C:488:TYR:N	1:C:489:PRO:CD	2.61	0.52
1:A:155:LYS:HE2	1:A:195:GLN:HG2	1.92	0.52
1:B:167:TYR:CE2	1:B:169:ASN:HA	2.45	0.51
1:A:208:LEU:HD12	1:A:209:ASN:H	1.76	0.51
1:B:36:ILE:HA	1:B:292:LEU:HD22	1.92	0.51
1:C:123:LYS:HG2	1:C:131:THR:HG21	1.92	0.51
1:B:476:GLU:HA	1:B:476:GLU:OE2	2.11	0.51
1:B:7:ILE:HG12	1:B:8:CYS:H	1.76	0.50
1:C:208:LEU:HD12	1:C:209:ASN:H	1.77	0.50
1:A:155:LYS:HE3	1:A:192:THR:O	2.11	0.50
1:B:334:ALA:HB3	1:B:441:ASP:OD2	2.11	0.50
1:B:89:PRO:O	1:B:90:ARG:HB3	2.12	0.50
1:C:215:GLU:O	1:C:219:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ILE:HD12	1:B:262:ARG:HH22	1.77	0.50
1:C:42:ASN:O	1:C:44:LYS:HG3	2.12	0.50
1:B:196:ASN:ND2	1:B:196:ASN:H	2.09	0.50
1:B:208:LEU:HD12	1:B:209:ASN:H	1.77	0.50
1:A:399:PHE:CE2	1:A:407:GLU:HA	2.46	0.50
1:A:55:GLU:HB2	1:A:75:LEU:HD12	1.93	0.49
1:A:61:ILE:HD12	1:A:106:LYS:HD2	1.95	0.49
1:B:54:LEU:HD12	1:B:55:GLU:N	2.28	0.49
1:B:194:TYR:O	1:B:196:ASN:N	2.39	0.49
1:A:248:GLY:O	1:A:249:ASN:HB2	2.13	0.49
1:C:355:HIS:HB2	1:C:478:MET:SD	2.53	0.49
1:A:334:ALA:HB3	1:A:441:ASP:OD2	2.13	0.49
1:C:399:PHE:CE2	1:C:407:GLU:HA	2.46	0.49
1:A:399:PHE:CD2	1:A:407:GLU:HB2	2.48	0.49
1:B:471:HIS:ND1	1:B:490:LYS:HE2	2.28	0.49
1:C:479:ASN:O	1:C:483:ASN:HB2	2.13	0.49
1:C:155:LYS:HE2	1:C:195:GLN:HG2	1.95	0.49
1:C:399:PHE:CD2	1:C:407:GLU:HB2	2.48	0.49
1:A:194:TYR:O	1:A:196:ASN:N	2.42	0.48
1:B:153:LEU:HD12	1:B:250:LEU:HD23	1.95	0.48
1:C:61:ILE:HD12	1:C:106:LYS:HD2	1.95	0.48
1:B:493:GLU:N	1:B:494:GLU:CA	2.76	0.48
1:B:399:PHE:CE2	1:B:407:GLU:HA	2.48	0.48
1:A:120:ILE:HG22	1:A:167:TYR:CE1	2.49	0.48
1:A:184:PRO:HG2	1:A:190:GLN:HE21	1.79	0.48
1:C:62:ALA:O	1:C:66:LEU:HB2	2.14	0.48
1:C:89:PRO:O	1:C:90:ARG:HB3	2.14	0.48
1:A:186:ASP:C	1:A:188:LYS:H	2.17	0.47
1:B:461:GLU:O	1:C:456:ARG:NH2	2.47	0.47
1:B:493:GLU:N	1:B:494:GLU:CG	2.75	0.47
1:C:487:ASP:CA	1:C:488:TYR:CB	2.88	0.47
1:C:461:GLU:HG3	1:C:467:PHE:CE2	2.49	0.47
1:A:320:LEU:HD23	1:A:320:LEU:H	1.80	0.47
1:B:123:LYS:HG2	1:B:131:THR:HG21	1.97	0.47
1:B:479:ASN:O	1:B:483:ASN:HB2	2.15	0.47
1:A:176:LEU:HA	1:A:235:LEU:HD23	1.96	0.47
1:B:489:PRO:O	1:B:490:LYS:HD2	2.15	0.47
1:C:354:HIS:ND1	1:C:362:GLY:O	2.44	0.47
1:A:89:PRO:O	1:A:90:ARG:HB3	2.15	0.47
1:B:320:LEU:HA	1:B:440:HIS:CD2	2.49	0.47
1:C:36:ILE:HA	1:C:292:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LYS:HB2	1:A:262:ARG:CB	2.45	0.47
1:C:186:ASP:C	1:C:188:LYS:H	2.18	0.47
1:C:102:TYR:CZ	1:C:106:LYS:HD3	2.49	0.47
1:B:43:GLY:HA2	1:B:285:LEU:O	2.15	0.47
1:B:487:ASP:CA	1:B:488:TYR:CB	2.87	0.46
1:A:211:ARG:HH11	1:C:216:ILE:H	1.63	0.46
1:C:491:TYR:CD2	1:C:492:GLU:CB	2.99	0.46
1:B:8:CYS:O	1:B:353:TYR:CA	2.61	0.46
1:B:461:GLU:HG3	1:B:467:PHE:CE2	2.50	0.46
1:C:357:ASN:ND2	1:C:475:ASP:OD1	2.49	0.46
1:B:12:HIS:CG	1:B:13:ALA:N	2.84	0.46
1:C:334:ALA:HB3	1:C:441:ASP:OD2	2.16	0.46
1:B:208:LEU:HD12	1:B:209:ASN:N	2.30	0.46
1:B:307:LYS:HG2	1:B:421:TRP:NE1	2.29	0.46
1:B:424:ASN:HD21	1:C:424:ASN:ND2	2.14	0.46
1:B:248:GLY:O	1:B:249:ASN:HB2	2.14	0.46
1:B:320:LEU:CD2	1:B:350:TRP:CD1	2.99	0.46
1:B:354:HIS:O	1:B:355:HIS:O	2.33	0.46
1:C:120:ILE:HG22	1:C:167:TYR:CE1	2.51	0.46
1:B:248:GLY:C	1:B:249:ASN:HD22	2.19	0.46
1:A:158:SER:O	1:A:195:GLN:HG3	2.17	0.45
1:B:12:HIS:HB2	1:B:350:TRP:HA	1.98	0.45
1:A:241:THR:HB	1:C:220:PRO:HG3	1.98	0.45
1:B:66:LEU:HB3	1:B:147:PHE:CD2	2.51	0.45
1:C:54:LEU:HD12	1:C:55:GLU:N	2.31	0.45
1:C:184:PRO:HG2	1:C:190:GLN:NE2	2.30	0.45
1:A:215:GLU:O	1:A:219:ARG:NH2	2.49	0.45
1:B:215:GLU:O	1:B:219:ARG:NH2	2.49	0.45
1:C:338:PHE:CE1	1:C:339:ILE:HG13	2.52	0.45
1:B:9:ILE:CD1	1:B:451:VAL:HG21	2.31	0.45
1:B:261:LYS:HB2	1:B:262:ARG:CB	2.43	0.45
1:C:358:ASP:OD1	1:C:472:LYS:HE2	2.16	0.45
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.78	0.45
1:B:220:PRO:HG3	1:C:241:THR:HB	1.98	0.45
1:B:338:PHE:CE1	1:B:339:ILE:HG13	2.52	0.45
1:C:66:LEU:HB3	1:C:147:PHE:CD2	2.52	0.45
1:C:153:LEU:HD12	1:C:250:LEU:HD23	1.98	0.45
1:C:208:LEU:HD12	1:C:209:ASN:N	2.32	0.45
1:A:208:LEU:HD12	1:A:209:ASN:N	2.31	0.45
1:B:427:LEU:HD12	1:B:427:LEU:HA	1.77	0.45
1:A:299:PRO:O	1:A:395:VAL:HG11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.82	0.45
1:B:492:GLU:HA	1:B:493:GLU:HA	1.44	0.45
1:C:43:GLY:HA2	1:C:285:LEU:O	2.16	0.45
1:A:44:LYS:O	1:A:286:GLY:HA2	2.16	0.45
1:A:222:VAL:O	1:A:223:ASN:HB2	2.17	0.45
1:B:44:LYS:O	1:B:286:GLY:HA2	2.17	0.45
1:B:261:LYS:CA	1:B:262:ARG:HB2	2.34	0.45
1:B:455:LEU:O	1:B:456:ARG:HB2	2.17	0.45
1:B:455:LEU:O	1:B:456:ARG:CB	2.65	0.45
1:A:53:PRO:HG3	1:A:82:TYR:CE2	2.53	0.44
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.72	0.44
1:B:184:PRO:HG2	1:B:190:GLN:NE2	2.32	0.44
1:C:490:LYS:CA	1:C:491:TYR:HB3	2.42	0.44
1:A:31:THR:C	1:A:32:HIS:ND1	2.70	0.44
1:C:261:LYS:CB	1:C:262:ARG:HB3	2.42	0.44
1:A:66:LEU:HB3	1:A:147:PHE:CD2	2.52	0.44
1:C:123:LYS:HG2	1:C:131:THR:CG2	2.46	0.44
1:A:51:ILE:HG23	1:A:52:PRO:HD2	1.99	0.44
1:B:176:LEU:HA	1:B:235:LEU:HD23	1.99	0.44
1:C:248:GLY:C	1:C:249:ASN:HD22	2.19	0.44
1:C:261:LYS:HB2	1:C:262:ARG:CB	2.41	0.44
1:C:31:THR:C	1:C:32:HIS:ND1	2.71	0.44
1:B:493:GLU:H	1:B:494:GLU:CG	2.28	0.44
1:B:103:GLU:OE1	1:B:400:SER:HB3	2.18	0.44
1:C:152:TRP:C	1:C:152:TRP:CD1	2.91	0.44
1:B:399:PHE:CD2	1:B:407:GLU:HB2	2.53	0.44
1:A:161:PRO:O	1:A:162:VAL:C	2.56	0.44
1:C:136:ARG:HD2	1:C:136:ARG:HA	1.79	0.44
1:B:22:THR:HB	1:B:434:GLU:HB3	2.00	0.43
1:B:53:PRO:HG3	1:B:82:TYR:CE2	2.53	0.43
1:A:66:LEU:O	1:A:147:PHE:HB3	2.19	0.43
1:A:153:LEU:HD12	1:A:250:LEU:HD23	1.99	0.43
1:A:293:PRO:HB3	1:A:388:MET:HG2	2.00	0.43
1:B:355:HIS:HD2	1:B:478:MET:HG3	1.84	0.43
1:C:12:HIS:CG	1:C:13:ALA:N	2.86	0.43
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.87	0.43
1:B:123:LYS:HG2	1:B:131:THR:CG2	2.48	0.43
1:B:158:SER:O	1:B:195:GLN:HG3	2.19	0.43
1:A:183:HIS:HB3	1:A:215:GLU:O	2.19	0.43
1:B:377:ILE:HD13	1:B:377:ILE:HA	1.86	0.43
1:B:61:ILE:HG22	1:B:61:ILE:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLU:HG3	1:A:467:PHE:CE2	2.54	0.43
1:B:112:VAL:CA	1:B:262:ARG:HD3	2.49	0.43
1:B:154:THR:HG21	1:B:193:LEU:HD22	2.00	0.42
1:B:298:HIS:HA	1:B:299:PRO:HD3	1.86	0.42
1:A:43:GLY:HA2	1:A:285:LEU:O	2.19	0.42
1:B:5:ASP:HA	1:B:356:SER:O	2.18	0.42
1:C:176:LEU:HA	1:C:235:LEU:HD23	2.00	0.42
1:C:455:LEU:O	1:C:456:ARG:CB	2.67	0.42
1:C:427:LEU:HD12	1:C:427:LEU:HA	1.75	0.42
1:A:152:TRP:C	1:A:152:TRP:CD1	2.93	0.42
1:B:6:GLN:O	1:B:6:GLN:CG	2.66	0.42
1:B:361:SER:HB3	1:B:362:GLY:H	1.66	0.42
1:B:488:TYR:O	1:B:488:TYR:CD2	2.72	0.42
1:A:423:TYR:CE1	1:B:388:MET:HB2	2.55	0.42
1:A:423:TYR:HD1	1:B:388:MET:HA	1.84	0.42
1:C:132:THR:O	1:C:133:GLY:C	2.58	0.42
1:A:338:PHE:CE1	1:A:339:ILE:HG13	2.54	0.42
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.87	0.42
1:B:53:PRO:HG3	1:B:82:TYR:CZ	2.55	0.42
1:B:424:ASN:HD21	1:C:424:ASN:HD21	1.68	0.42
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.78	0.42
1:C:320:LEU:H	1:C:320:LEU:HD23	1.84	0.42
1:B:31:THR:C	1:B:32:HIS:ND1	2.74	0.42
1:C:64:TRP:CD1	1:C:74:LEU:HD12	2.55	0.41
1:A:66:LEU:HD12	1:A:93:LEU:CD2	2.50	0.41
1:A:479:ASN:O	1:A:483:ASN:HB2	2.20	0.41
1:C:66:LEU:O	1:C:147:PHE:HB3	2.20	0.41
1:C:310:LYS:HG2	1:C:310:LYS:O	2.20	0.41
1:A:54:LEU:HD12	1:A:55:GLU:H	1.84	0.41
1:B:62:ALA:O	1:B:66:LEU:HB2	2.20	0.41
1:A:123:LYS:HG2	1:A:131:THR:HG21	2.00	0.41
1:A:292:LEU:HA	1:A:293:PRO:HD3	1.86	0.41
1:A:298:HIS:HA	1:A:299:PRO:HD3	1.85	0.41
1:A:335:ILE:O	1:A:336:ALA:HB3	2.20	0.41
1:C:78:PRO:O	1:C:114:HIS:HA	2.19	0.41
1:A:211:ARG:HH11	1:C:216:ILE:N	2.18	0.41
1:A:412:LYS:HE2	1:B:414:GLU:OE2	2.20	0.41
1:C:299:PRO:HG3	1:C:308:TYR:CZ	2.55	0.41
1:C:489:PRO:C	1:C:490:LYS:HG2	2.40	0.41
1:A:8:CYS:HA	1:A:466:CYS:HA	2.01	0.41
1:C:123:LYS:HD3	1:C:131:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH1	1:C:216:ILE:HB	2.33	0.41
1:C:8:CYS:HA	1:C:466:CYS:HA	2.03	0.41
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.68	0.41
1:A:64:TRP:CD1	1:A:74:LEU:HD12	2.55	0.41
1:A:102:TYR:CZ	1:A:106:LYS:HD3	2.56	0.41
1:A:132:THR:O	1:A:133:GLY:C	2.58	0.41
1:B:38:GLU:HG2	1:B:290:THR:HG21	2.02	0.41
1:B:64:TRP:CD1	1:B:74:LEU:HD12	2.55	0.41
1:B:136:ARG:HA	1:B:136:ARG:HD2	1.84	0.41
1:C:38:GLU:HG2	1:C:290:THR:HG21	2.03	0.41
1:C:77:VAL:HG23	1:C:79:GLU:N	2.29	0.41
1:C:161:PRO:O	1:C:162:VAL:C	2.56	0.41
1:A:78:PRO:O	1:A:114:HIS:HA	2.21	0.41
1:B:261:LYS:CB	1:B:262:ARG:HB3	2.48	0.41
1:A:123:LYS:HG2	1:A:131:THR:CG2	2.51	0.40
1:B:8:CYS:HB2	1:B:354:HIS:HB3	2.03	0.40
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.68	0.40
1:C:354:HIS:O	1:C:355:HIS:CG	2.73	0.40
1:B:102:TYR:CZ	1:B:106:LYS:HD3	2.57	0.40
1:B:217:ALA:O	1:B:219:ARG:HG3	2.21	0.40
1:A:26:ARG:NH1	1:B:386:GLU:OE1	2.54	0.40
1:A:412:LYS:NZ	1:B:395:VAL:HG22	2.37	0.40
1:B:399:PHE:CE1	1:B:406:LEU:HG	2.56	0.40
1:A:377:ILE:HD13	1:A:377:ILE:HA	1.80	0.40
1:C:357:ASN:HB3	1:C:360:GLY:O	2.22	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	A	466/505 (92%)	423 (91%)	35 (8%)	8 (2%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	482/505 (95%)	433 (90%)	39 (8%)	10 (2%)	7	33
1	C	477/505 (94%)	430 (90%)	35 (7%)	12 (2%)	5	28
All	All	1425/1515 (94%)	1286 (90%)	109 (8%)	30 (2%)	7	33

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ARG
1	A	488	TYR
1	B	6	GLN
1	B	262	ARG
1	B	355	HIS
1	B	488	TYR
1	C	262	ARG
1	C	355	HIS
1	C	488	TYR
1	B	171	SER
1	B	456	ARG
1	C	456	ARG
1	A	264	SER
1	A	456	ARG
1	B	264	SER
1	C	264	SER
1	C	491	TYR
1	C	492	GLU
1	A	76	SER
1	A	171	SER
1	B	76	SER
1	C	76	SER
1	C	171	SER
1	C	195	GLN
1	C	489	PRO
1	A	489	PRO
1	B	489	PRO
1	A	88	ASN
1	B	88	ASN
1	C	88	ASN

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	A	410/442 (93%)	377 (92%)	33 (8%)	12	40
1	B	423/442 (96%)	388 (92%)	35 (8%)	11	39
1	C	418/442 (95%)	388 (93%)	30 (7%)	14	45
All	All	1251/1326 (94%)	1153 (92%)	98 (8%)	12	42

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	25	GLU
1	A	26	ARG
1	A	34	LYS
1	A	40	THR
1	A	73	ARG
1	A	76	SER
1	A	77	VAL
1	A	82	TYR
1	A	99	PHE
1	A	109	LEU
1	A	118	VAL
1	A	131	THR
1	A	186	ASP
1	A	196	ASN
1	A	202	SER
1	A	218	THR
1	A	246	SER
1	A	268	MET
1	A	283	THR
1	A	291	THR
1	A	309	VAL
1	A	313	LYS
1	A	316	LEU
1	A	320	LEU
1	A	351	TYR

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Mol	Chain	Res	Type
1	A	390	THR
1	A	409	LEU
1	A	427	LEU
1	A	434	GLU
1	A	477	CYS
1	A	480	SER
1	A	487	ASP
1	B	6	GLN
1	B	17	THR
1	B	25	GLU
1	B	26	ARG
1	B	34	LYS
1	B	40	THR
1	B	73	ARG
1	B	76	SER
1	B	77	VAL
1	B	99	PHE
1	B	109	LEU
1	B	118	VAL
1	B	131	THR
1	B	186	ASP
1	B	196	ASN
1	B	202	SER
1	B	218	THR
1	B	246	SER
1	B	262	ARG
1	B	268	MET
1	B	283	THR
1	B	291	THR
1	B	316	LEU
1	B	320	LEU
1	B	351	TYR
1	B	355	HIS
1	B	357	ASN
1	B	358	ASP
1	B	390	THR
1	B	409	LEU
1	B	427	LEU
1	B	434	GLU
1	B	477	CYS
1	B	480	SER
1	B	487	ASP

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Mol	Chain	Res	Type
1	C	17	THR
1	C	25	GLU
1	C	26	ARG
1	C	34	LYS
1	C	40	THR
1	C	73	ARG
1	C	76	SER
1	C	77	VAL
1	C	99	PHE
1	C	109	LEU
1	C	118	VAL
1	C	131	THR
1	C	186	ASP
1	C	196	ASN
1	C	202	SER
1	C	218	THR
1	C	268	MET
1	C	283	THR
1	C	291	THR
1	C	316	LEU
1	C	320	LEU
1	C	351	TYR
1	C	390	THR
1	C	409	LEU
1	C	427	LEU
1	C	434	GLU
1	C	477	CYS
1	C	480	SER
1	C	487	ASP
1	C	491	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	129	HIS
1	A	190	GLN
1	A	195	GLN
1	A	196	ASN
1	A	249	ASN
1	A	424	ASN
1	A	454	GLN

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Mol	Chain	Res	Type
1	B	49	ASN
1	B	129	HIS
1	B	190	GLN
1	B	195	GLN
1	B	196	ASN
1	B	249	ASN
1	B	355	HIS
1	B	359	GLN
1	B	454	GLN
1	C	49	ASN
1	C	128	GLN
1	C	129	HIS
1	C	190	GLN
1	C	195	GLN
1	C	196	ASN
1	C	249	ASN
1	C	359	GLN
1	C	424	ASN
1	C	454	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	472/505 (93%)	-0.30	1 (0%)	95	87	13, 53, 101, 173	0
1	B	486/505 (96%)	-0.33	7 (1%)	75	49	20, 50, 92, 199	0
1	C	481/505 (95%)	-0.07	14 (2%)	51	23	20, 62, 127, 193	0
All	All	1439/1515 (94%)	-0.23	22 (1%)	73	46	13, 55, 111, 199	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	GLY	7.1
1	C	132	THR	6.5
1	B	141	SER	5.2
1	B	487	ASP	5.1
1	C	356	SER	4.6
1	C	141	SER	4.3
1	B	143	ASN	3.2
1	C	487	ASP	3.1
1	C	136	ARG	3.1
1	C	15	ASN	2.8
1	C	90	ARG	2.8
1	C	355	HIS	2.8
1	B	140	VAL	2.8
1	C	476	GLU	2.5
1	B	476	GLU	2.4
1	C	289	ASN	2.3
1	A	325	GLN	2.3
1	C	158	SER	2.2
1	B	187	GLU	2.2
1	C	361	SER	2.1
1	C	262	ARG	2.1
1	B	128	GLN	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 monosaccharides 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.