



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:04 am GMT

PDB ID : 3T1E
Title : The structure of the Newcastle disease virus hemagglutinin-neuraminidase (HN) ectodomain reveals a 4-helix bundle stalk
Authors : Yuan, P.; Swanson, K.; Leser, G.P.; Paterson, R.G.; Lamb, R.A.; Jardetzky, T.S.
Deposited on : 2011-07-21
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

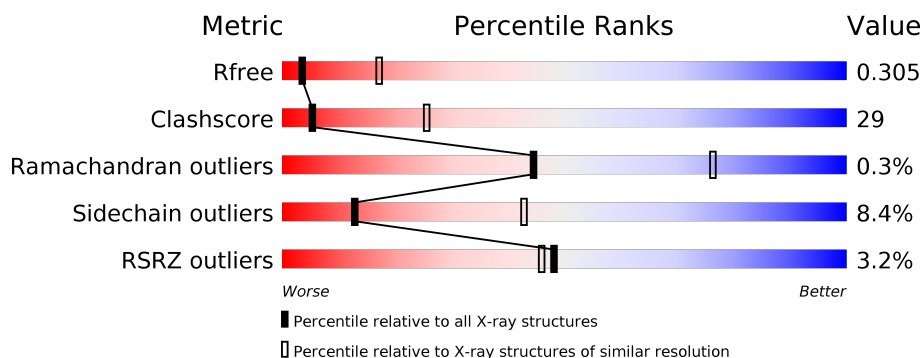
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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

Mol	Chain	Length	Quality of chain
1	A	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 50%, green 31%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 50% 31% 17% </div> </div>
1	B	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 48%, green 31%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 48% 31% 17% </div> </div>
1	E	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 93%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> • • • 93% </div> </div>
1	F	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 93%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> • • • 93% </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6976 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3204	1989	549	646	20			
1	B	445	Total	C	N	O	S	0	0	0
			3194	1983	546	646	19			
1	E	37	Total	C	N	O	S	0	0	0
			289	184	46	58	1			
1	F	37	Total	C	N	O	S	0	0	0
			289	184	46	58	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	EXPRESSION TAG	UNP P12554
A	35	MET	-	EXPRESSION TAG	UNP P12554
A	36	ALA	-	EXPRESSION TAG	UNP P12554
A	37	HIS	-	EXPRESSION TAG	UNP P12554
A	38	HIS	-	EXPRESSION TAG	UNP P12554
A	39	HIS	-	EXPRESSION TAG	UNP P12554
A	40	HIS	-	EXPRESSION TAG	UNP P12554
A	41	HIS	-	EXPRESSION TAG	UNP P12554
A	42	HIS	-	EXPRESSION TAG	UNP P12554
A	43	LEU	-	EXPRESSION TAG	UNP P12554
A	44	VAL	-	EXPRESSION TAG	UNP P12554
A	45	PRO	-	EXPRESSION TAG	UNP P12554
A	46	ARG	-	EXPRESSION TAG	UNP P12554
A	47	GLY	-	EXPRESSION TAG	UNP P12554
A	48	SER	-	EXPRESSION TAG	UNP P12554
A	328	ALA	GLY	SEE REMARK 999	UNP P12554
B	34	ALA	-	EXPRESSION TAG	UNP P12554
B	35	MET	-	EXPRESSION TAG	UNP P12554
B	36	ALA	-	EXPRESSION TAG	UNP P12554
B	37	HIS	-	EXPRESSION TAG	UNP P12554
B	38	HIS	-	EXPRESSION TAG	UNP P12554

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Chain	Residue	Modelled	Actual	Comment	Reference
B	39	HIS	-	EXPRESSION TAG	UNP P12554
B	40	HIS	-	EXPRESSION TAG	UNP P12554
B	41	HIS	-	EXPRESSION TAG	UNP P12554
B	42	HIS	-	EXPRESSION TAG	UNP P12554
B	43	LEU	-	EXPRESSION TAG	UNP P12554
B	44	VAL	-	EXPRESSION TAG	UNP P12554
B	45	PRO	-	EXPRESSION TAG	UNP P12554
B	46	ARG	-	EXPRESSION TAG	UNP P12554
B	47	GLY	-	EXPRESSION TAG	UNP P12554
B	48	SER	-	EXPRESSION TAG	UNP P12554
B	328	ALA	GLY	SEE REMARK 999	UNP P12554
E	34	ALA	-	EXPRESSION TAG	UNP P12554
E	35	MET	-	EXPRESSION TAG	UNP P12554
E	36	ALA	-	EXPRESSION TAG	UNP P12554
E	37	HIS	-	EXPRESSION TAG	UNP P12554
E	38	HIS	-	EXPRESSION TAG	UNP P12554
E	39	HIS	-	EXPRESSION TAG	UNP P12554
E	40	HIS	-	EXPRESSION TAG	UNP P12554
E	41	HIS	-	EXPRESSION TAG	UNP P12554
E	42	HIS	-	EXPRESSION TAG	UNP P12554
E	43	LEU	-	EXPRESSION TAG	UNP P12554
E	44	VAL	-	EXPRESSION TAG	UNP P12554
E	45	PRO	-	EXPRESSION TAG	UNP P12554
E	46	ARG	-	EXPRESSION TAG	UNP P12554
E	47	GLY	-	EXPRESSION TAG	UNP P12554
E	48	SER	-	EXPRESSION TAG	UNP P12554
E	328	ALA	GLY	SEE REMARK 999	UNP P12554
F	34	ALA	-	EXPRESSION TAG	UNP P12554
F	35	MET	-	EXPRESSION TAG	UNP P12554
F	36	ALA	-	EXPRESSION TAG	UNP P12554
F	37	HIS	-	EXPRESSION TAG	UNP P12554
F	38	HIS	-	EXPRESSION TAG	UNP P12554
F	39	HIS	-	EXPRESSION TAG	UNP P12554
F	40	HIS	-	EXPRESSION TAG	UNP P12554
F	41	HIS	-	EXPRESSION TAG	UNP P12554
F	42	HIS	-	EXPRESSION TAG	UNP P12554
F	43	LEU	-	EXPRESSION TAG	UNP P12554
F	44	VAL	-	EXPRESSION TAG	UNP P12554
F	45	PRO	-	EXPRESSION TAG	UNP P12554
F	46	ARG	-	EXPRESSION TAG	UNP P12554
F	47	GLY	-	EXPRESSION TAG	UNP P12554
F	48	SER	-	EXPRESSION TAG	UNP P12554

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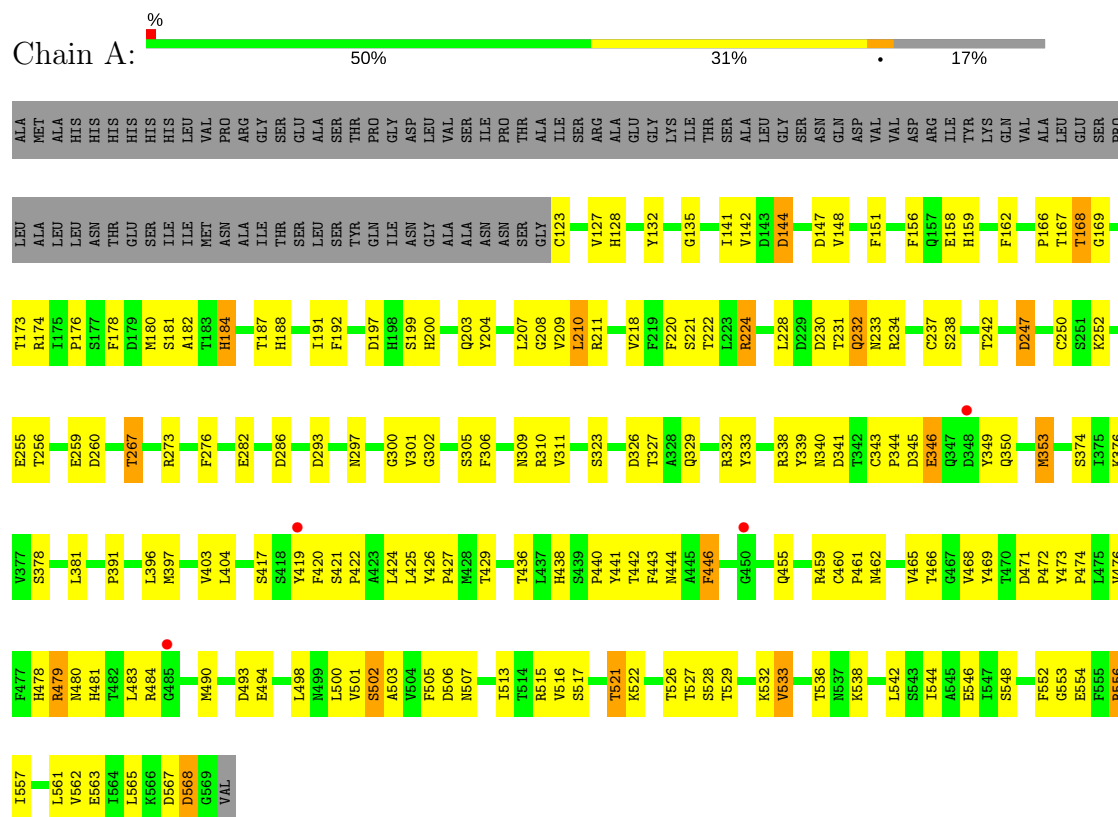
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Chain	Residue	Modelled	Actual	Comment	Reference
F	328	ALA	GLY	SEE REMARK 999	UNP P12554

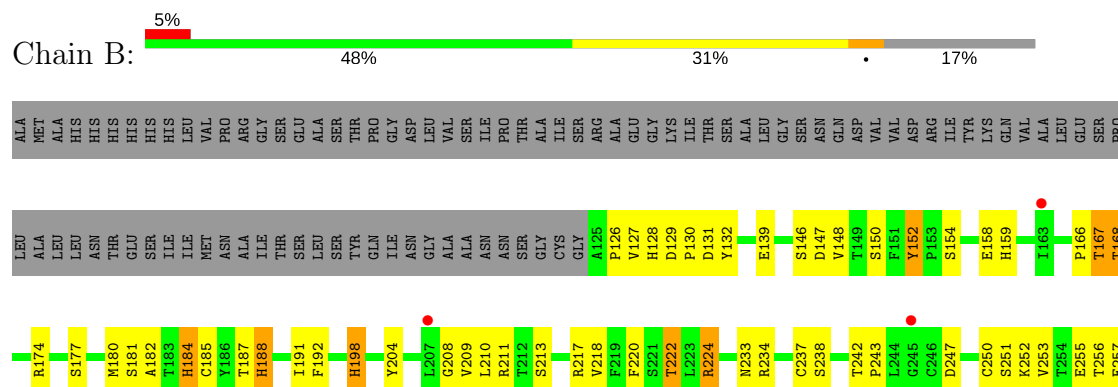
3 Residue-property plots

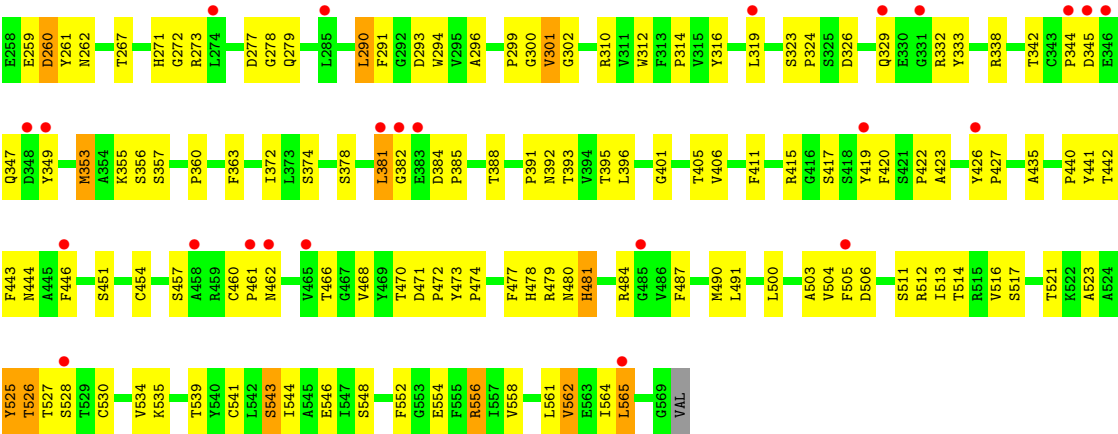
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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-neuraminidase

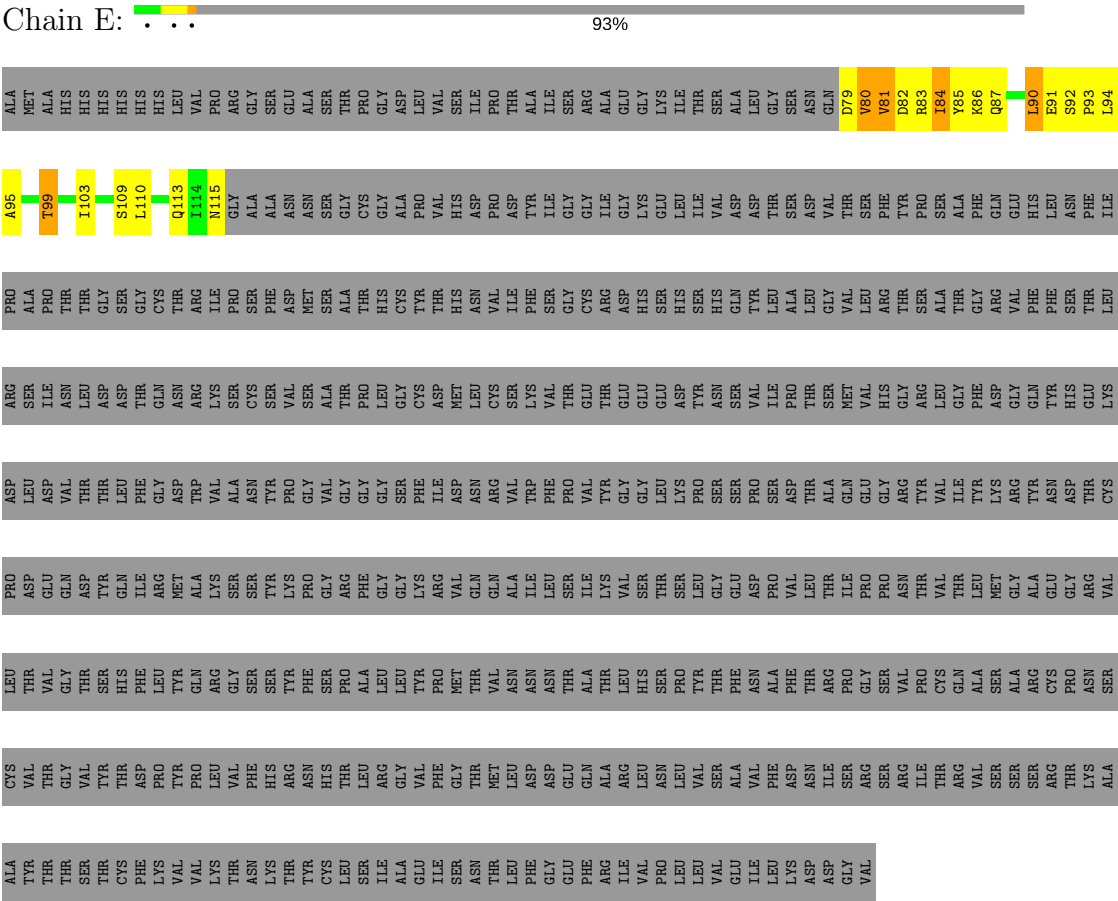


• Molecule 1: Hemagglutinin-neuraminidase

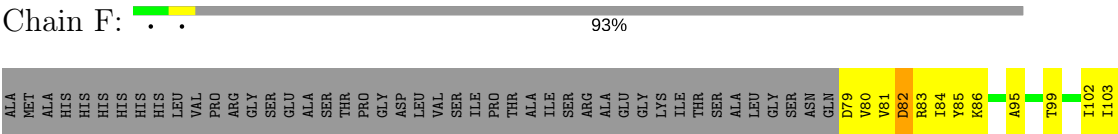




● Molecule 1: Hemagglutinin-neuraminidase



● Molecule 1: Hemagglutinin-neuraminidase



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.29Å 138.29Å 167.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.89 – 3.30 48.89 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.89-3.30) 100.0 (48.89-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.248 , 0.310 0.239 , 0.305	Depositor DCC
R_{free} test set	1240 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	126.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 117.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6976	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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 [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	0.30	0/3288	0.52	0/4502
1	B	0.29	0/3278	0.51	0/4490
1	E	0.29	0/291	0.46	0/396
1	F	0.28	0/291	0.51	0/396
All	All	0.30	0/7148	0.51	0/9784

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3204	0	2730	165	0
1	B	3194	0	2719	180	0
1	E	289	0	299	19	0
1	F	289	0	299	29	0
All	All	6976	0	6047	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 29.

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:B:451:SER:H	1:B:466:THR:HG21	1.16	1.06
1:A:224:ARG:HG3	1:A:224:ARG:HH11	1.22	1.04
1:B:152:TYR:HE2	1:B:565:LEU:HB2	1.23	1.02
1:B:471:ASP:HB2	1:B:527:THR:HA	1.49	0.95
1:B:152:TYR:CE2	1:B:565:LEU:HB2	2.03	0.94
1:B:128:HIS:HD2	1:B:210:LEU:HB2	1.33	0.94
1:B:198:HIS:O	1:B:233:ASN:ND2	2.01	0.93
1:B:423:ALA:HB2	1:B:446:PHE:HD2	1.35	0.91
1:B:333:TYR:CE1	1:B:355:LYS:HA	2.06	0.90
1:A:158:GLU:HG2	1:B:168:THR:HG21	1.55	0.89
1:A:419:TYR:CD1	1:A:461:PRO:HA	2.08	0.88
1:A:224:ARG:CG	1:A:224:ARG:HH11	1.86	0.87
1:E:85:TYR:HE2	1:F:85:TYR:HB3	1.38	0.86
1:B:198:HIS:NE2	1:B:253:VAL:O	2.09	0.85
1:E:95:ALA:O	1:E:99:THR:HG23	1.77	0.85
1:B:353:MET:O	1:B:356:SER:N	2.10	0.84
1:B:347:GLN:N	1:B:347:GLN:OE1	2.12	0.82
1:F:79:ASP:OD2	1:F:80:VAL:HG23	1.79	0.82
1:E:82:ASP:OD1	1:E:83:ARG:N	2.11	0.82
1:B:198:HIS:CD2	1:B:198:HIS:C	2.54	0.81
1:B:128:HIS:HA	1:B:209:VAL:HG13	1.63	0.80
1:B:147:ASP:O	1:B:150:SER:OG	1.98	0.80
1:A:191:ILE:HG22	1:A:192:PHE:H	1.47	0.79
1:A:128:HIS:HA	1:A:209:VAL:HG13	1.65	0.78
1:B:261:TYR:HD2	1:B:363:PHE:HB3	1.50	0.77
1:A:167:THR:HG21	1:B:159:HIS:CD2	2.19	0.77
1:A:343:CYS:SG	1:A:350:GLN:NE2	2.58	0.76
1:A:329:GLN:HA	1:A:332:ARG:HD3	1.68	0.76
1:E:85:TYR:CE2	1:F:85:TYR:HB3	2.21	0.74
1:F:81:VAL:HG13	1:F:82:ASP:H	1.52	0.74
1:A:199:SER:O	1:A:233:ASN:ND2	2.20	0.74
1:B:126:PRO:O	1:B:127:VAL:HG13	1.89	0.73
1:F:80:VAL:HG22	1:F:83:ARG:HH22	1.54	0.72
1:E:85:TYR:OH	1:F:86:LYS:HA	1.89	0.72
1:B:349:TYR:CZ	1:B:353:MET:HE1	2.25	0.72
1:B:256:THR:N	1:B:259:GLU:OE2	2.16	0.71
1:A:522:LYS:HG3	1:A:548:SER:HB2	1.72	0.71
1:B:128:HIS:HA	1:B:209:VAL:CG1	2.20	0.70
1:A:503:ALA:HB2	1:A:513:ILE:HG22	1.72	0.70
1:B:423:ALA:HB2	1:B:446:PHE:CD2	2.24	0.70
1:A:282:GLU:HA	1:A:381:LEU:HD22	1.73	0.70
1:A:427:PRO:HG2	1:A:438:HIS:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HD2	1:B:556:ARG:NH1	2.07	0.70
1:B:552:PHE:CD1	1:B:558:VAL:HG21	2.25	0.70
1:B:294:TRP:HA	1:B:319:LEU:HA	1.74	0.69
1:A:273:ARG:NH2	1:A:378:SER:O	2.25	0.69
1:A:344:PRO:HD2	1:A:460:CYS:SG	2.33	0.69
1:A:533:VAL:HG22	1:A:536:THR:HG22	1.75	0.69
1:B:148:VAL:HG23	1:B:484:ARG:NE	2.07	0.69
1:B:344:PRO:HD2	1:B:460:CYS:SG	2.34	0.68
1:B:503:ALA:HB2	1:B:513:ILE:HG22	1.74	0.68
1:A:192:PHE:HE2	1:B:158:GLU:HG2	1.58	0.68
1:A:224:ARG:HG3	1:A:224:ARG:NH1	1.97	0.68
1:A:563:GLU:HG2	1:A:565:LEU:HD21	1.74	0.68
1:B:310:ARG:HB2	1:B:312:TRP:NE1	2.09	0.67
1:A:552:PHE:O	1:B:556:ARG:NH2	2.24	0.67
1:A:158:GLU:CG	1:B:168:THR:HG21	2.23	0.67
1:B:198:HIS:HD2	1:B:198:HIS:C	1.97	0.67
1:B:511:SER:OG	1:B:512:ARG:O	2.13	0.67
1:A:267:THR:OG1	1:A:297:ASN:N	2.27	0.67
1:B:198:HIS:O	1:B:198:HIS:HD2	1.78	0.66
1:E:85:TYR:HE2	1:F:85:TYR:CB	2.07	0.66
1:B:148:VAL:HG21	1:B:484:ARG:HB3	1.77	0.66
1:A:473:TYR:CD1	1:A:529:THR:HA	2.30	0.66
1:B:146:SER:O	1:B:484:ARG:NH2	2.27	0.66
1:F:95:ALA:O	1:F:99:THR:HG23	1.97	0.65
1:A:425:LEU:HD11	1:A:472:PRO:HG2	1.77	0.65
1:A:191:ILE:HG22	1:A:192:PHE:N	2.10	0.65
1:B:388:THR:HG21	1:B:435:ALA:HB3	1.77	0.65
1:A:441:TYR:CE2	1:A:483:LEU:HB3	2.32	0.65
1:B:198:HIS:O	1:B:198:HIS:CD2	2.50	0.64
1:B:534:VAL:HG23	1:B:535:LYS:N	2.12	0.64
1:B:564:ILE:HD12	1:B:564:ILE:N	2.12	0.64
1:B:323:SER:H	1:B:326:ASP:HB3	1.62	0.64
1:A:522:LYS:CG	1:A:548:SER:HB2	2.28	0.64
1:A:417:SER:HA	1:A:466:THR:O	1.98	0.64
1:A:493:ASP:OD1	1:A:494:GLU:N	2.31	0.64
1:A:353:MET:SD	1:A:461:PRO:O	2.55	0.64
1:F:81:VAL:HG13	1:F:82:ASP:N	2.13	0.63
1:B:255:GLU:HB3	1:B:259:GLU:HG3	1.79	0.63
1:B:310:ARG:NH2	1:B:374:SER:O	2.32	0.63
1:B:548:SER:HA	1:B:554:GLU:O	1.98	0.63
1:A:247:ASP:OD1	1:A:273:ARG:HD3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASP:OD1	1:B:324:PRO:HD2	1.99	0.63
1:A:446:PHE:CE1	1:A:490:MET:HB3	2.33	0.62
1:B:147:ASP:HA	1:B:484:ARG:HH22	1.63	0.62
1:B:451:SER:H	1:B:466:THR:CG2	2.04	0.62
1:E:81:VAL:HA	1:E:84:ILE:HG22	1.80	0.62
1:F:109:SER:O	1:F:112:TYR:HB2	1.98	0.62
1:A:461:PRO:O	1:A:462:ASN:ND2	2.32	0.62
1:B:237:CYS:O	1:B:301:VAL:HA	1.99	0.62
1:A:148:VAL:HG23	1:A:484:ARG:CZ	2.28	0.62
1:A:192:PHE:HB2	1:A:200:HIS:NE2	2.14	0.62
1:F:114:ILE:O	1:F:114:ILE:HG13	1.99	0.62
1:B:487:PHE:HD1	1:B:503:ALA:O	1.83	0.61
1:A:242:THR:OG1	1:A:247:ASP:OD1	2.17	0.61
1:B:261:TYR:HE1	1:B:296:ALA:HB3	1.66	0.61
1:A:350:GLN:HG2	1:A:353:MET:HE3	1.82	0.61
1:A:238:SER:HB2	1:A:302:GLY:O	2.01	0.61
1:B:446:PHE:CE1	1:B:490:MET:HB3	2.36	0.61
1:B:491:LEU:HD11	1:B:523:ALA:HB3	1.83	0.61
1:A:345:ASP:HB2	1:A:350:GLN:HE21	1.65	0.60
1:B:406:VAL:HG21	1:B:474:PRO:HG2	1.83	0.60
1:B:233:ASN:O	1:B:252:LYS:HA	2.02	0.60
1:F:102:ILE:HD12	1:F:103:ILE:N	2.17	0.60
1:B:147:ASP:HA	1:B:484:ARG:NH2	2.17	0.60
1:A:168:THR:HG22	1:A:169:GLY:H	1.67	0.59
1:B:451:SER:N	1:B:466:THR:HG21	2.02	0.59
1:A:329:GLN:O	1:A:332:ARG:HG2	2.02	0.59
1:B:500:LEU:O	1:B:516:VAL:HG23	2.03	0.59
1:B:552:PHE:CE1	1:B:558:VAL:HG21	2.38	0.59
1:B:504:VAL:HG22	1:B:511:SER:HB3	1.85	0.59
1:A:174:ARG:HG2	1:A:546:GLU:CD	2.24	0.58
1:B:131:ASP:O	1:B:534:VAL:HG22	2.03	0.58
1:B:391:PRO:O	1:B:395:THR:HG22	2.03	0.58
1:A:306:PHE:CZ	1:A:309:ASN:HA	2.38	0.58
1:B:128:HIS:CD2	1:B:210:LEU:HB2	2.25	0.58
1:A:224:ARG:NH1	1:A:224:ARG:CG	2.57	0.58
1:B:419:TYR:HA	1:B:454:CYS:SG	2.42	0.58
1:E:92:SER:N	1:E:93:PRO:HD2	2.19	0.58
1:B:415:ARG:NE	1:B:417:SER:OG	2.37	0.57
1:B:242:THR:HB	1:B:243:PRO:HD2	1.86	0.57
1:A:455:GLN:OE1	1:A:455:GLN:N	2.31	0.57
1:A:192:PHE:HD1	1:A:200:HIS:HD2	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TYR:O	1:B:353:MET:HG2	2.04	0.57
1:B:541:CYS:SG	1:B:564:ILE:HD11	2.45	0.57
1:A:267:THR:HG1	1:A:297:ASN:H	1.51	0.57
1:A:349:TYR:CD2	1:A:353:MET:HE1	2.40	0.57
1:B:187:THR:HA	1:B:204:TYR:O	2.04	0.57
1:B:261:TYR:CD2	1:B:363:PHE:HB3	2.36	0.57
1:A:553:GLY:HA3	1:A:556:ARG:NH1	2.20	0.56
1:B:191:ILE:HG22	1:B:192:PHE:H	1.70	0.56
1:A:141:ILE:O	1:A:476:VAL:HA	2.06	0.56
1:A:350:GLN:HA	1:A:353:MET:HE2	1.88	0.56
1:A:526:THR:HA	1:A:544:ILE:O	2.06	0.56
1:B:273:ARG:HB3	1:B:381:LEU:HD21	1.87	0.56
1:B:444:ASN:C	1:B:446:PHE:H	2.09	0.56
1:F:80:VAL:O	1:F:80:VAL:HG12	2.05	0.56
1:A:234:ARG:HB3	1:A:250:CYS:HB3	1.86	0.55
1:E:91:GLU:O	1:E:94:LEU:HB2	2.06	0.55
1:B:471:ASP:CB	1:B:528:SER:H	2.18	0.55
1:A:498:LEU:HD23	1:A:522:LYS:HA	1.88	0.55
1:A:167:THR:O	1:A:167:THR:HG22	2.06	0.54
1:A:548:SER:HA	1:A:554:GLU:O	2.08	0.54
1:B:564:ILE:O	1:B:565:LEU:HD23	2.07	0.54
1:A:349:TYR:HD2	1:A:353:MET:CE	2.21	0.54
1:A:192:PHE:CE2	1:B:158:GLU:HG2	2.41	0.54
1:B:174:ARG:NH1	1:B:546:GLU:OE2	2.41	0.54
1:B:446:PHE:HD1	1:B:505:PHE:CZ	2.25	0.54
1:A:181:SER:OG	1:A:182:ALA:N	2.39	0.54
1:A:349:TYR:CD2	1:A:353:MET:CE	2.91	0.54
1:B:349:TYR:CE1	1:B:353:MET:HE1	2.43	0.54
1:A:187:THR:HA	1:A:204:TYR:O	2.08	0.54
1:B:271:HIS:CD2	1:B:382:GLY:H	2.26	0.54
1:B:191:ILE:HG22	1:B:192:PHE:N	2.23	0.54
1:B:277:ASP:OD1	1:B:279:GLN:N	2.41	0.54
1:B:419:TYR:CD2	1:B:461:PRO:HA	2.43	0.54
1:B:319:LEU:HD13	1:B:326:ASP:HB2	1.89	0.53
1:A:203:GLN:NE2	1:A:237:CYS:SG	2.80	0.53
1:B:166:PRO:HD2	1:B:556:ARG:HH12	1.71	0.53
1:B:261:TYR:CE1	1:B:296:ALA:HB3	2.43	0.53
1:E:109:SER:O	1:E:113:GLN:HG3	2.09	0.53
1:B:333:TYR:HE1	1:B:355:LYS:HA	1.71	0.53
1:A:142:VAL:O	1:A:142:VAL:HG23	2.07	0.53
1:A:162:PHE:CD1	1:A:220:PHE:HB2	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:HIS:CD2	1:B:210:LEU:H	2.27	0.52
1:A:339:TYR:H	1:A:444:ASN:ND2	2.08	0.52
1:B:423:ALA:HB3	1:B:443:PHE:HB2	1.92	0.52
1:A:184:HIS:CE1	1:A:222:THR:HG22	2.44	0.52
1:F:82:ASP:OD1	1:F:83:ARG:HG3	2.09	0.52
1:A:191:ILE:CG2	1:A:192:PHE:H	2.21	0.52
1:A:461:PRO:O	1:A:462:ASN:CG	2.47	0.52
1:F:113:GLN:O	1:F:114:ILE:C	2.48	0.52
1:A:506:ASP:OD1	1:A:507:ASN:N	2.40	0.51
1:A:478:HIS:HB3	1:A:480:ASN:HB2	1.91	0.51
1:A:144:ASP:OD1	1:A:479:ARG:HG2	2.10	0.51
1:A:350:GLN:HA	1:A:353:MET:CE	2.39	0.51
1:A:471:ASP:HB2	1:A:528:SER:H	1.76	0.51
1:B:238:SER:HB2	1:B:302:GLY:O	2.11	0.51
1:A:256:THR:HG23	1:A:259:GLU:OE1	2.11	0.51
1:A:224:ARG:NE	1:A:276:PHE:O	2.41	0.51
1:B:561:LEU:HD12	1:B:562:VAL:H	1.75	0.51
1:F:81:VAL:CG1	1:F:82:ASP:H	2.20	0.51
1:A:132:TYR:OH	1:A:218:VAL:HG22	2.11	0.50
1:E:84:ILE:O	1:E:87:GLN:HG2	2.11	0.50
1:F:80:VAL:HG13	1:F:83:ARG:HH12	1.76	0.50
1:A:396:LEU:HD22	1:A:419:TYR:HE2	1.77	0.50
1:B:480:ASN:O	1:B:481:HIS:HB2	2.12	0.50
1:B:411:PHE:CE1	1:B:441:TYR:HE2	2.28	0.50
1:A:339:TYR:H	1:A:444:ASN:HD21	1.60	0.50
1:A:397:MET:CE	1:A:465:VAL:HG22	2.42	0.50
1:B:152:TYR:CE2	1:B:565:LEU:HD12	2.47	0.50
1:B:132:TYR:OH	1:B:218:VAL:HG22	2.12	0.50
1:B:426:TYR:CD2	1:B:440:PRO:HB3	2.46	0.50
1:A:192:PHE:CD1	1:A:200:HIS:HD2	2.29	0.50
1:B:384:ASP:N	1:B:385:PRO:HD3	2.27	0.49
1:A:563:GLU:HG2	1:A:565:LEU:CD2	2.42	0.49
1:B:267:THR:HG23	1:B:296:ALA:HA	1.95	0.49
1:B:262:ASN:C	1:B:262:ASN:OD1	2.51	0.49
1:A:419:TYR:H	1:A:419:TYR:HD2	1.59	0.49
1:B:329:GLN:HA	1:B:329:GLN:OE1	2.13	0.49
1:A:188:HIS:CD2	1:A:188:HIS:C	2.85	0.49
1:A:479:ARG:C	1:A:481:HIS:H	2.15	0.49
1:A:300:GLY:C	1:A:302:GLY:H	2.16	0.49
1:E:86:LYS:O	1:E:86:LYS:HD3	2.13	0.49
1:B:392:ASN:HA	1:B:395:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:HIS:NE2	1:B:484:ARG:HG3	2.28	0.49
1:B:471:ASP:HB3	1:B:528:SER:H	1.78	0.49
1:F:83:ARG:HB3	1:F:86:LYS:HZ1	1.78	0.49
1:A:556:ARG:CZ	1:A:556:ARG:HB2	2.43	0.48
1:B:180:MET:HE1	1:B:220:PHE:HE2	1.78	0.48
1:B:256:THR:HG23	1:B:259:GLU:OE2	2.12	0.48
1:B:333:TYR:O	1:B:393:THR:HA	2.13	0.48
1:B:473:TYR:CD2	1:B:530:CYS:HB2	2.48	0.48
1:B:534:VAL:CG2	1:B:535:LYS:N	2.74	0.48
1:A:132:TYR:CE1	1:A:210:LEU:HD22	2.47	0.48
1:A:501:VAL:HG12	1:A:515:ARG:HG2	1.95	0.48
1:E:90:LEU:O	1:E:94:LEU:HD13	2.14	0.48
1:A:158:GLU:CD	1:B:168:THR:HG21	2.34	0.48
1:A:341:ASP:CB	1:A:459:ARG:CZ	2.92	0.48
1:A:230:ASP:OD1	1:A:232:GLN:HB2	2.14	0.48
1:B:345:ASP:HB3	1:B:349:TYR:HD2	1.78	0.48
1:A:323:SER:H	1:A:326:ASP:HB3	1.79	0.47
1:B:487:PHE:HB2	1:B:504:VAL:HG12	1.96	0.47
1:B:174:ARG:HG2	1:B:546:GLU:OE2	2.14	0.47
1:A:527:THR:HG22	1:A:544:ILE:HB	1.96	0.47
1:B:255:GLU:HB3	1:B:259:GLU:CG	2.43	0.47
1:B:411:PHE:HE1	1:B:427:PRO:HG3	1.79	0.47
1:A:231:THR:OG1	1:A:232:GLN:N	2.47	0.47
1:A:233:ASN:O	1:A:252:LYS:HA	2.14	0.47
1:B:420:PHE:CZ	1:B:422:PRO:HB2	2.49	0.47
1:B:419:TYR:HB3	1:B:462:ASN:O	2.14	0.47
1:B:184:HIS:O	1:B:184:HIS:ND1	2.48	0.47
1:B:338:ARG:NH1	1:B:457:SER:HA	2.29	0.47
1:E:82:ASP:OD1	1:E:83:ARG:HG3	2.15	0.47
1:A:238:SER:CB	1:A:302:GLY:O	2.63	0.46
1:B:148:VAL:CG2	1:B:484:ARG:HB3	2.45	0.46
1:B:312:TRP:CE3	1:B:374:SER:HB3	2.49	0.46
1:A:127:VAL:HG11	1:F:108:THR:HG23	1.97	0.46
1:F:113:GLN:C	1:F:113:GLN:CD	2.74	0.46
1:A:568:ASP:OD1	1:A:568:ASP:N	2.47	0.46
1:B:388:THR:O	1:B:388:THR:HG23	2.16	0.46
1:A:479:ARG:C	1:A:481:HIS:N	2.67	0.46
1:A:191:ILE:CG2	1:A:192:PHE:N	2.79	0.46
1:A:255:GLU:HB3	1:A:259:GLU:OE1	2.15	0.46
1:A:517:SER:HB3	1:A:521:THR:HG21	1.98	0.46
1:B:129:ASP:HB3	1:B:130:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:A:327:THR:HG23	2.15	0.46
1:A:247:ASP:OD2	1:A:273:ARG:NH1	2.48	0.46
1:A:151:PHE:HA	1:A:565:LEU:O	2.16	0.46
1:F:82:ASP:O	1:F:85:TYR:N	2.36	0.46
1:B:188:HIS:C	1:B:188:HIS:ND1	2.69	0.46
1:B:257:GLU:O	1:B:260:ASP:N	2.49	0.46
1:A:536:THR:HG23	1:A:538:LYS:HG3	1.97	0.45
1:A:473:TYR:HB2	1:A:528:SER:O	2.16	0.45
1:B:446:PHE:CD1	1:B:505:PHE:CE1	3.04	0.45
1:A:156:PHE:HZ	1:A:502:SER:HG	1.64	0.45
1:A:478:HIS:HB3	1:A:480:ASN:H	1.82	0.45
1:B:213:SER:OG	1:B:217:ARG:HB2	2.17	0.45
1:A:178:PHE:HZ	1:A:180:MET:HE2	1.81	0.45
1:A:132:TYR:OH	1:A:211:ARG:O	2.31	0.45
1:B:272:GLY:HA2	1:B:381:LEU:HD22	1.98	0.45
1:B:396:LEU:HD12	1:B:396:LEU:N	2.31	0.45
1:B:405:THR:HG23	1:B:405:THR:O	2.17	0.45
1:A:341:ASP:CB	1:A:459:ARG:NE	2.80	0.44
1:F:83:ARG:O	1:F:86:LYS:HG3	2.17	0.44
1:B:470:THR:O	1:B:472:PRO:HD3	2.17	0.44
1:F:103:ILE:O	1:F:106:ALA:HB3	2.17	0.44
1:A:381:LEU:N	1:A:381:LEU:HD12	2.32	0.44
1:A:426:TYR:CD2	1:A:440:PRO:HB3	2.53	0.44
1:B:319:LEU:HD12	1:B:319:LEU:O	2.18	0.44
1:B:139:GLU:HB3	1:B:477:PHE:CD2	2.53	0.44
1:A:167:THR:HG21	1:B:159:HIS:NE2	2.32	0.44
1:A:168:THR:HG22	1:A:169:GLY:N	2.33	0.44
1:A:166:PRO:HG3	1:A:173:THR:HG23	1.98	0.44
1:B:349:TYR:CE1	1:B:353:MET:CE	3.01	0.44
1:F:81:VAL:CG1	1:F:82:ASP:N	2.79	0.44
1:B:128:HIS:HE1	1:B:182:ALA:C	2.21	0.44
1:B:446:PHE:CD1	1:B:490:MET:HB3	2.52	0.44
1:A:197:ASP:CB	1:A:200:HIS:CE1	3.00	0.43
1:A:421:SER:HB3	1:A:422:PRO:HD3	2.00	0.43
1:B:132:TYR:OH	1:B:211:ARG:O	2.36	0.43
1:B:471:ASP:HB2	1:B:528:SER:H	1.83	0.43
1:B:564:ILE:N	1:B:564:ILE:CD1	2.81	0.43
1:B:224:ARG:HD3	1:B:224:ARG:HA	1.84	0.43
1:B:273:ARG:NH2	1:B:378:SER:O	2.51	0.43
1:B:528:SER:HB2	1:B:543:SER:OG	2.19	0.43
1:A:506:ASP:O	1:A:507:ASN:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:HIS:CE1	1:B:253:VAL:O	2.68	0.43
1:A:553:GLY:HA3	1:A:556:ARG:HH12	1.83	0.43
1:B:487:PHE:CE2	1:B:541:CYS:CB	3.01	0.43
1:A:479:ARG:H	1:A:479:ARG:HG2	1.51	0.43
1:A:490:MET:HG2	1:A:505:PHE:HZ	1.84	0.43
1:B:210:LEU:HD21	1:B:220:PHE:CE2	2.54	0.43
1:E:79:ASP:C	1:E:81:VAL:H	2.21	0.43
1:E:103:ILE:HD13	1:F:103:ILE:HG21	2.00	0.43
1:B:479:ARG:O	1:B:481:HIS:ND1	2.52	0.43
1:E:94:LEU:O	1:E:95:ALA:C	2.57	0.43
1:A:333:TYR:CD2	1:A:333:TYR:N	2.87	0.43
1:A:349:TYR:HD2	1:A:353:MET:HE1	1.79	0.43
1:A:561:LEU:HD12	1:A:562:VAL:H	1.84	0.43
1:A:144:ASP:OD2	1:A:478:HIS:ND1	2.45	0.43
1:A:429:THR:HG22	1:A:436:THR:OG1	2.18	0.43
1:B:517:SER:HB3	1:B:521:THR:OG1	2.19	0.43
1:A:188:HIS:CD2	1:A:188:HIS:O	2.72	0.43
1:B:146:SER:O	1:B:484:ARG:NH1	2.52	0.43
1:B:154:SER:O	1:B:514:THR:HG21	2.17	0.43
1:B:372:ILE:O	1:B:388:THR:HG22	2.19	0.42
1:A:220:PHE:CZ	1:A:542:LEU:HD22	2.54	0.42
1:B:255:GLU:HB3	1:B:259:GLU:CD	2.40	0.42
1:A:207:LEU:HD23	1:A:208:GLY:N	2.35	0.42
1:A:311:VAL:O	1:A:374:SER:HA	2.20	0.42
1:A:419:TYR:CD2	1:A:419:TYR:N	2.88	0.42
1:B:277:ASP:OD1	1:B:278:GLY:N	2.52	0.42
1:B:174:ARG:HG2	1:B:546:GLU:CD	2.39	0.42
1:A:349:TYR:CE2	1:A:353:MET:HE1	2.54	0.42
1:A:443:PHE:N	1:A:443:PHE:CD1	2.88	0.42
1:B:310:ARG:HB2	1:B:312:TRP:CE2	2.54	0.42
1:B:561:LEU:HD12	1:B:562:VAL:N	2.34	0.42
1:A:346:GLU:O	1:A:349:TYR:HB3	2.18	0.42
1:A:474:PRO:HB3	1:A:483:LEU:HD11	2.01	0.42
1:B:504:VAL:CG2	1:B:511:SER:HB3	2.49	0.42
1:A:425:LEU:HD11	1:A:472:PRO:CG	2.46	0.42
1:A:468:VAL:HG12	1:A:469:TYR:N	2.35	0.42
1:A:346:GLU:H	1:A:346:GLU:HG3	1.41	0.42
1:A:420:PHE:HD2	1:A:424:LEU:HD11	1.85	0.42
1:B:314:PRO:HG3	1:B:401:GLY:O	2.20	0.42
1:B:353:MET:C	1:B:355:LYS:N	2.70	0.42
1:A:197:ASP:CB	1:A:200:HIS:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:OE1	1:A:391:PRO:HA	2.19	0.42
1:A:142:VAL:CG2	1:A:142:VAL:O	2.67	0.41
1:A:404:LEU:HD23	1:A:404:LEU:N	2.35	0.41
1:A:338:ARG:NH2	1:A:444:ASN:O	2.53	0.41
1:B:181:SER:OG	1:B:182:ALA:N	2.45	0.41
1:B:256:THR:O	1:B:259:GLU:HG2	2.20	0.41
1:A:127:VAL:CG1	1:F:108:THR:HG23	2.50	0.41
1:A:305:SER:HB2	1:A:403:VAL:O	2.19	0.41
1:B:177:SER:HB3	1:B:187:THR:HG22	2.02	0.41
1:F:81:VAL:O	1:F:84:ILE:HG13	2.20	0.41
1:B:468:VAL:HG12	1:B:470:THR:HG23	2.02	0.41
1:B:526:THR:HA	1:B:544:ILE:O	2.21	0.41
1:F:80:VAL:HA	1:F:83:ARG:CZ	2.51	0.41
1:A:135:GLY:HA3	1:A:532:LYS:O	2.20	0.41
1:A:242:THR:HG22	1:A:306:PHE:HB2	2.03	0.41
1:B:208:GLY:HA3	1:B:222:THR:HA	2.02	0.41
1:A:338:ARG:NH2	1:A:444:ASN:OD1	2.53	0.41
1:A:404:LEU:H	1:A:404:LEU:HD23	1.85	0.41
1:A:293:ASP:OD1	1:A:323:SER:HB2	2.20	0.41
1:B:234:ARG:HA	1:B:251:SER:O	2.21	0.41
1:B:290:LEU:HG	1:B:291:PHE:CD1	2.56	0.41
1:B:332:ARG:C	1:B:333:TYR:CD2	2.94	0.41
1:A:500:LEU:O	1:A:516:VAL:HG23	2.20	0.41
1:B:300:GLY:N	1:B:314:PRO:O	2.51	0.41
1:B:310:ARG:NH1	1:B:384:ASP:OD2	2.52	0.41
1:A:159:HIS:CE1	1:B:167:THR:HG21	2.56	0.41
1:B:478:HIS:CD2	1:B:484:ARG:HG3	2.55	0.41
1:E:79:ASP:OD2	1:E:80:VAL:HG23	2.21	0.41
1:A:173:THR:O	1:A:174:ARG:HG3	2.21	0.41
1:A:340:ASN:O	1:A:340:ASN:OD1	2.38	0.41
1:F:81:VAL:O	1:F:84:ILE:CG1	2.69	0.41
1:A:176:PRO:HB3	1:A:557:ILE:HD13	2.04	0.40
1:B:357:SER:O	1:B:360:PRO:HD3	2.20	0.40
1:A:180:MET:HE3	1:A:220:PHE:HE2	1.86	0.40
1:A:192:PHE:HB2	1:A:200:HIS:CD2	2.56	0.40
1:A:527:THR:CG2	1:A:544:ILE:HB	2.51	0.40
1:B:128:HIS:CE1	1:B:182:ALA:C	2.95	0.40
1:B:271:HIS:NE2	1:B:381:LEU:HD23	2.36	0.40
1:A:349:TYR:CD2	1:A:353:MET:HE2	2.56	0.40
1:B:187:THR:OG1	1:B:204:TYR:O	2.27	0.40
1:E:85:TYR:C	1:E:87:GLN:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:HG2	1:A:376:LYS:HA	2.02	0.40
1:B:152:TYR:HD2	1:B:152:TYR:H	1.69	0.40
1:B:250:CYS:HA	1:B:299:PRO:HG2	2.04	0.40
1:A:180:MET:CE	1:A:220:PHE:HE2	2.35	0.40
1:B:247:ASP:OD2	1:B:273:ARG:NH1	2.54	0.40
1:B:525:TYR:CD1	1:B:525:TYR:N	2.88	0.40
1:B:564:ILE:C	1:B:565:LEU:HD23	2.42	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	445/537 (83%)	413 (93%)	31 (7%)	1 (0%)	51	81
1	B	443/537 (82%)	406 (92%)	36 (8%)	1 (0%)	51	81
1	E	35/537 (6%)	29 (83%)	5 (14%)	1 (3%)	5	31
1	F	35/537 (6%)	28 (80%)	7 (20%)	0	100	100
All	All	958/2148 (45%)	876 (91%)	79 (8%)	3 (0%)	44	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	VAL
1	B	301	VAL
1	E	80	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	A	313/463 (68%)	288 (92%)	25 (8%)	14	45
1	B	313/463 (68%)	288 (92%)	25 (8%)	14	45
1	E	34/463 (7%)	28 (82%)	6 (18%)	2	10
1	F	34/463 (7%)	32 (94%)	2 (6%)	23	58
All	All	694/1852 (38%)	636 (92%)	58 (8%)	13	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	CYS
1	A	144	ASP
1	A	147	ASP
1	A	168	THR
1	A	184	HIS
1	A	210	LEU
1	A	221	SER
1	A	224	ARG
1	A	228	LEU
1	A	232	GLN
1	A	247	ASP
1	A	260	ASP
1	A	267	THR
1	A	286	ASP
1	A	346	GLU
1	A	353	MET
1	A	442	THR
1	A	446	PHE
1	A	479	ARG
1	A	502	SER
1	A	521	THR
1	A	533	VAL
1	A	556	ARG
1	A	567	ASP
1	A	568	ASP
1	B	152	TYR
1	B	167	THR
1	B	168	THR

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Mol	Chain	Res	Type
1	B	184	HIS
1	B	185	CYS
1	B	188	HIS
1	B	198	HIS
1	B	222	THR
1	B	224	ARG
1	B	260	ASP
1	B	290	LEU
1	B	316	TYR
1	B	342	THR
1	B	353	MET
1	B	381	LEU
1	B	442	THR
1	B	481	HIS
1	B	506	ASP
1	B	525	TYR
1	B	526	THR
1	B	539	THR
1	B	543	SER
1	B	556	ARG
1	B	562	VAL
1	B	565	LEU
1	E	81	VAL
1	E	84	ILE
1	E	90	LEU
1	E	99	THR
1	E	110	LEU
1	E	115	ASN
1	F	82	ASP
1	F	113	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	HIS
1	A	340	ASN
1	A	350	GLN
1	A	462	ASN
1	B	128	HIS
1	B	271	HIS

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 carbohydrates 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	A	447/537 (83%)	0.08	4 (0%) 84 83	83, 111, 163, 215	0
1	B	445/537 (82%)	0.23	27 (6%) 22 21	83, 144, 200, 255	0
1	E	37/537 (6%)	0.02	0 100 100	100, 132, 177, 191	0
1	F	37/537 (6%)	-0.16	0 100 100	103, 133, 203, 212	0
All	All	966/2148 (44%)	0.14	31 (3%) 48 46	83, 129, 190, 255	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	GLY	4.5
1	A	485	GLY	3.6
1	B	274	LEU	3.5
1	B	383	GLU	3.3
1	B	345	ASP	3.1
1	B	462	ASN	3.0
1	B	461	PRO	3.0
1	B	348	ASP	3.0
1	A	419	TYR	2.9
1	B	419	TYR	2.9
1	B	346	GLU	2.8
1	B	485	GLY	2.8
1	B	465	VAL	2.6
1	B	245	GLY	2.6
1	B	329	GLN	2.6
1	B	344	PRO	2.5
1	B	349	TYR	2.4
1	B	458	ALA	2.4
1	B	446	PHE	2.3
1	B	426	TYR	2.2
1	B	528	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLY	2.2
1	B	319	LEU	2.2
1	B	207	LEU	2.1
1	B	565	LEU	2.1
1	B	505	PHE	2.1
1	B	381	LEU	2.1
1	B	163	ILE	2.1
1	A	450	GLY	2.1
1	A	348	ASP	2.0
1	B	285	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.