



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:44 AM UTC

PDB ID : 3T1E / pdb_00003t1e
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

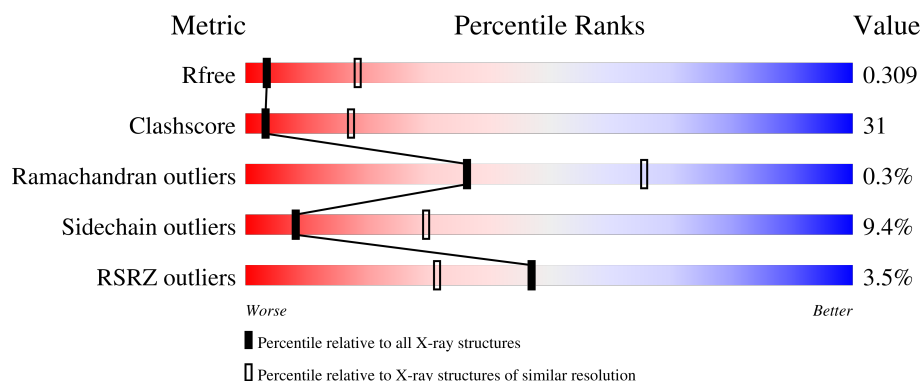
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	537	2% 49% 31% • 17%
1	B	537	4% 44% 34% • 17%
1	E	537	• • • 93%
1	F	537	• • • 93%

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

Continued on next page...

Continued from previous page...

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

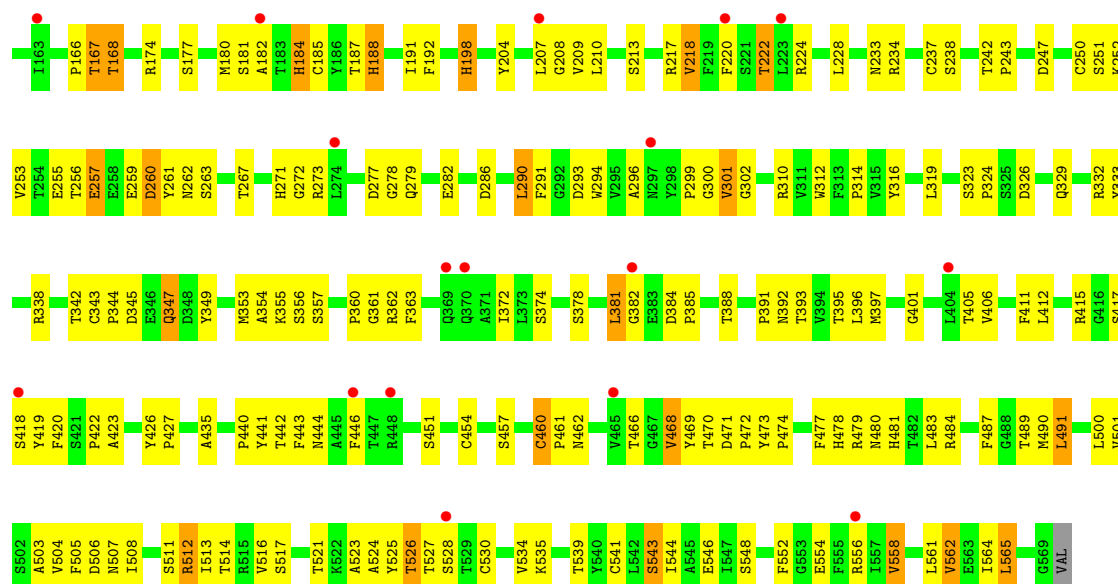
Continued on next page...

Continued from previous page...

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

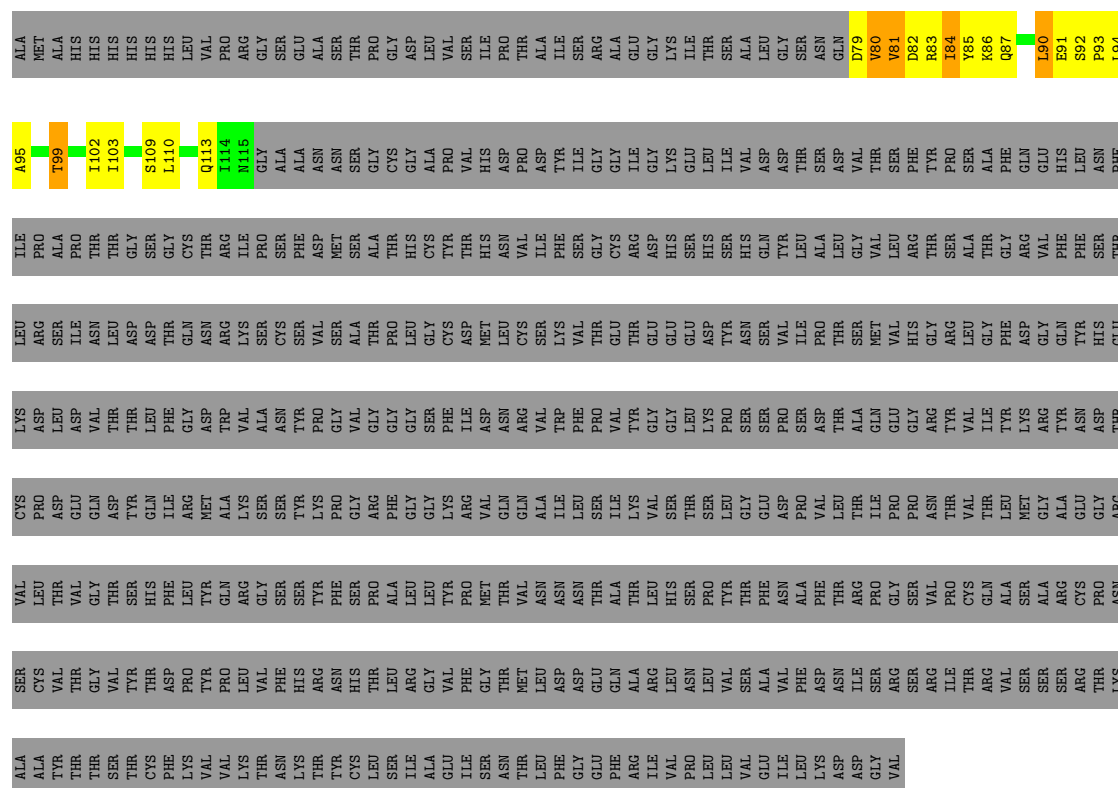
- Molecule 1: Hemagglutinin-neuraminidase





● Molecule 1: Hemagglutinin-neuraminidase

Chain E: . . . 93%



● Molecule 1: Hemagglutinin-neuraminidase

Chain F: . . . 93%



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) 99.9 (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 0.244 , 0.309	Depositor DCC
R_{free} test set	1241 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	126.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 160.2	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/3288	0.86	4/4502 (0.1%)
1	B	0.39	0/3278	0.89	7/4490 (0.2%)
1	E	0.39	0/291	0.76	0/396
1	F	0.37	0/291	0.82	0/396
All	All	0.39	0/7148	0.87	11/9784 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ARG	N-CA-C	-6.33	102.34	110.19
1	B	343	CYS	CA-C-N	6.17	125.73	119.19
1	B	343	CYS	C-N-CA	6.17	125.73	119.19
1	B	558	VAL	N-CA-C	5.52	114.02	107.73
1	B	155	ALA	N-CA-C	-5.49	103.38	110.19
1	B	460	CYS	CA-C-N	5.39	125.15	119.76
1	B	460	CYS	C-N-CA	5.39	125.15	119.76
1	A	389	ILE	CA-C-N	5.38	125.93	120.38
1	A	389	ILE	C-N-CA	5.38	125.93	120.38
1	A	508	ILE	N-CA-C	5.30	116.78	111.00
1	A	155	ALA	N-CA-C	-5.05	103.92	110.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3204	0	2730	168	0
1	B	3194	0	2719	197	0
1	E	289	0	299	19	0
1	F	289	0	299	31	0
All	All	6976	0	6047	399	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 31.

All (399) 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:A:397:MET:HE1	1:A:465:VAL:HG22	1.51	0.91
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:HH11	1:A:224:ARG:CG	1.86	0.87
1:E:85:TYR:HE2	1:F:85:TYR:HB3	1.38	0.86
1:B:198:HIS:C	1:B:198:HIS:CD2	2.54	0.85
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: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:A:349:TYR:CD2	1:A:353:MET:HE2	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:HIS:C	1:B:198:HIS:HD2	1.97	0.71
1:B:256:THR:N	1:B:259:GLU:OE2	2.16	0.71
1:A:180:MET:HE1	1:A:220:PHE:HE2	1.55	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
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:158:GLU:CG	1:B:168:THR:HG21	2.23	0.67
1:A:552:PHE:O	1:B:556:ARG:NH2	2.24	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:A:350:GLN:HA	1:A:353:MET:HE3	1.75	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:178:PHE:HZ	1:A:180:MET:HE3	1.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:260:ASP:O	1:B:263:SER:OG	2.10	0.63
1:B:534:VAL:HG23	1:B:535:LYS:N	2.12	0.63
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:A:349:TYR:HD2	1:A:353:MET:HE2	1.62	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:174:ARG:HG2	1:A:546:GLU:CD	2.24	0.63
1:A:247:ASP:OD1	1:A:273:ARG:HD3	1.97	0.63
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:349:TYR:CE1	1:B:353:MET:HE1	2.34	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:HG13	1:F:114:ILE:O	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:444:ASN:C	1:B:446:PHE:H	2.09	0.59
1:B:504:VAL:HG22	1:B:511:SER:HB3	1.85	0.59
1:A:178:PHE:CZ	1:A:180:MET:HE3	2.38	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:CG	1:A:224:ARG:NH1	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
1:B:349:TYR:O	1:B:353:MET:HG2	2.04	0.57
1:A:461:PRO:O	1:A:462:ASN:CG	2.47	0.57
1:B:541:CYS:SG	1:B:564:ILE:HD11	2.45	0.57
1:B:187:THR:HA	1:B:204:TYR:O	2.04	0.57
1:B:349:TYR:CZ	1:B:353:MET:HE1	2.39	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:F:113:GLN:O	1:F:114:ILE:C	2.48	0.56
1:A:141:ILE:O	1:A:476:VAL:HA	2.06	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:A:267:THR:HG1	1:A:297:ASN:H	1.52	0.56
1:F:80:VAL:HG12	1:F:80:VAL:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE2	1:B:158:GLU:HG2	2.41	0.54
1:A:349:TYR:HD2	1:A:353:MET:CE	2.21	0.54
1:B:174:ARG:NH1	1:B:546:GLU:OE2	2.41	0.54
1:B:262:ASN:OD1	1:B:262:ASN:C	2.51	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:188:HIS:C	1:A:188:HIS:CD2	2.85	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:A:300:GLY:C	1:A:302:GLY:H	2.16	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:A:479:ARG:C	1:A:481:HIS:H	2.15	0.53
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:F:113:GLN:C	1:F:113:GLN:CD	2.74	0.53
1:A:349:TYR:CD2	1:A:353:MET:CE	2.91	0.53
1:B:333:TYR:HE1	1:B:355:LYS:HA	1.71	0.53
1:A:142:VAL:HG23	1:A:142:VAL:O	2.07	0.53
1:A:158:GLU:CD	1:B:168:THR:HG21	2.34	0.53
1:A:162:PHE:CD1	1:A:220:PHE:HB2	2.45	0.53
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: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: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:224:ARG:NE	1:A:276:PHE:O	2.41	0.51
1:A:256:THR:HG23	1:A:259:GLU:OE1	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:OD2	1:A:353:MET:HE1	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:350:GLN:HG2	1:A:353:MET:HE3	1.92	0.50
1:B:188:HIS:C	1:B:188:HIS:ND1	2.69	0.50
1:A:396:LEU:HD22	1:A:419:TYR:HE2	1.77	0.50
1:A:479:ARG:C	1:A:481:HIS:N	2.67	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:B:132:TYR:OH	1:B:218:VAL:HG22	2.12	0.50
1:B:152:TYR:CE2	1:B:565:LEU:HD12	2.47	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:A:350:GLN:HA	1:A:353:MET:CE	2.39	0.49
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:A:419:TYR:HD2	1:A:419:TYR:H	1.59	0.49
1:B:329:GLN:HA	1:B:329:GLN:OE1	2.13	0.49
1:A:471:ASP:OD2	1:A:527:THR:OG1	2.29	0.49
1:E:86:LYS:HD3	1:E:86:LYS:O	2.13	0.49
1:B:392:ASN:HA	1:B:395:THR:HG22	1.93	0.49
1:B:471:ASP:HB3	1:B:528:SER:H	1.78	0.49
1:B:478:HIS:NE2	1:B:484:ARG:HG3	2.28	0.49
1:A:556:ARG:HB2	1:A:556:ARG:CZ	2.43	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:B:128:HIS:HE1	1:B:182:ALA:C	2.21	0.48
1:A:506:ASP:O	1:A:507:ASN:C	2.55	0.48
1:E:90:LEU:O	1:E:94:LEU:HD13	2.14	0.48
1:A:341:ASP:CB	1:A:459:ARG:CZ	2.92	0.48
1:E:79:ASP:C	1:E:81:VAL:H	2.21	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:E:94:LEU:O	1:E:95:ALA:C	2.57	0.48
1:A:323:SER:H	1:A:326:ASP:HB3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:PHE:HB2	1:B:504:VAL:HG12	1.96	0.47
1:F:83:ARG:HB3	1:F:86:LYS:HZ1	1.79	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:174:ARG:HG2	1:B:546:GLU:CD	2.39	0.47
1:B:184:HIS:O	1:B:184:HIS:ND1	2.48	0.47
1:B:255:GLU:HB3	1:B:259:GLU:CD	2.40	0.47
1:B:419:TYR:HB3	1:B:462:ASN:O	2.14	0.47
1:B:420:PHE:CZ	1:B:422:PRO:HB2	2.49	0.47
1:B:338:ARG:NH1	1:B:457:SER:HA	2.29	0.47
1:B:180:MET:HE1	1:B:220:PHE:HE2	1.79	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:397:MET:HE2	1:B:418:SER:HB2	1.97	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:A:568:ASP:OD1	1:A:568:ASP:N	2.47	0.46
1:B:388:THR:HG23	1:B:388:THR:O	2.16	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
1:B:353:MET:C	1:B:355:LYS:N	2.70	0.46
1:A:323:SER:O	1:A:327:THR:HG23	2.15	0.46
1:A:151:PHE:HA	1:A:565:LEU:O	2.16	0.46
1:A:247:ASP:OD2	1:A:273:ARG:NH1	2.48	0.46
1:F:82:ASP:O	1:F:85:TYR:N	2.36	0.46
1:B:257:GLU:O	1:B:260:ASP:N	2.49	0.46
1:B:332:ARG:C	1:B:333:TYR:CD2	2.94	0.46
1:A:536:THR:HG23	1:A:538:LYS:HG3	1.97	0.45
1:B:444:ASN:C	1:B:446:PHE:N	2.74	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:B:128:HIS:CE1	1:B:182:ALA:C	2.95	0.45
1:A:478:HIS:HB3	1:A:480:ASN:H	1.82	0.45
1:E:85:TYR:C	1:E:87:GLN:N	2.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:OG	1:B:217:ARG:HB2	2.17	0.45
1:B:564:ILE:C	1:B:565:LEU:HD23	2.42	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:B:187:THR:OG1	1:B:204:TYR:O	2.27	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:B:353:MET:O	1:B:354:ALA:C	2.60	0.44
1:A:166:PRO:HG3	1:A:173:THR:HG23	1.98	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:184:HIS:ND1	1:A:184:HIS:C	2.75	0.44
1:F:81:VAL:CG1	1:F:82:ASP:N	2.79	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: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:349:TYR:CD2	1:B:353:MET:HE3	2.52	0.43
1:B:528:SER:HB2	1:B:543:SER:OG	2.19	0.43
1:B:198:HIS:CE1	1:B:253:VAL:O	2.68	0.43
1:A:247:ASP:CG	1:A:273:ARG:HH11	2.25	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:B:524:ALA:C	1:B:525:TYR:CD1	2.97	0.43
1:A:479:ARG:HG2	1:A:479:ARG:H	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:B:483:LEU:HD23	1:B:483:LEU:C	2.43	0.43
1:B:469:TYR:C	1:B:469:TYR:CD2	2.95	0.43
1:E:103:ILE:HD13	1:F:103:ILE:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:GLY:C	1:B:302:GLY:H	2.27	0.43
1:B:479:ARG:O	1:B:481:HIS:ND1	2.52	0.43
1:F:113:GLN:CD	1:F:114:ILE:N	2.77	0.43
1:A:333:TYR:N	1:A:333:TYR:CD2	2.87	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: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:A:443:PHE:CD1	1:A:443:PHE:N	2.88	0.42
1:B:286:ASP:C	1:B:286:ASP:OD1	2.61	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:F:85:TYR:C	1:F:87:GLN:N	2.77	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:146:SER:C	1:B:484:ARG:HH22	2.23	0.42
1:B:314:PRO:HG3	1:B:401:GLY:O	2.20	0.42
1:B:506:ASP:C	1:B:508:ILE:N	2.76	0.42
1:A:197:ASP:CB	1:A:200:HIS:HE1	2.32	0.42
1:A:329:GLN:OE1	1:A:391:PRO:HA	2.19	0.42
1:A:142:VAL:O	1:A:142:VAL:CG2	2.67	0.41
1:A:404:LEU:HD23	1:A:404:LEU:N	2.35	0.41
1:B:506:ASP:O	1:B:507:ASN:C	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:438:HIS:O	1:A:439:SER:C	2.64	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:184:HIS:ND1	1:B:184:HIS:C	2.78	0.41
1:B:208:GLY:HA3	1:B:222:THR:HA	2.02	0.41
1:B:361:GLY:O	1:B:362:ARG:C	2.62	0.41
1:A:338:ARG:NH2	1:A:444:ASN:OD1	2.53	0.41
1:A:404:LEU:HD23	1:A:404:LEU:H	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:A:159:HIS:CE1	1:B:167:THR:HG21	2.56	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: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:OD1	1:A:340:ASN:O	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:192:PHE:HB2	1:A:200:HIS:CD2	2.56	0.40
1:A:524:ALA:HB3	1:A:546:GLU:CD	2.46	0.40
1:A:527:THR:CG2	1:A:544:ILE:HB	2.51	0.40
1:B:271:HIS:NE2	1:B:381:LEU:HD23	2.36	0.40
1:B:180:MET:HE2	1:B:184:HIS:HB3	2.03	0.40
1:B:489:THR:HG23	1:B:501:VAL:C	2.46	0.40
1:A:310:ARG:HG2	1:A:376:LYS:HA	2.02	0.40
1:B:152:TYR:H	1:B:152:TYR:HD2	1.69	0.40
1:B:250:CYS:HA	1:B:299:PRO:HG2	2.04	0.40
1:B:349:TYR:CE1	1:B:353:MET:CE	3.01	0.40
1:B:207:LEU:HD23	1:B:207:LEU:C	2.47	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/537 (83%)	413 (93%)	31 (7%)	1 (0%)	43	71
1	B	443/537 (82%)	406 (92%)	36 (8%)	1 (0%)	43	71
1	E	35/537 (6%)	29 (83%)	5 (14%)	1 (3%)	3	21
1	F	35/537 (6%)	28 (80%)	7 (20%)	0	100	100
All	All	958/2148 (45%)	876 (91%)	79 (8%)	3 (0%)	36	65

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

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%)	285 (91%)	28 (9%)	9	32
1	B	313/463 (68%)	285 (91%)	28 (9%)	9	32
1	E	34/463 (7%)	28 (82%)	6 (18%)	2	9
1	F	34/463 (7%)	31 (91%)	3 (9%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	694/1852 (38%)	629 (91%)	65 (9%)	8 30

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	CYS
1	A	142	VAL
1	A	147	ASP
1	A	168	THR
1	A	184	HIS
1	A	209	VAL
1	A	210	LEU
1	A	218	VAL
1	A	221	SER
1	A	224	ARG
1	A	226	ILE
1	A	228	LEU
1	A	232	GLN
1	A	256	THR
1	A	267	THR
1	A	286	ASP
1	A	329	GLN
1	A	346	GLU
1	A	404	LEU
1	A	442	THR
1	A	479	ARG
1	A	502	SER
1	A	521	THR
1	A	533	VAL
1	A	539	THR
1	A	556	ARG
1	A	562	VAL
1	A	568	ASP
1	B	142	VAL
1	B	152	TYR
1	B	167	THR
1	B	168	THR
1	B	184	HIS
1	B	185	CYS
1	B	188	HIS
1	B	198	HIS
1	B	218	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	THR
1	B	228	LEU
1	B	257	GLU
1	B	260	ASP
1	B	282	GLU
1	B	290	LEU
1	B	316	TYR
1	B	342	THR
1	B	347	GLN
1	B	381	LEU
1	B	412	LEU
1	B	442	THR
1	B	468	VAL
1	B	491	LEU
1	B	526	THR
1	B	539	THR
1	B	543	SER
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	102	ILE
1	E	110	LEU
1	F	82	ASP
1	F	84	ILE
1	F	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	HIS
1	A	227	ASN
1	A	279	GLN
1	A	340	ASN
1	A	350	GLN
1	A	462	ASN
1	B	128	HIS
1	B	271	HIS
1	B	350	GLN
1	B	410	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/537 (83%)	0.14	13 (2%) 53 35	83, 111, 163, 215	0
1	B	445/537 (82%)	0.34	19 (4%) 40 25	83, 144, 200, 255	0
1	E	37/537 (6%)	0.27	0 100 100	100, 132, 177, 191	0
1	F	37/537 (6%)	0.43	2 (5%) 31 21	103, 133, 203, 212	0
All	All	966/2148 (44%)	0.25	34 (3%) 47 31	83, 129, 190, 255	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	4.2
1	B	369	GLN	4.0
1	A	499	ASN	3.9
1	B	370	GLN	3.7
1	B	382	GLY	3.3
1	B	448	ARG	3.1
1	A	369	GLN	3.1
1	B	404	LEU	2.8
1	A	226	ILE	2.8
1	B	207	LEU	2.7
1	A	183	THR	2.7
1	B	465	VAL	2.6
1	A	308	ASP	2.5
1	F	108	THR	2.5
1	B	446	PHE	2.5
1	A	194	GLY	2.5
1	B	136	ILE	2.4
1	B	528	SER	2.4
1	B	163	ILE	2.4
1	B	556	ARG	2.4
1	B	223	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	418	SER	2.4
1	A	370	GLN	2.3
1	B	182	ALA	2.3
1	B	274	LEU	2.3
1	B	297	ASN	2.3
1	F	89	ALA	2.3
1	A	528	SER	2.2
1	B	160	LEU	2.1
1	A	555	PHE	2.0
1	B	220	PHE	2.0
1	A	546	GLU	2.0
1	A	524	ALA	2.0
1	A	529	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.