



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 PM UTC

PDB ID : 4EDB / pdb_00004edb
Title : Structures of monomeric hemagglutinin and its complex with an Fab fragment of a neutralizing antibody that binds to H1 subtype influenza viruses: molecular basis of infectivity of 2009 pandemic H1N1 influenza A viruses
Authors : Kim, K.H.; Cho, K.J.; Lee, J.H.; Park, Y.H.; Khan, T.G.; Lee, J.Y.; Kang, S.H.; Alam, I.
Deposited on : 2012-03-27
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

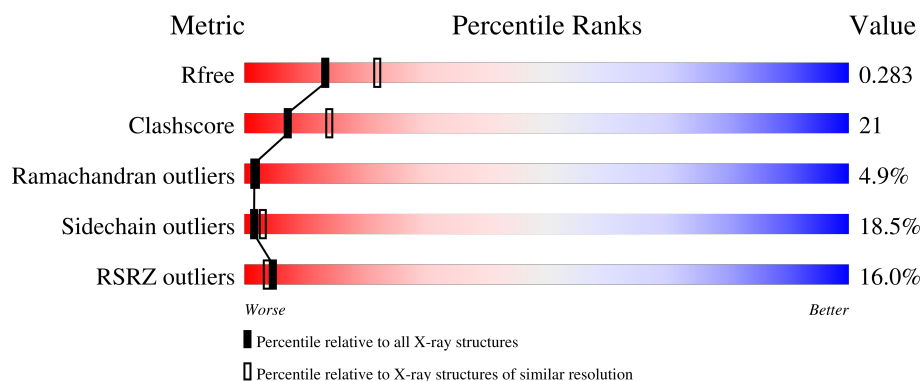
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	330	25% 49% 36% 12% ..
1	C	330	15% 51% 37% 10% .
1	E	330	10% 48% 38% 11% ..
2	B	182	8% 43% 33% 12% 12%
2	D	182	23% 39% 35% 13% . 12%

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Mol	Chain	Length	Quality of chain
2	F	182	7% 54% 26% 8% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11449 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
1	A	323	Total	C	N	O	S	0	0	0
			2530	1598	438	482	12			
1	C	323	Total	C	N	O	S	0	0	0
			2530	1598	438	482	12			
1	E	323	Total	C	N	O	S	0	0	0
			2530	1598	438	482	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP A7LI25
A	-2	ASP	-	expression tag	UNP A7LI25
A	-1	PRO	-	expression tag	UNP A7LI25
A	0	GLY	-	expression tag	UNP A7LI25
C	-3	ALA	-	expression tag	UNP A7LI25
C	-2	ASP	-	expression tag	UNP A7LI25
C	-1	PRO	-	expression tag	UNP A7LI25
C	0	GLY	-	expression tag	UNP A7LI25
E	-3	ALA	-	expression tag	UNP A7LI25
E	-2	ASP	-	expression tag	UNP A7LI25
E	-1	PRO	-	expression tag	UNP A7LI25
E	0	GLY	-	expression tag	UNP A7LI25

- Molecule 2 is a protein called Hemagglutinin.

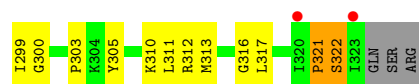
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1281	804	218	252	7			
2	D	160	Total	C	N	O	S	0	0	0
			1281	804	218	252	7			
2	F	160	Total	C	N	O	S	0	0	0
			1281	804	218	252	7			

There are 18 discrepancies between the modelled and reference sequences:

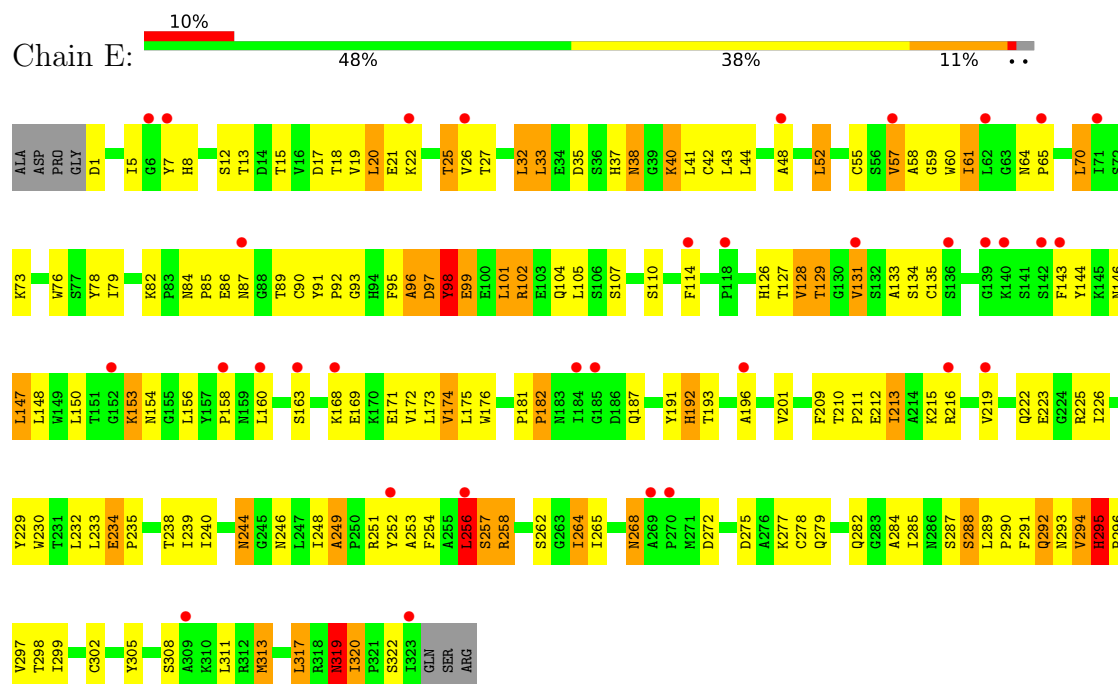
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	expression tag	UNP A7LI25
B	178	SER	-	expression tag	UNP A7LI25
B	179	LEU	-	expression tag	UNP A7LI25
B	180	VAL	-	expression tag	UNP A7LI25
B	181	PRO	-	expression tag	UNP A7LI25
B	182	ARG	-	expression tag	UNP A7LI25
D	177	ARG	-	expression tag	UNP A7LI25
D	178	SER	-	expression tag	UNP A7LI25
D	179	LEU	-	expression tag	UNP A7LI25
D	180	VAL	-	expression tag	UNP A7LI25
D	181	PRO	-	expression tag	UNP A7LI25
D	182	ARG	-	expression tag	UNP A7LI25
F	177	ARG	-	expression tag	UNP A7LI25
F	178	SER	-	expression tag	UNP A7LI25
F	179	LEU	-	expression tag	UNP A7LI25
F	180	VAL	-	expression tag	UNP A7LI25
F	181	PRO	-	expression tag	UNP A7LI25
F	182	ARG	-	expression tag	UNP A7LI25

- Molecule 3 is water.

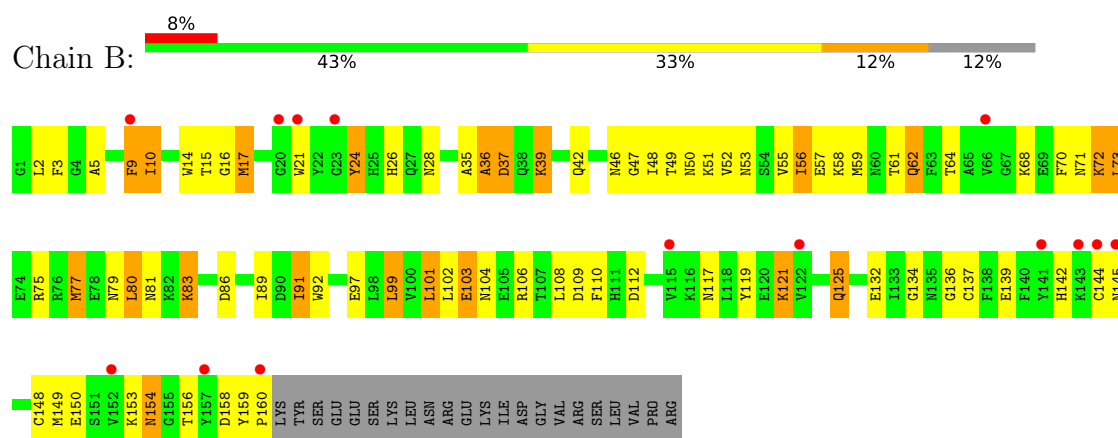
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	D	2	Total O 2 2	0	0
3	E	2	Total O 2 2	0	0
3	F	1	Total O 1 1	0	0



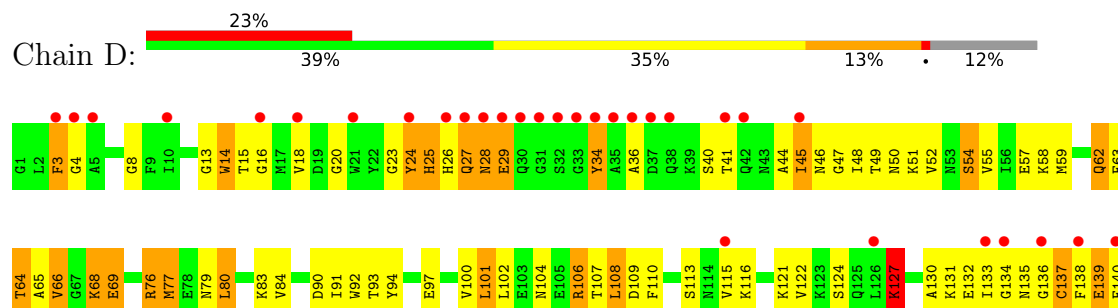
• Molecule 1: Hemagglutinin

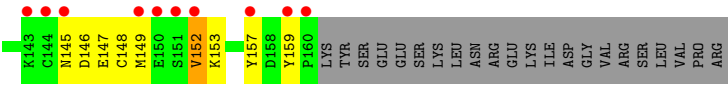


• Molecule 2: Hemagglutinin

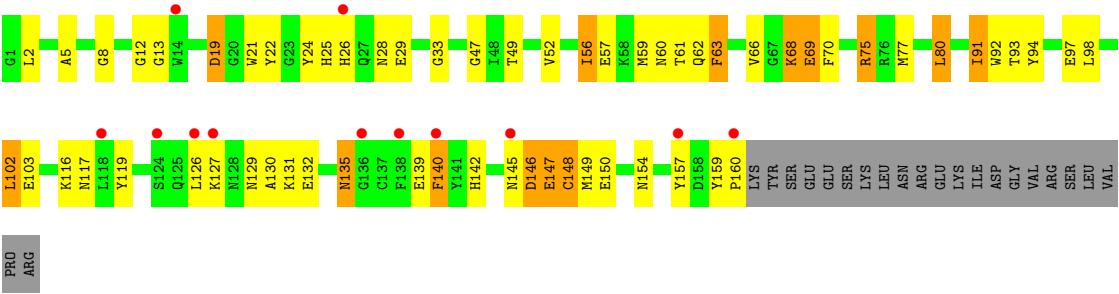


• Molecule 2: Hemagglutinin





● Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	217.12Å 217.12Å 266.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.34 – 2.50 44.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.34-2.50) 99.5 (44.34-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.239 , 0.274 0.252 , 0.283	Depositor DCC
R_{free} test set	4113 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.085 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.085 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.077 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
Reported twinning fraction	0.249 for H, K, L 0.250 for -2/3H-1/3K+2/3L, -1/3H-2/3K-2/3L, 2/3H-2/3K+1/ 0.247 for -1/3H+1/3K-2/3L, -K, -4/3H-2/3K+1/3L 0.254 for -H, 1/3H-1/3K+2/3L, 2/3H+4/3K+1/3L	Depositor
Outliers	1 of 83091 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11449	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.66	0/2596	0.88	2/3532 (0.1%)
1	C	0.65	0/2596	0.86	6/3532 (0.2%)
1	E	0.65	0/2596	0.89	9/3532 (0.3%)
2	B	0.59	0/1307	0.85	0/1759
2	D	0.60	0/1307	0.85	2/1759 (0.1%)
2	F	0.58	0/1307	0.85	0/1759
All	All	0.63	0/11709	0.87	19/15873 (0.1%)

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	E	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	256	LEU	N-CA-C	6.15	117.89	108.12
1	E	249	ALA	CA-C-N	5.81	125.83	119.90
1	E	249	ALA	C-N-CA	5.81	125.83	119.90
1	E	99	GLU	N-CA-C	-5.80	98.45	110.80
1	C	141	SER	N-CA-C	5.69	117.41	110.41
1	E	295	HIS	CA-C-N	5.63	125.31	119.56
1	E	295	HIS	C-N-CA	5.63	125.31	119.56
1	C	289	LEU	CA-C-N	5.53	125.20	119.56
1	C	289	LEU	C-N-CA	5.53	125.20	119.56
1	E	213	ILE	N-CA-C	5.47	115.73	107.80
1	E	13	THR	N-CA-C	-5.41	107.33	114.31
1	A	196	ALA	N-CA-C	5.39	117.89	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASN	N-CA-C	5.34	116.89	107.61
2	D	134	GLY	N-CA-C	5.23	120.21	114.40
1	E	319	ASN	N-CA-C	5.15	117.88	109.59
1	C	8	HIS	N-CA-C	5.13	117.14	110.43
1	C	216	ARG	CA-C-N	5.07	126.18	119.84
1	C	216	ARG	C-N-CA	5.07	126.18	119.84
2	D	136	GLY	N-CA-C	-5.04	107.87	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	98	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2530	0	2455	104	0
1	C	2530	0	2455	115	0
1	E	2530	0	2455	123	0
2	B	1281	0	1209	67	0
2	D	1281	0	1209	75	0
2	F	1281	0	1209	51	0
3	A	8	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
All	All	11449	0	10992	467	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 21.

All (467) 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)
2:B:59:MET:HB2	2:F:94:TYR:CD1	2.03	0.93
1:E:37:HIS:HD2	1:E:294:VAL:HG21	1.36	0.89
1:E:101:LEU:HA	1:E:104:GLN:OE1	1.75	0.85
2:B:59:MET:HB2	2:F:94:TYR:HD1	1.39	0.85
1:C:3:ILE:O	2:D:137:CYS:HA	1.74	0.85
1:E:48:ALA:O	1:E:76:TRP:HA	1.77	0.83
2:D:14:TRP:HB2	2:D:34:TYR:OH	1.77	0.83
2:F:145:ASN:CG	2:F:146:ASP:H	1.87	0.83
1:A:176:TRP:HH2	1:A:231:THR:HG22	1.42	0.83
1:E:42:CYS:HB3	1:E:272:ASP:O	1.78	0.83
1:E:37:HIS:CD2	1:E:294:VAL:HG21	2.14	0.82
1:C:218:LYS:HA	1:C:223:GLU:HG3	1.62	0.81
1:E:256:LEU:HD12	1:E:257:SER:H	1.45	0.81
2:D:24:TYR:O	2:D:25:HIS:HB3	1.81	0.80
1:C:216:ARG:HB2	1:C:217:PRO:HD2	1.64	0.78
1:C:28:HIS:CE1	1:C:316:GLY:HA3	2.18	0.78
1:C:174:VAL:HG13	1:C:231:THR:HG22	1.67	0.77
1:C:179:HIS:HA	1:C:226:ILE:HG22	1.67	0.76
2:B:99:LEU:O	2:B:103:GLU:HB2	1.85	0.76
2:B:2:LEU:HD12	2:D:113:SER:HB3	1.67	0.76
1:A:316:GLY:HA2	2:B:21:TRP:HZ2	1.50	0.76
1:C:292:GLN:HB3	1:C:303:PRO:HB2	1.68	0.76
1:E:59:GLY:HA3	1:E:64:ASN:HB2	1.68	0.75
1:E:298:THR:H	2:F:66:VAL:CG2	2.00	0.75
2:B:24:TYR:CE1	2:B:153:LYS:HD3	2.22	0.74
1:A:82:LYS:HB2	1:A:85:PRO:HD3	1.69	0.74
1:C:184:ILE:HD13	1:C:213:ILE:HG12	1.69	0.74
1:C:84:ASN:N	1:C:85:PRO:HD3	2.02	0.74
1:E:57:VAL:HG21	1:E:102:ARG:HD2	1.71	0.73
1:E:256:LEU:O	1:E:257:SER:HB2	1.90	0.72
2:D:14:TRP:N	2:D:14:TRP:CD1	2.58	0.71
2:B:79:ASN:O	2:B:83:LYS:HB2	1.90	0.71
2:B:36:ALA:O	2:B:37:ASP:HB2	1.89	0.71
1:E:1:ASP:HB3	2:F:140:PHE:HE1	1.55	0.71
2:B:39:LYS:NZ	2:B:39:LYS:HA	2.06	0.70
2:B:91:ILE:HG13	2:D:92:TRP:CZ2	2.28	0.69
1:A:34:GLU:HB2	1:A:292:GLN:HA	1.74	0.69
1:A:20:LEU:HD11	2:D:110:PHE:CE1	2.27	0.68
1:E:96:ALA:C	1:E:98:TYR:H	2.01	0.68
1:E:298:THR:H	2:F:66:VAL:HG21	1.59	0.68
1:C:292:GLN:HG3	1:C:294:VAL:HG12	1.74	0.68
2:D:14:TRP:CD1	2:D:14:TRP:H	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:HB2	1:A:230:TRP:HE1	1.59	0.67
1:C:20:LEU:O	2:F:47:GLY:HA2	1.94	0.67
1:C:97:ASP:HB2	1:C:230:TRP:HE1	1.59	0.67
1:A:96:ALA:HB2	1:A:229:TYR:CD2	2.30	0.66
1:C:43:LEU:HD23	1:C:271:MET:HE1	1.76	0.66
1:E:1:ASP:HB3	2:F:140:PHE:CE1	2.30	0.66
1:C:90:CYS:SG	1:C:91:TYR:N	2.69	0.66
1:E:57:VAL:O	1:E:61:ILE:HG13	1.96	0.66
1:A:33:LEU:HB2	1:A:311:LEU:HB2	1.77	0.65
1:E:35:ASP:HA	1:E:293:ASN:HB3	1.79	0.65
1:C:173:LEU:HB3	1:C:254:PHE:HB2	1.77	0.65
1:A:201:VAL:HB	1:A:240:ILE:HB	1.78	0.65
1:C:3:ILE:HG23	2:D:27:GLN:HB3	1.77	0.65
2:F:28:ASN:HD21	2:F:145:ASN:HA	1.62	0.65
1:A:55:CYS:O	1:A:85:PRO:HB3	1.96	0.65
2:F:77:MET:HA	2:F:80:LEU:HB3	1.78	0.64
1:A:17:ASP:HB2	2:B:101:LEU:HD22	1.78	0.64
2:B:86:ASP:HA	2:B:89:ILE:HB	1.79	0.64
1:A:116:MET:HE2	1:A:253:ALA:HB3	1.78	0.64
1:C:3:ILE:HB	2:D:138:PHE:HB2	1.79	0.64
1:C:19:VAL:HG23	2:D:101:LEU:HB3	1.80	0.64
1:A:31:ASN:O	1:A:33:LEU:N	2.31	0.63
1:A:32:LEU:HA	1:A:289:LEU:HD22	1.81	0.63
1:E:146:ASN:HA	1:E:252:TYR:HD1	1.63	0.63
2:B:24:TYR:HE1	2:B:153:LYS:HD3	1.64	0.63
1:A:81:GLU:HB3	1:A:266:ASN:HB3	1.80	0.63
1:C:231:THR:HG23	1:C:232:LEU:N	2.14	0.63
2:D:14:TRP:H	2:D:14:TRP:HD1	1.46	0.63
1:C:19:VAL:HG12	1:C:20:LEU:HD22	1.81	0.62
2:D:4:GLY:HA3	2:F:117:ASN:HD21	1.64	0.62
1:E:133:ALA:C	1:E:135:CYS:H	2.08	0.62
1:C:282:GLN:HG3	1:C:295:HIS:HB2	1.82	0.62
1:C:91:TYR:HB3	1:C:226:ILE:HD11	1.82	0.61
1:E:290:PRO:HD3	2:F:56:ILE:HG13	1.82	0.61
1:C:33:LEU:HB2	1:C:311:LEU:HD12	1.83	0.61
2:D:25:HIS:CE1	2:D:34:TYR:HB3	2.35	0.61
1:E:277:LYS:HB3	1:E:287:SER:OG	2.01	0.61
2:D:54:SER:O	2:D:58:LYS:HB2	2.01	0.61
2:D:104:ASN:HA	2:D:107:THR:HG22	1.80	0.61
1:A:104:GLN:HG3	2:F:75:ARG:HG2	1.83	0.60
1:A:125:ASN:C	1:A:125:ASN:HD22	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HB	2:D:25:HIS:HE1	1.66	0.60
1:E:27:THR:HG1	1:E:317:LEU:H	1.47	0.60
1:A:19:VAL:O	2:D:51:LYS:HG3	2.00	0.60
1:A:84:ASN:N	1:A:85:PRO:HD2	2.17	0.60
1:C:216:ARG:HE	1:C:225:ARG:HB2	1.67	0.60
1:E:182:PRO:HG3	1:E:223:GLU:HB2	1.81	0.60
1:E:294:VAL:HG13	1:E:295:HIS:N	2.16	0.60
1:C:60:TRP:HD1	1:C:70:LEU:HD13	1.64	0.60
1:A:57:VAL:O	1:A:61:ILE:HG13	2.01	0.60
1:A:96:ALA:HB3	1:A:229:TYR:HA	1.83	0.60
2:F:146:ASP:C	2:F:148:CYS:H	2.10	0.60
1:A:123:TRP:CZ3	1:A:148:LEU:HD12	2.37	0.60
1:A:117:PHE:HD1	1:A:250:PRO:O	1.84	0.60
1:E:107:SER:HB3	1:E:262:SER:HB2	1.84	0.59
1:E:298:THR:O	2:F:66:VAL:HG22	2.02	0.59
1:C:148:LEU:HD11	1:C:249:ALA:H	1.67	0.59
1:E:294:VAL:HG13	1:E:295:HIS:H	1.67	0.59
1:A:290:PRO:HD3	2:B:56:ILE:HG13	1.83	0.59
1:C:292:GLN:O	1:C:305:TYR:HA	2.03	0.58
2:D:76:ARG:NH1	2:F:69:GLU:O	2.36	0.58
1:C:125:ASN:C	1:C:153:LYS:HG2	2.28	0.58
1:E:110:SER:O	1:E:256:LEU:HA	2.03	0.58
1:A:75:SER:HA	1:A:108:VAL:HG12	1.85	0.58
1:C:196:ALA:HB1	1:C:244:ASN:HB2	1.85	0.58
1:C:313:MET:HA	2:D:104:ASN:HD21	1.67	0.58
1:A:193:THR:HG21	1:A:196:ALA:HB2	1.86	0.58
1:C:32:LEU:HD11	2:D:55:VAL:HG11	1.85	0.58
1:E:40:LYS:HG2	1:E:272:ASP:HB2	1.85	0.58
1:E:15:THR:HG22	1:E:25:THR:HA	1.86	0.58
2:D:93:THR:O	2:D:97:GLU:HG3	2.03	0.58
2:D:79:ASN:O	2:D:83:LYS:HB2	2.04	0.58
1:A:79:ILE:HB	1:A:264:ILE:HG23	1.87	0.57
1:C:300:GLY:HA2	2:D:63:PHE:CE2	2.39	0.57
2:D:29:GLU:OE2	2:D:145:ASN:O	2.22	0.57
1:A:181:PRO:HG2	1:A:187:GLN:HB2	1.86	0.57
1:A:43:LEU:HB2	1:A:48:ALA:HA	1.86	0.57
2:B:75:ARG:HB3	1:C:100:GLU:OE1	2.05	0.57
1:C:292:GLN:CG	1:C:294:VAL:HG12	2.34	0.57
1:A:317:LEU:HG	2:B:21:TRP:HE1	1.70	0.56
2:B:47:GLY:HA2	1:E:20:LEU:O	2.04	0.56
2:B:154:ASN:H	2:B:154:ASN:HD22	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:TYR:CE2	1:E:102:ARG:HD3	2.40	0.56
1:A:272:ASP:HB3	1:A:274:CYS:SG	2.45	0.56
1:C:321:PRO:O	1:C:322:SER:HB2	2.04	0.56
2:D:50:ASN:O	2:D:54:SER:HB2	2.04	0.56
2:D:130:ALA:HA	2:D:140:PHE:HA	1.87	0.56
1:A:43:LEU:HA	1:A:49:PRO:HD3	1.88	0.56
1:E:285:ILE:HD11	1:E:294:VAL:HG11	1.87	0.56
1:C:152:GLY:HA3	1:C:190:LEU:O	2.04	0.56
1:A:41:LEU:HA	1:A:279:GLN:NE2	2.20	0.55
2:D:26:HIS:O	2:D:27:GLN:CB	2.54	0.55
1:A:44:LEU:HA	1:A:276:ALA:O	2.07	0.55
1:A:67:CYS:C	1:A:69:LEU:H	2.14	0.55
2:B:49:THR:O	2:B:53:ASN:HB2	2.05	0.55
1:E:91:TYR:CD1	1:E:226:ILE:HG12	2.40	0.55
1:C:84:ASN:N	1:C:85:PRO:CD	2.70	0.54
1:E:211:PRO:HG2	1:E:246:ASN:HD22	1.73	0.54
1:E:37:HIS:HD2	1:E:294:VAL:CG2	2.13	0.54
1:E:147:LEU:HD12	1:E:248:ILE:HG22	1.90	0.54
1:A:37:HIS:HB3	1:A:294:VAL:HG21	1.89	0.54
2:B:26:HIS:HB2	2:B:149:MET:HE3	1.90	0.54
2:D:25:HIS:HD2	2:D:149:MET:HE2	1.73	0.54
2:B:5:ALA:O	2:B:10:ILE:HG22	2.06	0.54
1:C:3:ILE:HA	2:D:27:GLN:HG2	1.89	0.54
1:A:38:ASN:HB3	1:A:284:ALA:H	1.73	0.54
1:A:316:GLY:HA2	2:B:21:TRP:CZ2	2.37	0.54
1:E:78:TYR:CE1	1:E:265:ILE:HD12	2.43	0.54
2:D:26:HIS:HB2	2:D:122:VAL:CG1	2.38	0.54
1:A:218:LYS:HD3	1:A:223:GLU:HG3	1.91	0.53
2:D:14:TRP:N	2:D:14:TRP:HD1	2.03	0.53
1:E:27:THR:HG23	1:E:319:ASN:HB3	1.89	0.53
1:C:300:GLY:HA2	2:D:63:PHE:HE2	1.72	0.53
2:D:131:LYS:HG2	2:D:139:GLU:HB3	1.88	0.53
2:F:145:ASN:CG	2:F:146:ASP:N	2.57	0.53
1:C:125:ASN:HB2	1:C:158:PRO:HG2	1.91	0.53
2:B:9:PHE:CD1	2:B:10:ILE:N	2.77	0.53
1:E:176:TRP:HE1	1:E:209:PHE:HE1	1.55	0.53
1:C:175:LEU:HA	1:C:230:TRP:HA	1.90	0.53
1:C:216:ARG:CB	1:C:217:PRO:HD2	2.32	0.53
1:E:98:TYR:HE2	1:E:102:ARG:HD3	1.72	0.53
1:A:62:LEU:C	1:A:146:ASN:HD21	2.16	0.53
1:E:313:MET:HE2	2:F:103:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:HIS:CD2	1:C:294:VAL:HG23	2.44	0.52
2:B:9:PHE:HD1	2:B:10:ILE:N	2.06	0.52
1:A:128:VAL:O	1:A:148:LEU:HD11	2.10	0.52
1:C:148:LEU:HD21	1:C:249:ALA:HB3	1.90	0.52
1:E:129:THR:HB	1:E:131:VAL:HG12	1.91	0.52
1:E:320:ILE:O	2:F:13:GLY:N	2.42	0.52
2:B:36:ALA:O	2:B:37:ASP:CB	2.58	0.52
1:C:95:PHE:HB3	1:C:98:TYR:HB2	1.90	0.52
1:A:183:ASN:HD22	1:A:185:GLY:H	1.55	0.52
1:E:37:HIS:NE2	1:E:282:GLN:HB3	2.24	0.52
1:E:201:VAL:HG13	1:E:240:ILE:HB	1.92	0.52
1:A:18:THR:HG22	2:B:104:ASN:HB3	1.92	0.52
1:A:50:LEU:HB3	1:A:79:ILE:HA	1.92	0.52
2:D:48:ILE:O	2:D:52:VAL:HG23	2.10	0.52
1:E:59:GLY:CA	1:E:64:ASN:HB2	2.40	0.52
1:C:19:VAL:HG21	2:D:102:LEU:HD23	1.90	0.52
1:E:96:ALA:O	1:E:98:TYR:N	2.43	0.52
2:F:68:LYS:HB3	2:F:70:PHE:CE1	2.44	0.52
1:E:181:PRO:HD2	1:E:213:ILE:HG12	1.92	0.51
2:B:53:ASN:HB3	2:B:57:GLU:OE2	2.11	0.51
1:C:84:ASN:H	1:C:85:PRO:HD3	1.72	0.51
1:E:70:LEU:H	1:E:70:LEU:HD22	1.75	0.51
1:A:40:LYS:HA	1:A:269:ALA:HB1	1.92	0.51
1:A:216:ARG:O	1:A:223:GLU:HG2	2.10	0.51
1:A:35:ASP:OD1	1:A:35:ASP:N	2.39	0.51
1:A:96:ALA:HB2	1:A:229:TYR:HD2	1.74	0.51
1:A:202:SER:HB3	1:A:205:TYR:HB3	1.92	0.51
1:E:82:LYS:HB3	1:E:85:PRO:HD3	1.93	0.51
1:A:179:HIS:CD2	1:A:226:ILE:HD11	2.46	0.51
2:B:28:ASN:ND2	2:B:145:ASN:HA	2.26	0.51
1:E:96:ALA:C	1:E:98:TYR:N	2.69	0.51
1:E:114:PHE:CZ	1:E:253:ALA:HB3	2.46	0.51
2:B:39:LYS:HA	2:B:39:LYS:HZ2	1.75	0.51
1:E:256:LEU:CD1	1:E:257:SER:H	2.22	0.51
1:A:213:ILE:HA	1:A:216:ARG:HH12	1.76	0.51
1:E:297:VAL:HA	2:F:66:VAL:HG21	1.93	0.51
1:C:108:VAL:HG11	1:C:111:PHE:CD2	2.46	0.50
2:B:42:GLN:O	2:B:46:ASN:HB2	2.11	0.50
2:B:92:TRP:CZ2	2:F:91:ILE:HD12	2.46	0.50
2:F:52:VAL:O	2:F:56:ILE:HD12	2.11	0.50
2:B:62:GLN:CD	2:B:62:GLN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ALA:HB2	1:E:229:TYR:HA	1.92	0.50
1:E:191:TYR:O	1:E:192:HIS:HB2	2.10	0.50
1:A:123:TRP:HZ3	1:A:148:LEU:HD12	1.75	0.50
1:C:128:VAL:C	1:C:130:GLY:H	2.19	0.50
1:A:97:ASP:CB	1:A:230:TRP:HE1	2.24	0.50
1:E:8:HIS:HB2	2:F:21:TRP:HA	1.92	0.50
1:A:2:THR:HG22	2:B:139:GLU:HB3	1.93	0.50
1:A:220:ARG:O	1:A:221:ASP:HB3	2.12	0.50
2:D:133:ILE:HB	2:D:137:CYS:HB3	1.93	0.50
2:F:130:ALA:HA	2:F:140:PHE:HA	1.94	0.50
1:A:292:GLN:HG2	1:A:293:ASN:N	2.27	0.49
1:E:279:GLN:O	1:E:298:THR:HA	2.12	0.49
2:F:62:GLN:O	2:F:63:PHE:C	2.55	0.49
1:C:26:VAL:HG12	1:C:27:THR:H	1.76	0.49
2:B:106:ARG:HD3	2:D:106:ARG:HH12	1.77	0.49
1:E:89:THR:HG21	1:E:93:GLY:O	2.11	0.49
1:A:199:SER:HB3	1:A:242:GLU:HB2	1.93	0.49
2:D:25:HIS:CG	2:D:26:HIS:N	2.80	0.49
1:E:291:PHE:HE2	2:F:92:TRP:CE3	2.30	0.49
2:B:39:LYS:HA	2:B:39:LYS:HZ3	1.78	0.49
1:A:102:ARG:O	1:A:106:SER:OG	2.30	0.49
2:D:26:HIS:NE2	2:D:152:VAL:HG13	2.27	0.49
1:C:148:LEU:HG	1:C:249:ALA:O	2.13	0.49
1:A:5:ILE:O	2:B:10:ILE:HD11	2.13	0.49
2:B:159:TYR:HB2	2:B:160:PRO:HD2	1.95	0.49
1:E:172:VAL:HA	1:E:254:PHE:O	2.13	0.49
1:E:17:ASP:HB3	1:E:22:LYS:HD2	1.95	0.48
1:E:292:GLN:OE1	1:E:305:TYR:HD1	1.96	0.48
1:A:50:LEU:HD23	1:A:79:ILE:HG12	1.95	0.48
1:C:243:ALA:HB2	1:C:247:LEU:HD13	1.96	0.48
1:E:234:GLU:HG2	1:E:235:PRO:HD3	1.96	0.48
1:A:67:CYS:C	1:A:69:LEU:N	2.72	0.48
1:C:128:VAL:O	1:C:130:GLY:N	2.46	0.48
1:E:278:CYS:HB3	1:E:285:ILE:HB	1.93	0.48
1:C:28:HIS:CE1	1:C:316:GLY:CA	2.95	0.48
1:C:292:GLN:NE2	1:C:303:PRO:O	2.47	0.48
2:D:132:GLU:HB2	2:F:127:LYS:HE2	1.95	0.48
1:E:148:LEU:HB3	1:E:251:ARG:HD2	1.95	0.48
2:B:109:ASP:HA	2:B:112:ASP:HB2	1.96	0.48
1:C:33:LEU:HD11	1:C:293:ASN:HB3	1.95	0.48
1:C:292:GLN:HG3	1:C:294:VAL:CG1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:LYS:O	1:E:169:GLU:HB2	2.14	0.48
1:C:8:HIS:NE2	1:C:10:ASN:HB3	2.29	0.48
1:C:56:SER:O	1:C:58:ALA:N	2.47	0.48
1:E:256:LEU:O	1:E:257:SER:CB	2.62	0.48
2:B:71:ASN:HD21	2:B:73:LEU:HB2	1.78	0.47
1:E:76:TRP:NE1	1:E:105:LEU:O	2.44	0.47
1:E:295:HIS:HA	1:E:296:PRO:HD3	1.79	0.47
1:C:65:PRO:HA	1:C:145:LYS:HE3	1.96	0.47
1:C:179:HIS:O	1:C:246:ASN:HB3	2.15	0.47
2:D:3:PHE:HE1	2:D:109:ASP:O	1.97	0.47
1:C:80:VAL:HG12	1:C:81:GLU:N	2.29	0.47
1:C:277:LYS:HD2	1:C:277:LYS:N	2.30	0.47
1:C:28:HIS:HE1	1:C:316:GLY:HA3	1.76	0.47
1:C:280:THR:C	1:C:282:GLN:H	2.22	0.47
2:D:26:HIS:O	2:D:27:GLN:HB2	2.13	0.47
2:D:140:PHE:HD1	2:D:140:PHE:H	1.61	0.47
1:A:160:LEU:HD21	1:A:243:ALA:HB3	1.95	0.47
1:C:57:VAL:HG21	1:C:102:ARG:HG2	1.96	0.47
1:C:166:ASN:HD22	1:C:236:GLY:H	1.63	0.47
1:E:163:SER:HB2	1:E:238:THR:CG2	2.44	0.47
1:A:176:TRP:CH2	1:A:231:THR:HG22	2.33	0.47
1:E:182:PRO:HA	1:E:215:LYS:HA	1.95	0.47
1:E:211:PRO:HG2	1:E:246:ASN:ND2	2.29	0.47
1:E:322:SER:HB2	2:F:12:GLY:HA3	1.97	0.47
2:F:131:LYS:N	2:F:139:GLU:O	2.35	0.47
2:D:26:HIS:CE1	2:D:152:VAL:HG13	2.49	0.47
1:E:232:LEU:HD21	1:E:256:LEU:HD21	1.97	0.47
2:B:9:PHE:CD1	2:B:9:PHE:C	2.92	0.47
1:A:58:ALA:HB2	1:A:98:TYR:CE1	2.51	0.46
1:C:33:LEU:HD23	1:C:310:LYS:HA	1.97	0.46
1:A:313:MET:HE3	2:B:52:VAL:HG22	1.97	0.46
2:D:130:ALA:HB1	2:D:138:PHE:HB3	1.96	0.46
2:D:23:GLY:HA2	2:D:40:SER:HB2	1.98	0.46
2:B:125:GLN:H	2:B:125:GLN:HE21	1.63	0.46
1:C:111:PHE:HA	1:C:255:ALA:O	2.16	0.46
1:C:201:VAL:HG13	1:C:206:SER:HB3	1.97	0.46
2:B:3:PHE:HD1	2:B:112:ASP:HB3	1.79	0.46
1:A:98:TYR:O	1:A:99:GLU:HG2	2.15	0.46
2:D:45:ILE:O	2:D:49:THR:OG1	2.22	0.46
2:D:113:SER:O	2:D:116:LYS:HB3	2.16	0.46
1:E:84:ASN:N	1:E:85:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:VAL:HG11	1:E:239:ILE:HG21	1.97	0.46
1:E:196:ALA:HB2	1:E:211:PRO:HD2	1.98	0.46
1:A:118:PRO:HD2	1:A:122:SER:HB2	1.98	0.46
2:B:14:TRP:C	2:B:16:GLY:H	2.22	0.46
1:A:137:HIS:O	1:A:140:LYS:HG2	2.16	0.45
1:C:231:THR:CG2	1:C:232:LEU:N	2.78	0.45
1:E:85:PRO:C	1:E:87:ASN:H	2.24	0.45
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.98	0.45
1:A:104:GLN:CG	2:F:75:ARG:HG2	2.45	0.45
2:D:3:PHE:CE1	2:D:113:SER:HB2	2.52	0.45
1:A:84:ASN:N	1:A:85:PRO:CD	2.79	0.45
1:C:79:ILE:HD11	1:C:105:LEU:O	2.16	0.45
1:E:38:ASN:HD21	1:E:284:ALA:HB3	1.81	0.45
1:E:104:GLN:HE22	1:E:230:TRP:HH2	1.63	0.45
1:E:92:PRO:O	1:E:225:ARG:HA	2.17	0.45
2:B:103:GLU:OE1	2:B:103:GLU:HA	2.16	0.45
2:B:150:GLU:HA	2:B:153:LYS:HE2	1.98	0.45
1:C:83:PRO:HG3	1:C:266:ASN:HB3	1.98	0.45
1:C:226:ILE:HD13	1:C:228:TYR:CZ	2.52	0.45
1:E:289:LEU:HB3	1:E:290:PRO:HD2	1.97	0.45
1:E:298:THR:HG21	1:E:302:CYS:SG	2.57	0.45
1:E:308:SER:HB3	2:F:93:THR:HG23	1.98	0.45
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.51	0.45
2:F:98:LEU:O	2:F:102:LEU:HB2	2.17	0.45
1:C:151:THR:HG23	1:C:190:LEU:HB3	1.98	0.45
1:C:216:ARG:HH11	1:E:201:VAL:HG21	1.81	0.45
1:C:86:GLU:HA	1:C:86:GLU:OE2	2.17	0.44
1:E:79:ILE:HB	1:E:264:ILE:HG23	1.99	0.44
2:D:77:MET:HE3	2:D:77:MET:H	1.82	0.44
2:D:94:TYR:CE1	2:F:59:MET:HB2	2.52	0.44
1:C:216:ARG:HB2	1:C:217:PRO:CD	2.42	0.44
2:D:107:THR:HA	2:D:110:PHE:HB3	1.99	0.44
1:A:50:LEU:HD13	1:A:73:LYS:HD2	1.98	0.44
1:A:120:GLU:O	1:A:121:SER:HB3	2.17	0.44
2:D:91:ILE:HD13	2:F:91:ILE:HG21	2.00	0.44
1:E:33:LEU:HD22	1:E:311:LEU:HB2	2.00	0.44
1:A:20:LEU:HA	2:D:47:GLY:HA2	1.99	0.44
1:A:280:THR:HG22	1:A:298:THR:HG22	1.99	0.44
1:A:174:VAL:HB	1:A:176:TRP:HZ3	1.82	0.44
1:C:34:GLU:HG3	1:C:286:ASN:O	2.17	0.44
1:C:49:PRO:HA	1:C:76:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HB3	1:C:55:CYS:O	2.18	0.44
2:D:90:ASP:OD1	2:F:61:THR:HA	2.18	0.44
1:E:37:HIS:CE1	1:E:282:GLN:HB3	2.53	0.44
1:E:104:GLN:HB3	1:E:258:ARG:HH11	1.83	0.44
2:B:5:ALA:HA	2:B:9:PHE:CD1	2.53	0.44
1:C:111:PHE:CE1	1:C:256:LEU:HB3	2.53	0.44
1:E:52:LEU:HD21	1:E:60:TRP:HB2	1.99	0.44
1:E:234:GLU:HG2	1:E:235:PRO:CD	2.48	0.44
1:E:146:ASN:HA	1:E:252:TYR:CD1	2.49	0.44
1:A:81:GLU:HB3	1:A:266:ASN:CB	2.47	0.43
1:A:197:TYR:HB2	1:A:208:LYS:NZ	2.32	0.43
1:A:230:TRP:HZ3	1:A:232:LEU:HG	1.83	0.43
1:C:60:TRP:HE3	1:C:61:ILE:HG23	1.83	0.43
1:E:93:GLY:HA3	1:E:226:ILE:O	2.18	0.43
1:E:268:ASN:OD1	1:E:268:ASN:N	2.50	0.43
1:C:61:ILE:H	1:C:61:ILE:HG13	1.56	0.43
1:C:218:LYS:HD3	1:C:218:LYS:C	2.44	0.43
2:D:41:THR:O	2:D:44:ALA:HB3	2.18	0.43
1:A:63:GLY:O	1:A:145:LYS:N	2.46	0.43
2:B:35:ALA:CB	2:B:153:LYS:HE3	2.49	0.43
2:B:134:GLY:HA2	2:D:124:SER:OG	2.18	0.43
1:C:34:GLU:HG2	1:C:289:LEU:HD12	2.00	0.43
1:A:79:ILE:HG22	1:A:80:VAL:N	2.33	0.43
1:C:201:VAL:HB	1:C:240:ILE:HG22	1.99	0.43
2:D:26:HIS:NE2	2:D:149:MET:HA	2.34	0.43
2:D:62:GLN:NE2	2:D:64:THR:OG1	2.51	0.43
1:E:7:TYR:HA	2:F:21:TRP:O	2.18	0.43
1:A:180:HIS:CE1	1:A:211:PRO:HA	2.53	0.43
2:B:77:MET:HE2	2:B:80:LEU:HD12	2.01	0.43
1:C:97:ASP:HB2	1:C:230:TRP:NE1	2.32	0.43
1:C:219:VAL:H	1:C:223:GLU:CD	2.27	0.43
2:D:24:TYR:HB3	2:D:121:LYS:HE2	2.01	0.43
2:D:36:ALA:HB1	2:D:41:THR:HG21	2.01	0.43
1:E:95:PHE:O	1:E:96:ALA:O	2.37	0.43
1:A:292:GLN:HB3	1:A:303:PRO:HB2	1.99	0.43
1:C:179:HIS:HB3	1:C:246:ASN:HA	2.00	0.43
1:E:84:ASN:O	1:E:86:GLU:N	2.52	0.43
1:E:298:THR:HB	1:E:302:CYS:SG	2.58	0.43
2:F:56:ILE:HG22	2:F:57:GLU:N	2.33	0.43
1:A:314:VAL:HG11	2:B:108:LEU:CD2	2.48	0.42
2:D:104:ASN:O	2:D:108:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TYR:O	1:A:99:GLU:CG	2.67	0.42
1:E:187:GLN:O	1:E:191:TYR:N	2.49	0.42
2:F:146:ASP:O	2:F:148:CYS:N	2.51	0.42
1:E:5:ILE:HD11	2:F:119:TYR:HA	2.01	0.42
1:E:153:LYS:HE3	1:E:158:PRO:HD2	2.00	0.42
2:F:126:LEU:HB2	2:F:129:ASN:HB2	2.00	0.42
1:C:32:LEU:HA	1:C:289:LEU:HD22	2.02	0.42
2:D:14:TRP:CB	2:D:34:TYR:OH	2.58	0.42
1:E:175:LEU:HD23	1:E:230:TRP:HB3	2.02	0.42
2:F:19:ASP:OD1	2:F:19:ASP:N	2.43	0.42
1:E:27:THR:HG23	1:E:319:ASN:CB	2.49	0.42
1:E:163:SER:HB2	1:E:238:THR:HG22	2.01	0.42
2:B:70:PHE:CE1	2:B:81:ASN:HB2	2.54	0.42
2:B:79:ASN:HD21	1:C:261:GLY:HA3	1.85	0.42
2:B:106:ARG:O	2:B:110:PHE:N	2.52	0.42
1:E:175:LEU:HA	1:E:229:TYR:O	2.19	0.42
1:A:272:ASP:C	1:A:274:CYS:H	2.27	0.42
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.85	0.42
1:E:216:ARG:HB3	1:E:225:ARG:NH1	2.34	0.42
1:A:97:ASP:HB2	1:A:230:TRP:NE1	2.29	0.42
1:A:97:ASP:CG	1:A:230:TRP:HE1	2.28	0.42
1:C:297:VAL:HA	2:D:66:VAL:HG22	2.02	0.42
2:D:80:LEU:O	2:D:84:VAL:HG23	2.19	0.42
1:E:32:LEU:O	1:E:290:PRO:HD2	2.20	0.42
2:F:147:GLU:HA	2:F:150:GLU:HB2	2.01	0.42
2:B:83:LYS:HE3	2:D:66:VAL:HG12	2.01	0.42
2:B:97:GLU:O	2:B:101:LEU:HG	2.20	0.42
1:C:265:ILE:HG13	1:C:299:ILE:HD12	2.02	0.42
1:E:84:ASN:N	1:E:85:PRO:HD2	2.35	0.42
2:F:28:ASN:CG	2:F:29:GLU:N	2.78	0.42
1:C:171:GLU:HG2	1:C:234:GLU:HA	2.02	0.42
1:E:26:VAL:HG12	1:E:27:THR:N	2.34	0.42
1:A:32:LEU:HG	1:A:313:MET:HB2	2.02	0.41
2:B:142:HIS:O	2:B:142:HIS:CG	2.72	0.41
1:C:8:HIS:HB3	1:C:317:LEU:HD11	2.02	0.41
1:C:40:LYS:NZ	1:C:272:ASP:OD2	2.45	0.41
2:D:68:LYS:O	2:D:69:GLU:HB2	2.19	0.41
1:E:143:PHE:CG	1:E:144:TYR:N	2.88	0.41
2:F:140:PHE:HB2	2:F:142:HIS:H	1.84	0.41
2:B:51:LYS:HE2	2:B:103:GLU:HG3	2.02	0.41
1:C:321:PRO:O	1:C:322:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:ASP:OD1	2:F:60:ASN:O	2.38	0.41
1:A:175:LEU:O	1:A:250:PRO:HA	2.20	0.41
1:A:196:ALA:HB1	1:A:244:ASN:HB3	2.02	0.41
2:D:26:HIS:CD2	2:D:152:VAL:HG13	2.54	0.41
2:D:145:ASN:C	2:D:147:GLU:H	2.27	0.41
1:A:130:GLY:O	1:A:143:PHE:HB2	2.20	0.41
2:B:28:ASN:HD21	2:B:145:ASN:HA	1.85	0.41
1:C:168:LYS:O	1:C:170:LYS:N	2.53	0.41
1:C:285:ILE:HG13	1:C:294:VAL:HG11	2.01	0.41
1:E:317:LEU:HD21	2:F:21:TRP:HB3	2.01	0.41
1:A:96:ALA:CB	1:A:229:TYR:HA	2.47	0.41
1:C:60:TRP:CE3	1:C:61:ILE:HG23	2.55	0.41
1:C:80:VAL:CG1	1:C:81:GLU:N	2.83	0.41
1:E:244:ASN:O	1:E:244:ASN:ND2	2.54	0.41
1:A:321:PRO:HB2	1:A:322:SER:H	1.54	0.41
2:B:92:TRP:CZ2	2:F:91:ILE:CD1	3.04	0.41
1:C:8:HIS:ND1	2:D:16:GLY:O	2.54	0.41
1:C:58:ALA:HA	1:C:61:ILE:HD11	2.02	0.41
1:C:184:ILE:H	1:C:184:ILE:HG12	1.66	0.41
1:C:299:ILE:HG12	2:D:65:ALA:CB	2.50	0.41
2:D:25:HIS:CD2	2:D:149:MET:HE2	2.53	0.41
1:E:18:THR:OG1	1:E:21:GLU:O	2.37	0.41
1:E:61:ILE:HG22	1:E:175:LEU:HD11	2.02	0.41
2:F:131:LYS:HG2	2:F:132:GLU:H	1.86	0.41
2:B:132:GLU:HB3	2:D:127:LYS:HE3	2.03	0.41
1:C:7:TYR:HB2	1:C:317:LEU:HD22	2.02	0.41
1:C:7:TYR:HD1	1:C:317:LEU:HD13	1.86	0.41
2:F:159:TYR:HA	2:F:160:PRO:HD3	1.93	0.41
1:A:45:LYS:HE2	1:A:277:LYS:HG2	2.02	0.41
1:A:119:LYS:HG3	1:A:128:VAL:HB	2.02	0.41
1:A:134:SER:HB2	1:A:222:GLN:HG2	2.02	0.41
1:A:218:LYS:CD	1:A:223:GLU:HG3	2.51	0.41
1:C:256:LEU:HD12	1:C:258:ARG:HD2	2.02	0.41
1:A:55:CYS:HB3	1:A:56:SER:H	1.64	0.41
1:A:127:THR:N	1:A:153:LYS:HG2	2.36	0.41
2:B:102:LEU:HD23	2:B:103:GLU:OE1	2.21	0.41
1:E:222:GLN:HA	1:E:222:GLN:HE21	1.85	0.41
2:F:26:HIS:CE1	2:F:33:GLY:H	2.39	0.41
1:A:4:CYS:HA	2:B:137:CYS:HA	2.02	0.41
2:B:72:LYS:H	2:B:72:LYS:HG2	1.61	0.41
1:C:157:TYR:CZ	1:C:245:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:THR:HG23	1:C:232:LEU:H	1.86	0.41
1:C:14:ASP:OD2	1:C:14:ASP:N	2.54	0.40
1:E:148:LEU:HG	1:E:249:ALA:O	2.20	0.40
1:A:157:TYR:N	1:A:157:TYR:CD2	2.89	0.40
1:A:179:HIS:HE1	1:A:181:PRO:HB3	1.86	0.40
1:C:106:SER:HB2	1:C:262:SER:HB3	2.02	0.40
1:E:58:ALA:HA	1:E:95:PHE:HE2	1.86	0.40
1:C:52:LEU:HD23	1:C:80:VAL:O	2.22	0.40
1:E:64:ASN:OD1	1:E:65:PRO:HD2	2.21	0.40
1:E:98:TYR:O	1:E:98:TYR:CG	2.73	0.40
1:A:80:VAL:HA	1:A:265:ILE:O	2.21	0.40
2:B:117:ASN:O	2:B:121:LYS:HB2	2.22	0.40
1:E:64:ASN:HA	1:E:65:PRO:HD2	1.92	0.40
1:E:128:VAL:O	1:E:129:THR:C	2.64	0.40
1:E:298:THR:CG2	1:E:302:CYS:SG	3.10	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	321/330 (97%)	262 (82%)	44 (14%)	15 (5%)	2	2
1	C	321/330 (97%)	256 (80%)	45 (14%)	20 (6%)	1	1
1	E	321/330 (97%)	251 (78%)	55 (17%)	15 (5%)	2	2
2	B	158/182 (87%)	124 (78%)	31 (20%)	3 (2%)	6	11
2	D	158/182 (87%)	120 (76%)	27 (17%)	11 (7%)	1	1
2	F	158/182 (87%)	128 (81%)	23 (15%)	7 (4%)	2	2
All	All	1437/1536 (94%)	1141 (79%)	225 (16%)	71 (5%)	1	2

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	258	ARG
2	B	36	ALA
2	B	37	ASP
1	C	169	GLU
1	C	205	TYR
1	C	220	ARG
2	D	24	TYR
2	D	27	GLN
1	E	96	ALA
1	E	97	ASP
1	E	129	THR
1	A	55	CYS
1	A	220	ARG
1	A	321	PRO
2	B	17	MET
1	C	57	VAL
1	C	128	VAL
1	C	129	THR
1	C	221	ASP
2	D	8	GLY
2	D	20	GLY
1	E	90	CYS
1	E	98	TYR
1	E	134	SER
1	E	192	HIS
1	E	193	THR
1	E	219	VAL
1	E	257	SER
1	E	288	SER
2	F	8	GLY
2	F	56	ILE
2	F	135	ASN
1	A	85	PRO
1	A	88	GLY
1	A	115	GLU
1	A	121	SER
1	A	214	ALA
1	A	262	SER
1	C	90	CYS
1	C	99	GLU
1	C	115	GLU
1	C	138	ASN

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Mol	Chain	Res	Type
1	C	222	GLN
1	C	322	SER
2	D	28	ASN
2	D	29	GLU
1	E	154	ASN
2	F	5	ALA
1	A	45	LYS
1	A	182	PRO
1	C	125	ASN
1	C	182	PRO
2	D	13	GLY
2	D	127	LYS
1	E	294	VAL
2	F	63	PHE
2	F	69	GLU
1	A	71	ILE
1	C	84	ASN
1	C	154	ASN
1	C	321	PRO
2	D	18	VAL
2	D	69	GLU
1	E	182	PRO
2	F	147	GLU
1	C	259	GLY
2	D	146	ASP
1	A	259	GLY
1	C	219	VAL
1	E	128	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	283/288 (98%)	226 (80%)	57 (20%)	1	2
1	C	283/288 (98%)	240 (85%)	43 (15%)	3	5
1	E	283/288 (98%)	233 (82%)	50 (18%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	136/157 (87%)	106 (78%)	30 (22%)	1	2
2	D	136/157 (87%)	104 (76%)	32 (24%)	1	1
2	F	136/157 (87%)	116 (85%)	20 (15%)	3	6
All	All	1257/1335 (94%)	1025 (82%)	232 (18%)	1	3

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	10	ASN
1	A	13	THR
1	A	17	ASP
1	A	20	LEU
1	A	32	LEU
1	A	35	ASP
1	A	43	LEU
1	A	47	ILE
1	A	50	LEU
1	A	52	LEU
1	A	55	CYS
1	A	61	ILE
1	A	69	LEU
1	A	71	ILE
1	A	80	VAL
1	A	82	LYS
1	A	87	ASN
1	A	94	HIS
1	A	97	ASP
1	A	101	LEU
1	A	106	SER
1	A	119	LYS
1	A	123	TRP
1	A	125	ASN
1	A	131	VAL
1	A	135	CYS
1	A	143	PHE
1	A	146	ASN
1	A	147	LEU
1	A	148	LEU
1	A	151	THR
1	A	153	LYS

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Mol	Chain	Res	Type
1	A	157	TYR
1	A	160	LEU
1	A	162	LYS
1	A	168	LYS
1	A	170	LYS
1	A	173	LEU
1	A	175	LEU
1	A	183	ASN
1	A	213	ILE
1	A	223	GLU
1	A	226	ILE
1	A	248	ILE
1	A	251	ARG
1	A	252	TYR
1	A	258	ARG
1	A	265	ILE
1	A	273	GLU
1	A	274	CYS
1	A	285	ILE
1	A	292	GLN
1	A	293	ASN
1	A	304	LYS
1	A	315	THR
1	A	317	LEU
2	B	9	PHE
2	B	10	ILE
2	B	15	THR
2	B	17	MET
2	B	24	TYR
2	B	39	LYS
2	B	48	ILE
2	B	50	ASN
2	B	55	VAL
2	B	56	ILE
2	B	61	THR
2	B	62	GLN
2	B	64	THR
2	B	68	LYS
2	B	72	LYS
2	B	73	LEU
2	B	77	MET
2	B	80	LEU

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Mol	Chain	Res	Type
2	B	83	LYS
2	B	91	ILE
2	B	99	LEU
2	B	101	LEU
2	B	103	GLU
2	B	121	LYS
2	B	125	GLN
2	B	144	CYS
2	B	148	CYS
2	B	154	ASN
2	B	156	THR
2	B	158	ASP
1	C	4	CYS
1	C	5	ILE
1	C	10	ASN
1	C	14	ASP
1	C	19	VAL
1	C	26	VAL
1	C	28	HIS
1	C	32	LEU
1	C	61	ILE
1	C	62	LEU
1	C	66	GLU
1	C	68	GLU
1	C	69	LEU
1	C	82	LYS
1	C	89	THR
1	C	90	CYS
1	C	112	GLU
1	C	140	LYS
1	C	147	LEU
1	C	150	LEU
1	C	160	LEU
1	C	170	LYS
1	C	174	VAL
1	C	184	ILE
1	C	187	GLN
1	C	193	THR
1	C	194	GLU
1	C	197	TYR
1	C	210	THR
1	C	212	GLU

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Mol	Chain	Res	Type
1	C	220	ARG
1	C	226	ILE
1	C	231	THR
1	C	240	ILE
1	C	271	MET
1	C	272	ASP
1	C	274	CYS
1	C	277	LYS
1	C	282	GLN
1	C	285	ILE
1	C	292	GLN
1	C	294	VAL
1	C	312	ARG
2	D	3	PHE
2	D	14	TRP
2	D	15	THR
2	D	25	HIS
2	D	28	ASN
2	D	34	TYR
2	D	45	ILE
2	D	46	ASN
2	D	54	SER
2	D	57	GLU
2	D	59	MET
2	D	62	GLN
2	D	64	THR
2	D	66	VAL
2	D	68	LYS
2	D	76	ARG
2	D	77	MET
2	D	80	LEU
2	D	100	VAL
2	D	101	LEU
2	D	106	ARG
2	D	108	LEU
2	D	115	VAL
2	D	127	LYS
2	D	135	ASN
2	D	137	CYS
2	D	139	GLU
2	D	148	CYS
2	D	152	VAL

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Mol	Chain	Res	Type
2	D	153	LYS
2	D	157	TYR
2	D	159	TYR
1	E	12	SER
1	E	19	VAL
1	E	20	LEU
1	E	25	THR
1	E	32	LEU
1	E	33	LEU
1	E	38	ASN
1	E	40	LYS
1	E	41	LEU
1	E	43	LEU
1	E	44	LEU
1	E	52	LEU
1	E	55	CYS
1	E	57	VAL
1	E	61	ILE
1	E	70	LEU
1	E	73	LYS
1	E	97	ASP
1	E	99	GLU
1	E	101	LEU
1	E	102	ARG
1	E	126	HIS
1	E	127	THR
1	E	131	VAL
1	E	147	LEU
1	E	150	LEU
1	E	153	LYS
1	E	156	LEU
1	E	160	LEU
1	E	171	GLU
1	E	173	LEU
1	E	174	VAL
1	E	210	THR
1	E	212	GLU
1	E	233	LEU
1	E	234	GLU
1	E	244	ASN
1	E	256	LEU
1	E	258	ARG

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Mol	Chain	Res	Type
1	E	264	ILE
1	E	268	ASN
1	E	275	ASP
1	E	288	SER
1	E	292	GLN
1	E	295	HIS
1	E	299	ILE
1	E	313	MET
1	E	317	LEU
1	E	319	ASN
1	E	320	ILE
2	F	2	LEU
2	F	19	ASP
2	F	22	TYR
2	F	24	TYR
2	F	25	HIS
2	F	49	THR
2	F	68	LYS
2	F	75	ARG
2	F	80	LEU
2	F	91	ILE
2	F	97	GLU
2	F	102	LEU
2	F	116	LYS
2	F	135	ASN
2	F	140	PHE
2	F	146	ASP
2	F	148	CYS
2	F	149	MET
2	F	154	ASN
2	F	157	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	125	ASN
1	A	146	ASN
1	A	179	HIS
1	A	183	ASN
1	A	187	GLN
1	A	246	ASN

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Mol	Chain	Res	Type
1	A	266	ASN
2	B	81	ASN
2	B	111	HIS
2	B	125	GLN
2	B	154	ASN
1	C	10	ASN
1	C	37	HIS
1	C	94	HIS
1	C	187	GLN
1	C	266	ASN
1	C	282	GLN
1	C	292	GLN
2	D	25	HIS
2	D	28	ASN
2	D	53	ASN
2	D	62	GLN
2	D	79	ASN
1	E	28	HIS
1	E	84	ASN
1	E	125	ASN
1	E	146	ASN
1	E	179	HIS
1	E	195	ASN
1	E	227	ASN
1	E	246	ASN
1	E	286	ASN
1	E	295	HIS
2	F	27	GLN
2	F	28	ASN
2	F	117	ASN
2	F	129	ASN
2	F	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	323/330 (97%)	1.40	83 (25%)	1 1	37, 51, 65, 80	0
1	C	323/330 (97%)	1.04	48 (14%)	5 4	27, 48, 58, 67	0
1	E	323/330 (97%)	0.95	34 (10%)	11 10	28, 45, 59, 64	0
2	B	160/182 (87%)	0.93	14 (8%)	15 14	29, 48, 63, 70	0
2	D	160/182 (87%)	1.22	41 (25%)	1 1	20, 56, 79, 87	0
2	F	160/182 (87%)	0.78	12 (7%)	20 18	27, 45, 58, 71	0
All	All	1449/1536 (94%)	1.08	232 (16%)	5 4	20, 49, 64, 87	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	PRO	6.2
2	D	30	GLN	5.8
1	C	197	TYR	5.2
1	A	69	LEU	4.9
1	A	198	VAL	4.5
2	D	32	SER	4.4
1	C	241	PHE	4.3
2	D	27	GLN	4.2
2	D	26	HIS	4.0
2	D	145	ASN	4.0
2	D	16	GLY	3.9
2	D	10	ILE	3.9
2	D	31	GLY	3.9
1	A	175	LEU	3.9
1	A	261	GLY	3.7
1	A	320	ILE	3.7
1	E	256	LEU	3.7
1	A	238	THR	3.7
2	D	36	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	28	ASN	3.6
1	C	240	ILE	3.6
1	C	2	THR	3.5
2	B	122	VAL	3.5
1	A	152	GLY	3.5
1	C	270	PRO	3.5
2	B	152	VAL	3.5
1	E	152	GLY	3.5
1	A	278	CYS	3.5
1	C	261	GLY	3.5
1	C	5	ILE	3.5
1	E	269	ALA	3.4
1	A	323	ILE	3.4
1	C	173	LEU	3.4
1	A	9	ALA	3.4
1	E	270	PRO	3.4
1	C	152	GLY	3.4
2	D	33	GLY	3.3
2	B	143	LYS	3.3
1	C	252	TYR	3.3
1	A	150	LEU	3.3
2	D	4	GLY	3.3
1	A	239	ILE	3.3
1	C	243	ALA	3.2
1	C	142	SER	3.2
2	D	149	MET	3.2
2	D	18	VAL	3.1
1	A	3	ILE	3.1
1	E	184	ILE	3.1
1	A	235	PRO	3.1
2	D	138	PHE	3.1
1	A	259	GLY	3.1
1	E	219	VAL	3.1
1	C	187	GLN	3.1
1	A	144	TYR	3.0
1	A	321	PRO	3.0
1	C	155	GLY	3.0
2	D	152	VAL	3.0
1	C	248	ILE	3.0
2	D	136	GLY	3.0
1	A	247	LEU	3.0
1	E	136	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	6	GLY	3.0
1	A	255	ALA	2.9
1	E	142	SER	2.9
2	D	160	PRO	2.9
1	C	260	PHE	2.9
2	D	151	SER	2.9
1	A	260	PHE	2.9
1	C	256	LEU	2.9
1	E	62	LEU	2.9
2	D	21	TRP	2.9
1	A	170	LYS	2.8
1	A	177	GLY	2.8
1	A	107	SER	2.8
2	F	14	TRP	2.8
1	A	274	CYS	2.8
2	D	133	ILE	2.8
1	A	256	LEU	2.8
1	A	168	LYS	2.8
2	D	150	GLU	2.8
1	A	5	ILE	2.7
1	A	71	ILE	2.7
1	A	85	PRO	2.7
1	E	158	PRO	2.7
1	A	224	GLY	2.7
1	E	22	LYS	2.7
1	E	140	LYS	2.7
1	E	143	PHE	2.7
2	B	23	GLY	2.7
2	D	34	TYR	2.7
2	B	144	CYS	2.7
2	B	145	ASN	2.7
1	A	114	PHE	2.6
1	A	264	ILE	2.6
1	E	160	LEU	2.6
1	A	253	ALA	2.6
1	A	95	PHE	2.6
1	A	143	PHE	2.6
1	A	257	SER	2.6
1	C	91	TYR	2.6
1	E	323	ILE	2.6
1	A	88	GLY	2.6
1	A	226	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	66	VAL	2.6
1	C	133	ALA	2.6
1	A	258	ARG	2.5
1	A	1	ASP	2.5
1	A	236	GLY	2.5
2	B	160	PRO	2.5
1	C	215	LYS	2.5
1	E	163	SER	2.5
2	F	126	LEU	2.5
1	C	214	ALA	2.5
2	B	157	TYR	2.5
2	F	157	TYR	2.5
1	C	63	GLY	2.5
1	E	185	GLY	2.5
2	D	37	ASP	2.5
1	A	70	LEU	2.5
1	A	294	VAL	2.5
1	E	139	GLY	2.4
1	A	197	TYR	2.4
2	B	141	TYR	2.4
1	A	26	VAL	2.4
1	A	172	VAL	2.4
2	D	41	THR	2.4
2	F	136	GLY	2.4
1	E	216	ARG	2.4
1	C	123	TRP	2.4
2	F	127	LYS	2.4
2	D	134	GLY	2.4
1	A	62	LEU	2.4
1	C	147	LEU	2.4
1	A	299	ILE	2.4
2	B	9	PHE	2.4
1	A	266	ASN	2.4
1	C	141	SER	2.3
1	A	232	LEU	2.3
1	C	69	LEU	2.3
2	D	29	GLU	2.3
2	D	35	ALA	2.3
1	C	250	PRO	2.3
1	A	285	ILE	2.3
1	C	323	ILE	2.3
2	D	38	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	26	HIS	2.3
2	D	140	PHE	2.3
2	D	144	CYS	2.3
1	A	228	TYR	2.3
1	E	57	VAL	2.3
1	E	131	VAL	2.3
2	B	20	GLY	2.3
2	F	124	SER	2.3
2	B	21	TRP	2.3
2	D	126	LEU	2.3
1	C	153	LYS	2.3
2	B	115	VAL	2.3
1	E	118	PRO	2.3
1	C	255	ALA	2.2
1	A	52	LEU	2.2
1	A	233	LEU	2.2
1	C	136	SER	2.2
1	E	71	ILE	2.2
1	A	174	VAL	2.2
1	C	128	VAL	2.2
1	E	26	VAL	2.2
2	D	115	VAL	2.2
2	F	145	ASN	2.2
1	E	7	TYR	2.2
1	A	46	GLY	2.2
1	A	109	SER	2.2
1	C	265	ILE	2.2
2	D	3	PHE	2.2
1	C	148	LEU	2.2
1	C	79	ILE	2.2
1	A	141	SER	2.2
1	A	322	SER	2.2
1	E	65	PRO	2.2
1	A	133	ALA	2.2
1	E	196	ALA	2.2
1	C	156	LEU	2.2
2	D	45	ILE	2.2
1	C	209	PHE	2.2
1	A	57	VAL	2.1
1	A	173	LEU	2.1
2	D	143	LYS	2.1
1	C	249	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	87	ASN	2.1
1	C	247	LEU	2.1
1	E	6	GLY	2.1
1	A	164	TYR	2.1
2	D	24	TYR	2.1
1	A	75	SER	2.1
1	E	168	LYS	2.1
1	A	131	VAL	2.1
2	D	42	GLN	2.1
1	E	48	ALA	2.1
1	A	64	ASN	2.1
1	C	263	GLY	2.1
1	C	264	ILE	2.1
1	C	320	ILE	2.1
1	A	229	TYR	2.1
2	D	159	TYR	2.1
1	A	24	VAL	2.1
1	A	297	VAL	2.1
1	A	43	LEU	2.1
1	A	53	GLY	2.1
1	A	78	TYR	2.1
2	D	157	TYR	2.1
1	A	262	SER	2.1
1	C	174	VAL	2.0
1	A	113	ARG	2.0
1	A	50	LEU	2.0
2	F	118	LEU	2.0
1	A	263	GLY	2.0
1	A	2	THR	2.0
1	C	231	THR	2.0
1	C	144	TYR	2.0
1	A	220	ARG	2.0
1	C	251	ARG	2.0
1	E	114	PHE	2.0
2	F	138	PHE	2.0
2	F	140	PHE	2.0
1	E	309	ALA	2.0
2	D	5	ALA	2.0
1	A	82	LYS	2.0
1	A	89	THR	2.0
1	C	238	THR	2.0
1	A	65	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	2.0
1	A	142	SER	2.0
1	E	252	TYR	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.