Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:16 pm BST

PDB ID	:	4EDB
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 (i) symbol.

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

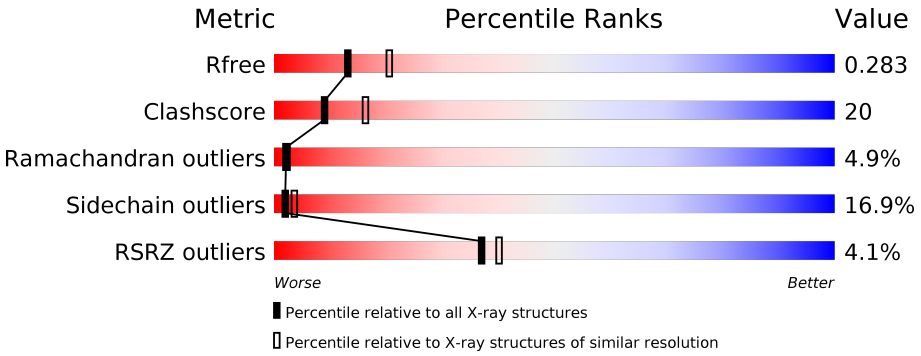
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	5% 50% 38% 9%
1	C	330	4% 50% 40% 8%
1	E	330	3% 48% 39% 11%
2	B	182	3% 46% 34% 8% 12%
2	D	182	7% 42% 34% 12% 12%
2	F	182	% 54% 27% 7% 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.

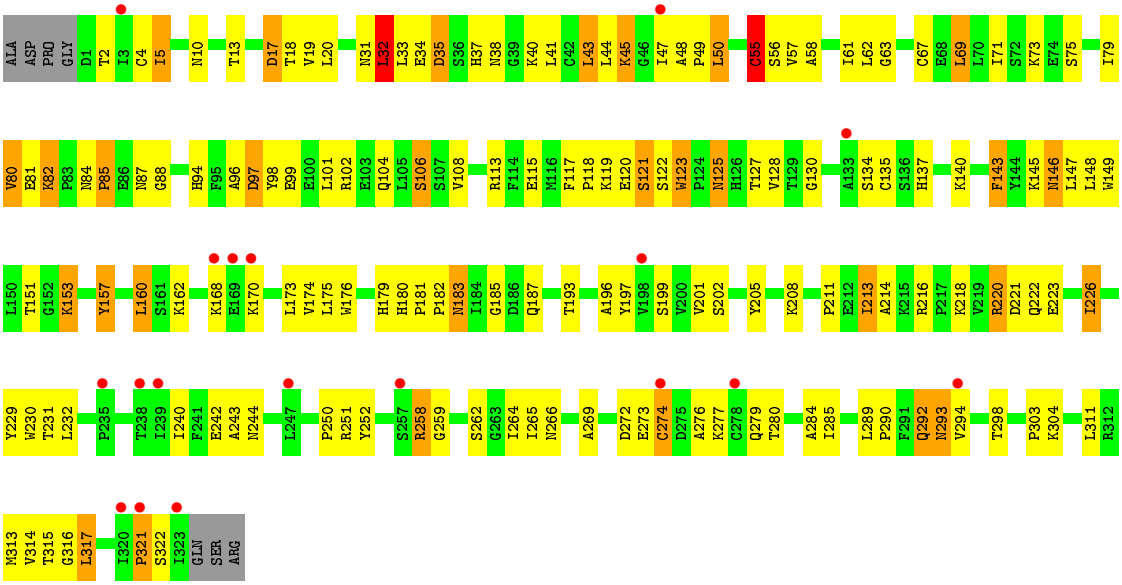
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	D	2	Total O 2 2	0	0
3	E	2	Total O 2 2	0	0
3	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

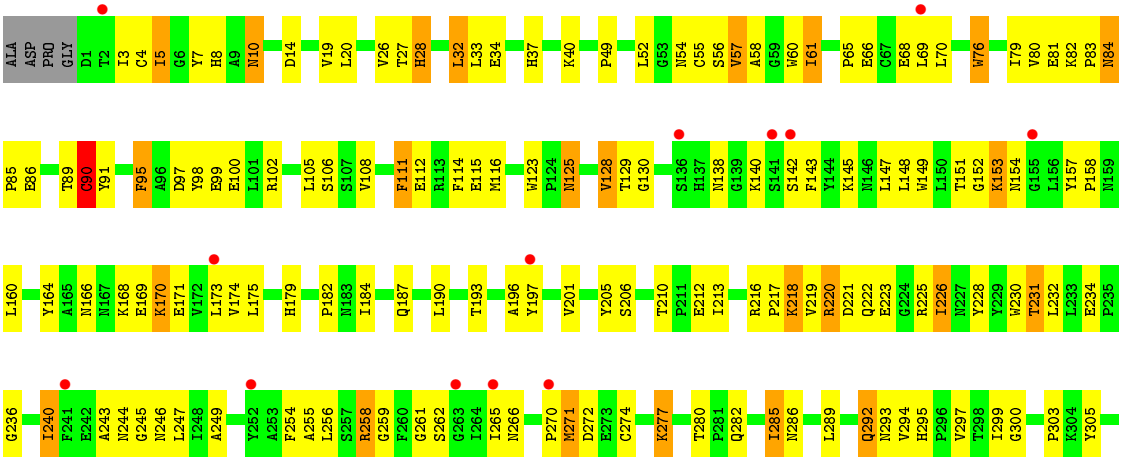
- Molecule 1: Hemagglutinin

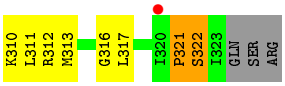
Chain A:



- Molecule 1: Hemagglutinin

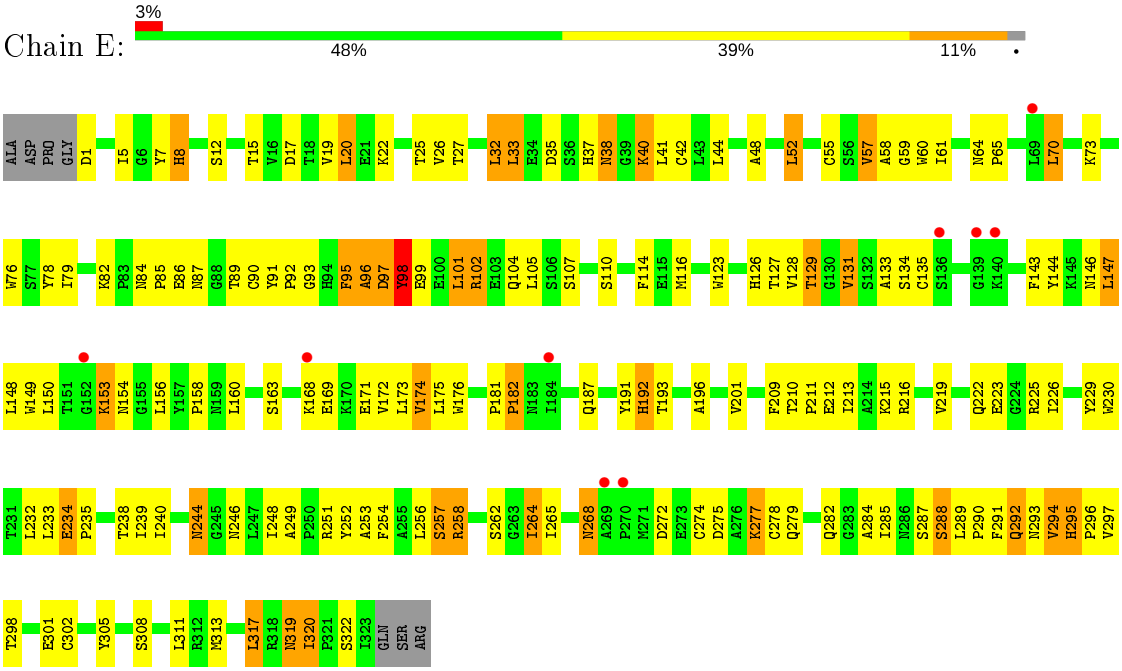
Chain C:





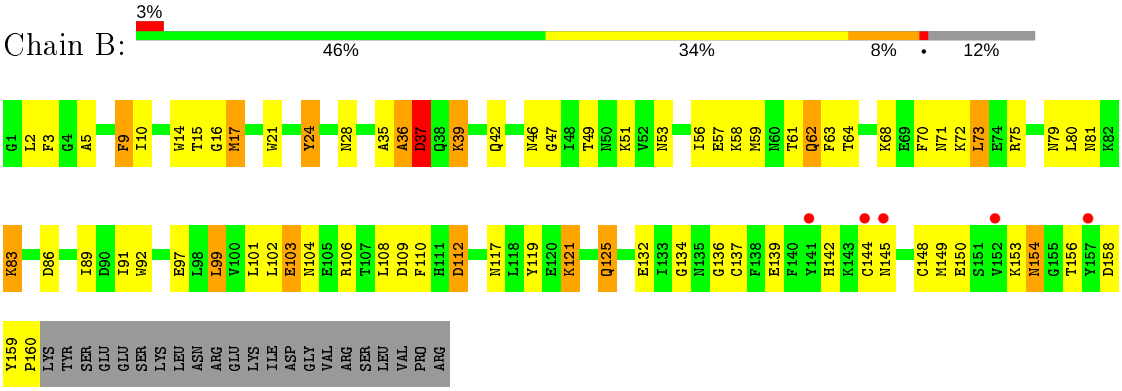
- Molecule 1: Hemagglutinin

Chain E:



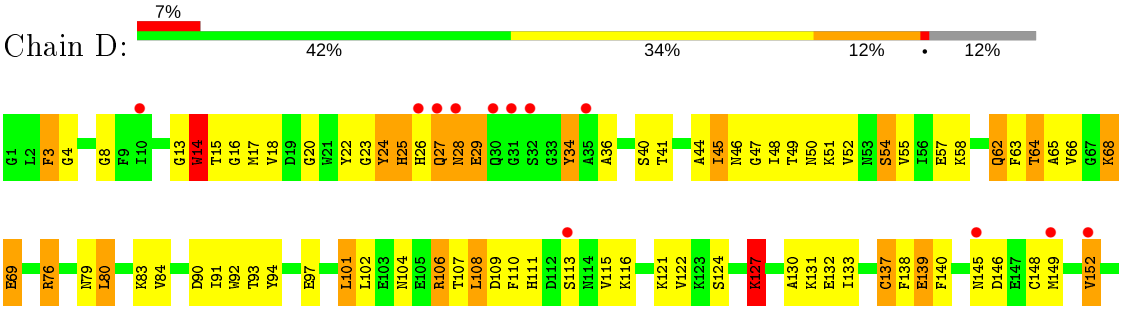
- Molecule 2: Hemagglutinin

Chain B:



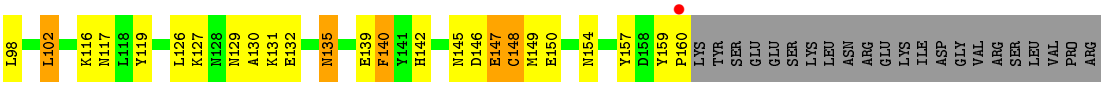
- Molecule 2: Hemagglutinin

Chain D:



- Molecule 2: Hemagglutinin

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.35 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.49	0/2596	0.60	0/3532
1	C	0.49	2/2596 (0.1%)	0.58	0/3532
1	E	0.49	2/2596 (0.1%)	0.62	0/3532
2	B	0.47	0/1307	0.56	0/1759
2	D	0.49	1/1307 (0.1%)	0.56	0/1759
2	F	0.47	0/1307	0.54	0/1759
All	All	0.49	5/11709 (0.0%)	0.59	0/15873

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	14	TRP	CD2-CE2	5.21	1.47	1.41
1	C	149	TRP	CD2-CE2	5.17	1.47	1.41
1	C	76	TRP	CD2-CE2	5.11	1.47	1.41
1	E	123	TRP	CD2-CE2	5.10	1.47	1.41
1	E	149	TRP	CD2-CE2	5.04	1.47	1.41

There are no bond angle outliers.

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 (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	2530	0	2455	100	0
1	C	2530	0	2455	115	0
1	E	2530	0	2455	119	0
2	B	1281	0	1209	63	0
2	D	1281	0	1209	72	0
2	F	1281	0	1209	49	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	452	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 20.

All (452) 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
1:C:3:ILE:O	2:D:137:CYS:HA	1.74	0.85
2:B:59:MET:HB2	2:F:94:TYR:HD1	1.39	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
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
2:F:145:ASN:CG	2:F:146:ASP:H	1.87	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:HA	2:B:89:ILE:HB	1.79	0.64
1:C:19:VAL:HG23	2:D:101:LEU:HB3	1.80	0.64
1:C:3:ILE:HB	2:D:138:PHE:HB2	1.79	0.64
1:E:96:ALA:C	1:E:98:TYR:H	2.01	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:HD1	2:D:14:TRP:H	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: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:104:ASN:HA	2:D:107:THR:HG22	1.80	0.61
2:D:54:SER:O	2:D:58:LYS:HB2	2.01	0.61
2:B:39:LYS:HZ3	2:B:39:LYS:HA	1.66	0.60
1:C:5:ILE:HB	2:D:25:HIS:HE1	1.66	0.60
1:A:104:GLN:HG3	2:F:75:ARG:HG2	1.83	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:A:19:VAL:O	2:D:51:LYS:HG3	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ASN:CG	2:F:146:ASP:N	2.57	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:E:133:ALA:C	1:E:135:CYS:H	2.08	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:154:ASN:H	2:B:154:ASN:HD22	1.52	0.56
2:B:47:GLY:HA2	1:E:20:LEU:O	2.04	0.56
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:A:125:ASN:HD22	1:A:125:ASN:C	2.09	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
2:F:146:ASP:C	2:F:148:CYS:H	2.10	0.55
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:HIS:HB3	1:A:294:VAL:HG21	1.89	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:C:125:ASN:C	1:C:153:LYS:HG2	2.28	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
2:D:131:LYS:HG2	2:D:139:GLU:HB3	1.88	0.53
1:C:300:GLY:HA2	2:D:63:PHE:HE2	1.72	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:216:ARG:CB	1:C:217:PRO:HD2	2.32	0.53
1:C:175:LEU:HA	1:C:230:TRP:HA	1.90	0.53
1:E:98:TYR:HE2	1:E:102:ARG:HD3	1.72	0.53
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:201:VAL:HG13	1:E:240:ILE:HB	1.92	0.52
1:E:37:HIS:NE2	1:E:282:GLN:HB3	2.24	0.52
1:A:50:LEU:HB3	1:A:79:ILE:HA	1.92	0.52
1:A:18:THR:HG22	2:B:104:ASN:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:14:TRP:HB2	2:D:34:TYR:HH	1.73	0.51
1:A:202:SER:HB3	1:A:205:TYR:HB3	1.92	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: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:114:PHE:CZ	1:E:253:ALA:HB3	2.46	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:A:67:CYS:C	1:A:69:LEU:H	2.14	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:F:52:VAL:O	2:F:56:ILE:HD12	2.11	0.50
2:B:92:TRP:CZ2	2:F:91:ILE:HD12	2.46	0.50
1:E:191:TYR:O	1:E:192:HIS:HB2	2.10	0.50
1:E:96:ALA:HB2	1:E:229:TYR:HA	1.92	0.50
1:A:123:TRP:HZ3	1:A:148:LEU:HD12	1.75	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:220:ARG:O	1:A:221:ASP:HB3	2.12	0.50
1:A:2:THR:HG22	2:B:139:GLU:HB3	1.93	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:62:LEU:C	1:A:146:ASN:HD21	2.16	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
2:D:45:ILE:O	2:D:49:THR:OG1	2.22	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
1:E:168:LYS:O	1:E:169:GLU:HB2	2.14	0.48
1:C:56:SER:O	1:C:58:ALA:N	2.47	0.48
1:C:8:HIS:NE2	1:C:10:ASN:HB3	2.29	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:114:PHE:HE1	1:C:164:TYR:HH	1.62	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:277:LYS:N	1:C:277:LYS:HD2	2.30	0.47
1:C:80:VAL:HG12	1:C:81:GLU:N	2.29	0.47
1:C:28:HIS:HE1	1:C:316:GLY:HA3	1.76	0.47
2:D:140:PHE:H	2:D:140:PHE:HD1	1.61	0.47
2:D:26:HIS:O	2:D:27:GLN:HB2	2.13	0.47
1:A:160:LEU:HD21	1:A:243:ALA:HB3	1.95	0.47
1:C:166:ASN:HD22	1:C:236:GLY:H	1.63	0.47
1:C:57:VAL:HG21	1:C:102:ARG:HG2	1.96	0.47
1:E:163:SER:HB2	1:E:238:THR:CG2	2.44	0.47
1:E:211:PRO:HG2	1:E:246:ASN:ND2	2.29	0.47
1:E:182:PRO:HA	1:E:215:LYS:HA	1.95	0.47
2:F:131:LYS:N	2:F:139:GLU:O	2.35	0.47
1:A:176:TRP:CH2	1:A:231:THR:HG22	2.33	0.47
1:E:322:SER:HB2	2:F:12:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:E:96:ALA:C	1:E:98:TYR:N	2.69	0.46
2:B:125:GLN:HE21	2:B:125:GLN:H	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:113:SER:O	2:D:116:LYS:HB3	2.16	0.46
1:E:196:ALA:HB2	1:E:211:PRO:HD2	1.98	0.46
1:E:174:VAL:HG11	1:E:239:ILE:HG21	1.97	0.46
1:E:84:ASN:N	1:E:85:PRO:CD	2.78	0.46
1:A:118:PRO:HD2	1:A:122:SER:HB2	1.98	0.46
2:B:62:GLN:H	2:B:62:GLN:CD	2.20	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:A:130:GLY:HA3	1:A:149:TRP:HB3	1.98	0.45
1:C:128:VAL:C	1:C:130:GLY:H	2.19	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:104:GLN:HE22	1:E:230:TRP:HH2	1.63	0.45
1:E:38:ASN:HD21	1:E:284:ALA:HB3	1.81	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:F:62:GLN:O	2:F:63:PHE:C	2.55	0.45
2:B:150:GLU:HA	2:B:153:LYS:HE2	1.98	0.45
1:C:226:ILE:HD13	1:C:228:TYR:CZ	2.52	0.45
1:C:83:PRO:HG3	1:C:266:ASN:HB3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLU:OE2	1:C:86:GLU:HA	2.17	0.44
1:E:79:ILE:HB	1:E:264:ILE:HG23	1.99	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:120:GLU:O	1:A:121:SER:HB3	2.17	0.44
1:A:50:LEU:HD13	1:A:73:LYS:HD2	1.98	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:52:LEU:HB3	1:C:55:CYS:O	2.18	0.44
1:C:49:PRO:HA	1:C:76:TRP:HB2	2.00	0.44
1:E:104:GLN:HB3	1:E:258:ARG:HH11	1.83	0.44
1:E:37:HIS:CE1	1:E:282:GLN:HB3	2.53	0.44
2:D:90:ASP:OD1	2:F:61:THR:HA	2.18	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:C:40:LYS:HZ3	1:C:270:PRO:HB2	1.82	0.44
1:E:146:ASN:HA	1:E:252:TYR:CD1	2.49	0.44
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:A:81:GLU:HB3	1:A:266:ASN:CB	2.47	0.43
1:C:60:TRP:HE3	1:C:61:ILE:HG23	1.83	0.43
1:E:268:ASN:N	1:E:268:ASN:OD1	2.50	0.43
1:E:93:GLY:HA3	1:E:226:ILE:O	2.18	0.43
1:C:61:ILE:HG13	1:C:61:ILE:H	1.56	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:134:GLY:HA2	2:D:124:SER:OG	2.18	0.43
2:B:35:ALA:CB	2:B:153:LYS:HE3	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:HIS:CE1	1:A:211:PRO:HA	2.53	0.43
1:C:97:ASP:HB2	1:C:230:TRP:NE1	2.32	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:C:49:PRO:HD2	1:C:271:MET:HE3	2.01	0.43
1:E:298:THR:HB	1:E:302:CYS:SG	2.58	0.43
1:E:84:ASN:O	1:E:86:GLU:N	2.52	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
1:C:280:THR:C	1:C:282:GLN:H	2.22	0.42
2:D:104:ASN:O	2:D:108:LEU:HB2	2.19	0.42
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:A:67:CYS:C	1:A:69:LEU:N	2.72	0.42
2:D:22:TYR:HH	2:D:111:HIS:CE1	2.37	0.42
1:E:153:LYS:HE3	1:E:158:PRO:HD2	2.00	0.42
1:E:5:ILE:HD11	2:F:119:TYR:HA	2.01	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:N	2:F:19:ASP:OD1	2.43	0.42
1:E:143:PHE:CG	1:E:144:TYR:N	2.88	0.42
1:E:163:SER:HB2	1:E:238:THR:HG22	2.01	0.42
1:E:27:THR:HG23	1:E:319:ASN:CB	2.49	0.42
2:B:106:ARG:O	2:B:110:PHE:N	2.52	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
1:E:175:LEU:HA	1:E:229:TYR:O	2.19	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
2:B:9:PHE:CD1	2:B:9:PHE:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLU:O	2:B:101:LEU:HG	2.20	0.42
2:B:83:LYS:HE3	2:D:66:VAL:HG12	2.01	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
1:E:98:TYR:O	1:E:98:TYR:CG	2.73	0.42
2:B:14:TRP:C	2:B:16:GLY:H	2.22	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:CG	2:B:142:HIS:O	2.72	0.41
1:C:8:HIS:HB3	1:C:317:LEU:HD11	2.02	0.41
2:D:68:LYS:O	2:D:69:GLU:HB2	2.19	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
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
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: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
1:C:58:ALA:HA	1:C:61:ILE:HD11	2.02	0.41
1:C:8:HIS:ND1	2:D:16:GLY:O	2.54	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
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:B:132:GLU:HB3	2:D:127:LYS:HE3	2.03	0.41
2:F:159:TYR:HA	2:F:160:PRO:HD3	1.93	0.41
1:A:119:LYS:HG3	1:A:128:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:45:LYS:HE2	1:A:277:LYS:HG2	2.02	0.41
1:C:256:LEU:HD12	1:C:258:ARG:HD2	2.02	0.41
1:A:127:THR:N	1:A:153:LYS:HG2	2.36	0.41
1:C:142:SER:OG	1:C:143:PHE:N	2.54	0.41
1:E:85:PRO:C	1:E:87:ASN:H	2.24	0.41
2:F:26:HIS:CE1	2:F:33:GLY:H	2.39	0.41
1:A:55:CYS:HB3	1:A:56:SER:H	1.64	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
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:231:THR:HG23	1:C:232:LEU:H	1.86	0.41
1:C:157:TYR:CZ	1:C:245:GLY:HA2	2.56	0.41
1:C:14:ASP:N	1:C:14:ASP:OD2	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: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:298:THR:CG2	1:E:302:CYS:SG	3.10	0.40
1:E:64:ASN:HA	1:E:65:PRO:HD2	1.92	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	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%)	8 13
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 3
All	All	1437/1536 (94%)	1141 (79%)	225 (16%)	71 (5%)	2 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

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Mol	Chain	Res	Type
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
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 (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	283/288 (98%)	236 (83%)	47 (17%)	2	4
1	C	283/288 (98%)	242 (86%)	41 (14%)	3	6
1	E	283/288 (98%)	231 (82%)	52 (18%)	1	2
2	B	136/157 (87%)	111 (82%)	25 (18%)	1	2
2	D	136/157 (87%)	109 (80%)	27 (20%)	1	2
2	F	136/157 (87%)	116 (85%)	20 (15%)	3	5
All	All	1257/1335 (94%)	1045 (83%)	212 (17%)	2	3

All (212) 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	32	LEU
1	A	35	ASP
1	A	43	LEU
1	A	47	ILE
1	A	50	LEU
1	A	55	CYS
1	A	69	LEU
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	113	ARG
1	A	123	TRP
1	A	125	ASN
1	A	135	CYS

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Mol	Chain	Res	Type
1	A	143	PHE
1	A	146	ASN
1	A	147	LEU
1	A	151	THR
1	A	153	LYS
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	183	ASN
1	A	213	ILE
1	A	226	ILE
1	A	251	ARG
1	A	252	TYR
1	A	258	ARG
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	15	THR
2	B	17	MET
2	B	24	TYR
2	B	37	ASP
2	B	39	LYS
2	B	61	THR
2	B	62	GLN
2	B	63	PHE
2	B	64	THR
2	B	68	LYS
2	B	73	LEU
2	B	80	LEU
2	B	83	LYS
2	B	99	LEU
2	B	103	GLU
2	B	112	ASP

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Mol	Chain	Res	Type
2	B	121	LYS
2	B	125	GLN
2	B	144	CYS
2	B	148	CYS
2	B	149	MET
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	28	HIS
1	C	32	LEU
1	C	54	ASN
1	C	61	ILE
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	95	PHE
1	C	111	PHE
1	C	112	GLU
1	C	116	MET
1	C	123	TRP
1	C	140	LYS
1	C	147	LEU
1	C	153	LYS
1	C	160	LEU
1	C	170	LYS
1	C	187	GLN
1	C	193	THR
1	C	197	TYR
1	C	210	THR
1	C	212	GLU
1	C	218	LYS
1	C	220	ARG
1	C	226	ILE
1	C	231	THR
1	C	240	ILE
1	C	258	ARG

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Mol	Chain	Res	Type
1	C	271	MET
1	C	272	ASP
1	C	274	CYS
1	C	277	LYS
1	C	285	ILE
1	C	292	GLN
1	C	312	ARG
2	D	3	PHE
2	D	14	TRP
2	D	15	THR
2	D	17	MET
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	62	GLN
2	D	64	THR
2	D	68	LYS
2	D	76	ARG
2	D	80	LEU
2	D	101	LEU
2	D	106	ARG
2	D	108	LEU
2	D	115	VAL
2	D	127	LYS
2	D	137	CYS
2	D	139	GLU
2	D	148	CYS
2	D	152	VAL
2	D	157	TYR
2	D	159	TYR
1	E	8	HIS
1	E	12	SER
1	E	19	VAL
1	E	20	LEU
1	E	32	LEU
1	E	33	LEU
1	E	38	ASN
1	E	40	LYS

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Mol	Chain	Res	Type
1	E	41	LEU
1	E	44	LEU
1	E	52	LEU
1	E	55	CYS
1	E	57	VAL
1	E	70	LEU
1	E	73	LYS
1	E	95	PHE
1	E	97	ASP
1	E	98	TYR
1	E	99	GLU
1	E	101	LEU
1	E	102	ARG
1	E	116	MET
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	258	ARG
1	E	264	ILE
1	E	268	ASN
1	E	274	CYS
1	E	275	ASP
1	E	277	LYS
1	E	288	SER
1	E	292	GLN
1	E	295	HIS
1	E	301	GLU
1	E	313	MET
1	E	317	LEU

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Mol	Chain	Res	Type
1	E	319	ASN
1	E	320	ILE
2	F	9	PHE
2	F	19	ASP
2	F	22	TYR
2	F	24	TYR
2	F	25	HIS
2	F	43	ASN
2	F	49	THR
2	F	68	LYS
2	F	72	LYS
2	F	75	ARG
2	F	80	LEU
2	F	97	GLU
2	F	102	LEU
2	F	116	LYS
2	F	135	ASN
2	F	140	PHE
2	F	148	CYS
2	F	149	MET
2	F	154	ASN
2	F	157	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	146	ASN
1	A	183	ASN
1	A	187	GLN
1	A	246	ASN
1	A	282	GLN
2	B	26	HIS
2	B	28	ASN
2	B	111	HIS
2	B	125	GLN
1	C	10	ASN
1	C	37	HIS
1	C	187	GLN
1	C	227	ASN
1	C	292	GLN
2	D	25	HIS

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Mol	Chain	Res	Type
2	D	28	ASN
2	D	53	ASN
2	D	62	GLN
2	D	79	ASN
1	E	28	HIS
1	E	125	ASN
1	E	227	ASN
1	E	246	ASN
1	E	286	ASN
1	E	293	ASN
1	E	295	HIS
2	F	28	ASN
2	F	117	ASN
2	F	135	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/330 (97%)	0.38	18 (5%) 24 25	37, 51, 65, 80	0
1	C	323/330 (97%)	0.22	14 (4%) 35 38	27, 48, 58, 67	0
1	E	323/330 (97%)	0.10	9 (2%) 53 56	28, 45, 59, 64	0
2	B	160/182 (87%)	0.31	5 (3%) 49 52	29, 48, 63, 70	0
2	D	160/182 (87%)	0.56	12 (7%) 14 14	20, 56, 79, 87	0
2	F	160/182 (87%)	0.25	1 (0%) 89 90	27, 45, 58, 71	0
All	All	1449/1536 (94%)	0.28	59 (4%) 37 40	20, 49, 64, 87	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	32	SER	8.3
2	D	30	GLN	6.5
2	F	160	PRO	6.4
2	D	28	ASN	5.8
2	D	26	HIS	5.5
2	D	31	GLY	5.1
2	D	27	GLN	3.8
1	E	184	ILE	3.6
1	C	2	THR	3.4
1	C	155	GLY	3.3
1	E	140	LYS	3.1
1	C	173	LEU	3.0
1	A	274	CYS	3.0
1	C	69	LEU	3.0
1	C	241	PHE	2.9
1	A	238	THR	2.8
2	B	145	ASN	2.8
1	A	168	LYS	2.8
1	A	239	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	294	VAL	2.8
1	A	320	ILE	2.8
2	B	144	CYS	2.7
1	C	141	SER	2.7
1	C	270	PRO	2.7
1	A	170	LYS	2.6
1	E	69	LEU	2.5
1	C	252	TYR	2.5
1	A	169	GLU	2.5
1	A	198	VAL	2.4
1	E	136	SER	2.4
2	B	157	TYR	2.4
2	D	10	ILE	2.4
2	B	141	TYR	2.4
1	C	136	SER	2.3
1	A	235	PRO	2.3
1	C	142	SER	2.3
1	C	197	TYR	2.3
1	E	269	ALA	2.2
2	D	152	VAL	2.2
1	A	323	ILE	2.2
1	A	257	SER	2.2
2	D	149	MET	2.2
1	E	139	GLY	2.2
1	E	168	LYS	2.2
1	A	133	ALA	2.2
1	C	320	ILE	2.1
2	D	145	ASN	2.1
1	C	263	GLY	2.1
1	A	247	LEU	2.1
2	D	113	SER	2.1
2	B	152	VAL	2.1
1	E	270	PRO	2.1
2	D	35	ALA	2.1
1	A	47	ILE	2.1
1	A	278	CYS	2.1
1	A	3	ILE	2.0
1	C	265	ILE	2.0
1	E	152	GLY	2.0
1	A	321	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.