Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:18 AM GMT

PDB ID	:	3HW6
Title	:	Crystal structure of avian influenza virus PA_N in complex with Mn
Authors	:	Zhao, C.; Lou, Z.; Guo, Y.; Ma, M.; Chen, Y.; Rao, Z.
Deposited on	:	2009-06-17
Resolution	:	2.50 Å(reported)

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

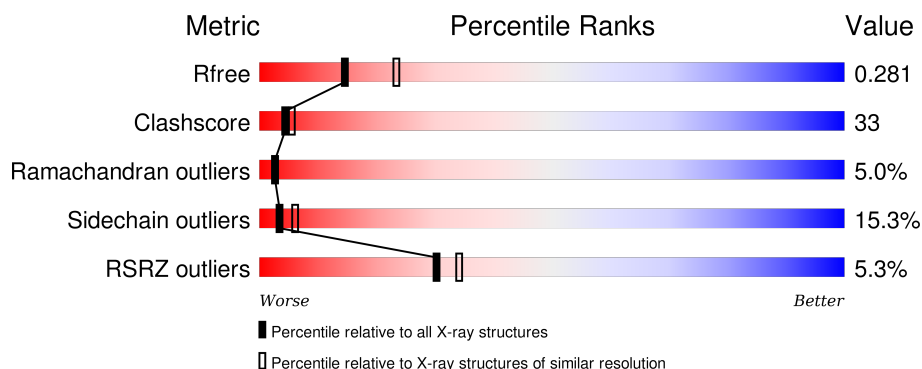|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	Percentile Ranks	Value
Rfree		0.281
Clashscore		33
Ramachandran outliers		5.0%
Sidechain outliers		15.3%
RSRZ outliers		5.3%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	261	36% 26% 5% 33%
1	B	261	3% 29% 27% 9% • 33%
1	C	261	7% 28% 29% 10% • 33%
1	D	261	4% 28% 32% 7% 33%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5922 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			
1	B	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			
1	C	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			
1	D	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
A	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
A	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
B	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
B	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
B	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
C	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
C	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
C	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
C	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
D	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
D	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
D	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	25	Total O 25 25	0	0
3	C	42	Total O 42 42	0	0
3	D	25	Total O 25 25	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
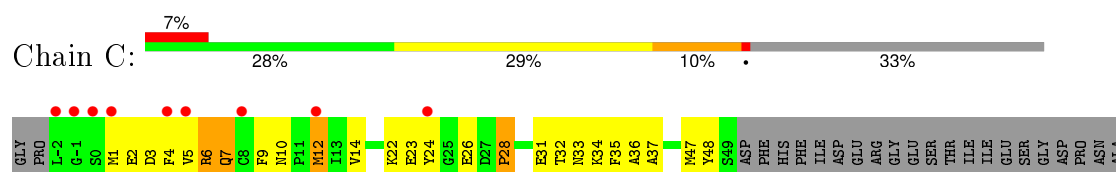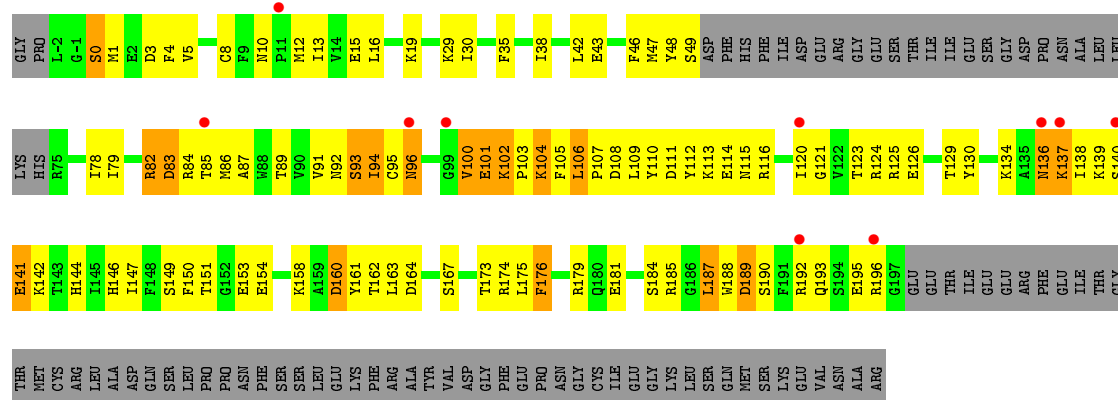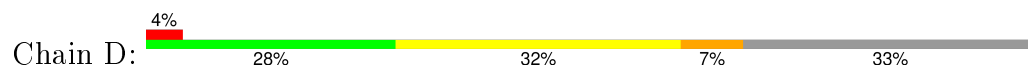
- Molecule 1: Polymerase acidic protein
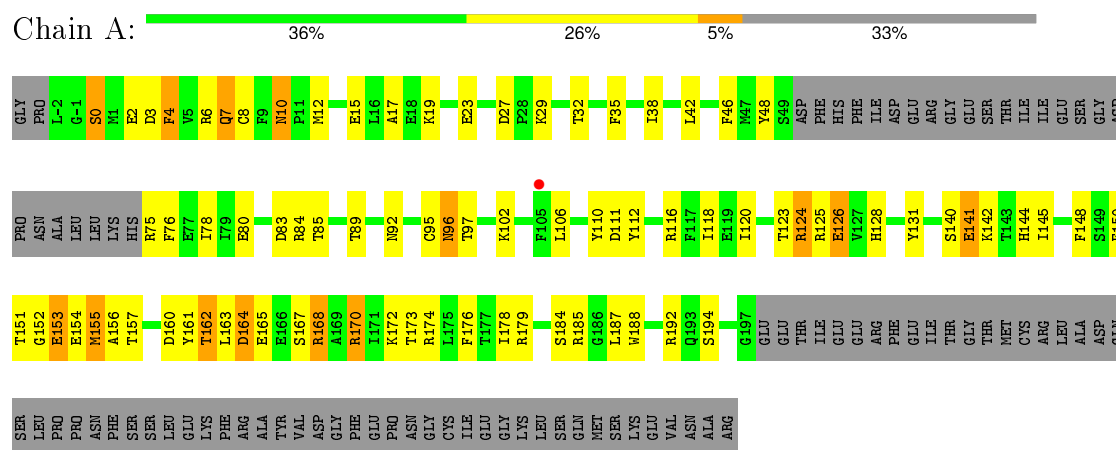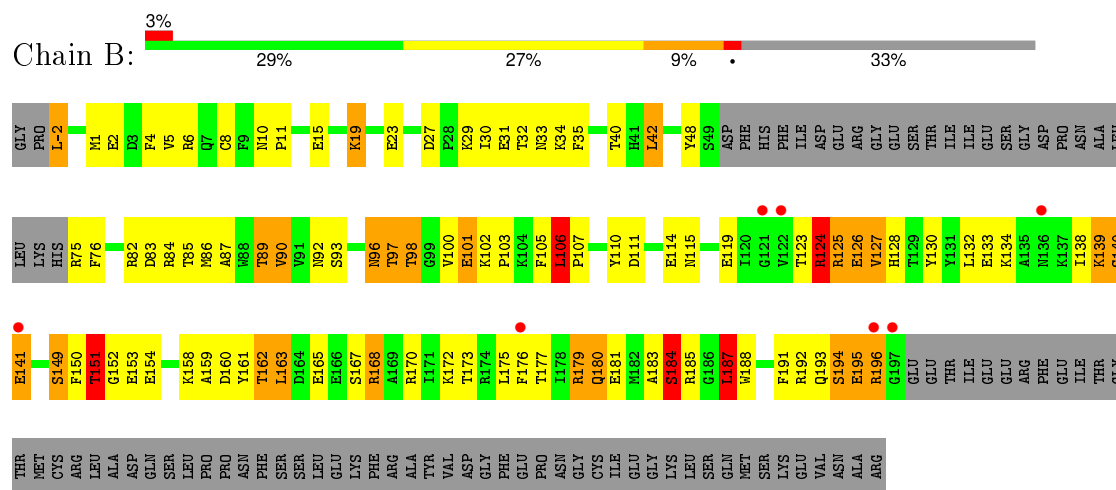
- Molecule 1: Polymerase acidic protein

- Molecule 1: Polymerase acidic protein

• Molecule 1: Polymerase acidic protein

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.50Å 60.21Å 67.22Å 96.06° 96.49° 109.66°	Depositor
Resolution (Å)	30.00 – 2.50 29.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.8 (30.00-2.50) 72.5 (29.44-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.240 , 0.289 0.236 , 0.281	Depositor DCC
R_{free} test set	971 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 18991 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5922	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.89	0/1474	0.90	0/1977
1	B	0.95	0/1474	0.93	5/1977 (0.3%)
1	C	0.96	1/1474 (0.1%)	0.96	1/1977 (0.1%)
1	D	0.89	0/1474	0.86	1/1977 (0.1%)
All	All	0.92	1/5896 (0.0%)	0.92	7/7908 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	GLU	CG-CD	5.42	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	124	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	124	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	42	LEU	CA-CB-CG	6.22	129.61	115.30
1	B	163	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	187	LEU	CA-CB-CG	5.97	129.03	115.30
1	C	111	ASP	CB-CG-OD2	5.26	123.04	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1446	0	1422	80	0
1	B	1446	0	1422	95	0
1	C	1446	0	1422	132	0
1	D	1446	0	1422	72	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	38	0	0	15	0
3	B	25	0	0	16	0
3	C	42	0	0	22	0
3	D	25	0	0	5	0
All	All	5922	0	5688	376	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 33.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:HA	3:A:284:HOH:O	1.18	1.35
1:C:151:THR:HA	3:C:298:HOH:O	1.19	1.28
1:D:158:LYS:HE3	3:D:281:HOH:O	1.40	1.21
1:B:175:LEU:HB3	3:B:271:HOH:O	1.41	1.19
1:A:15:GLU:O	1:A:19:LYS:HG2	1.53	1.08
1:A:2:GLU:O	1:A:6:ARG:HG3	1.55	1.07
1:C:9:PHE:HA	3:C:296:HOH:O	1.54	1.07
1:A:170:ARG:HH11	1:A:170:ARG:HG3	1.09	1.07
1:B:158:LYS:HA	3:B:275:HOH:O	1.53	1.06
1:B:150:PHE:HA	3:B:271:HOH:O	1.61	1.01
1:A:85:THR:O	1:A:89:THR:HG23	1.60	1.01
1:A:32:THR:HA	3:A:296:HOH:O	1.61	1.01
1:A:92:ASN:HD21	1:A:102:LYS:NZ	1.62	0.97
1:C:126:GLU:HG3	3:C:295:HOH:O	1.63	0.97
1:C:125:ARG:HH11	1:C:195:GLU:HB3	1.24	0.97
1:A:89:THR:HG22	1:B:23:GLU:HA	1.44	0.95
1:C:126:GLU:OE1	1:C:129:THR:OG1	1.85	0.92
1:C:185:ARG:HB2	1:C:187:LEU:HD21	1.50	0.92
1:C:125:ARG:NH1	1:C:195:GLU:HB3	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HB3	3:B:280:HOH:O	1.72	0.89
1:A:96:ASN:HD22	1:A:97:THR:N	1.71	0.88
1:B:98:THR:OG1	1:B:100:VAL:HG23	1.72	0.88
1:C:5:VAL:C	1:C:7:GLN:H	1.75	0.88
1:D:8:CYS:HB2	3:D:279:HOH:O	1.73	0.87
1:C:187:LEU:HD22	1:C:187:LEU:H	1.38	0.86
1:B:105:PHE:O	1:B:106:LEU:HB2	1.77	0.84
1:A:170:ARG:NH1	1:A:170:ARG:HG3	1.90	0.84
1:A:42:LEU:HG	1:A:46:PHE:HE2	1.43	0.84
1:A:32:THR:CA	3:A:296:HOH:O	2.21	0.83
1:A:92:ASN:HD21	1:A:102:LYS:HZ2	1.26	0.82
1:C:3:ASP:HB3	3:C:291:HOH:O	1.78	0.82
1:C:124:ARG:HG2	1:C:191:PHE:CD2	2.16	0.81
1:C:116:ARG:HD2	1:C:144:HIS:HB2	1.63	0.80
1:C:4:PHE:HB3	3:C:297:HOH:O	1.80	0.80
1:A:92:ASN:ND2	1:A:102:LYS:HZ2	1.80	0.80
1:D:83:ASP:HB2	1:D:86:MET:CB	2.12	0.79
1:C:125:ARG:HH11	1:C:195:GLU:CB	1.96	0.79
1:C:1:MET:HG3	3:C:297:HOH:O	1.84	0.78
1:D:185:ARG:HG3	1:D:187:LEU:HD22	1.66	0.77
1:C:141:GLU:HG3	1:C:142:LYS:H	1.49	0.77
1:A:170:ARG:CG	1:A:170:ARG:HH11	1.95	0.77
1:C:121:GLY:HA3	1:C:130:TYR:HE2	1.49	0.76
1:B:173:THR:HA	3:B:273:HOH:O	1.84	0.76
1:D:83:ASP:HB2	1:D:86:MET:HB3	1.66	0.76
1:B:165:GLU:HG2	1:B:168:ARG:NH2	2.00	0.76
1:D:116:ARG:HD2	1:D:144:HIS:HB2	1.67	0.75
1:B:185:ARG:HB2	1:B:187:LEU:HD22	1.69	0.75
1:A:144:HIS:CE1	1:A:160:ASP:HB3	2.22	0.74
1:C:168:ARG:HH11	1:C:168:ARG:CB	2.00	0.74
1:C:177:THR:HG22	3:C:299:HOH:O	1.87	0.74
1:C:76:PHE:HA	1:C:110:TYR:O	1.88	0.74
1:C:5:VAL:O	1:C:7:GLN:N	2.21	0.73
1:B:139:LYS:O	1:B:139:LYS:HG2	1.88	0.73
1:A:92:ASN:ND2	1:A:102:LYS:NZ	2.32	0.73
1:C:187:LEU:N	1:C:187:LEU:HD22	2.04	0.72
1:D:95:CYS:SG	1:D:102:LYS:HA	2.28	0.72
1:B:124:ARG:HG3	1:B:192:ARG:HA	1.71	0.72
1:C:141:GLU:HB3	3:C:260:HOH:O	1.90	0.71
1:C:4:PHE:CE2	1:C:182:MET:HG3	2.25	0.71
1:D:29:LYS:HB2	1:D:30:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:HA	1:B:110:TYR:O	1.92	0.70
1:D:85:THR:O	1:D:89:THR:HG23	1.91	0.70
1:B:85:THR:O	1:B:89:THR:HG23	1.90	0.70
1:C:5:VAL:C	1:C:7:GLN:N	2.41	0.69
1:A:170:ARG:O	1:A:173:THR:HG22	1.91	0.69
1:C:191:PHE:HB2	3:C:274:HOH:O	1.91	0.69
1:B:125:ARG:HG3	1:B:195:GLU:OE1	1.93	0.69
1:B:75:ARG:HG2	1:B:75:ARG:O	1.91	0.69
1:B:179:ARG:HB2	1:B:188:TRP:CZ3	2.28	0.69
1:C:47:MET:HE1	1:C:174:ARG:HB3	1.74	0.69
1:B:92:ASN:HD21	1:B:102:LYS:NZ	1.91	0.69
1:A:161:TYR:O	1:A:163:LEU:N	2.23	0.69
1:D:101:GLU:HG2	1:D:102:LYS:H	1.58	0.68
1:B:196:ARG:HG3	3:B:269:HOH:O	1.93	0.68
1:A:96:ASN:HD22	1:A:96:ASN:C	1.96	0.68
1:C:144:HIS:CE1	1:C:157:THR:HB	2.28	0.68
1:C:182:MET:O	1:C:188:TRP:N	2.27	0.67
1:C:126:GLU:HG2	1:C:128:HIS:H	1.60	0.67
1:C:124:ARG:NH2	1:C:194:SER:OG	2.28	0.66
1:A:42:LEU:HG	1:A:46:PHE:CE2	2.27	0.66
1:B:130:TYR:O	1:B:133:GLU:HB2	1.94	0.66
1:B:165:GLU:HG2	1:B:168:ARG:HH22	1.58	0.66
1:D:196:ARG:HB3	3:D:263:HOH:O	1.95	0.65
1:A:118:ILE:HG22	3:A:290:HOH:O	1.95	0.65
1:C:32:THR:HA	1:C:35:PHE:HB3	1.78	0.65
1:A:17:ALA:HB1	1:A:38:ILE:HG22	1.79	0.65
1:C:126:GLU:CG	3:C:295:HOH:O	2.29	0.65
1:A:32:THR:CB	3:A:296:HOH:O	2.44	0.65
1:C:28:PRO:O	1:C:32:THR:HG23	1.95	0.65
1:D:15:GLU:O	1:D:19:LYS:HG2	1.97	0.65
1:C:182:MET:O	1:C:188:TRP:CA	2.45	0.65
1:A:128:HIS:HA	1:A:155:MET:HE1	1.80	0.64
1:C:187:LEU:CD2	1:C:187:LEU:H	2.09	0.64
1:A:35:PHE:HB3	3:A:296:HOH:O	1.98	0.64
1:A:3:ASP:HB3	1:A:7:GLN:NE2	2.12	0.64
1:C:111:ASP:HB2	1:C:118:ILE:HD11	1.78	0.64
1:C:181:GLU:HG3	3:C:299:HOH:O	1.98	0.64
1:C:179:ARG:HG2	1:C:188:TRP:CH2	2.33	0.64
1:D:10:ASN:HB3	1:D:13:ILE:HD13	1.78	0.64
1:A:92:ASN:HD21	1:A:102:LYS:HZ1	1.45	0.63
1:B:161:TYR:HB3	1:B:168:ARG:NE	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ILE:HA	1:D:109:LEU:HD23	1.80	0.63
1:B:175:LEU:CB	3:B:271:HOH:O	2.18	0.63
1:D:42:LEU:O	1:D:46:PHE:CD2	2.51	0.63
1:B:165:GLU:HB3	3:B:282:HOH:O	1.99	0.63
1:C:141:GLU:HG3	1:C:142:LYS:N	2.13	0.63
1:D:111:ASP:O	1:D:115:ASN:HA	1.99	0.62
1:B:96:ASN:HD22	1:B:97:THR:N	1.97	0.62
1:D:108:ASP:OD2	1:D:120:ILE:N	2.30	0.62
1:C:141:GLU:CG	1:C:142:LYS:H	2.12	0.62
1:A:151:THR:OG1	1:A:153:GLU:HB2	2.00	0.62
1:D:1:MET:O	1:D:4:PHE:HB3	2.00	0.62
1:B:149:SER:HB2	1:B:151:THR:HG23	1.82	0.62
1:D:181:GLU:O	1:D:184:SER:HB3	2.00	0.61
1:C:75:ARG:NE	1:C:111:ASP:OD2	2.29	0.61
1:D:105:PHE:O	1:D:106:LEU:HB2	1.99	0.61
1:D:107:PRO:HB3	3:D:282:HOH:O	2.00	0.61
1:D:164:ASP:OD2	1:D:167:SER:HB3	2.00	0.61
1:C:105:PHE:O	1:C:106:LEU:CB	2.47	0.61
1:D:83:ASP:HB2	1:D:86:MET:HB2	1.83	0.60
1:C:172:LYS:HG2	3:C:285:HOH:O	2.01	0.60
1:B:154:GLU:OE2	1:B:172:LYS:NZ	2.34	0.60
1:A:83:ASP:CG	1:B:85:THR:HB	2.21	0.60
1:A:42:LEU:O	1:A:46:PHE:HD2	1.84	0.60
1:B:96:ASN:C	1:B:96:ASN:HD22	2.04	0.60
1:C:152:GLY:HA2	3:C:289:HOH:O	2.01	0.60
1:A:116:ARG:HD2	1:A:144:HIS:HB2	1.84	0.60
1:C:95:CYS:SG	1:C:102:LYS:HA	2.42	0.60
1:D:110:TYR:HE2	1:D:112:TYR:CD1	2.20	0.60
1:C:124:ARG:NH1	1:C:195:GLU:H	2.00	0.59
1:C:182:MET:O	1:C:188:TRP:HA	2.03	0.59
1:B:150:PHE:HD2	1:B:179:ARG:HB3	1.67	0.59
1:B:165:GLU:CB	3:B:282:HOH:O	2.51	0.59
1:D:79:ILE:O	1:D:82:ARG:HG3	2.01	0.59
1:A:152:GLY:HA2	1:A:172:LYS:HD3	1.85	0.59
1:C:161:TYR:HB3	1:C:168:ARG:HE	1.68	0.58
1:C:105:PHE:O	1:C:106:LEU:HB3	2.02	0.58
1:D:181:GLU:O	1:D:185:ARG:HG2	2.04	0.58
1:B:111:ASP:OD1	1:B:114:GLU:HB2	2.04	0.58
1:C:114:GLU:HG3	1:C:116:ARG:NH2	2.19	0.57
1:D:95:CYS:SG	1:D:103:PRO:HD3	2.44	0.57
1:C:124:ARG:HH12	1:C:195:GLU:H	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:32:THR:HB	1.87	0.57
1:D:179:ARG:C	1:D:179:ARG:HD2	2.25	0.57
1:B:-2:LEU:HD22	1:B:-2:LEU:N	2.20	0.57
1:C:86:MET:O	1:C:90:VAL:HG23	2.04	0.57
1:C:47:MET:CE	1:C:174:ARG:HG2	2.35	0.56
1:C:3:ASP:O	1:C:7:GLN:NE2	2.38	0.56
1:C:116:ARG:CD	1:C:144:HIS:HB2	2.32	0.56
1:B:48:TYR:O	1:B:48:TYR:CD1	2.58	0.56
1:B:27:ASP:HB3	1:B:30:ILE:HD13	1.88	0.56
1:B:97:THR:HG22	1:B:98:THR:N	2.20	0.56
1:C:2:GLU:HG3	1:C:6:ARG:HE	1.70	0.56
1:C:1:MET:CE	1:C:33:ASN:ND2	2.69	0.55
1:A:154:GLU:OE1	1:A:168:ARG:NH1	2.39	0.55
1:D:179:ARG:HG2	1:D:188:TRP:CE3	2.41	0.55
1:A:27:ASP:OD2	1:A:29:LYS:HE3	2.07	0.55
1:B:172:LYS:CB	3:B:280:HOH:O	2.41	0.55
1:A:141:GLU:N	3:A:284:HOH:O	2.31	0.55
1:C:124:ARG:HD2	1:C:124:ARG:H	1.71	0.55
1:B:82:ARG:HB2	1:B:87:ALA:HB2	1.89	0.55
1:A:170:ARG:O	1:A:173:THR:CG2	2.56	0.54
1:D:190:SER:HA	1:D:193:GLN:HB2	1.90	0.54
1:C:140:SER:HB2	1:C:143:THR:O	2.06	0.54
1:A:3:ASP:C	1:A:7:GLN:HE21	2.11	0.54
1:C:182:MET:HB3	1:C:188:TRP:CE3	2.43	0.53
1:C:148:PHE:CE1	1:C:171:ILE:HG21	2.42	0.53
1:C:180:GLN:O	1:C:184:SER:N	2.41	0.53
1:C:181:GLU:CG	3:C:299:HOH:O	2.55	0.53
1:C:191:PHE:CB	3:C:287:HOH:O	2.55	0.53
1:D:100:VAL:HG12	1:D:101:GLU:O	2.08	0.53
1:C:1:MET:HB3	1:C:32:THR:HB	1.91	0.53
1:D:147:ILE:O	1:D:154:GLU:HB2	2.09	0.53
1:B:124:ARG:HB2	1:B:188:TRP:CH2	2.44	0.52
1:B:194:SER:O	1:B:196:ARG:N	2.42	0.52
1:B:107:PRO:HA	1:B:119:GLU:HG2	1.90	0.52
1:B:172:LYS:CA	3:B:280:HOH:O	2.57	0.52
1:C:1:MET:HB3	1:C:32:THR:CB	2.39	0.52
1:A:83:ASP:OD2	1:B:85:THR:HB	2.09	0.52
1:A:17:ALA:CB	1:A:38:ILE:HG22	2.39	0.52
1:B:10:ASN:OD1	1:B:11:PRO:HD2	2.09	0.52
1:A:4:PHE:O	1:A:8:CYS:HB2	2.08	0.52
1:D:43:GLU:O	1:D:47:MET:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASP:OD1	1:D:114:GLU:HB2	2.10	0.52
1:C:189:ASP:OD1	1:C:192:ARG:NH1	2.42	0.52
1:B:100:VAL:HG12	1:B:101:GLU:N	2.24	0.52
1:B:124:ARG:HD2	1:B:191:PHE:O	2.10	0.51
1:D:181:GLU:OE2	1:D:181:GLU:HA	2.06	0.51
1:B:161:TYR:O	1:B:163:LEU:N	2.43	0.51
1:C:168:ARG:HH11	1:C:168:ARG:HB2	1.75	0.51
1:C:140:SER:CB	1:C:143:THR:O	2.58	0.51
1:A:144:HIS:HE1	1:A:160:ASP:HB3	1.70	0.51
1:B:15:GLU:O	1:B:19:LYS:HG2	2.10	0.51
1:C:181:GLU:C	1:C:183:ALA:H	2.14	0.51
1:C:2:GLU:CG	1:C:6:ARG:HE	2.24	0.51
1:C:75:ARG:N	3:C:282:HOH:O	2.44	0.51
1:A:152:GLY:O	1:A:153:GLU:C	2.49	0.51
1:A:164:ASP:OD2	1:A:167:SER:HB2	2.11	0.50
1:B:98:THR:OG1	1:B:100:VAL:CG2	2.51	0.50
1:D:124:ARG:HH21	1:D:195:GLU:CG	2.24	0.50
1:A:140:SER:CA	3:A:284:HOH:O	2.04	0.50
1:C:33:ASN:OD1	1:C:191:PHE:HD1	1.94	0.50
1:C:37:ALA:HB2	1:C:191:PHE:HZ	1.77	0.50
1:C:154:GLU:OE1	1:C:168:ARG:NH1	2.45	0.50
1:D:150:PHE:O	1:D:176:PHE:CE2	2.65	0.50
1:D:140:SER:C	1:D:142:LYS:H	2.15	0.50
1:A:0:SER:O	1:A:3:ASP:HB2	2.11	0.50
1:B:48:TYR:O	1:B:48:TYR:HD1	1.94	0.50
1:C:77:GLU:O	1:C:109:LEU:HA	2.12	0.50
1:C:91:VAL:CG1	1:C:103:PRO:HD2	2.41	0.50
1:B:188:TRP:HE1	1:B:192:ARG:HH11	1.60	0.50
1:B:138:ILE:HG13	1:B:140:SER:H	1.77	0.50
1:C:94:ILE:O	1:C:98:THR:HG23	2.11	0.50
1:D:79:ILE:N	1:D:79:ILE:HD13	2.26	0.50
1:C:191:PHE:HB3	3:C:287:HOH:O	2.12	0.49
1:C:32:THR:HG22	1:C:35:PHE:HD1	1.77	0.49
1:B:184:SER:OG	1:B:184:SER:O	2.30	0.49
1:A:170:ARG:C	1:A:173:THR:HG22	2.32	0.49
1:C:10:ASN:OD1	1:C:12:MET:HB3	2.12	0.49
1:B:2:GLU:O	1:B:6:ARG:HG2	2.11	0.49
1:B:33:ASN:HD22	1:B:194:SER:HB3	1.77	0.49
1:A:128:HIS:HA	1:A:155:MET:CE	2.43	0.49
1:A:140:SER:HB2	3:A:295:HOH:O	2.13	0.49
1:A:170:ARG:CG	1:A:170:ARG:NH1	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:CD1	1:A:80:GLU:HG3	2.42	0.49
1:A:126:GLU:CG	3:A:281:HOH:O	2.60	0.49
1:B:160:ASP:HB3	3:B:272:HOH:O	2.11	0.49
1:D:87:ALA:O	1:D:91:VAL:HG23	2.13	0.49
1:A:48:TYR:OH	1:A:162:THR:HB	2.12	0.49
1:C:184:SER:O	1:C:184:SER:OG	2.30	0.49
1:C:191:PHE:N	3:C:287:HOH:O	2.44	0.49
1:B:15:GLU:HG2	1:B:19:LYS:NZ	2.27	0.49
1:C:6:ARG:HB2	1:C:7:GLN:NE2	2.28	0.48
1:B:150:PHE:O	1:B:152:GLY:N	2.46	0.48
1:C:168:ARG:HB3	1:C:168:ARG:HH11	1.77	0.48
1:B:4:PHE:O	1:B:8:CYS:N	2.43	0.48
1:C:116:ARG:HD2	1:C:144:HIS:CB	2.38	0.48
1:C:107:PRO:HG2	1:C:117:PHE:HB3	1.94	0.48
1:C:1:MET:O	1:C:4:PHE:HB3	2.14	0.48
1:A:185:ARG:HG3	3:A:286:HOH:O	2.13	0.48
1:D:10:ASN:ND2	1:D:12:MET:H	2.11	0.48
1:B:31:GLU:HB3	1:B:34:LYS:CG	2.43	0.48
1:C:183:ALA:HB2	1:C:188:TRP:HB2	1.95	0.48
1:A:23:GLU:CD	1:A:84:ARG:HH21	2.17	0.48
1:C:47:MET:HE1	1:C:174:ARG:CB	2.41	0.47
1:B:92:ASN:HD21	1:B:102:LYS:HZ2	1.61	0.47
1:A:75:ARG:O	1:A:112:TYR:HD2	1.97	0.47
1:C:124:ARG:NH1	1:C:191:PHE:O	2.47	0.47
1:C:1:MET:HE1	1:C:33:ASN:ND2	2.29	0.47
1:D:30:ILE:N	1:D:30:ILE:HD12	2.28	0.47
1:D:78:ILE:HG12	1:D:109:LEU:CD2	2.45	0.47
1:D:126:GLU:OE1	1:D:129:THR:OG1	2.32	0.47
1:D:179:ARG:HG2	1:D:188:TRP:CZ3	2.48	0.47
1:A:126:GLU:HA	3:A:271:HOH:O	2.13	0.47
1:D:93:SER:O	1:D:94:ILE:HG13	2.14	0.47
1:C:2:GLU:HB2	1:C:32:THR:HG21	1.95	0.47
1:B:123:THR:O	1:B:149:SER:HA	2.15	0.47
1:A:188:TRP:HE1	1:A:192:ARG:HD3	1.79	0.47
1:B:196:ARG:HB2	3:B:269:HOH:O	2.13	0.47
1:D:116:ARG:NH2	1:D:160:ASP:OD2	2.48	0.46
1:D:111:ASP:O	1:D:115:ASN:CA	2.63	0.46
1:B:123:THR:HG23	1:B:149:SER:HB3	1.97	0.46
1:C:188:TRP:NE1	1:C:192:ARG:NH2	2.63	0.46
1:A:157:THR:HA	3:A:283:HOH:O	2.15	0.46
1:A:75:ARG:NE	1:A:111:ASP:OD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:33:ASN:ND2	2.29	0.46
1:B:15:GLU:HG2	1:B:19:LYS:HZ3	1.80	0.46
1:C:1:MET:HE3	1:C:33:ASN:HD22	1.80	0.46
1:A:170:ARG:HA	1:A:173:THR:HG22	1.98	0.46
1:D:121:GLY:HA3	1:D:130:TYR:HE2	1.79	0.46
1:B:196:ARG:CG	3:B:269:HOH:O	2.60	0.46
1:D:104:LYS:CE	1:D:104:LYS:H	2.28	0.46
1:D:150:PHE:O	1:D:176:PHE:CD2	2.69	0.46
1:B:92:ASN:HD21	1:B:102:LYS:HZ1	1.64	0.46
1:D:136:ASN:O	1:D:138:ILE:N	2.49	0.45
1:D:149:SER:OG	1:D:153:GLU:HB2	2.17	0.45
1:B:126:GLU:HG3	1:B:126:GLU:H	1.59	0.45
1:C:5:VAL:CG2	1:C:36:ALA:HB2	2.47	0.45
1:A:118:ILE:CG2	3:A:290:HOH:O	2.59	0.45
1:D:47:MET:O	1:D:48:TYR:C	2.54	0.45
1:D:78:ILE:HG12	1:D:109:LEU:HD21	1.98	0.45
1:D:0:SER:O	1:D:3:ASP:HB2	2.17	0.45
1:C:47:MET:HE2	1:C:174:ARG:HG2	1.98	0.45
1:A:76:PHE:HA	1:A:110:TYR:O	2.16	0.45
1:C:151:THR:C	1:C:176:PHE:HE1	2.20	0.45
1:C:1:MET:O	3:C:297:HOH:O	2.21	0.45
1:B:1:MET:O	1:B:5:VAL:HG23	2.17	0.45
1:D:125:ARG:HA	3:D:280:HOH:O	2.16	0.45
1:C:180:GLN:O	1:C:183:ALA:HB3	2.17	0.45
1:A:144:HIS:HE1	1:A:157:THR:O	1.99	0.45
1:C:141:GLU:CG	1:C:142:LYS:N	2.75	0.45
1:D:192:ARG:NH2	1:D:193:GLN:HE21	2.14	0.44
1:C:125:ARG:HH22	1:C:133:GLU:HG3	1.82	0.44
1:A:7:GLN:NE2	1:A:185:ARG:HH22	2.16	0.44
1:C:186:GLY:N	1:C:187:LEU:HD22	2.32	0.44
1:C:4:PHE:CB	3:C:297:HOH:O	2.53	0.44
1:A:144:HIS:CE1	1:A:157:THR:O	2.71	0.44
1:D:150:PHE:HD2	1:D:175:LEU:O	2.00	0.44
1:D:136:ASN:O	1:D:137:LYS:C	2.56	0.44
1:B:196:ARG:CB	3:B:269:HOH:O	2.64	0.44
1:C:170:ARG:O	1:C:171:ILE:C	2.55	0.44
1:B:128:HIS:O	1:B:132:LEU:HG	2.17	0.44
1:A:150:PHE:O	1:A:179:ARG:NH2	2.46	0.44
1:C:115:ASN:ND2	3:C:288:HOH:O	2.43	0.44
1:B:188:TRP:HE1	1:B:192:ARG:NH1	2.16	0.44
1:A:96:ASN:ND2	1:A:96:ASN:C	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ALA:N	1:C:187:LEU:HD23	2.32	0.43
1:C:124:ARG:HH11	1:C:192:ARG:HA	1.83	0.43
1:B:31:GLU:O	1:B:35:PHE:HB2	2.18	0.43
1:C:90:VAL:O	1:C:91:VAL:C	2.57	0.43
1:A:131:TYR:HE1	1:A:145:ILE:HB	1.83	0.43
1:C:176:PHE:CE2	1:C:179:ARG:NH2	2.87	0.43
1:D:189:ASP:O	1:D:192:ARG:HB3	2.18	0.43
1:D:161:TYR:O	1:D:163:LEU:N	2.51	0.43
1:B:179:ARG:HG2	1:B:179:ARG:O	2.16	0.43
1:B:165:GLU:HG2	1:B:168:ARG:CZ	2.48	0.43
1:D:150:PHE:CD2	1:D:179:ARG:HB2	2.54	0.43
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.31	0.43
1:A:124:ARG:NH1	1:A:194:SER:OG	2.52	0.43
1:B:176:PHE:O	1:B:177:THR:C	2.56	0.43
1:B:158:LYS:CA	3:B:275:HOH:O	2.31	0.43
1:A:10:ASN:HD22	1:A:12:MET:N	2.16	0.43
1:B:102:LYS:HD3	1:B:103:PRO:HD2	2.01	0.43
1:D:150:PHE:HD2	1:D:179:ARG:HB2	1.83	0.43
1:D:92:ASN:C	1:D:94:ILE:H	2.21	0.43
1:B:6:ARG:HG2	1:B:6:ARG:H	1.57	0.42
1:C:22:LYS:HE3	1:C:22:LYS:HB2	1.80	0.42
1:D:111:ASP:O	1:D:115:ASN:N	2.52	0.42
1:B:167:SER:OG	1:B:170:ARG:NH2	2.52	0.42
1:C:1:MET:HG2	1:C:32:THR:C	2.40	0.42
1:B:40:THR:C	1:B:42:LEU:N	2.71	0.42
1:C:124:ARG:CG	1:C:191:PHE:CD2	2.95	0.42
1:B:23:GLU:OE2	1:B:84:ARG:NH2	2.43	0.42
1:C:83:ASP:O	1:C:84:ARG:C	2.58	0.42
1:C:32:THR:HG22	1:C:35:PHE:CD1	2.55	0.42
1:A:15:GLU:HG2	1:A:19:LYS:NZ	2.35	0.42
1:B:150:PHE:CD2	1:B:179:ARG:HB3	2.51	0.42
1:A:164:ASP:O	1:A:165:GLU:C	2.58	0.42
1:C:178:ILE:O	1:C:180:GLN:N	2.53	0.42
1:D:151:THR:OG1	1:D:153:GLU:HB2	2.19	0.42
1:C:149:SER:O	1:C:175:LEU:HD12	2.20	0.42
1:C:189:ASP:HA	1:C:192:ARG:HH12	1.85	0.42
1:B:138:ILE:O	1:B:139:LYS:C	2.57	0.42
1:D:16:LEU:HA	1:D:16:LEU:HD23	1.85	0.42
1:B:141:GLU:CD	1:B:141:GLU:N	2.73	0.42
1:A:123:THR:HG23	1:A:125:ARG:H	1.85	0.42
1:B:105:PHE:O	1:B:106:LEU:CB	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG2	1:C:33:ASN:N	2.35	0.41
1:C:1:MET:HB3	1:C:32:THR:OG1	2.20	0.41
1:C:119:GLU:HG3	3:C:292:HOH:O	2.20	0.41
1:C:130:TYR:CE1	1:C:195:GLU:OE2	2.74	0.41
1:A:156:ALA:HB1	1:A:160:ASP:O	2.20	0.41
1:A:174:ARG:HE	1:A:178:ILE:HD11	1.85	0.41
1:D:96:ASN:C	1:D:96:ASN:HD22	2.23	0.41
1:C:182:MET:HB3	1:C:188:TRP:HE3	1.85	0.41
1:C:188:TRP:CE2	1:C:192:ARG:NH2	2.89	0.41
1:B:138:ILE:C	1:B:140:SER:N	2.73	0.41
1:D:5:VAL:HG11	1:D:35:PHE:CE1	2.56	0.41
1:C:124:ARG:HD2	1:C:195:GLU:OE1	2.21	0.41
1:C:125:ARG:HB3	1:C:126:GLU:H	1.71	0.41
1:C:183:ALA:HA	1:C:188:TRP:H	1.86	0.41
1:B:15:GLU:CG	1:B:19:LYS:NZ	2.83	0.41
1:D:124:ARG:HH21	1:D:195:GLU:HG3	1.85	0.41
1:C:10:ASN:O	1:C:14:VAL:HG23	2.20	0.41
1:B:176:PHE:O	1:B:180:GLN:HG3	2.20	0.41
1:B:150:PHE:C	1:B:152:GLY:N	2.75	0.40
1:C:140:SER:C	1:C:141:GLU:HG2	2.42	0.40
1:D:140:SER:O	1:D:142:LYS:N	2.54	0.40
1:B:86:MET:O	1:B:90:VAL:HG12	2.21	0.40
1:A:32:THR:HB	3:A:296:HOH:O	2.16	0.40
1:B:193:GLN:O	1:B:195:GLU:N	2.54	0.40
1:C:121:GLY:CA	1:C:130:TYR:HE2	2.26	0.40
1:B:183:ALA:C	1:B:185:ARG:H	2.24	0.40
1:A:173:THR:O	1:A:176:PHE:HB2	2.21	0.40
1:A:188:TRP:NE1	1:A:192:ARG:HD3	2.37	0.40
1:B:127:VAL:HG11	1:B:153:GLU:CG	2.50	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	171/261 (66%)	148 (86%)	21 (12%)	2 (1%)	16	29
1	B	171/261 (66%)	143 (84%)	17 (10%)	11 (6%)	2	1
1	C	171/261 (66%)	141 (82%)	17 (10%)	13 (8%)	1	1
1	D	171/261 (66%)	143 (84%)	20 (12%)	8 (5%)	3	3
All	All	684/1044 (66%)	575 (84%)	75 (11%)	34 (5%)	3	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	B	97	THR
1	B	106	LEU
1	B	151	THR
1	C	141	GLU
1	C	188	TRP
1	D	100	VAL
1	D	137	LYS
1	A	162	THR
1	B	125	ARG
1	B	184	SER
1	B	195	GLU
1	C	6	ARG
1	C	179	ARG
1	C	189	ASP
1	D	94	ILE
1	D	101	GLU
1	D	141	GLU
1	B	93	SER
1	B	162	THR
1	C	140	SER
1	D	93	SER
1	B	194	SER
1	C	106	LEU
1	C	125	ARG
1	C	139	LYS
1	C	162	THR
1	C	195	GLU
1	D	106	LEU
1	D	162	THR
1	B	140	SER
1	B	159	ALA
1	C	28	PRO

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Mol	Chain	Res	Type
1	C	107	PRO

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	157/232 (68%)	137 (87%)	20 (13%)	5	10
1	B	157/232 (68%)	130 (83%)	27 (17%)	2	4
1	C	157/232 (68%)	129 (82%)	28 (18%)	2	3
1	D	157/232 (68%)	136 (87%)	21 (13%)	5	9
All	All	628/928 (68%)	532 (85%)	96 (15%)	3	6

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	4	PHE
1	A	7	GLN
1	A	10	ASN
1	A	78	ILE
1	A	95	CYS
1	A	96	ASN
1	A	120	ILE
1	A	124	ARG
1	A	126	GLU
1	A	141	GLU
1	A	142	LYS
1	A	148	PHE
1	A	153	GLU
1	A	155	MET
1	A	164	ASP
1	A	168	ARG
1	A	170	ARG
1	A	184	SER
1	A	187	LEU

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Mol	Chain	Res	Type
1	B	-2	LEU
1	B	19	LYS
1	B	29	LYS
1	B	83	ASP
1	B	89	THR
1	B	90	VAL
1	B	96	ASN
1	B	98	THR
1	B	101	GLU
1	B	106	LEU
1	B	115	ASN
1	B	124	ARG
1	B	126	GLU
1	B	127	VAL
1	B	134	LYS
1	B	139	LYS
1	B	141	GLU
1	B	149	SER
1	B	151	THR
1	B	162	THR
1	B	168	ARG
1	B	179	ARG
1	B	180	GLN
1	B	181	GLU
1	B	184	SER
1	B	187	LEU
1	B	196	ARG
1	C	7	GLN
1	C	12	MET
1	C	24	TYR
1	C	26	GLU
1	C	31	GLU
1	C	34	LYS
1	C	48	TYR
1	C	92	ASN
1	C	96	ASN
1	C	98	THR
1	C	102	LYS
1	C	104	LYS
1	C	106	LEU
1	C	119	GLU
1	C	124	ARG

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Mol	Chain	Res	Type
1	C	134	LYS
1	C	138	ILE
1	C	139	LYS
1	C	142	LYS
1	C	143	THR
1	C	168	ARG
1	C	176	PHE
1	C	180	GLN
1	C	182	MET
1	C	187	LEU
1	C	189	ASP
1	C	191	PHE
1	C	196	ARG
1	D	0	SER
1	D	38	ILE
1	D	49	SER
1	D	82	ARG
1	D	83	ASP
1	D	84	ARG
1	D	96	ASN
1	D	102	LYS
1	D	104	LYS
1	D	113	LYS
1	D	123	THR
1	D	134	LYS
1	D	136	ASN
1	D	139	LYS
1	D	141	GLU
1	D	146	HIS
1	D	173	THR
1	D	174	ARG
1	D	176	PHE
1	D	187	LEU
1	D	189	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	10	ASN
1	A	92	ASN
1	A	96	ASN

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Mol	Chain	Res	Type
1	B	92	ASN
1	B	96	ASN
1	B	136	ASN
1	C	7	GLN
1	C	33	ASN
1	D	10	ASN
1	D	92	ASN
1	D	96	ASN
1	D	115	ASN
1	D	136	ASN
1	D	193	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	175/261 (67%)	-0.24	1 (0%)	90	91	20, 34, 46, 50	0
1	B	175/261 (67%)	0.16	7 (4%)	42	47	25, 40, 63, 74	0
1	C	175/261 (67%)	0.39	19 (10%)	7	7	24, 41, 90, 98	0
1	D	175/261 (67%)	0.32	10 (5%)	27	31	30, 48, 65, 80	0
All	All	700/1044 (67%)	0.16	37 (5%)	30	34	20, 40, 66, 98	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	GLY	6.9
1	C	4	PHE	5.9
1	C	183	ALA	5.0
1	C	0	SER	4.4
1	C	196	ARG	3.9
1	C	8	CYS	3.5
1	B	196	ARG	3.3
1	B	141	GLU	3.3
1	C	192	ARG	3.2
1	B	122	VAL	3.2
1	D	96	ASN	3.1
1	C	1	MET	3.0
1	C	189	ASP	2.9
1	D	140	SER	2.7
1	C	-1	GLY	2.7
1	D	11	PRO	2.6
1	C	194	SER	2.5
1	C	24	TYR	2.5
1	C	-2	LEU	2.5
1	D	192	ARG	2.4
1	D	99	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	136	ASN	2.3
1	D	137	LYS	2.3
1	C	105	PHE	2.3
1	C	191	PHE	2.2
1	C	182	MET	2.2
1	A	105	PHE	2.2
1	D	196	ARG	2.1
1	C	12	MET	2.1
1	C	5	VAL	2.1
1	B	121	GLY	2.1
1	B	197	GLY	2.1
1	D	85	THR	2.1
1	D	136	ASN	2.1
1	D	120	ILE	2.1
1	B	176	PHE	2.1
1	C	190	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	A	258	1/1	0.95	0.18	1.60	41,41,41,41	0
2	MN	C	257	1/1	0.97	0.20	0.52	33,33,33,33	0
2	MN	C	258	1/1	0.98	0.18	0.21	44,44,44,44	0
2	MN	B	257	1/1	0.95	0.18	0.05	37,37,37,37	0
2	MN	A	257	1/1	0.99	0.15	-0.39	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	B	258	1/1	0.97	0.15	-1.45	35,35,35,35	0
2	MN	D	258	1/1	0.97	0.18	-2.22	55,55,55,55	0
2	MN	D	257	1/1	0.98	0.16	-3.69	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.