Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:38 AM GMT

PDB ID	:	2NNW
Title	:	Alternative conformations of Nop56/58-fibrillarin complex and implication for induced-fit assenly of box C/D RNPs
Authors	:	Oruganti, S.; Zhang, Y.; Terns, R.; Terns, M.P.; Li, H.
Deposited on	:	2006-10-24
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

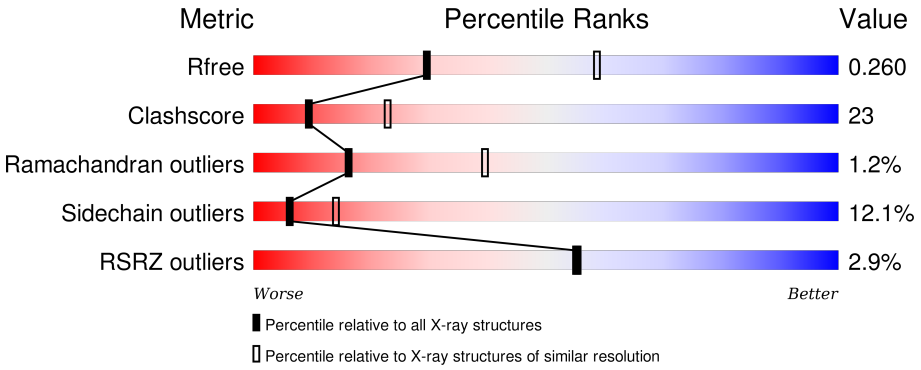
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	376	2% 61% 28% • 7%
1	C	376	2% 57% 31% • 7%
2	B	234	4% 54% 33% 9% •
2	D	234	3% 53% 36% 9% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9336 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 NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2846	1815	491	533	7			
1	C	350	Total	C	N	O	S	0	0	0
			2846	1815	491	533	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	CLONING ARTIFACT	UNP Q8U4M1
A	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	0	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	2	VAL	-	CLONING ARTIFACT	UNP Q8U4M1
A	3	MET	-	CLONING ARTIFACT	UNP Q8U4M1
A	4	ILE	-	CLONING ARTIFACT	UNP Q8U4M1
C	-5	MET	-	CLONING ARTIFACT	UNP Q8U4M1
C	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	0	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	2	VAL	-	CLONING ARTIFACT	UNP Q8U4M1
C	3	MET	-	CLONING ARTIFACT	UNP Q8U4M1
C	4	ILE	-	CLONING ARTIFACT	UNP Q8U4M1

- Molecule 2 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			
2	D	227	Total	C	N	O	S	0	0	0
			1822	1174	312	334	2			

There are 14 discrepancies between the modelled and reference sequences:

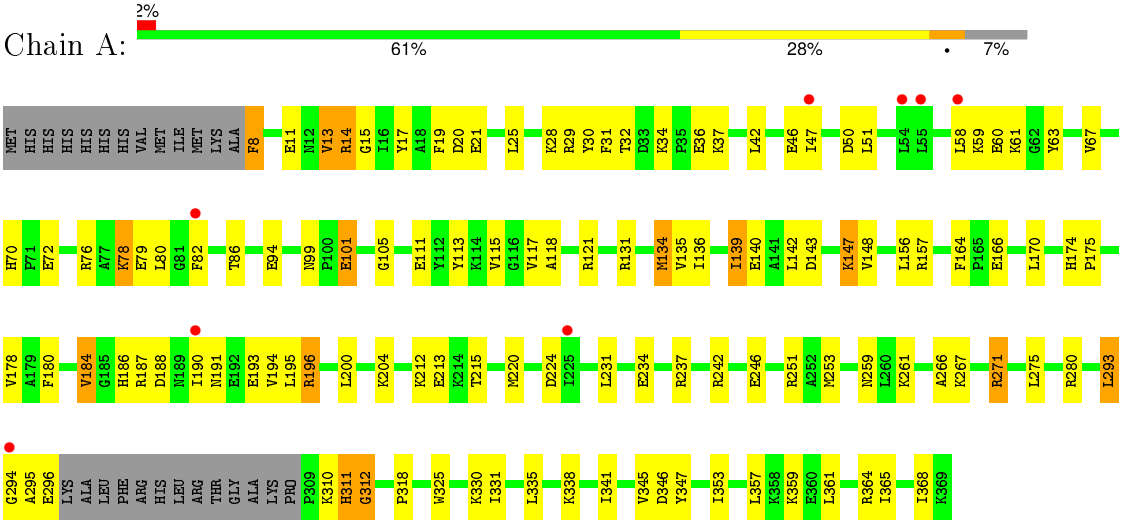
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	CLONING ARTIFACT	UNP Q8U4M2
B	-5	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M2
B	0	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	-6	MET	-	CLONING ARTIFACT	UNP Q8U4M2
D	-5	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M2
D	0	HIS	-	EXPRESSION TAG	UNP Q8U4M2

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 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.

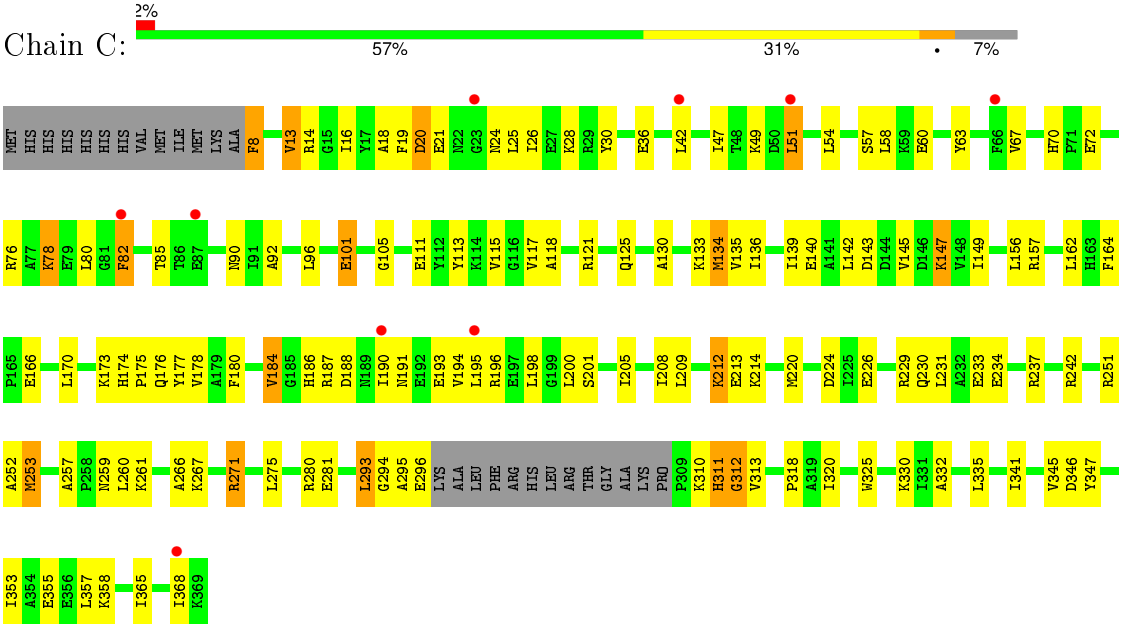
- Molecule 1: NOP5/NOP56 related protein

Chain A:



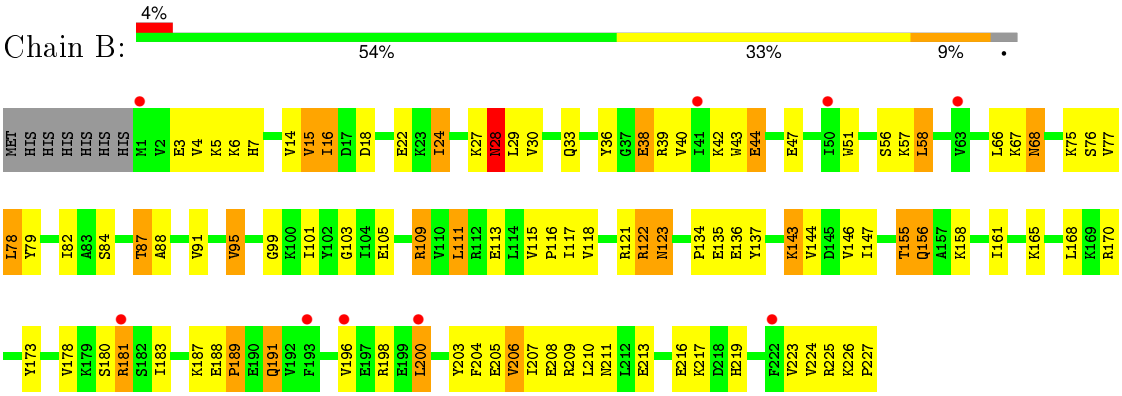
- Molecule 1: NOP5/NOP56 related protein

Chain C:



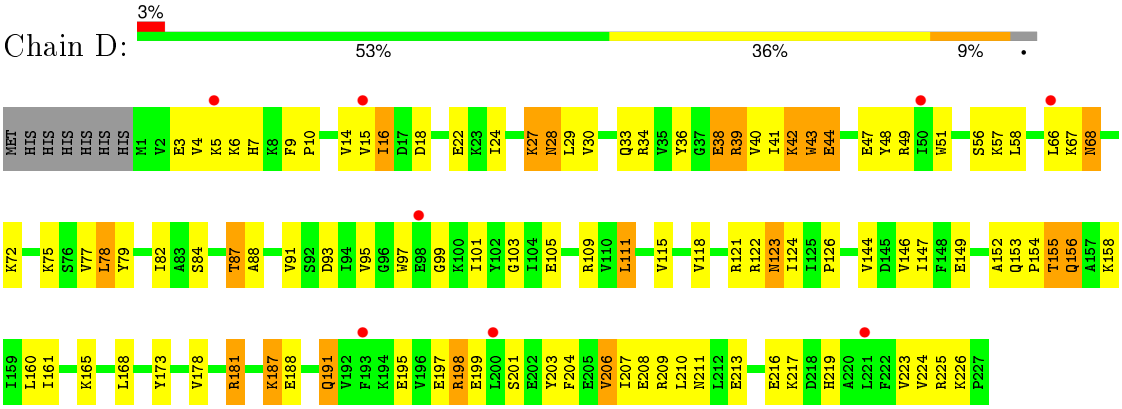
- Molecule 2: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

Chain B:



- Molecule 2: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	120.71Å 120.71Å 297.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.33 – 2.70 49.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.33-2.70) 92.9 (49.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.265 0.233 , 0.260	Depositor DCC
R_{free} test set	3290 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 71252 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9336	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.67	1/2896 (0.0%)	0.72	1/3896 (0.0%)
1	C	0.80	2/2896 (0.1%)	0.81	0/3896
2	B	0.62	0/1861	0.74	1/2515 (0.0%)
2	D	0.76	0/1861	0.81	1/2515 (0.0%)
All	All	0.72	3/9514 (0.0%)	0.77	3/12822 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	MET	SD-CE	-6.28	1.42	1.77
1	A	134	MET	SD-CE	-5.45	1.47	1.77
1	C	253	MET	SD-CE	-5.36	1.47	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	MET	CG-SD-CE	5.26	108.62	100.20
2	B	109	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	D	109	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2846	0	2877	107	2
1	C	2846	0	2877	116	2
2	B	1822	0	1869	101	0
2	D	1822	0	1869	107	0
All	All	9336	0	9492	426	4

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 23.

All (426) 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:135:VAL:HG11	1:A:253:MET:HE1	1.17	1.13
2:D:181:ARG:HD3	2:D:181:ARG:H	1.14	1.10
2:B:211:ASN:HD21	2:B:213:GLU:HG2	1.24	0.99
1:C:330:LYS:HD3	1:C:368:ILE:HD12	1.38	0.98
1:A:157:ARG:HH11	1:A:174:HIS:HD2	1.17	0.92
2:B:24:ILE:HG22	2:B:51:TRP:HB3	1.50	0.92
2:D:68:ASN:N	2:D:68:ASN:HD22	1.66	0.92
2:D:5:LYS:NZ	2:D:16:ILE:HD12	1.83	0.92
1:A:330:LYS:HD3	1:A:368:ILE:HD12	1.54	0.90
1:C:345:VAL:HG11	1:C:353:ILE:HD11	1.55	0.89
2:B:207:ILE:HD11	2:B:225:ARG:HB2	1.55	0.89
1:A:135:VAL:HG11	1:A:253:MET:CE	2.02	0.88
1:C:157:ARG:HH11	1:C:174:HIS:HD2	1.21	0.88
1:A:345:VAL:HG11	1:A:353:ILE:HD11	1.56	0.87
2:B:211:ASN:HD22	2:B:213:GLU:H	1.22	0.87
2:D:211:ASN:HD21	2:D:213:GLU:HG2	1.40	0.87
1:C:8:PHE:HB2	1:C:67:VAL:HG12	1.58	0.86
2:B:181:ARG:HD3	2:B:181:ARG:H	1.43	0.84
1:A:261:LYS:HD2	1:A:266:ALA:HB2	1.56	0.83
1:A:295:ALA:HB3	1:A:312:GLY:H	1.42	0.83
1:C:295:ALA:HB1	1:C:311:HIS:HA	1.58	0.83
2:D:161:ILE:O	2:D:165:LYS:HG2	1.79	0.82
1:A:135:VAL:CG1	1:A:253:MET:HE1	2.07	0.82
2:D:16:ILE:HD13	2:D:16:ILE:H	1.44	0.81
2:B:68:ASN:N	2:B:68:ASN:HD22	1.80	0.80
2:B:56:SER:OG	2:B:87:THR:HB	1.82	0.79
2:D:156:GLN:NE2	2:D:178:VAL:HA	1.97	0.78
2:B:211:ASN:ND2	2:B:213:GLU:HG2	1.97	0.78
1:C:295:ALA:HB3	1:C:312:GLY:H	1.49	0.78
1:C:13:VAL:CG2	1:C:115:VAL:HB	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:THR:HG22	2:B:158:LYS:HE2	1.66	0.78
1:A:8:PHE:HB2	1:A:67:VAL:HG12	1.66	0.78
2:B:33:GLN:HE22	2:B:121:ARG:HE	1.31	0.78
1:A:275:LEU:HD13	1:A:294:GLY:HA3	1.65	0.77
2:B:16:ILE:H	2:B:16:ILE:HD13	1.49	0.77
2:D:5:LYS:HZ1	2:D:16:ILE:HD12	1.48	0.76
1:C:275:LEU:HD13	1:C:294:GLY:HA3	1.68	0.76
2:D:173:TYR:CZ	2:D:225:ARG:HD2	2.20	0.76
2:D:33:GLN:HE22	2:D:121:ARG:HE	1.33	0.75
2:D:156:GLN:HE22	2:D:178:VAL:HA	1.51	0.75
1:C:330:LYS:CD	1:C:368:ILE:HD12	2.16	0.75
2:D:68:ASN:N	2:D:68:ASN:ND2	2.34	0.74
1:C:135:VAL:HG11	1:C:253:MET:HE1	1.69	0.74
1:C:135:VAL:HG11	1:C:253:MET:CE	2.16	0.74
1:A:13:VAL:CG2	1:A:115:VAL:HB	2.17	0.74
1:A:47:ILE:HG23	1:A:51:LEU:HD12	1.70	0.74
2:B:156:GLN:HE22	2:B:178:VAL:HA	1.52	0.74
2:D:56:SER:OG	2:D:87:THR:HB	1.88	0.74
2:D:211:ASN:ND2	2:D:213:GLU:HG2	2.04	0.73
1:C:78:LYS:HA	1:C:82:PHE:O	1.89	0.72
2:B:211:ASN:ND2	2:B:213:GLU:H	1.87	0.71
2:D:155:THR:HG22	2:D:158:LYS:HE2	1.74	0.70
2:D:203:TYR:OH	2:D:226:LYS:HE3	1.92	0.70
2:D:207:ILE:HB	2:D:223:VAL:HG23	1.71	0.70
2:D:187:LYS:NZ	2:D:187:LYS:HB2	2.06	0.70
2:D:181:ARG:HD3	2:D:181:ARG:N	1.98	0.70
2:D:6:LYS:HD2	2:D:7:HIS:H	1.56	0.69
1:C:220:MET:HG2	1:C:224:ASP:HB2	1.73	0.69
2:B:68:ASN:N	2:B:68:ASN:ND2	2.40	0.69
2:D:5:LYS:HZ2	2:D:16:ILE:HD12	1.57	0.69
1:C:135:VAL:HG21	1:C:253:MET:HE2	1.75	0.69
1:A:295:ALA:HB3	1:A:312:GLY:N	2.08	0.68
2:D:24:ILE:HG22	2:D:51:TRP:HB3	1.72	0.68
1:C:251:ARG:HH11	1:C:251:ARG:HG2	1.59	0.68
1:C:242:ARG:HG3	1:C:242:ARG:HH11	1.58	0.68
2:D:68:ASN:OD1	2:D:207:ILE:HG22	1.93	0.68
2:B:207:ILE:HD11	2:B:225:ARG:CB	2.24	0.68
1:C:275:LEU:HB3	1:C:293:LEU:HD22	1.76	0.68
2:D:121:ARG:C	2:D:123:ASN:H	1.93	0.68
1:A:295:ALA:HB1	1:A:311:HIS:HA	1.75	0.67
2:B:121:ARG:C	2:B:123:ASN:H	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ALA:CB	1:C:311:HIS:HA	2.24	0.67
2:B:156:GLN:NE2	2:B:178:VAL:HA	2.08	0.67
1:A:131:ARG:HA	1:A:134:MET:CE	2.23	0.67
1:A:13:VAL:HG22	1:A:115:VAL:HG21	1.76	0.67
2:B:95:VAL:HG22	2:B:99:GLY:HA3	1.77	0.66
2:B:170:ARG:HA	2:B:226:LYS:HD3	1.77	0.66
1:C:58:LEU:O	1:C:63:TYR:HB2	1.96	0.65
2:B:173:TYR:CZ	2:B:225:ARG:HD2	2.31	0.65
1:A:186:HIS:CD2	1:A:188:ASP:H	2.14	0.65
2:B:5:LYS:NZ	2:B:16:ILE:HD12	2.11	0.65
1:C:237:ARG:HH21	1:C:237:ARG:HG2	1.62	0.65
1:C:365:ILE:HA	1:C:368:ILE:HG12	1.79	0.64
1:C:345:VAL:HG11	1:C:353:ILE:CD1	2.26	0.64
1:C:13:VAL:HG22	1:C:115:VAL:CB	2.26	0.64
2:D:72:LYS:HB2	2:D:75:LYS:HZ3	1.61	0.64
1:A:237:ARG:NH2	1:A:237:ARG:HG2	2.13	0.63
2:D:181:ARG:H	2:D:181:ARG:CD	1.95	0.63
1:A:294:GLY:O	1:A:295:ALA:HB2	1.99	0.63
1:A:275:LEU:HB3	1:A:293:LEU:HD22	1.79	0.63
2:D:6:LYS:CD	2:D:7:HIS:H	2.11	0.63
1:C:220:MET:HG2	1:C:224:ASP:CB	2.29	0.63
1:A:186:HIS:HD2	1:A:188:ASP:H	1.47	0.63
1:A:131:ARG:HA	1:A:134:MET:HE3	1.79	0.62
2:D:68:ASN:OD1	2:D:207:ILE:CG2	2.47	0.62
2:D:6:LYS:HE3	2:D:7:HIS:O	1.98	0.62
2:D:42:LYS:H	2:D:42:LYS:CD	2.13	0.62
2:B:161:ILE:HG22	2:B:165:LYS:HE3	1.81	0.62
1:C:13:VAL:HG22	1:C:115:VAL:HG21	1.82	0.61
2:D:77:VAL:HG12	2:D:146:VAL:HB	1.82	0.61
1:A:157:ARG:HH11	1:A:174:HIS:CD2	2.08	0.61
1:C:295:ALA:HB1	1:C:311:HIS:CA	2.30	0.61
1:A:78:LYS:HA	1:A:82:PHE:O	2.00	0.61
1:A:237:ARG:HH21	1:A:237:ARG:HG2	1.65	0.61
1:A:13:VAL:HG22	1:A:115:VAL:CB	2.30	0.61
2:B:205:GLU:O	2:B:207:ILE:HG13	2.00	0.61
2:B:216:GLU:HB3	2:B:219:HIS:CD2	2.36	0.61
2:B:78:LEU:HB2	2:B:144:VAL:HG21	1.82	0.61
2:D:105:GLU:HB3	2:D:111:LEU:HG	1.82	0.61
2:B:211:ASN:HD21	2:B:213:GLU:CG	2.06	0.61
1:A:28:LYS:HD3	1:A:30:TYR:CE2	2.36	0.60
2:D:208:GLU:HB3	2:D:223:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:HB2	1:A:67:VAL:CG1	2.30	0.60
1:A:131:ARG:HG3	1:A:134:MET:HE3	1.82	0.60
2:D:43:TRP:HB3	2:D:44:GLU:OE1	2.00	0.60
2:B:67:LYS:HB2	2:B:208:GLU:OE1	2.01	0.59
1:A:13:VAL:HG22	1:A:115:VAL:CG2	2.32	0.59
2:B:161:ILE:O	2:B:165:LYS:HG2	2.02	0.59
1:C:47:ILE:HG23	1:C:51:LEU:HD12	1.85	0.59
2:D:28:ASN:ND2	2:D:30:VAL:H	2.01	0.59
2:B:68:ASN:OD1	2:B:207:ILE:HG22	2.03	0.59
2:B:43:TRP:HB3	2:B:44:GLU:OE1	2.02	0.59
2:D:42:LYS:H	2:D:42:LYS:HD3	1.68	0.58
2:D:3:GLU:HB3	2:D:16:ILE:HD11	1.84	0.58
1:C:280:ARG:HG3	1:C:347:TYR:OH	2.02	0.58
2:B:204:PHE:HB3	2:B:224:VAL:HB	1.84	0.58
2:D:121:ARG:O	2:D:123:ASN:N	2.36	0.58
1:C:8:PHE:HB2	1:C:67:VAL:CG1	2.30	0.58
1:C:180:PHE:O	1:C:184:VAL:HG13	2.03	0.58
1:A:346:ASP:O	2:B:109:ARG:NH2	2.30	0.58
2:B:105:GLU:HB3	2:B:111:LEU:HG	1.85	0.57
2:B:33:GLN:NE2	2:B:121:ARG:HE	2.01	0.57
2:B:111:LEU:O	2:B:111:LEU:HD22	2.04	0.57
2:D:77:VAL:HG22	2:D:101:ILE:HG12	1.87	0.57
1:C:170:LEU:HD23	1:C:208:ILE:HG12	1.86	0.57
1:A:94:GLU:OE1	2:B:143:LYS:HE3	2.05	0.57
2:B:16:ILE:HG22	2:B:22:GLU:HA	1.85	0.57
1:C:13:VAL:HG22	1:C:115:VAL:CG2	2.35	0.57
2:B:5:LYS:HZ1	2:B:16:ILE:HD12	1.68	0.57
2:B:211:ASN:ND2	2:B:213:GLU:CG	2.67	0.57
2:D:211:ASN:HD21	2:D:213:GLU:CG	2.15	0.57
2:B:168:LEU:O	2:B:226:LYS:HE3	2.04	0.57
2:D:42:LYS:N	2:D:42:LYS:HD3	2.19	0.57
1:C:237:ARG:NH2	1:C:237:ARG:HG2	2.19	0.56
2:B:40:VAL:CG1	2:B:47:GLU:HG2	2.35	0.56
2:D:211:ASN:HD22	2:D:213:GLU:H	1.51	0.56
1:A:295:ALA:HB1	1:A:311:HIS:CA	2.36	0.56
1:A:113:TYR:O	1:A:117:VAL:HG23	2.05	0.56
2:B:147:ILE:HG13	2:B:168:LEU:HD13	1.88	0.55
2:B:88:ALA:HA	2:B:91:VAL:HG13	1.89	0.55
2:D:204:PHE:HB3	2:D:224:VAL:HB	1.88	0.55
2:B:206:VAL:HA	2:B:224:VAL:HG12	1.88	0.55
1:C:13:VAL:HG21	1:C:115:VAL:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ILE:O	1:C:190:ILE:HG22	2.06	0.55
1:C:186:HIS:CD2	1:C:188:ASP:H	2.23	0.55
2:B:6:LYS:HD2	2:B:7:HIS:H	1.70	0.55
2:B:6:LYS:HE3	2:B:7:HIS:O	2.06	0.55
1:A:330:LYS:CD	1:A:368:ILE:HG23	2.36	0.55
1:C:196:ARG:HG2	1:C:196:ARG:HH11	1.71	0.55
2:D:3:GLU:O	2:D:16:ILE:HD13	2.06	0.54
2:D:188:GLU:HB3	2:D:191:GLN:HB2	1.88	0.54
1:C:180:PHE:HZ	1:C:190:ILE:HD11	1.72	0.54
2:D:27:LYS:HE3	2:D:93:ASP:O	2.07	0.54
1:A:280:ARG:HG3	1:A:347:TYR:OH	2.08	0.54
1:A:295:ALA:CB	1:A:311:HIS:HA	2.37	0.54
2:D:198:ARG:HH21	2:D:199:GLU:HA	1.73	0.54
1:C:295:ALA:CB	1:C:312:GLY:H	2.19	0.54
1:A:330:LYS:HD2	1:A:368:ILE:HG23	1.88	0.54
2:D:211:ASN:ND2	2:D:213:GLU:H	2.05	0.54
2:D:40:VAL:CG1	2:D:47:GLU:HG2	2.37	0.54
1:A:345:VAL:HG11	1:A:353:ILE:CD1	2.34	0.54
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.73	0.54
1:C:70:HIS:CE1	1:C:72:GLU:HB3	2.43	0.54
1:A:331:ILE:HG23	1:A:365:ILE:HD11	1.90	0.54
1:C:16:ILE:HG21	1:C:51:LEU:HD23	1.90	0.53
1:A:280:ARG:HG3	1:A:347:TYR:CZ	2.42	0.53
1:C:135:VAL:HG11	1:C:253:MET:HE2	1.89	0.53
1:C:13:VAL:HG22	1:C:115:VAL:HB	1.87	0.53
1:C:82:PHE:N	1:C:82:PHE:CD1	2.75	0.53
1:A:174:HIS:HB2	1:A:175:PRO:HD3	1.90	0.53
2:D:211:ASN:ND2	2:D:213:GLU:CG	2.70	0.53
1:C:13:VAL:CG2	1:C:115:VAL:CB	2.83	0.53
1:A:259:ASN:ND2	1:A:346:ASP:OD1	2.39	0.52
2:D:207:ILE:HD11	2:D:225:ARG:HB2	1.91	0.52
2:D:43:TRP:CE3	2:D:43:TRP:HA	2.45	0.52
1:C:295:ALA:CB	1:C:312:GLY:N	2.73	0.52
2:D:78:LEU:HB2	2:D:144:VAL:HG21	1.91	0.52
1:C:311:HIS:CD2	1:C:311:HIS:N	2.77	0.52
2:D:88:ALA:HA	2:D:91:VAL:HG13	1.90	0.52
2:D:3:GLU:HA	2:D:43:TRP:CH2	2.44	0.52
1:A:70:HIS:CE1	1:A:72:GLU:HB3	2.45	0.52
1:C:295:ALA:HB3	1:C:312:GLY:N	2.22	0.51
2:B:16:ILE:N	2:B:16:ILE:HD13	2.22	0.51
1:A:135:VAL:HG21	1:A:253:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:O	1:A:178:VAL:HG23	2.10	0.51
2:B:135:GLU:CD	2:B:135:GLU:H	2.13	0.51
2:D:115:VAL:O	2:D:118:VAL:HG22	2.10	0.51
1:A:11:GLU:HG2	1:A:42:LEU:HD13	1.91	0.51
1:C:341:ILE:O	1:C:345:VAL:HG12	2.11	0.51
2:D:216:GLU:HB3	2:D:219:HIS:CD2	2.46	0.51
1:A:14:ARG:HD2	1:C:325:TRP:CD1	2.46	0.51
2:D:43:TRP:HA	2:D:43:TRP:HE3	1.74	0.51
2:B:121:ARG:O	2:B:123:ASN:N	2.38	0.51
2:D:41:ILE:HG13	2:D:41:ILE:O	2.10	0.51
1:C:259:ASN:ND2	1:C:346:ASP:OD1	2.43	0.51
1:C:136:ILE:O	1:C:140:GLU:HG2	2.11	0.51
2:B:3:GLU:O	2:B:16:ILE:HD13	2.11	0.51
2:D:67:LYS:C	2:D:68:ASN:HD22	2.14	0.51
2:B:207:ILE:HB	2:B:223:VAL:HG23	1.92	0.51
1:A:13:VAL:HG21	1:A:115:VAL:HB	1.92	0.51
2:D:38:GLU:OE2	2:D:49:ARG:NH2	2.38	0.51
2:B:51:TRP:CH2	2:B:58:LEU:HD13	2.46	0.50
2:B:77:VAL:HG22	2:B:101:ILE:HG12	1.94	0.50
1:A:13:VAL:HG22	1:A:115:VAL:HB	1.88	0.50
2:D:187:LYS:HZ2	2:D:187:LYS:HB2	1.73	0.50
2:D:77:VAL:HA	2:D:146:VAL:O	2.11	0.50
2:B:7:HIS:HB2	2:B:14:VAL:HG23	1.93	0.50
2:D:152:ALA:O	2:D:153:GLN:HG2	2.12	0.50
1:A:295:ALA:CB	1:A:312:GLY:N	2.74	0.50
2:D:187:LYS:HG2	2:D:191:GLN:HB3	1.93	0.50
1:A:157:ARG:NH1	1:A:174:HIS:HD2	1.97	0.50
1:C:174:HIS:HB2	1:C:175:PRO:HD3	1.93	0.50
1:A:166:GLU:O	1:A:170:LEU:HD13	2.12	0.50
2:B:173:TYR:CD1	2:B:225:ARG:HG3	2.47	0.50
2:B:77:VAL:HA	2:B:146:VAL:O	2.11	0.50
2:B:208:GLU:HB3	2:B:223:VAL:HG22	1.94	0.49
2:B:187:LYS:HG2	2:B:191:GLN:HB3	1.94	0.49
1:A:180:PHE:HZ	1:A:190:ILE:HD11	1.76	0.49
1:A:275:LEU:HD13	1:A:294:GLY:CA	2.41	0.49
1:C:280:ARG:HG3	1:C:347:TYR:CZ	2.47	0.49
1:C:174:HIS:O	1:C:178:VAL:HG23	2.12	0.49
2:D:42:LYS:H	2:D:42:LYS:HZ3	1.60	0.49
1:A:246:GLU:HG2	1:A:267:LYS:NZ	2.28	0.49
1:C:8:PHE:HA	1:C:19:PHE:O	2.12	0.49
1:A:13:VAL:CG2	1:A:115:VAL:CB	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:VAL:HG11	2:B:47:GLU:HG2	1.95	0.49
1:C:275:LEU:HD13	1:C:294:GLY:CA	2.40	0.49
2:D:6:LYS:NZ	2:D:10:PRO:HA	2.28	0.49
1:C:117:VAL:O	1:C:121:ARG:HG3	2.13	0.49
2:B:29:LEU:HG	2:B:29:LEU:O	2.13	0.49
1:A:215:THR:HG23	1:A:215:THR:O	2.13	0.49
2:D:16:ILE:HG12	2:D:16:ILE:O	2.12	0.49
2:D:95:VAL:HG22	2:D:99:GLY:HA3	1.95	0.49
2:B:51:TRP:HH2	2:B:58:LEU:HD13	1.78	0.49
2:D:29:LEU:HD11	2:D:97:TRP:NE1	2.28	0.48
2:D:66:LEU:HA	2:D:210:LEU:HD22	1.95	0.48
2:D:4:VAL:HG22	2:D:15:VAL:HB	1.95	0.48
1:A:220:MET:HG2	1:A:224:ASP:HB3	1.95	0.48
1:A:131:ARG:HG3	1:A:134:MET:CE	2.43	0.48
2:B:75:LYS:O	2:B:95:VAL:CG2	2.62	0.48
1:C:113:TYR:O	1:C:117:VAL:HG23	2.13	0.48
2:B:187:LYS:HD3	2:B:191:GLN:NE2	2.29	0.48
2:D:56:SER:HG	2:D:87:THR:HB	1.79	0.48
1:C:186:HIS:HD2	1:C:187:ARG:N	2.12	0.48
1:C:125:GLN:HG3	1:C:251:ARG:HH12	1.79	0.47
2:B:36:TYR:CE1	2:B:38:GLU:HG2	2.49	0.47
1:A:194:VAL:HG23	1:A:195:LEU:N	2.29	0.47
1:A:186:HIS:HD2	1:A:187:ARG:N	2.12	0.47
1:C:28:LYS:HD3	1:C:30:TYR:CE2	2.49	0.47
1:C:143:ASP:OD2	1:C:271:ARG:NH1	2.48	0.47
2:B:173:TYR:CE1	2:B:225:ARG:HG3	2.48	0.47
1:A:78:LYS:HB3	1:A:78:LYS:HZ2	1.78	0.47
1:C:101:GLU:HA	1:C:105:GLY:O	2.15	0.47
1:C:198:LEU:HB2	1:C:200:LEU:HD13	1.96	0.47
2:D:207:ILE:HD11	2:D:225:ARG:HD3	1.97	0.47
2:D:16:ILE:HD13	2:D:16:ILE:N	2.20	0.47
2:B:16:ILE:O	2:B:16:ILE:HG12	2.15	0.47
2:B:3:GLU:HB3	2:B:16:ILE:HD11	1.95	0.47
2:D:121:ARG:C	2:D:123:ASN:N	2.66	0.47
1:A:186:HIS:CD2	1:A:187:ARG:N	2.82	0.47
1:A:78:LYS:HB3	1:A:78:LYS:NZ	2.30	0.47
1:C:101:GLU:H	1:C:101:GLU:CD	2.18	0.47
2:D:147:ILE:HG13	2:D:168:LEU:HD13	1.96	0.47
2:D:6:LYS:CG	2:D:7:HIS:N	2.78	0.47
1:C:125:GLN:HG3	1:C:251:ARG:NH1	2.30	0.47
1:A:246:GLU:HG2	1:A:267:LYS:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LYS:HD2	1:C:266:ALA:HB2	1.95	0.47
1:A:341:ILE:O	1:A:345:VAL:HG12	2.15	0.46
2:D:111:LEU:HD22	2:D:111:LEU:O	2.15	0.46
1:A:117:VAL:O	1:A:121:ARG:HG3	2.15	0.46
2:D:40:VAL:HG12	2:D:47:GLU:HG2	1.97	0.46
2:D:197:GLU:HG3	2:D:206:VAL:HG21	1.97	0.46
1:A:101:GLU:HA	1:A:105:GLY:O	2.16	0.46
1:A:365:ILE:HA	1:A:368:ILE:HG12	1.97	0.46
1:C:242:ARG:HH11	1:C:242:ARG:CG	2.24	0.46
2:D:82:ILE:HD13	2:D:103:GLY:HA3	1.98	0.46
2:D:82:ILE:HG22	2:D:105:GLU:HB2	1.97	0.46
1:C:194:VAL:HG23	1:C:195:LEU:N	2.30	0.46
2:D:208:GLU:HG2	2:D:209:ARG:N	2.31	0.46
2:B:43:TRP:CD1	2:B:44:GLU:HG3	2.51	0.46
2:D:72:LYS:HD3	2:D:75:LYS:HZ3	1.80	0.46
2:D:72:LYS:HD3	2:D:75:LYS:NZ	2.31	0.46
1:C:20:ASP:OD1	1:C:24:ASN:HB2	2.15	0.46
2:D:7:HIS:HB2	2:D:14:VAL:HG23	1.98	0.46
2:D:6:LYS:HD2	2:D:7:HIS:N	2.29	0.46
2:D:41:ILE:HA	2:D:42:LYS:HZ2	1.81	0.46
1:C:275:LEU:CB	1:C:293:LEU:HD22	2.44	0.46
2:B:33:GLN:HE22	2:B:121:ARG:NE	2.06	0.46
1:C:242:ARG:NH1	1:C:242:ARG:CG	2.79	0.46
1:A:359:LYS:HE2	2:B:183:ILE:O	2.16	0.46
1:C:191:ASN:HD22	1:C:194:VAL:HG13	1.80	0.45
1:A:58:LEU:O	1:A:63:TYR:HB2	2.16	0.45
1:A:8:PHE:HA	1:A:19:PHE:O	2.16	0.45
2:D:75:LYS:O	2:D:95:VAL:CG2	2.64	0.45
2:D:6:LYS:HZ3	2:D:10:PRO:HA	1.81	0.45
1:A:15:GLY:HA2	1:A:31:PHE:CE1	2.50	0.45
2:B:208:GLU:HG2	2:B:209:ARG:N	2.32	0.45
2:B:6:LYS:CD	2:B:7:HIS:H	2.29	0.45
2:D:34:ARG:NH1	2:D:38:GLU:O	2.49	0.45
1:A:29:ARG:HH11	1:A:32:THR:CG2	2.29	0.45
1:C:20:ASP:HA	1:C:26:ILE:HD11	1.99	0.45
1:C:281:GLU:H	1:C:281:GLU:CD	2.18	0.45
1:A:17:TYR:CD1	1:A:17:TYR:N	2.84	0.45
1:C:157:ARG:NH1	1:C:174:HIS:HD2	2.02	0.45
1:A:131:ARG:HA	1:A:134:MET:HE2	1.96	0.45
1:A:78:LYS:HG3	1:A:79:GLU:N	2.32	0.45
2:D:187:LYS:HZ3	2:D:187:LYS:HB2	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:LEU:HA	2:D:111:LEU:HD23	1.73	0.45
1:C:36:GLU:HG2	1:C:118:ALA:HB1	1.99	0.45
1:A:134:MET:HB2	1:A:134:MET:HE3	1.80	0.44
2:B:187:LYS:HD3	2:B:191:GLN:HE21	1.82	0.44
1:C:226:GLU:HA	1:C:226:GLU:OE1	2.17	0.44
2:B:24:ILE:CG2	2:B:51:TRP:HB3	2.35	0.44
1:C:16:ILE:HD11	1:C:42:LEU:HD11	1.98	0.44
1:C:205:ILE:HG22	1:C:209:LEU:HD12	1.98	0.44
1:A:36:GLU:HG2	1:A:118:ALA:HB1	2.00	0.44
1:C:311:HIS:CD2	1:C:311:HIS:H	2.35	0.44
1:C:57:SER:HA	1:C:60:GLU:HG2	1.97	0.44
1:C:16:ILE:HG22	1:C:54:LEU:CD2	2.48	0.44
1:A:29:ARG:HH11	1:A:32:THR:HG21	1.82	0.44
1:C:21:GLU:HG2	1:C:21:GLU:O	2.16	0.44
1:C:145:VAL:O	1:C:149:ILE:HG13	2.18	0.44
1:A:59:LYS:C	1:A:61:LYS:H	2.20	0.44
1:A:364:ARG:O	1:A:368:ILE:HG12	2.16	0.44
2:B:76:SER:OG	2:B:144:VAL:HA	2.18	0.44
2:B:155:THR:CG2	2:B:158:LYS:HE2	2.41	0.44
2:B:67:LYS:HB2	2:B:208:GLU:CD	2.39	0.43
1:C:113:TYR:OH	2:D:118:VAL:O	2.26	0.43
1:A:135:VAL:HG21	1:A:253:MET:CE	2.48	0.43
2:B:180:SER:OG	2:B:189:PRO:HA	2.18	0.43
2:B:196:VAL:O	2:B:200:LEU:HB2	2.17	0.43
2:B:24:ILE:HD13	2:B:24:ILE:HA	1.79	0.43
2:D:43:TRP:HB2	2:D:48:TYR:CE1	2.53	0.43
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.84	0.43
1:C:8:PHE:O	1:C:18:ALA:HA	2.18	0.43
1:C:201:SER:O	1:C:205:ILE:HG13	2.18	0.43
2:B:16:ILE:HG22	2:B:22:GLU:CA	2.49	0.43
2:D:6:LYS:CG	2:D:7:HIS:H	2.30	0.43
2:B:82:ILE:HG22	2:B:105:GLU:HB2	2.01	0.43
1:C:166:GLU:O	1:C:170:LEU:HD13	2.18	0.43
1:C:14:ARG:HD3	1:C:111:GLU:OE2	2.19	0.43
1:A:34:LYS:HB2	1:A:37:LYS:HG3	2.01	0.43
2:D:210:LEU:HD12	2:D:211:ASN:N	2.33	0.43
1:A:70:HIS:HE1	1:A:72:GLU:HB3	1.84	0.43
1:C:212:LYS:HD2	1:C:212:LYS:O	2.19	0.43
1:C:142:LEU:HG	1:C:242:ARG:HH12	1.84	0.43
1:C:226:GLU:O	1:C:230:GLN:HG2	2.19	0.42
1:A:338:LYS:HG3	1:A:361:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.31	0.42
1:C:186:HIS:CD2	1:C:187:ARG:N	2.87	0.42
2:D:36:TYR:CE1	2:D:38:GLU:HG2	2.55	0.42
1:A:311:HIS:NE2	1:A:325:TRP:HH2	2.17	0.42
2:D:9:PHE:HA	2:D:10:PRO:HD3	1.88	0.42
2:B:115:VAL:O	2:B:118:VAL:HG22	2.20	0.42
1:C:294:GLY:O	1:C:295:ALA:HB2	2.19	0.42
2:D:82:ILE:CD1	2:D:103:GLY:HA3	2.50	0.42
1:A:180:PHE:O	1:A:184:VAL:CG1	2.68	0.42
1:C:78:LYS:C	1:C:80:LEU:H	2.21	0.42
1:A:136:ILE:O	1:A:140:GLU:HG2	2.19	0.42
2:B:121:ARG:C	2:B:123:ASN:N	2.69	0.42
1:C:242:ARG:NH1	1:C:242:ARG:HG3	2.30	0.42
1:A:200:LEU:HD22	1:A:204:LYS:HD2	2.02	0.42
1:C:125:GLN:HE22	1:C:252:ALA:HA	1.83	0.42
2:B:161:ILE:CG2	2:B:165:LYS:HE3	2.48	0.42
1:A:220:MET:HG2	1:A:224:ASP:CB	2.50	0.42
1:A:237:ARG:HH21	1:A:237:ARG:CG	2.33	0.42
1:C:229:ARG:O	1:C:233:GLU:HG3	2.20	0.42
2:D:6:LYS:HG3	2:D:7:HIS:N	2.34	0.42
2:B:14:VAL:C	2:B:15:VAL:HG12	2.40	0.42
1:A:101:GLU:CD	1:A:101:GLU:H	2.24	0.42
2:B:134:PRO:HA	2:B:137:TYR:CZ	2.55	0.41
1:C:170:LEU:HD23	1:C:208:ILE:CG1	2.50	0.41
2:B:188:GLU:HB3	2:B:191:GLN:HB2	2.02	0.41
1:C:260:LEU:HA	1:C:260:LEU:HD23	1.71	0.41
1:C:320:ILE:HD11	1:C:332:ALA:HA	2.01	0.41
1:A:78:LYS:C	1:A:80:LEU:H	2.23	0.41
2:D:153:GLN:O	2:D:156:GLN:HB2	2.20	0.41
2:B:3:GLU:HA	2:B:43:TRP:CZ3	2.56	0.41
1:C:194:VAL:O	1:C:198:LEU:HG	2.20	0.41
2:B:66:LEU:HA	2:B:210:LEU:HD22	2.01	0.41
1:C:82:PHE:HD1	1:C:82:PHE:H	1.63	0.41
1:C:180:PHE:C	1:C:180:PHE:CD1	2.94	0.41
1:A:191:ASN:H	1:A:194:VAL:CG2	2.33	0.41
1:A:143:ASP:OD2	1:A:271:ARG:NH1	2.53	0.41
1:A:142:LEU:CD2	1:A:267:LYS:HE3	2.49	0.41
1:C:173:LYS:O	1:C:176:GLN:HB2	2.19	0.41
2:B:207:ILE:O	2:B:208:GLU:HB2	2.20	0.41
2:B:68:ASN:OD1	2:B:207:ILE:CG2	2.69	0.41
1:A:311:HIS:CE1	1:A:325:TRP:CH2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:THR:HG22	2:B:158:LYS:CE	2.43	0.41
1:A:180:PHE:O	1:A:184:VAL:HG13	2.20	0.41
2:B:28:ASN:ND2	2:B:30:VAL:H	2.19	0.41
2:B:4:VAL:HG12	2:B:5:LYS:N	2.35	0.41
2:B:82:ILE:HD13	2:B:103:GLY:HA3	2.02	0.41
1:C:214:LYS:HG2	1:C:214:LYS:O	2.20	0.41
1:C:186:HIS:HD2	1:C:188:ASP:H	1.65	0.41
1:C:257:ALA:HB1	1:C:260:LEU:HB2	2.03	0.41
1:C:130:ALA:O	1:C:134:MET:HG3	2.20	0.41
1:C:70:HIS:CE1	1:C:72:GLU:CB	3.04	0.41
1:A:14:ARG:HD3	1:A:111:GLU:OE2	2.21	0.41
1:C:90:ASN:OD1	1:C:92:ALA:HB3	2.21	0.41
2:B:203:TYR:O	2:B:227:PRO:HD3	2.21	0.41
1:A:330:LYS:HD3	1:A:368:ILE:HG23	2.03	0.40
1:C:157:ARG:NH2	1:C:177:TYR:CD1	2.89	0.40
2:B:113:GLU:O	2:B:116:PRO:HD2	2.21	0.40
2:D:149:GLU:OE1	2:D:160:LEU:HB2	2.21	0.40
2:B:24:ILE:HG22	2:B:51:TRP:CB	2.37	0.40
2:B:77:VAL:HG12	2:B:146:VAL:HB	2.04	0.40
2:D:39:ARG:CG	2:D:39:ARG:HH11	2.35	0.40
2:D:126:PRO:HG2	2:D:126:PRO:O	2.22	0.40
1:A:253:MET:HB3	1:A:261:LYS:HD3	2.04	0.40
2:B:207:ILE:HG22	2:B:207:ILE:O	2.21	0.40
2:D:118:VAL:HG12	2:D:124:ILE:HB	2.03	0.40
1:A:139:ILE:HA	1:A:139:ILE:HD13	1.87	0.40
1:A:46:GLU:HG2	1:A:76:ARG:HH12	1.86	0.40
1:C:295:ALA:HB1	1:C:310:LYS:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:OE2	1:A:234:GLU:OE2[4_775]	1.73	0.47
1:A:147:LYS:NZ	1:A:147:LYS:NZ[4_775]	1.87	0.33
1:C:147:LYS:NZ	1:C:147:LYS:NZ[6_576]	1.95	0.25
1:C:234:GLU:OE2	1:C:234:GLU:OE2[6_576]	2.00	0.20

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	346/376 (92%)	326 (94%)	17 (5%)	3 (1%)	21	49
1	C	346/376 (92%)	321 (93%)	22 (6%)	3 (1%)	21	49
2	B	225/234 (96%)	204 (91%)	16 (7%)	5 (2%)	8	22
2	D	225/234 (96%)	200 (89%)	22 (10%)	3 (1%)	15	37
All	All	1142/1220 (94%)	1051 (92%)	77 (7%)	14 (1%)	16	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	156	GLN
1	A	312	GLY
2	B	122	ARG
2	B	156	GLN
2	B	206	VAL
1	C	312	GLY
2	D	122	ARG
2	D	206	VAL
1	A	20	ASP
2	B	28	ASN
1	C	49	LYS
1	A	60	GLU
2	B	136	GLU
1	C	20	ASP

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	299/321 (93%)	269 (90%)	30 (10%)	9 22
1	C	299/321 (93%)	267 (89%)	32 (11%)	8 19
2	B	197/204 (97%)	167 (85%)	30 (15%)	3 9
2	D	197/204 (97%)	169 (86%)	28 (14%)	4 10
All	All	992/1050 (94%)	872 (88%)	120 (12%)	6 14

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	13	VAL
1	A	14	ARG
1	A	21	GLU
1	A	25	LEU
1	A	50	ASP
1	A	78	LYS
1	A	86	THR
1	A	99	ASN
1	A	101	GLU
1	A	139	ILE
1	A	147	LYS
1	A	148	VAL
1	A	156	LEU
1	A	164	PHE
1	A	184	VAL
1	A	193	GLU
1	A	196	ARG
1	A	212	LYS
1	A	213	GLU
1	A	231	LEU
1	A	242	ARG
1	A	271	ARG
1	A	293	LEU
1	A	296	GLU
1	A	310	LYS
1	A	311	HIS
1	A	318	PRO
1	A	335	LEU
1	A	357	LEU
2	B	15	VAL
2	B	16	ILE
2	B	18	ASP

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Mol	Chain	Res	Type
2	B	24	ILE
2	B	27	LYS
2	B	28	ASN
2	B	38	GLU
2	B	39	ARG
2	B	42	LYS
2	B	44	GLU
2	B	57	LYS
2	B	58	LEU
2	B	68	ASN
2	B	78	LEU
2	B	79	TYR
2	B	84	SER
2	B	87	THR
2	B	95	VAL
2	B	111	LEU
2	B	117	ILE
2	B	122	ARG
2	B	123	ASN
2	B	143	LYS
2	B	155	THR
2	B	181	ARG
2	B	189	PRO
2	B	191	GLN
2	B	198	ARG
2	B	200	LEU
2	B	217	LYS
1	C	8	PHE
1	C	13	VAL
1	C	25	LEU
1	C	51	LEU
1	C	76	ARG
1	C	78	LYS
1	C	82	PHE
1	C	85	THR
1	C	96	LEU
1	C	101	GLU
1	C	133	LYS
1	C	139	ILE
1	C	147	LYS
1	C	156	LEU
1	C	162	LEU

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Mol	Chain	Res	Type
1	C	164	PHE
1	C	184	VAL
1	C	193	GLU
1	C	212	LYS
1	C	213	GLU
1	C	231	LEU
1	C	267	LYS
1	C	271	ARG
1	C	293	LEU
1	C	296	GLU
1	C	311	HIS
1	C	313	VAL
1	C	318	PRO
1	C	335	LEU
1	C	355	GLU
1	C	357	LEU
1	C	358	LYS
2	D	16	ILE
2	D	18	ASP
2	D	22	GLU
2	D	27	LYS
2	D	28	ASN
2	D	38	GLU
2	D	39	ARG
2	D	42	LYS
2	D	43	TRP
2	D	44	GLU
2	D	57	LYS
2	D	58	LEU
2	D	68	ASN
2	D	78	LEU
2	D	79	TYR
2	D	84	SER
2	D	87	THR
2	D	111	LEU
2	D	123	ASN
2	D	154	PRO
2	D	155	THR
2	D	181	ARG
2	D	187	LYS
2	D	191	GLN
2	D	195	GLU

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Mol	Chain	Res	Type
2	D	198	ARG
2	D	201	SER
2	D	217	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	150	ASN
1	A	174	HIS
1	A	176	GLN
1	A	186	HIS
1	A	240	GLN
1	A	291	GLN
2	B	28	ASN
2	B	33	GLN
2	B	64	ASN
2	B	68	ASN
2	B	123	ASN
2	B	156	GLN
2	B	211	ASN
2	B	219	HIS
1	C	125	GLN
1	C	150	ASN
1	C	174	HIS
1	C	176	GLN
1	C	186	HIS
1	C	191	ASN
1	C	240	GLN
1	C	291	GLN
1	C	311	HIS
2	D	28	ASN
2	D	33	GLN
2	D	64	ASN
2	D	68	ASN
2	D	123	ASN
2	D	156	GLN
2	D	211	ASN
2	D	219	HIS

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	350/376 (93%)	0.49	8 (2%)	64	64	30, 58, 102, 115	0
1	C	350/376 (93%)	0.50	9 (2%)	59	59	32, 59, 103, 118	0
2	B	227/234 (97%)	0.51	9 (3%)	42	41	34, 64, 92, 127	0
2	D	227/234 (97%)	0.52	8 (3%)	48	48	34, 64, 94, 128	0
All	All	1154/1220 (94%)	0.50	34 (2%)	55	55	30, 61, 101, 128	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	PHE	4.2
1	A	54	LEU	4.0
2	D	221	LEU	3.4
2	D	200	LEU	3.3
1	C	42	LEU	3.2
2	B	200	LEU	3.2
2	D	5	LYS	3.0
1	A	58	LEU	2.9
1	C	368	ILE	2.9
2	B	1	MET	2.9
1	A	82	PHE	2.8
1	A	55	LEU	2.7
1	A	190	ILE	2.7
1	C	195	LEU	2.6
1	A	294	GLY	2.6
2	B	196	VAL	2.6
2	B	193	PHE	2.5
2	B	181	ARG	2.5
1	C	66	PHE	2.4
2	B	222	PHE	2.4
2	D	15	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	23	GLY	2.3
1	C	190	ILE	2.3
2	B	41	ILE	2.3
1	A	225	ILE	2.2
1	C	87	GLU	2.2
1	C	51	LEU	2.1
1	A	47	ILE	2.1
2	B	63	VAL	2.1
2	B	50	ILE	2.1
2	D	193	PHE	2.0
2	D	98	GLU	2.0
2	D	66	LEU	2.0
2	D	50	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.