WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:59 AM GMT

PDB ID : 2JLF
Title : STRUCTURAL EXPLANATION FOR THE ROLE OF MN IN THE ACTIV-
ITY OF PHI6 RNA-DEPENDENT RNA POLYMERASE
Authors : Poranen, M.M.; Salgado, P.S.; Koivunen, M.R.L.; Wright, S.; Bamford, D.H.;
Stuart, D.I.; Grimes, J.M.
Deposited on : 2008-09-08
Resolution : 3.20 Å(reported)

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

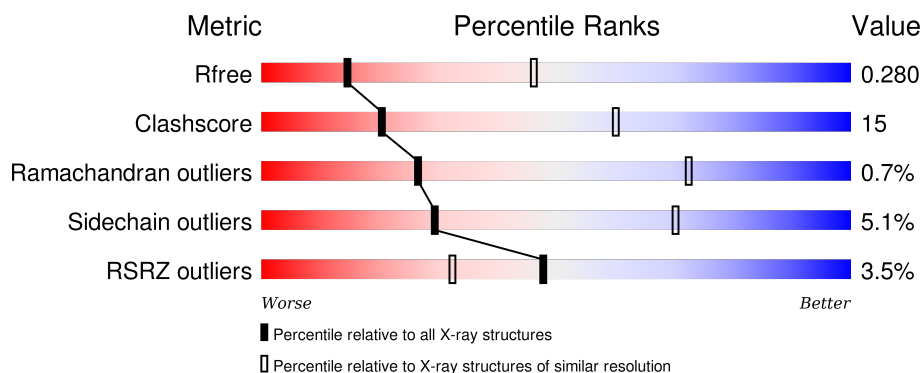|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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		0.280
Clashscore		15
Ramachandran outliers		0.7%
Sidechain outliers		5.1%
RSRZ outliers		3.5%

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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	664	67% 28% • •
1	B	664	2% 66% 30% •
1	C	664	8% 65% 30% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15610 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total 5186	C 3297	N 895	O 963	S 31	0	0	0
1	B	661	Total 5235	C 3325	N 906	O 972	S 32	0	0	0
1	C	654	Total 5187	C 3298	N 895	O 963	S 31	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	CONFLICT	UNP P11124
A	491	GLN	GLU	ENGINEERED MUTATION	UNP P11124
B	456	MET	ILE	CONFLICT	UNP P11124
B	491	GLN	GLU	ENGINEERED MUTATION	UNP P11124
C	456	MET	ILE	CONFLICT	UNP P11124
C	491	GLN	GLU	ENGINEERED MUTATION	UNP P11124

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 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 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: RNA-DIRECTED RNA POLYMERASE
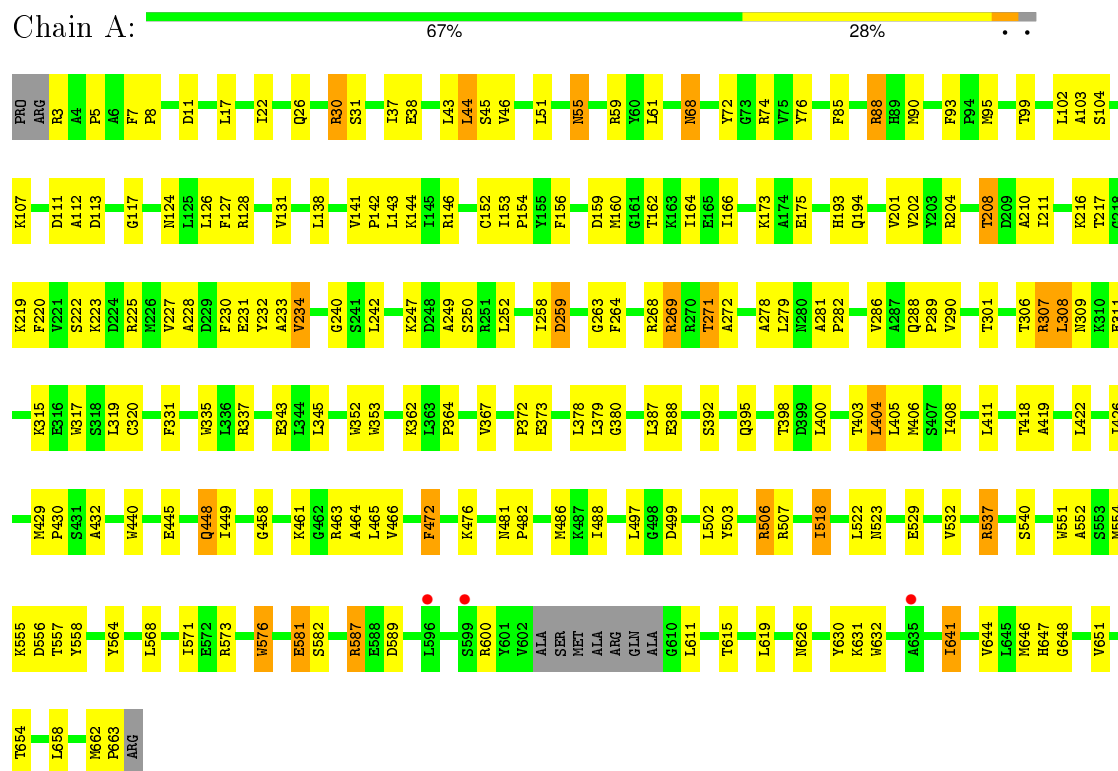
- Molecule 1: RNA-DIRECTED RNA POLYMERASE
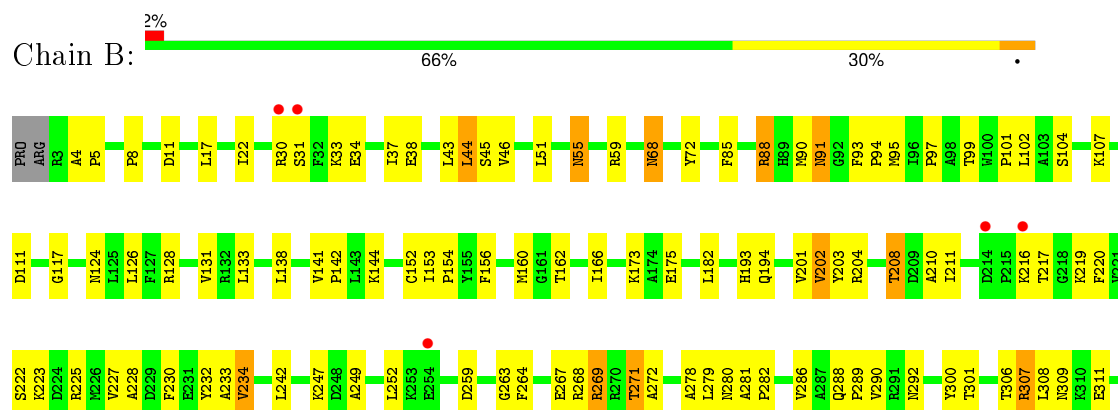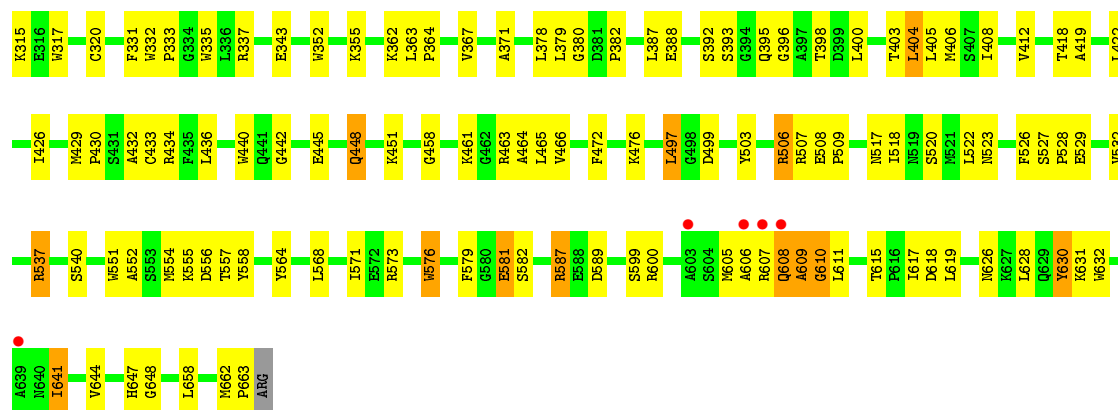
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

4   Data and refinement statistics (i)

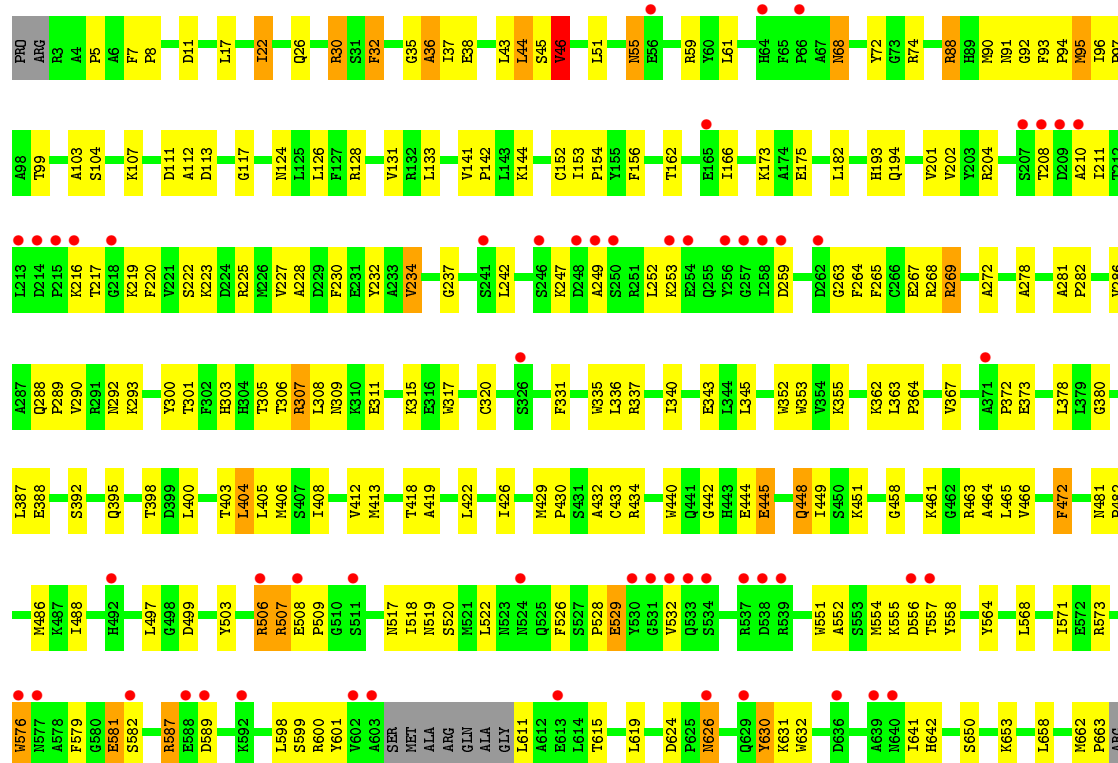| Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	110.04Å 110.04Å 159.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.02 – 3.20 18.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (18.02-3.20) 99.9 (18.02-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.21Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.228 , 0.286 0.217 , 0.280	Depositor DCC
R_{free} test set	1771 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
Estimated twinning fraction	0.017 for -h,-k,l 0.049 for h,-h-k,-l 0.031 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 35350 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15610	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.38	0/5315	0.79	15/7190 (0.2%)
1	B	0.38	0/5365	0.73	16/7258 (0.2%)
1	C	0.36	0/5316	0.68	14/7192 (0.2%)
All	All	0.37	0/15996	0.73	45/21640 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ARG	NE-CZ-NH2	19.49	130.05	120.30
1	A	506	ARG	NE-CZ-NH1	-18.51	111.05	120.30
1	A	269	ARG	NE-CZ-NH2	17.44	129.02	120.30
1	B	204	ARG	NE-CZ-NH1	-17.39	111.61	120.30
1	A	269	ARG	NE-CZ-NH1	-17.25	111.67	120.30
1	A	307	ARG	NE-CZ-NH1	-17.11	111.75	120.30
1	B	204	ARG	NE-CZ-NH2	16.78	128.69	120.30
1	C	88	ARG	NE-CZ-NH1	-16.25	112.17	120.30
1	A	307	ARG	NE-CZ-NH2	15.79	128.20	120.30
1	C	88	ARG	NE-CZ-NH2	15.79	128.20	120.30
1	B	30	ARG	NE-CZ-NH1	-13.19	113.71	120.30
1	B	30	ARG	NE-CZ-NH2	12.71	126.65	120.30
1	B	307	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	506	ARG	CD-NE-CZ	9.25	136.55	123.60
1	C	307	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	B	269	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	B	537	ARG	CB-CG-CD	8.98	134.94	111.60
1	B	88	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	C	269	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	B	269	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	C	506	ARG	NE-CZ-NH2	-8.61	115.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	C	307	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	269	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	88	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	B	307	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	88	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	204	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	88	ARG	CD-NE-CZ	8.18	135.06	123.60
1	B	506	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	506	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	204	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	204	ARG	CD-NE-CZ	7.88	134.63	123.60
1	A	307	ARG	CD-NE-CZ	7.82	134.55	123.60
1	A	269	ARG	CD-NE-CZ	7.80	134.52	123.60
1	C	204	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	88	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	506	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	30	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	30	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	30	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	30	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	628	LEU	CA-CB-CG	6.12	129.39	115.30
1	C	46	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	B	30	ARG	CD-NE-CZ	5.51	131.31	123.60

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	5186	0	5080	148	2
1	B	5235	0	5131	149	0
1	C	5187	0	5082	159	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15610	0	15293	452	2

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 15.

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)
1:B:364:PRO:HA	1:B:387:LEU:CD1	1.96	0.96
1:B:99:THR:HB	1:B:227:VAL:HG12	1.50	0.93
1:C:364:PRO:HA	1:C:387:LEU:CD1	1.99	0.91
1:B:364:PRO:HA	1:B:387:LEU:HD12	1.53	0.89
1:A:364:PRO:HA	1:A:387:LEU:CD1	2.01	0.89
1:C:364:PRO:HA	1:C:387:LEU:HD12	1.57	0.85
1:A:364:PRO:HA	1:A:387:LEU:HD12	1.56	0.85
1:B:126:LEU:HD21	1:B:426:ILE:HD13	1.58	0.84
1:C:461:LYS:HA	1:C:465:LEU:HD22	1.58	0.84
1:C:99:THR:HB	1:C:227:VAL:HG12	1.61	0.82
1:A:126:LEU:HD21	1:A:426:ILE:HD13	1.62	0.80
1:C:126:LEU:HD21	1:C:426:ILE:HD13	1.65	0.78
1:B:461:LYS:HA	1:B:465:LEU:HD22	1.64	0.77
1:C:220:PHE:CD2	1:C:263:GLY:HA3	2.19	0.77
1:A:461:LYS:HA	1:A:465:LEU:HD22	1.66	0.76
1:A:72:TYR:CZ	1:A:476:LYS:HE2	2.20	0.76
1:C:90:MET:HE2	1:C:264:PHE:HB3	1.68	0.75
1:C:35:GLY:HA2	1:C:93:PHE:CZ	2.21	0.75
1:A:202:VAL:HG23	1:A:272:ALA:HB3	1.68	0.73
1:C:202:VAL:HG23	1:C:272:ALA:HB3	1.69	0.73
1:A:93:PHE:CG	1:A:252:LEU:HD21	2.24	0.72
1:A:249:ALA:O	1:A:252:LEU:HB2	1.90	0.72
1:B:337:ARG:NH1	1:B:362:LYS:HG2	2.05	0.72
1:C:220:PHE:HD2	1:C:263:GLY:HA3	1.54	0.71
1:B:220:PHE:CD2	1:B:263:GLY:HA3	2.26	0.70
1:A:90:MET:HE2	1:A:264:PHE:HB3	1.71	0.70
1:B:95:MET:HE2	1:B:269:ARG:H	1.58	0.69
1:A:220:PHE:CD2	1:A:263:GLY:HA3	2.28	0.69
1:A:537:ARG:NH2	1:C:253:LYS:NZ	2.39	0.69
1:C:38:GLU:HB3	1:C:532:VAL:HG22	1.73	0.68
1:B:38:GLU:HB3	1:B:532:VAL:HG22	1.76	0.68
1:C:249:ALA:O	1:C:252:LEU:HB2	1.92	0.68
1:C:337:ARG:NH1	1:C:362:LYS:HG2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASN:O	1:C:128:ARG:HG3	1.94	0.67
1:B:552:ALA:HB3	1:B:619:LEU:HD13	1.74	0.67
1:C:107:LYS:HE3	1:C:111:ASP:OD2	1.95	0.67
1:A:552:ALA:HB3	1:A:619:LEU:HD13	1.76	0.67
1:C:131:VAL:HG11	1:C:343:GLU:HB3	1.77	0.66
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.31	0.65
1:B:93:PHE:CG	1:B:252:LEU:HD21	2.32	0.65
1:B:540:SER:HB2	1:B:644:VAL:O	1.97	0.65
1:C:307:ARG:HG2	1:C:499:ASP:OD2	1.96	0.65
1:A:17:LEU:HD11	1:A:378:LEU:HD22	1.78	0.65
1:A:537:ARG:NH2	1:C:253:LYS:HZ1	1.95	0.65
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.32	0.64
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.32	0.64
1:A:223:LYS:HD3	1:A:225:ARG:HH21	1.63	0.64
1:B:124:ASN:O	1:B:128:ARG:HG3	1.97	0.64
1:A:576:TRP:CD1	1:A:581:GLU:O	2.51	0.63
1:C:576:TRP:CD1	1:C:581:GLU:O	2.52	0.63
1:A:17:LEU:HB3	1:A:153:ILE:HD13	1.80	0.63
1:B:162:THR:O	1:B:166:ILE:HG13	1.98	0.63
1:A:38:GLU:HB3	1:A:532:VAL:HG22	1.80	0.63
1:B:107:LYS:HE3	1:B:111:ASP:OD2	1.99	0.63
1:C:223:LYS:HD3	1:C:225:ARG:HH21	1.63	0.63
1:B:131:VAL:HG11	1:B:343:GLU:HB3	1.80	0.63
1:C:395:GLN:O	1:C:398:THR:HG22	1.99	0.62
1:A:220:PHE:HD2	1:A:263:GLY:HA3	1.65	0.62
1:C:17:LEU:HD11	1:C:378:LEU:HD22	1.80	0.62
1:B:220:PHE:HD2	1:B:263:GLY:HA3	1.64	0.62
1:C:141:VAL:HG11	1:C:292:ASN:ND2	2.15	0.62
1:B:17:LEU:HD11	1:B:378:LEU:HD22	1.82	0.62
1:C:94:PRO:HB3	1:C:269:ARG:HH11	1.65	0.61
1:A:107:LYS:HE3	1:A:111:ASP:OD2	2.00	0.61
1:A:93:PHE:CD2	1:A:252:LEU:HD21	2.35	0.61
1:C:162:THR:O	1:C:166:ILE:HG13	2.00	0.61
1:A:124:ASN:O	1:A:128:ARG:HG3	2.00	0.61
1:A:17:LEU:O	1:A:153:ILE:HG23	1.99	0.61
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.36	0.61
1:A:8:PRO:HD2	1:A:11:ASP:HB2	1.81	0.61
1:B:230:PHE:O	1:B:234:VAL:HG22	2.00	0.61
1:C:17:LEU:HB3	1:C:153:ILE:HD13	1.83	0.61
1:B:202:VAL:HG12	1:B:272:ALA:HB3	1.81	0.60
1:C:230:PHE:O	1:C:234:VAL:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:TRP:CD1	1:B:581:GLU:O	2.55	0.60
1:A:88:ARG:HD3	1:A:263:GLY:O	2.02	0.60
1:A:138:LEU:HB2	1:A:662:MET:SD	2.42	0.60
1:A:131:VAL:HG11	1:A:343:GLU:HB3	1.83	0.60
1:C:8:PRO:HD2	1:C:11:ASP:HB2	1.83	0.60
1:C:17:LEU:O	1:C:153:ILE:HG23	2.01	0.59
1:B:249:ALA:O	1:B:252:LEU:HB2	2.03	0.59
1:C:95:MET:C	1:C:96:ILE:HG13	2.23	0.59
1:B:8:PRO:HD2	1:B:11:ASP:HB2	1.84	0.59
1:B:307:ARG:HG2	1:B:499:ASP:OD2	2.03	0.58
1:C:517:ASN:HB3	1:C:520:SER:OG	2.03	0.58
1:C:43:LEU:HD12	1:C:44:LEU:N	2.18	0.58
1:C:600:ARG:HG2	1:C:600:ARG:O	2.03	0.58
1:A:99:THR:HB	1:A:227:VAL:HG12	1.85	0.58
1:C:94:PRO:HB3	1:C:269:ARG:HD3	1.87	0.57
1:A:88:ARG:HB2	1:A:211:ILE:HD12	1.87	0.57
1:B:194:GLN:O	1:B:278:ALA:HB3	2.04	0.57
1:C:141:VAL:HG11	1:C:292:ASN:HD21	1.69	0.57
1:B:301:THR:HG23	1:B:440:TRP:O	2.05	0.57
1:C:306:THR:O	1:C:309:ASN:HB3	2.04	0.57
1:B:600:ARG:HG2	1:B:600:ARG:O	2.05	0.57
1:C:74:ARG:HH11	1:C:507:ARG:HB3	1.70	0.57
1:B:364:PRO:CA	1:B:387:LEU:HD12	2.30	0.56
1:C:91:ASN:HA	1:C:267:GLU:OE1	2.05	0.56
1:A:337:ARG:NH1	1:A:362:LYS:HG2	2.20	0.56
1:A:230:PHE:O	1:A:234:VAL:HG22	2.04	0.56
1:B:72:TYR:CE1	1:B:476:LYS:HE2	2.40	0.56
1:B:95:MET:CE	1:B:269:ARG:H	2.17	0.56
1:A:600:ARG:HG2	1:A:600:ARG:O	2.05	0.56
1:C:552:ALA:HB3	1:C:619:LEU:HD13	1.86	0.56
1:C:301:THR:HG22	1:C:448:GLN:O	2.05	0.56
1:A:117:GLY:HA2	1:A:335:TRP:CD2	2.40	0.55
1:A:208:THR:HG21	1:A:523:ASN:CG	2.26	0.55
1:A:162:THR:O	1:A:166:ILE:HG13	2.06	0.55
1:B:17:LEU:HB3	1:B:153:ILE:HD13	1.88	0.55
1:B:395:GLN:O	1:B:398:THR:HG22	2.07	0.55
1:B:306:THR:O	1:B:309:ASN:HB3	2.07	0.55
1:C:26:GLN:O	1:C:30:ARG:HG3	2.07	0.55
1:C:225:ARG:HD2	1:C:268:ARG:HD2	1.89	0.55
1:B:662:MET:HB3	1:B:663:PRO:CD	2.37	0.55
1:B:208:THR:HG21	1:B:523:ASN:CG	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:PRO:HB3	1:C:269:ARG:NH1	2.22	0.54
1:A:225:ARG:HD2	1:A:268:ARG:HD2	1.90	0.54
1:A:55:ASN:O	1:A:59:ARG:HG3	2.08	0.54
1:A:306:THR:O	1:A:309:ASN:HB3	2.08	0.54
1:A:95:MET:CE	1:A:269:ARG:H	2.21	0.54
1:B:223:LYS:HD3	1:B:225:ARG:HH21	1.70	0.54
1:C:35:GLY:O	1:C:36:ALA:O	2.25	0.54
1:C:55:ASN:O	1:C:59:ARG:HG3	2.07	0.54
1:B:232:TYR:CE1	1:B:242:LEU:HB2	2.43	0.54
1:B:317:TRP:CD2	1:B:458:GLY:HA3	2.42	0.54
1:B:286:VAL:C	1:B:289:PRO:HD2	2.28	0.54
1:A:141:VAL:HB	1:A:142:PRO:CD	2.38	0.54
1:C:36:ALA:HB1	1:C:45:SER:OG	2.09	0.53
1:B:88:ARG:HD3	1:B:263:GLY:O	2.07	0.53
1:A:210:ALA:HB3	1:A:223:LYS:HB2	1.89	0.53
1:A:317:TRP:CD2	1:A:458:GLY:HA3	2.44	0.53
1:B:599:SER:HB2	1:B:606:ALA:C	2.29	0.53
1:A:395:GLN:O	1:A:398:THR:HG22	2.08	0.53
1:C:551:TRP:CZ3	1:C:587:ARG:HG3	2.44	0.53
1:B:17:LEU:O	1:B:153:ILE:HG23	2.08	0.53
1:B:99:THR:HB	1:B:227:VAL:CG1	2.32	0.53
1:A:90:MET:HE2	1:A:264:PHE:CB	2.38	0.53
1:C:225:ARG:NH1	1:C:268:ARG:CZ	2.72	0.53
1:C:225:ARG:NH1	1:C:268:ARG:NH1	2.56	0.53
1:C:429:MET:O	1:C:432:ALA:HB3	2.09	0.53
1:C:317:TRP:CD2	1:C:458:GLY:HA3	2.44	0.53
1:C:662:MET:HB3	1:C:663:PRO:CD	2.39	0.53
1:C:94:PRO:HG3	1:C:269:ARG:NH1	2.24	0.52
1:A:301:THR:HG23	1:A:440:TRP:O	2.10	0.52
1:A:551:TRP:CZ3	1:A:587:ARG:HG3	2.44	0.52
1:B:301:THR:HG22	1:B:448:GLN:O	2.09	0.52
1:B:33:LYS:HD2	1:B:34:GLU:H	1.75	0.52
1:B:43:LEU:HD12	1:B:44:LEU:N	2.24	0.52
1:A:301:THR:HG22	1:A:448:GLN:O	2.08	0.52
1:C:94:PRO:CB	1:C:269:ARG:NH1	2.73	0.52
1:B:600:ARG:HH11	1:B:600:ARG:HB3	1.75	0.52
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.91	0.52
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.44	0.52
1:A:658:LEU:HG	1:A:662:MET:CE	2.39	0.52
1:A:217:THR:CG2	1:A:219:LYS:HB2	2.40	0.52
1:A:364:PRO:CA	1:A:387:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ALA:O	1:B:610:GLY:C	2.48	0.52
1:A:631:LYS:HE3	1:A:632:TRP:CZ2	2.45	0.52
1:C:103:ALA:HB1	1:C:387:LEU:CD2	2.39	0.52
1:C:364:PRO:CA	1:C:387:LEU:HD12	2.34	0.52
1:A:103:ALA:HB1	1:A:387:LEU:CD2	2.40	0.52
1:B:599:SER:OG	1:B:607:ARG:HG2	2.10	0.52
1:B:117:GLY:HA2	1:B:335:TRP:CD2	2.45	0.52
1:C:210:ALA:HB3	1:C:223:LYS:HB2	1.91	0.52
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.92	0.52
1:A:43:LEU:HD12	1:A:44:LEU:N	2.25	0.52
1:C:658:LEU:HG	1:C:662:MET:CE	2.40	0.51
1:A:286:VAL:C	1:A:289:PRO:HD2	2.31	0.51
1:A:160:MET:CE	1:A:647:HIS:HB3	2.40	0.51
1:A:232:TYR:CE1	1:A:242:LEU:HB2	2.46	0.51
1:B:210:ALA:HB3	1:B:223:LYS:HB2	1.92	0.51
1:A:600:ARG:HB3	1:A:600:ARG:HH11	1.75	0.51
1:B:551:TRP:CZ3	1:B:587:ARG:HG3	2.45	0.51
1:C:117:GLY:HA2	1:C:335:TRP:CD2	2.45	0.51
1:B:173:LYS:HB3	1:B:193:HIS:CE1	2.46	0.51
1:A:72:TYR:HB3	1:A:472:PHE:CZ	2.45	0.50
1:B:72:TYR:CZ	1:B:476:LYS:HE2	2.46	0.50
1:B:564:TYR:CZ	1:B:568:LEU:CD1	2.94	0.50
1:C:88:ARG:HB2	1:C:211:ILE:HD12	1.94	0.50
1:B:93:PHE:CD2	1:B:252:LEU:HD21	2.47	0.50
1:A:142:PRO:HG3	1:A:651:VAL:HG22	1.93	0.49
1:C:194:GLN:O	1:C:278:ALA:HB3	2.12	0.49
1:C:631:LYS:HE3	1:C:632:TRP:CZ2	2.47	0.49
1:A:429:MET:O	1:A:432:ALA:HB3	2.12	0.49
1:A:662:MET:HB3	1:A:663:PRO:CD	2.41	0.49
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.93	0.49
1:B:152:CYS:HA	1:B:156:PHE:CD1	2.47	0.49
1:A:5:PRO:HD2	1:A:380:GLY:HA2	1.95	0.49
1:B:201:VAL:HB	1:B:367:VAL:HA	1.93	0.49
1:B:337:ARG:HH11	1:B:362:LYS:HG2	1.75	0.49
1:B:141:VAL:HB	1:B:142:PRO:CD	2.43	0.49
1:C:152:CYS:HA	1:C:156:PHE:CD1	2.48	0.49
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.94	0.49
1:C:320:CYS:HB3	1:C:503:TYR:OH	2.13	0.49
1:C:141:VAL:HG21	1:C:288:GLN:HG3	1.94	0.49
1:C:600:ARG:HB3	1:C:600:ARG:HH11	1.76	0.49
1:A:76:TYR:HA	1:A:502:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:THR:CG2	1:C:219:LYS:HB2	2.43	0.49
1:B:225:ARG:NH1	1:B:268:ARG:CZ	2.76	0.49
1:C:144:LYS:HE3	1:C:642:HIS:CE1	2.48	0.49
1:C:37:ILE:HG12	1:C:45:SER:HB3	1.94	0.49
1:C:337:ARG:HH11	1:C:362:LYS:HG2	1.77	0.49
1:C:301:THR:HG23	1:C:440:TRP:O	2.13	0.49
1:C:281:ALA:HB3	1:C:282:PRO:HD3	1.94	0.49
1:C:90:MET:HE2	1:C:264:PHE:CB	2.42	0.48
1:B:631:LYS:HE3	1:B:632:TRP:CZ2	2.48	0.48
1:C:555:LYS:C	1:C:557:THR:H	2.17	0.48
1:C:222:SER:HB2	1:C:247:LYS:HD2	1.94	0.48
1:A:307:ARG:HG2	1:A:499:ASP:OD2	2.13	0.48
1:B:429:MET:O	1:B:432:ALA:HB3	2.14	0.48
1:A:290:VAL:HG11	1:A:400:LEU:HD13	1.96	0.48
1:B:605:MET:HG2	1:B:606:ALA:O	2.13	0.48
1:A:225:ARG:NH1	1:A:268:ARG:CZ	2.77	0.48
1:C:418:THR:O	1:C:464:ALA:HA	2.14	0.48
1:C:104:SER:HA	1:C:388:GLU:HB2	1.95	0.48
1:B:153:ILE:HA	1:B:154:PRO:HA	1.63	0.48
1:B:138:LEU:HB2	1:B:662:MET:SD	2.54	0.48
1:B:68:ASN:N	1:B:68:ASN:HD22	2.11	0.48
1:C:522:LEU:HD21	1:C:571:ILE:HD11	1.95	0.48
1:A:37:ILE:HG12	1:A:45:SER:HB3	1.95	0.48
1:C:95:MET:CE	1:C:269:ARG:H	2.25	0.47
1:B:451:LYS:HD3	1:B:630:TYR:O	2.14	0.47
1:B:97:PRO:HB3	1:B:371:ALA:HB2	1.96	0.47
1:C:641:ILE:HA	1:C:641:ILE:HD13	1.74	0.47
1:C:95:MET:O	1:C:96:ILE:HG13	2.14	0.47
1:A:46:VAL:HG12	1:A:90:MET:SD	2.55	0.47
1:B:599:SER:CB	1:B:607:ARG:HA	2.44	0.47
1:A:228:ALA:HB1	1:A:232:TYR:HB3	1.95	0.47
1:B:90:MET:HE2	1:B:264:PHE:HB3	1.95	0.47
1:C:599:SER:C	1:C:601:TYR:H	2.17	0.47
1:A:104:SER:HA	1:A:388:GLU:HB2	1.96	0.47
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.95	0.47
1:A:486:MET:HB2	1:A:488:ILE:HD11	1.96	0.47
1:C:32:PHE:CD2	1:C:32:PHE:O	2.67	0.47
1:B:217:THR:CG2	1:B:219:LYS:HB2	2.44	0.47
1:C:564:TYR:CZ	1:C:568:LEU:CD1	2.98	0.47
1:C:286:VAL:HG21	1:C:353:TRP:CE2	2.49	0.47
1:A:146:ARG:HD2	1:A:646:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:SER:HB2	1:B:606:ALA:O	2.14	0.47
1:C:93:PHE:HA	1:C:94:PRO:HD2	1.44	0.47
1:C:74:ARG:HH11	1:C:507:ARG:CB	2.27	0.47
1:B:606:ALA:HB3	1:B:608:GLN:HE21	1.80	0.47
1:B:104:SER:HA	1:B:388:GLU:HB2	1.96	0.47
1:C:72:TYR:HB3	1:C:472:PHE:CZ	2.49	0.47
1:C:173:LYS:HB3	1:C:193:HIS:CE1	2.50	0.47
1:A:194:GLN:O	1:A:278:ALA:HB3	2.15	0.47
1:C:201:VAL:HB	1:C:367:VAL:HA	1.97	0.47
1:C:141:VAL:HB	1:C:142:PRO:CD	2.45	0.47
1:B:658:LEU:HG	1:B:662:MET:CE	2.45	0.47
1:B:288:GLN:HB3	1:B:289:PRO:HD3	1.96	0.47
1:A:217:THR:HG22	1:A:219:LYS:HB2	1.97	0.47
1:B:506:ARG:O	1:B:507:ARG:C	2.53	0.47
1:B:133:LEU:HD12	1:B:436:LEU:HD23	1.96	0.47
1:B:160:MET:CE	1:B:647:HIS:HB3	2.45	0.47
1:B:228:ALA:HB1	1:B:232:TYR:HB3	1.97	0.46
1:C:551:TRP:CH2	1:C:554:MET:HE1	2.50	0.46
1:A:555:LYS:C	1:A:557:THR:H	2.19	0.46
1:A:201:VAL:HB	1:A:367:VAL:HA	1.97	0.46
1:A:152:CYS:HA	1:A:156:PHE:CD1	2.50	0.46
1:A:631:LYS:HG2	1:A:632:TRP:CE2	2.50	0.46
1:B:225:ARG:NH1	1:B:268:ARG:NH1	2.64	0.46
1:C:232:TYR:CE1	1:C:242:LEU:HB2	2.50	0.46
1:A:68:ASN:N	1:A:68:ASN:HD22	2.13	0.46
1:B:222:SER:HB2	1:B:247:LYS:HD2	1.97	0.46
1:A:103:ALA:HB1	1:A:387:LEU:HD22	1.98	0.46
1:A:88:ARG:HB2	1:A:211:ILE:CD1	2.45	0.46
1:B:279:LEU:O	1:B:282:PRO:HD2	2.16	0.46
1:B:332:TRP:HA	1:B:333:PRO:HD3	1.81	0.46
1:C:217:THR:C	1:C:219:LYS:H	2.19	0.46
1:B:608:GLN:O	1:B:610:GLY:N	2.49	0.46
1:B:522:LEU:HD21	1:B:571:ILE:HD11	1.97	0.46
1:A:222:SER:HB2	1:A:247:LYS:HD2	1.97	0.46
1:A:153:ILE:HA	1:A:154:PRO:HA	1.64	0.46
1:A:26:GLN:O	1:A:30:ARG:HG3	2.16	0.46
1:C:363:LEU:HG	1:C:364:PRO:HD2	1.98	0.45
1:B:202:VAL:CG1	1:B:272:ALA:HB3	2.47	0.45
1:B:37:ILE:HG12	1:B:45:SER:HB3	1.97	0.45
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.79	0.45
1:B:290:VAL:HG11	1:B:400:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PRO:HA	1:B:387:LEU:HD11	1.94	0.45
1:C:587:ARG:HD2	1:C:587:ARG:HA	1.66	0.45
1:A:258:ILE:HG22	1:A:259:ASP:N	2.31	0.45
1:A:481:ASN:HA	1:A:482:PRO:HD3	1.70	0.45
1:B:405:LEU:HG	1:B:406:MET:N	2.29	0.45
1:B:608:GLN:HB2	1:B:609:ALA:H	1.47	0.45
1:C:46:VAL:HA	1:C:51:LEU:HD21	1.98	0.45
1:B:517:ASN:HB3	1:B:520:SER:OG	2.17	0.45
1:A:143:LEU:HB2	1:A:654:THR:HG21	1.98	0.45
1:A:564:TYR:CZ	1:A:568:LEU:CD1	3.00	0.45
1:C:175:GLU:HA	1:C:352:TRP:CD2	2.51	0.45
1:A:518:ILE:HA	1:A:518:ILE:HD12	1.81	0.45
1:A:99:THR:HG22	1:A:271:THR:CG2	2.47	0.45
1:C:557:THR:HG22	1:C:558:TYR:CG	2.52	0.45
1:B:101:PRO:O	1:B:233:ALA:HB1	2.17	0.45
1:C:311:GLU:HG2	1:C:315:LYS:HE2	1.99	0.45
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.79	0.45
1:C:573:ARG:O	1:C:576:TRP:HB2	2.17	0.45
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.99	0.44
1:B:564:TYR:CZ	1:B:568:LEU:HD11	2.52	0.44
1:B:216:LYS:HE3	1:B:216:LYS:HB3	1.74	0.44
1:A:46:VAL:HA	1:A:51:LEU:HD21	1.99	0.44
1:B:46:VAL:HA	1:B:51:LEU:HD21	1.99	0.44
1:B:141:VAL:HG11	1:B:292:ASN:ND2	2.32	0.44
1:B:175:GLU:HA	1:B:352:TRP:CD2	2.52	0.44
1:A:225:ARG:NH1	1:A:268:ARG:NH1	2.65	0.44
1:C:228:ALA:HB1	1:C:232:TYR:HB3	1.99	0.44
1:C:68:ASN:N	1:C:68:ASN:HD22	2.15	0.44
1:C:222:SER:HB3	1:C:265:PHE:CD2	2.53	0.44
1:C:598:LEU:O	1:C:601:TYR:HB2	2.17	0.44
1:A:159:ASP:C	1:A:159:ASP:OD1	2.55	0.44
1:A:540:SER:HB2	1:A:644:VAL:O	2.18	0.44
1:B:463:ARG:O	1:B:466:VAL:HG12	2.18	0.44
1:A:311:GLU:HG2	1:A:315:LYS:HE2	2.00	0.44
1:B:573:ARG:O	1:B:576:TRP:HB2	2.18	0.44
1:C:658:LEU:HG	1:C:662:MET:HE2	1.99	0.44
1:C:508:GLU:HA	1:C:509:PRO:HD3	1.85	0.44
1:C:372:PRO:O	1:C:373:GLU:HB2	2.17	0.44
1:B:217:THR:C	1:B:219:LYS:H	2.21	0.44
1:C:579:PHE:C	1:C:581:GLU:H	2.22	0.43
1:A:551:TRP:CH2	1:A:554:MET:HE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LYS:HB2	1:A:555:LYS:HE2	1.87	0.43
1:A:126:LEU:HD13	1:A:411:LEU:CD2	2.48	0.43
1:B:631:LYS:HG2	1:B:632:TRP:CE2	2.53	0.43
1:B:379:LEU:O	1:B:387:LEU:HD11	2.17	0.43
1:C:506:ARG:O	1:C:507:ARG:C	2.56	0.43
1:B:217:THR:HG22	1:B:219:LYS:HB2	2.00	0.43
1:C:303:HIS:CD2	1:C:305:THR:HG23	2.53	0.43
1:C:517:ASN:OD1	1:C:519:ASN:N	2.52	0.43
1:C:345:LEU:HA	1:C:345:LEU:HD23	1.88	0.43
1:A:418:THR:O	1:A:464:ALA:HA	2.18	0.43
1:A:173:LYS:HB3	1:A:193:HIS:CE1	2.53	0.43
1:A:405:LEU:HG	1:A:406:MET:N	2.32	0.43
1:C:7:PHE:HA	1:C:8:PRO:HD3	1.85	0.43
1:C:217:THR:HG22	1:C:219:LYS:HB2	2.00	0.43
1:B:102:LEU:HD12	1:B:233:ALA:HA	2.00	0.43
1:C:336:LEU:HD21	1:C:404:LEU:HD12	2.00	0.43
1:C:481:ASN:HA	1:C:482:PRO:HD3	1.67	0.43
1:C:232:TYR:CE2	1:C:237:GLY:HA2	2.54	0.43
1:A:573:ARG:O	1:A:576:TRP:HB2	2.19	0.43
1:B:555:LYS:C	1:B:557:THR:H	2.20	0.43
1:C:405:LEU:HG	1:C:406:MET:N	2.31	0.43
1:A:522:LEU:HD21	1:A:571:ILE:HD11	1.99	0.43
1:C:182:LEU:HD21	1:C:355:LYS:HB2	2.01	0.43
1:C:554:MET:HE1	1:C:568:LEU:HD21	2.00	0.43
1:B:526:PHE:C	1:B:528:PRO:HD3	2.39	0.43
1:C:631:LYS:HG2	1:C:632:TRP:CE2	2.54	0.42
1:B:144:LYS:HA	1:B:648:GLY:HA2	2.01	0.42
1:C:133:LEU:O	1:C:293:LYS:HE2	2.19	0.42
1:B:518:ILE:HD12	1:B:518:ILE:HA	1.89	0.42
1:B:641:ILE:HA	1:B:641:ILE:HD13	1.74	0.42
1:C:290:VAL:HG11	1:C:400:LEU:HD13	2.01	0.42
1:B:363:LEU:HG	1:B:364:PRO:HD2	2.01	0.42
1:C:153:ILE:HA	1:C:154:PRO:HA	1.61	0.42
1:B:225:ARG:HD2	1:B:268:ARG:HD2	2.01	0.42
1:B:55:ASN:O	1:B:59:ARG:HG3	2.18	0.42
1:C:451:LYS:HD3	1:C:630:TYR:O	2.18	0.42
1:B:320:CYS:HB3	1:B:503:TYR:OH	2.19	0.42
1:A:85:PHE:O	1:A:211:ILE:HD12	2.18	0.42
1:B:429:MET:HB2	1:B:430:PRO:HD3	2.01	0.42
1:B:497:LEU:HA	1:B:497:LEU:HD12	1.80	0.42
1:C:22:ILE:HG12	1:C:22:ILE:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:HG2	1:B:315:LYS:HE2	2.01	0.42
1:C:37:ILE:HG23	1:C:92:GLY:HA3	2.01	0.42
1:A:463:ARG:O	1:A:466:VAL:HG12	2.19	0.42
1:A:372:PRO:O	1:A:373:GLU:HB2	2.20	0.42
1:A:102:LEU:HD12	1:A:233:ALA:HA	2.00	0.42
1:B:280:ASN:ND2	1:B:396:GLY:H	2.17	0.42
1:C:449:ILE:O	1:C:449:ILE:HG13	2.20	0.42
1:A:175:GLU:HA	1:A:352:TRP:CD2	2.55	0.42
1:A:317:TRP:CE3	1:A:458:GLY:HA3	2.55	0.42
1:B:617:ILE:O	1:B:618:ASP:C	2.58	0.42
1:C:624:ASP:OD1	1:C:626:ASN:HB2	2.20	0.42
1:A:419:ALA:HB1	1:A:422:LEU:HD12	2.00	0.42
1:C:463:ARG:O	1:C:466:VAL:HG12	2.20	0.42
1:B:508:GLU:HA	1:B:509:PRO:HD3	1.87	0.42
1:B:393:SER:O	1:B:398:THR:HG21	2.19	0.42
1:A:250:SER:C	1:A:252:LEU:N	2.73	0.42
1:B:606:ALA:CB	1:B:608:GLN:HE21	2.33	0.42
1:C:555:LYS:HB2	1:C:555:LYS:HE2	1.89	0.42
1:C:650:SER:OG	1:C:653:LYS:HD2	2.20	0.42
1:A:587:ARG:HA	1:A:587:ARG:HD2	1.73	0.42
1:A:320:CYS:HB3	1:A:503:TYR:OH	2.19	0.42
1:A:143:LEU:H	1:A:654:THR:HG21	1.85	0.42
1:A:449:ILE:HG13	1:A:449:ILE:O	2.20	0.42
1:C:486:MET:HB2	1:C:488:ILE:HD11	2.02	0.42
1:B:522:LEU:CD2	1:B:571:ILE:HD11	2.50	0.41
1:A:112:ALA:O	1:A:113:ASP:HB2	2.19	0.41
1:A:72:TYR:CE1	1:A:476:LYS:HE2	2.53	0.41
1:A:537:ARG:CZ	1:C:253:LYS:HE3	2.50	0.41
1:A:506:ARG:O	1:A:507:ARG:C	2.56	0.41
1:A:144:LYS:HA	1:A:648:GLY:HA2	2.01	0.41
1:C:96:ILE:HA	1:C:97:PRO:HA	1.81	0.41
1:A:7:PHE:HA	1:A:8:PRO:HD3	1.87	0.41
1:A:551:TRP:CE3	1:A:587:ARG:HG3	2.55	0.41
1:A:160:MET:O	1:A:164:ILE:HG12	2.20	0.41
1:A:429:MET:HB2	1:A:430:PRO:HD3	2.02	0.41
1:B:557:THR:HG22	1:B:558:TYR:CG	2.55	0.41
1:C:433:CYS:O	1:C:434:ARG:C	2.58	0.41
1:B:182:LEU:HD21	1:B:355:LYS:HB2	2.01	0.41
1:B:537:ARG:HD3	1:B:537:ARG:HH11	1.65	0.41
1:A:319:LEU:HD12	1:A:320:CYS:H	1.86	0.41
1:A:557:THR:HG22	1:A:558:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:SER:N	1:B:528:PRO:HD3	2.35	0.41
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.85	0.41
1:B:403:THR:O	1:B:404:LEU:C	2.58	0.41
1:A:286:VAL:HG21	1:A:353:TRP:CE2	2.56	0.41
1:A:429:MET:CB	1:A:430:PRO:HD3	2.50	0.41
1:A:143:LEU:N	1:A:654:THR:HG21	2.36	0.41
1:A:641:ILE:HD13	1:A:641:ILE:HA	1.71	0.41
1:B:551:TRP:CH2	1:B:554:MET:HE1	2.55	0.41
1:A:290:VAL:CG1	1:A:400:LEU:HD13	2.51	0.41
1:B:418:THR:O	1:B:464:ALA:HA	2.21	0.41
1:A:143:LEU:HB2	1:A:654:THR:CG2	2.50	0.41
1:B:433:CYS:O	1:B:434:ARG:C	2.57	0.41
1:B:300:TYR:CD1	1:B:442:GLY:HA3	2.56	0.41
1:B:91:ASN:HA	1:B:267:GLU:OE1	2.21	0.41
1:A:537:ARG:HH22	1:C:253:LYS:HZ1	1.67	0.41
1:C:74:ARG:NH1	1:C:507:ARG:CB	2.83	0.41
1:A:217:THR:C	1:A:219:LYS:H	2.23	0.41
1:A:279:LEU:O	1:A:282:PRO:HD2	2.21	0.41
1:B:152:CYS:HA	1:B:156:PHE:CE1	2.56	0.41
1:B:429:MET:CB	1:B:430:PRO:HD3	2.51	0.41
1:C:403:THR:O	1:C:404:LEU:C	2.59	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.84	0.41
1:C:5:PRO:HD2	1:C:380:GLY:HA2	2.03	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.88	0.41
1:B:94:PRO:CB	1:B:269:ARG:HG3	2.51	0.41
1:B:579:PHE:C	1:B:581:GLU:H	2.25	0.41
1:C:32:PHE:CD2	1:C:372:PRO:HG3	2.56	0.41
1:C:413:MET:HE1	1:C:488:ILE:HG21	2.02	0.41
1:C:442:GLY:C	1:C:444:GLU:H	2.24	0.41
1:A:403:THR:O	1:A:404:LEU:C	2.59	0.41
1:A:127:PHE:CE2	1:A:408:ILE:HB	2.56	0.41
1:A:379:LEU:O	1:A:387:LEU:HD11	2.21	0.40
1:B:317:TRP:CE3	1:B:458:GLY:HA3	2.56	0.40
1:C:429:MET:HB2	1:C:430:PRO:HD3	2.03	0.40
1:C:429:MET:CB	1:C:430:PRO:HD3	2.51	0.40
1:C:526:PHE:C	1:C:528:PRO:HD3	2.41	0.40
1:B:380:GLY:O	1:B:382:PRO:HD3	2.21	0.40
1:C:216:LYS:HB3	1:C:216:LYS:HE3	1.72	0.40
1:B:554:MET:HE1	1:B:568:LEU:HD21	2.04	0.40
1:C:408:ILE:O	1:C:412:VAL:HG23	2.20	0.40
1:A:216:LYS:HE3	1:A:216:LYS:HB3	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ALA:O	1:C:113:ASP:HB2	2.21	0.40
1:C:300:TYR:CD1	1:C:442:GLY:HA3	2.56	0.40
1:B:4:ALA:HA	1:B:5:PRO:HD3	1.90	0.40
1:B:85:PHE:O	1:B:211:ILE:HD12	2.21	0.40
1:C:131:VAL:HG21	1:C:340:ILE:HA	2.03	0.40
1:A:658:LEU:HG	1:A:662:MET:HE1	2.03	0.40
1:C:522:LEU:CD2	1:C:571:ILE:HD11	2.50	0.40
1:A:3:ARG:NH2	1:A:231:GLU:OE2	2.54	0.40
1:B:408:ILE:O	1:B:412:VAL:HG23	2.21	0.40

All (2) 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:506:ARG:NH2	1:C:445:GLU:N[3_544]	2.01	0.19
1:A:240:GLY:N	1:C:217:THR:O[2_554]	2.15	0.05

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	650/664 (98%)	589 (91%)	59 (9%)	2 (0%)	46	85
1	B	659/664 (99%)	586 (89%)	68 (10%)	5 (1%)	24	69
1	C	650/664 (98%)	575 (88%)	68 (10%)	7 (1%)	17	62
All	All	1959/1992 (98%)	1750 (89%)	195 (10%)	14 (1%)	26	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	609	ALA
1	C	36	ALA

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Mol	Chain	Res	Type
1	B	610	GLY
1	C	630	TYR
1	A	630	TYR
1	B	630	TYR
1	C	581	GLU
1	A	581	GLU
1	B	581	GLU
1	C	95	MET
1	C	507	ARG
1	C	529	GLU
1	B	91	ASN
1	C	32	PHE

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	550/557 (99%)	521 (95%)	29 (5%)	28	69
1	B	554/557 (100%)	525 (95%)	29 (5%)	29	69
1	C	550/557 (99%)	524 (95%)	26 (5%)	32	73
All	All	1654/1671 (99%)	1570 (95%)	84 (5%)	29	70

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	31	SER
1	A	44	LEU
1	A	55	ASN
1	A	68	ASN
1	A	208	THR
1	A	234	VAL
1	A	259	ASP
1	A	271	THR
1	A	308	LEU

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Mol	Chain	Res	Type
1	A	331	PHE
1	A	392	SER
1	A	404	LEU
1	A	445	GLU
1	A	448	GLN
1	A	472	PHE
1	A	497	LEU
1	A	518	ILE
1	A	529	GLU
1	A	537	ARG
1	A	556	ASP
1	A	576	TRP
1	A	582	SER
1	A	587	ARG
1	A	589	ASP
1	A	611	LEU
1	A	615	THR
1	A	626	ASN
1	A	641	ILE
1	B	22	ILE
1	B	31	SER
1	B	44	LEU
1	B	55	ASN
1	B	68	ASN
1	B	202	VAL
1	B	208	THR
1	B	234	VAL
1	B	259	ASP
1	B	271	THR
1	B	308	LEU
1	B	331	PHE
1	B	392	SER
1	B	404	LEU
1	B	445	GLU
1	B	448	GLN
1	B	472	PHE
1	B	497	LEU
1	B	529	GLU
1	B	556	ASP
1	B	576	TRP
1	B	582	SER
1	B	587	ARG

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Mol	Chain	Res	Type
1	B	589	ASP
1	B	608	GLN
1	B	611	LEU
1	B	615	THR
1	B	626	ASN
1	B	641	ILE
1	C	22	ILE
1	C	44	LEU
1	C	46	VAL
1	C	55	ASN
1	C	68	ASN
1	C	208	THR
1	C	234	VAL
1	C	259	ASP
1	C	308	LEU
1	C	331	PHE
1	C	392	SER
1	C	404	LEU
1	C	445	GLU
1	C	448	GLN
1	C	472	PHE
1	C	497	LEU
1	C	518	ILE
1	C	529	GLU
1	C	556	ASP
1	C	576	TRP
1	C	582	SER
1	C	587	ARG
1	C	589	ASP
1	C	611	LEU
1	C	615	THR
1	C	626	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	191	GLN
1	A	280	ASN
1	B	15	GLN
1	B	191	GLN
1	B	280	ASN

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Mol	Chain	Res	Type
1	B	608	GLN
1	C	15	GLN
1	C	55	ASN
1	C	191	GLN
1	C	280	ASN
1	C	626	ASN
1	C	642	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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	654/664 (98%)	-0.29	3 (0%)	91	87	9, 32, 66, 101	0
1	B	661/664 (99%)	-0.28	10 (1%)	76	63	9, 33, 68, 118	0
1	C	654/664 (98%)	0.26	56 (8%)	13	7	12, 38, 72, 132	0
All	All	1969/1992 (98%)	-0.10	69 (3%)	48	32	9, 34, 69, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	603	ALA	6.7
1	C	218	GLY	6.4
1	C	259	ASP	5.0
1	C	537	ARG	4.5
1	C	215	PRO	4.4
1	C	253	LYS	4.0
1	C	576	TRP	3.9
1	B	606	ALA	3.8
1	C	262	ASP	3.8
1	C	257	GLY	3.8
1	B	608	GLN	3.8
1	C	577	ASN	3.7
1	B	214	ASP	3.6
1	C	533	GLN	3.6
1	C	534	SER	3.3
1	C	506	ARG	3.2
1	C	602	VAL	3.2
1	C	208	THR	3.1
1	C	511	SER	3.1
1	C	66	PRO	3.1
1	C	531	GLY	3.0
1	C	213	LEU	3.0
1	C	592	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	635	ALA	2.8
1	C	556	ASP	2.8
1	B	603	ALA	2.8
1	C	210	ALA	2.8
1	C	254	GLU	2.8
1	C	258	ILE	2.8
1	C	241	SER	2.8
1	C	539	ARG	2.7
1	C	214	ASP	2.7
1	C	589	ASP	2.7
1	B	607	ARG	2.7
1	C	557	THR	2.7
1	B	30	ARG	2.6
1	C	209	ASP	2.5
1	C	371	ALA	2.5
1	B	639	ALA	2.5
1	C	64	HIS	2.4
1	C	492	HIS	2.4
1	C	56	GLU	2.4
1	A	596	LEU	2.4
1	C	626	ASN	2.4
1	C	165	GLU	2.4
1	C	216	LYS	2.3
1	C	532	VAL	2.3
1	B	31	SER	2.3
1	C	248	ASP	2.3
1	C	249	ALA	2.3
1	A	599	SER	2.3
1	C	640	ASN	2.3
1	C	508	GLU	2.2
1	C	256	TYR	2.2
1	C	246	SER	2.2
1	C	636	ASP	2.2
1	B	254	GLU	2.2
1	C	326	SER	2.2
1	C	250	SER	2.2
1	C	524	ASN	2.2
1	C	582	SER	2.1
1	B	216	LYS	2.1
1	C	588	GLU	2.1
1	C	629	GLN	2.1
1	C	613	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	538	ASP	2.1
1	C	530	TYR	2.0
1	C	207	SER	2.0
1	C	639	ALA	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	B	1664	1/1	0.98	0.14	-0.72	67,67,67,67	0
2	MN	A	1664	1/1	0.96	0.08	-1.74	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.