Full wwPDB EM Validation Report (i)

May 13, 2024 – 08:50 pm BST

PDB ID	:	6XZD
EMDB ID	:	EMD-10659
Title	:	Influenza C virus polymerase complex without chicken ANP32A - Subclass 2
Authors	:	Keown, J.R.; Carrique, L.; Fan, H.; Grimes, J.M.; Fodor, E.
Deposited on	:	2020-02-04
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

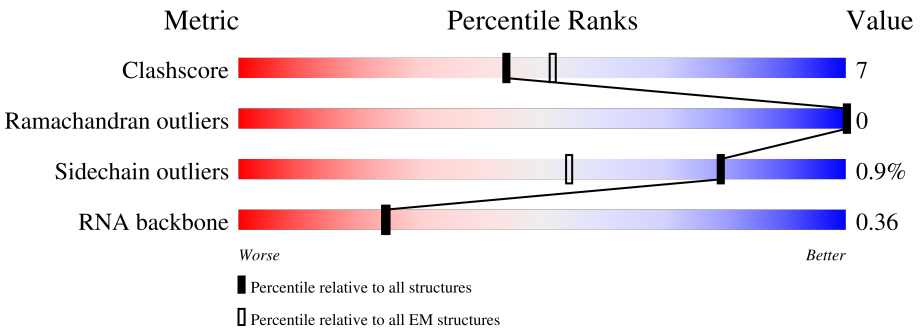
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	IN1	47	17% 17% 6% • 57%
2	AP1	709	87% 11% •
2	DP1	709	62% 12% 26%
3	BP1	754	82% 12% 6%
3	EP1	754	63% 18% • 18%
4	CP1	774	84% 16%
4	FP1	774	60% 17% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 63749 atoms, of which 31961 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (5'-R(*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*GP*CP*CP*CP*UP*GP*C)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	IN1	20	650	193	221	84	133	19	0	0

- Molecule 2 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AP1	696	11291	3599	5645	955	1049	43	0	0
2	DP1	525	8558	2710	4306	729	779	34	0	0

- Molecule 3 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	BP1	712	11444	3602	5761	960	1068	53	0	0
3	EP1	615	9855	3116	4961	822	911	45	0	0

- Molecule 4 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	CP1	772	12409	3888	6261	1080	1142	38	0	0
4	FP1	599	9542	3004	4806	820	884	28	0	0

3 Residue-property plots (i)

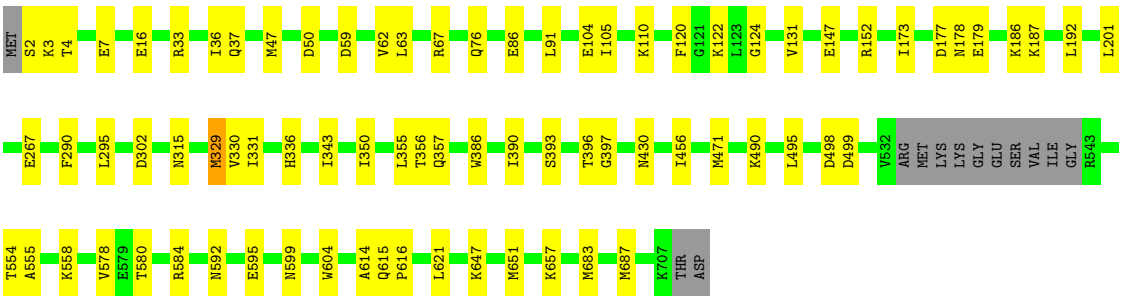
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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 (5'-R(*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*GP*CP*CP *CP*UP*GP*C)-3')

Chain IN1:

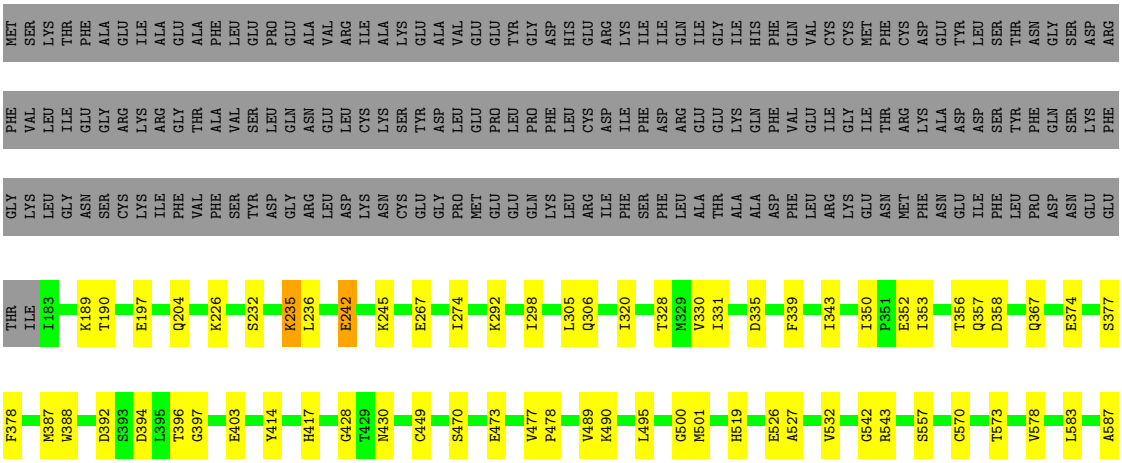
• Molecule 2: Polymerase acidic protein

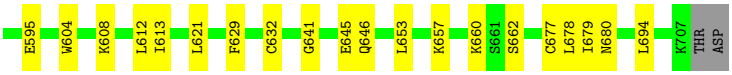
Chain AP1:



• Molecule 2: Polymerase acidic protein

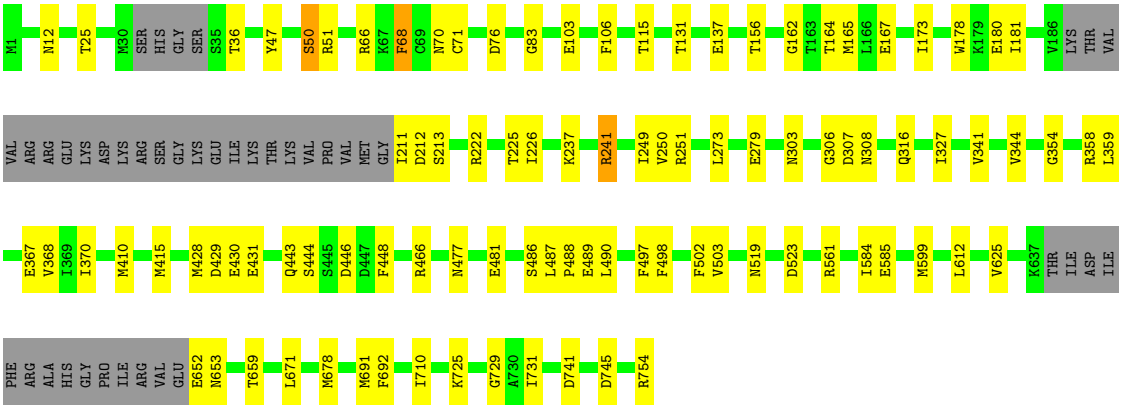
Chain DP1:





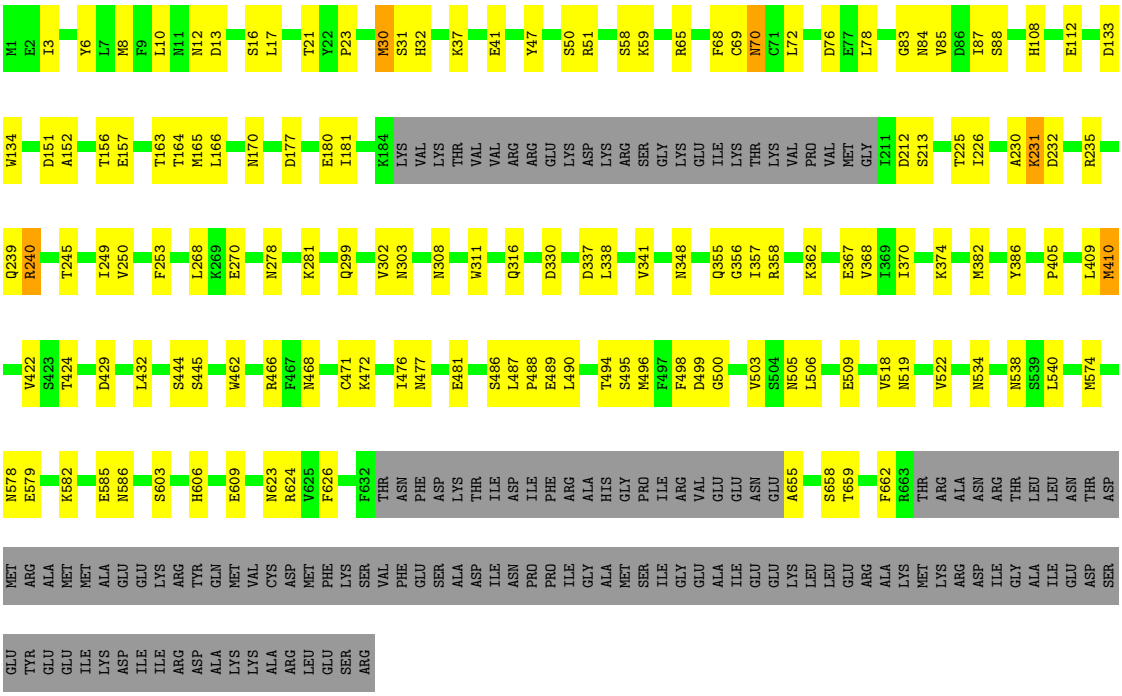
• Molecule 3: RNA-directed RNA polymerase catalytic subunit

Chain BP1:



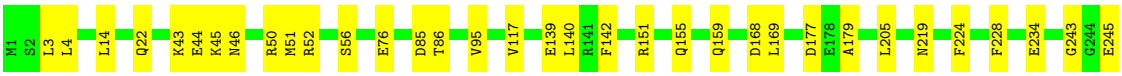
• Molecule 3: RNA-directed RNA polymerase catalytic subunit

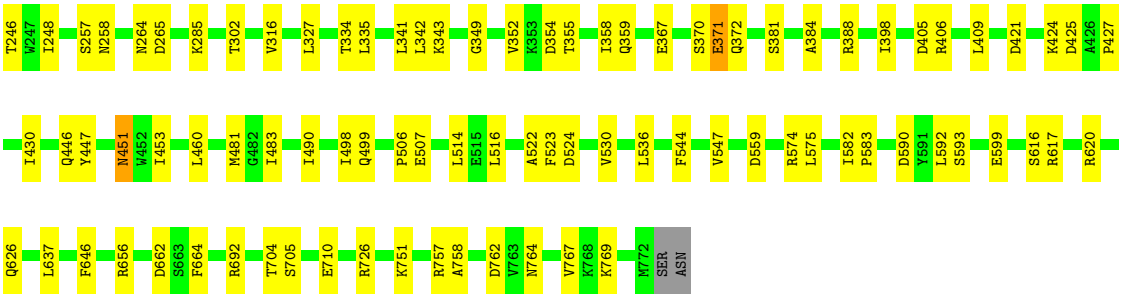
Chain EP1:



• Molecule 4: Polymerase basic protein 2

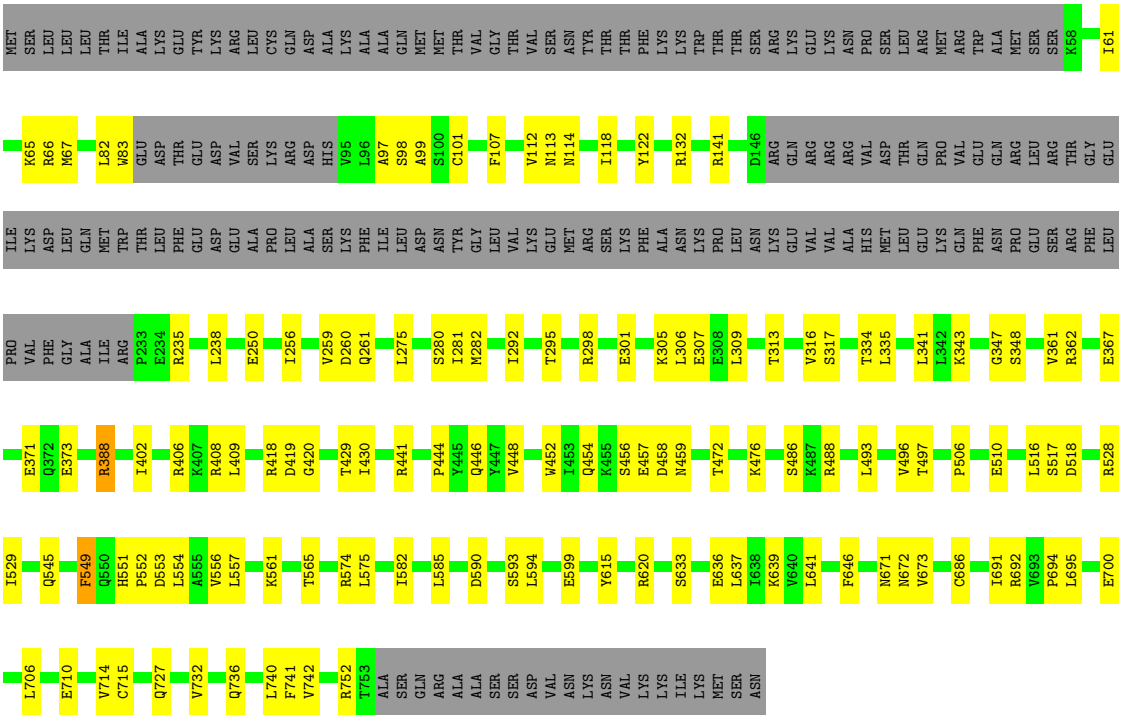
Chain CP1:





- Molecule 4: Polymerase basic protein 2

Chain FP1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.8	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	IN1	0.95	0/480	1.12	3/745 (0.4%)
2	AP1	0.68	0/5764	0.59	0/7746
2	DP1	0.65	0/4342	0.56	0/5835
3	BP1	0.69	0/5780	0.63	0/7762
3	EP1	0.43	0/4986	0.51	0/6707
4	CP1	0.65	0/6259	0.60	0/8425
4	FP1	0.31	0/4821	0.46	0/6493
All	All	0.60	0/32432	0.58	3/43713 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	IN1	39	G	O4'-C1'-N9	6.47	113.38	108.20
1	IN1	5	G	O4'-C1'-N9	5.29	112.43	108.20
1	IN1	39	G	C4-N9-C1'	5.04	133.05	126.50

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	IN1	429	221	221	7	0
2	AP1	5646	5645	5645	55	0
2	DP1	4252	4306	4305	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BP1	5683	5761	5759	63	0
3	EP1	4894	4961	4959	106	0
4	CP1	6148	6261	6261	83	0
4	FP1	4736	4806	4806	94	0
All	All	31788	31961	31956	439	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 7.

All (439) 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)
3:BP1:303:ASN:ND2	3:BP1:488:PRO:O	1.89	1.05
4:FP1:575:LEU:HD12	4:FP1:582:ILE:HD13	1.45	0.97
2:DP1:449:CYS:SG	2:DP1:490:LYS:NZ	2.45	0.89
3:BP1:237:LYS:NZ	3:BP1:307:ASP:OD1	2.06	0.88
4:CP1:44:GLU:OE1	4:CP1:50:ARG:NH2	2.06	0.88
4:FP1:710:GLU:OE1	4:FP1:710:GLU:N	2.06	0.88
3:EP1:609:GLU:OE1	3:EP1:609:GLU:N	2.11	0.82
2:AP1:59:ASP:OD2	4:CP1:769:LYS:NZ	2.13	0.81
3:EP1:299:GLN:O	4:FP1:488:ARG:NH1	2.13	0.81
3:EP1:489:GLU:OE1	3:EP1:489:GLU:N	2.13	0.81
2:AP1:498:ASP:OD1	2:AP1:499:ASP:N	2.13	0.81
4:CP1:575:LEU:HD13	4:CP1:582:ILE:HD11	1.62	0.81
2:AP1:86:GLU:N	2:AP1:86:GLU:OE1	2.13	0.80
4:CP1:367:GLU:OE1	4:CP1:367:GLU:N	2.16	0.79
2:DP1:242:GLU:O	2:DP1:245:LYS:NZ	2.17	0.76
4:FP1:66:ARG:NH2	4:FP1:67:MET:SD	2.59	0.75
3:BP1:103:GLU:N	3:BP1:103:GLU:OE1	2.20	0.75
2:AP1:110:LYS:NZ	2:AP1:177:ASP:OD2	2.20	0.75
4:CP1:151:ARG:NH2	4:CP1:507:GLU:OE2	2.19	0.74
3:EP1:166:LEU:O	3:EP1:170:ASN:ND2	2.20	0.74
3:EP1:65:ARG:NH2	3:EP1:348:ASN:OD1	2.20	0.74
4:CP1:245:GLU:HG3	4:CP1:246:THR:HG23	1.70	0.73
3:EP1:505:ASN:OD1	3:EP1:506:LEU:N	2.21	0.73
2:DP1:526:GLU:OE1	2:DP1:526:GLU:N	2.22	0.73
3:EP1:308:ASN:ND2	3:EP1:477:ASN:O	2.22	0.72
3:BP1:410:MET:SD	3:BP1:410:MET:N	2.62	0.72
2:DP1:356:THR:HG22	2:DP1:357:GLN:H	1.55	0.72
2:DP1:473:GLU:OE2	4:FP1:615:TYR:OH	2.07	0.71
4:FP1:727:GLN:N	4:FP1:727:GLN:OE1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CP1:44:GLU:OE2	4:CP1:46:ASN:N	2.23	0.71
2:AP1:578:VAL:HG21	2:AP1:621:LEU:HD22	1.71	0.71
2:DP1:189:LYS:O	2:DP1:189:LYS:NZ	2.23	0.71
3:BP1:481:GLU:OE1	3:BP1:481:GLU:N	2.24	0.70
3:EP1:481:GLU:N	3:EP1:481:GLU:OE1	2.23	0.70
2:DP1:694:LEU:HD22	3:EP1:6:TYR:HB3	1.74	0.69
4:CP1:258:ASN:O	4:CP1:258:ASN:ND2	2.26	0.69
3:EP1:424:THR:HG21	3:EP1:471:CYS:SG	2.33	0.68
4:CP1:575:LEU:CD1	4:CP1:582:ILE:HD11	2.22	0.68
4:CP1:620:ARG:NH2	4:CP1:646:PHE:O	2.27	0.68
4:FP1:371:GLU:OE1	4:FP1:371:GLU:N	2.28	0.67
2:AP1:33:ARG:NH2	2:AP1:173:ILE:O	2.27	0.67
3:EP1:410:MET:SD	3:EP1:410:MET:N	2.69	0.66
4:CP1:76:GLU:OE1	4:CP1:76:GLU:N	2.29	0.66
4:FP1:371:GLU:O	4:FP1:388:ARG:NH2	2.28	0.65
3:BP1:83:GLY:O	3:BP1:316:GLN:NE2	2.29	0.65
2:DP1:608:LYS:HB3	2:DP1:613:ILE:HD11	1.79	0.65
3:BP1:678:MET:SD	3:BP1:678:MET:N	2.70	0.65
1:IN1:7:A:O2'	1:IN1:8:A:OP2	2.13	0.64
4:FP1:295:THR:HG23	4:FP1:306:LEU:HB2	1.77	0.64
4:FP1:373:GLU:OE1	4:FP1:528:ARG:NH2	2.30	0.64
3:EP1:358:ARG:NH1	3:EP1:367:GLU:OE2	2.30	0.64
4:FP1:561:LYS:O	4:FP1:565:THR:HG23	1.97	0.64
2:AP1:657:LYS:NZ	3:BP1:12:ASN:O	2.32	0.63
3:BP1:358:ARG:NH1	3:BP1:367:GLU:OE2	2.30	0.63
4:FP1:732:VAL:O	4:FP1:752:ARG:NH1	2.32	0.63
2:AP1:50:ASP:OD1	2:AP1:152:ARG:NH2	2.32	0.63
4:CP1:159:GLN:OE1	4:CP1:302:THR:OG1	2.16	0.62
3:BP1:36:THR:HG23	3:BP1:354:GLY:O	1.99	0.62
3:BP1:212:ASP:OD1	3:BP1:213:SER:N	2.32	0.62
3:EP1:626:PHE:O	4:FP1:114:ASN:ND2	2.30	0.62
3:BP1:431:GLU:OE1	3:BP1:466:ARG:NH1	2.32	0.62
2:DP1:298:ILE:HG23	2:DP1:527:ALA:HB1	1.82	0.62
4:CP1:234:GLU:CG	4:CP1:257:SER:HB3	2.30	0.60
3:EP1:239:GLN:N	3:EP1:239:GLN:OE1	2.33	0.60
3:EP1:8:MET:O	3:EP1:12:ASN:ND2	2.34	0.60
3:BP1:25:THR:O	3:BP1:25:THR:HG22	2.01	0.60
2:AP1:578:VAL:CG2	2:AP1:621:LEU:HD22	2.32	0.60
4:FP1:620:ARG:NH2	4:FP1:646:PHE:O	2.32	0.59
4:FP1:590:ASP:OD2	4:FP1:593:SER:OG	2.16	0.59
4:CP1:371:GLU:O	4:CP1:388:ARG:NH2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:EP1:163:THR:HG22	3:EP1:163:THR:O	2.03	0.59
3:EP1:624:ARG:NH2	4:FP1:107:PHE:O	2.36	0.59
4:CP1:3:LEU:HD12	4:CP1:4:LEU:N	2.17	0.59
3:EP1:603:SER:OG	4:FP1:132:ARG:NH2	2.35	0.58
2:AP1:178:ASN:OD1	2:AP1:179:GLU:N	2.37	0.58
2:DP1:396:THR:HG23	2:DP1:428:GLY:HA2	1.84	0.57
3:EP1:355:GLN:OE1	3:EP1:356:GLY:N	2.36	0.57
2:AP1:50:ASP:O	4:CP1:757:ARG:NH2	2.38	0.57
2:DP1:356:THR:HG22	2:DP1:357:GLN:N	2.18	0.57
2:AP1:152:ARG:NH2	4:CP1:762:ASP:OD2	2.27	0.57
4:FP1:282:MET:SD	4:FP1:282:MET:N	2.77	0.57
3:EP1:108:HIS:NE2	3:EP1:112:GLU:OE2	2.38	0.57
3:BP1:237:LYS:NZ	3:BP1:446:ASP:OD1	2.37	0.57
3:EP1:579:GLU:O	3:EP1:582:LYS:NZ	2.38	0.57
4:CP1:285:LYS:NZ	4:CP1:516:LEU:O	2.36	0.57
4:FP1:112:VAL:HG12	4:FP1:113:ASN:N	2.20	0.56
2:DP1:197:GLU:OE2	3:EP1:65:ARG:NH2	2.38	0.56
4:FP1:565:THR:HG22	4:FP1:686:CYS:SG	2.45	0.56
4:CP1:544:PHE:HB3	4:CP1:547:VAL:HG21	1.88	0.56
3:EP1:30:MET:O	3:EP1:31:SER:OG	2.17	0.56
3:EP1:30:MET:SD	3:EP1:30:MET:N	2.80	0.55
3:BP1:211:ILE:O	3:BP1:211:ILE:HG22	2.06	0.55
2:DP1:204:GLN:N	2:DP1:204:GLN:OE1	2.40	0.55
4:CP1:427:PRO:HD2	4:CP1:430:ILE:HD12	1.88	0.55
3:EP1:23:PRO:O	3:EP1:235:ARG:NH1	2.40	0.55
3:BP1:131:THR:HG22	3:BP1:251:ARG:HH22	1.71	0.55
4:CP1:590:ASP:OD2	4:CP1:593:SER:OG	2.21	0.55
3:BP1:308:ASN:ND2	3:BP1:477:ASN:O	2.39	0.55
4:CP1:354:ASP:OD1	4:CP1:355:THR:N	2.35	0.55
3:BP1:671:LEU:HD13	3:BP1:671:LEU:O	2.07	0.55
2:DP1:657:LYS:NZ	3:EP1:12:ASN:O	2.40	0.55
3:EP1:32:HIS:O	3:EP1:230:ALA:HB1	2.06	0.55
2:AP1:2:SER:OG	2:AP1:3:LYS:N	2.37	0.54
3:BP1:429:ASP:OD1	3:BP1:430:GLU:N	2.37	0.54
4:CP1:316:VAL:HG23	4:CP1:316:VAL:O	2.07	0.54
2:DP1:339:PHE:O	2:DP1:343:ILE:HG23	2.07	0.54
3:EP1:83:GLY:O	3:EP1:316:GLN:NE2	2.41	0.54
2:AP1:456:ILE:HG23	2:AP1:490:LYS:O	2.07	0.54
4:FP1:740:LEU:HD12	4:FP1:741:PHE:H	1.71	0.54
2:AP1:356:THR:HG22	2:AP1:357:GLN:N	2.23	0.54
2:AP1:471:MET:SD	2:AP1:471:MET:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:250:VAL:HG12	3:BP1:250:VAL:O	2.07	0.54
4:CP1:656:ARG:HD2	4:CP1:664:PHE:CE1	2.43	0.54
4:CP1:85:ASP:O	4:CP1:86:THR:HG23	2.08	0.54
2:DP1:274:ILE:HD12	2:DP1:274:ILE:N	2.22	0.54
3:EP1:574:MET:O	3:EP1:578:ASN:N	2.39	0.54
3:EP1:330:ASP:OD1	3:EP1:330:ASP:N	2.37	0.53
2:DP1:190:THR:HG22	3:EP1:177:ASP:OD1	2.08	0.53
4:FP1:510:GLU:OE2	4:FP1:510:GLU:N	2.42	0.53
4:CP1:514:LEU:HD13	4:CP1:522:ALA:HB1	1.90	0.53
4:CP1:86:THR:H	4:CP1:95:VAL:HG23	1.73	0.53
2:DP1:320:ILE:HD11	2:DP1:489:VAL:CG2	2.38	0.53
2:DP1:694:LEU:HD11	3:EP1:10:LEU:HD21	1.90	0.53
4:FP1:316:VAL:O	4:FP1:317:SER:OG	2.23	0.53
2:DP1:353:ILE:H	2:DP1:353:ILE:HD12	1.73	0.53
4:CP1:234:GLU:HG2	4:CP1:257:SER:HB3	1.90	0.53
2:AP1:267:GLU:OE1	2:AP1:267:GLU:N	2.41	0.53
2:DP1:396:THR:HG22	2:DP1:397:GLY:H	1.74	0.53
4:FP1:408:ARG:NH2	4:FP1:454:GLN:OE1	2.42	0.53
4:CP1:592:LEU:HD23	4:CP1:592:LEU:O	2.09	0.52
3:EP1:180:GLU:C	3:EP1:181:ILE:HD12	2.29	0.52
4:FP1:82:LEU:HD22	4:FP1:101:CYS:HA	1.91	0.52
2:DP1:396:THR:HG22	2:DP1:397:GLY:N	2.25	0.52
4:CP1:44:GLU:OE2	4:CP1:45:LYS:N	2.43	0.52
2:DP1:653:LEU:C	2:DP1:653:LEU:HD23	2.30	0.52
2:DP1:660:LYS:HE2	3:EP1:489:GLU:HB2	1.92	0.51
3:BP1:156:THR:HG21	3:BP1:178:TRP:CZ3	2.44	0.51
2:DP1:267:GLU:OE1	2:DP1:519:HIS:NE2	2.43	0.51
2:DP1:678:LEU:O	2:DP1:679:ILE:HG23	2.11	0.51
4:FP1:281:ILE:HD12	4:FP1:281:ILE:N	2.26	0.51
3:BP1:51:ARG:NH1	3:BP1:76:ASP:O	2.40	0.51
3:EP1:13:ASP:OD1	3:EP1:16:SER:N	2.39	0.51
4:FP1:457:GLU:N	4:FP1:457:GLU:OE2	2.43	0.51
4:FP1:472:THR:HG23	4:FP1:476:LYS:HD2	1.92	0.51
3:BP1:599:MET:O	3:BP1:612:LEU:HD23	2.11	0.51
3:EP1:496:MET:SD	3:EP1:505:ASN:ND2	2.83	0.51
1:IN1:4:A:H1'	1:IN1:7:A:H61	1.75	0.51
2:AP1:16:GLU:OE2	4:CP1:767:VAL:HG11	2.11	0.51
3:BP1:279:GLU:N	3:BP1:279:GLU:OE1	2.43	0.51
4:CP1:490:ILE:N	4:CP1:490:ILE:HD12	2.26	0.51
2:DP1:335:ASP:OD1	2:DP1:335:ASP:N	2.43	0.51
3:EP1:432:LEU:HD13	3:EP1:462:TRP:HZ3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP1:489:GLU:OE1	3:BP1:489:GLU:HA	2.11	0.51
2:DP1:374:GLU:OE1	2:DP1:374:GLU:N	2.42	0.51
3:BP1:359:LEU:HD13	3:BP1:370:ILE:HD12	1.94	0.50
1:IN1:7:A:O2'	1:IN1:8:A:P	2.70	0.50
3:EP1:499:ASP:OD1	3:EP1:500:GLY:N	2.41	0.50
4:FP1:429:THR:OG1	4:FP1:452:TRP:NE1	2.45	0.50
2:DP1:470:SER:HB2	2:DP1:477:VAL:HG21	1.93	0.50
1:IN1:38:U:H2'	1:IN1:39:G:C4	2.47	0.50
4:FP1:82:LEU:O	4:FP1:83:TRP:HB3	2.11	0.50
4:FP1:672:ASN:OD1	4:FP1:673:VAL:N	2.45	0.50
4:FP1:740:LEU:HD12	4:FP1:741:PHE:N	2.27	0.50
3:BP1:487:LEU:HB3	3:BP1:488:PRO:CD	2.42	0.50
3:BP1:652:GLU:OE1	3:BP1:653:ASN:N	2.44	0.50
4:FP1:402:ILE:O	4:FP1:406:ARG:NE	2.45	0.50
2:AP1:355:LEU:HD23	2:AP1:356:THR:N	2.27	0.50
4:FP1:367:GLU:OE1	4:FP1:367:GLU:N	2.44	0.50
3:EP1:78:LEU:O	3:EP1:472:LYS:NZ	2.35	0.49
3:EP1:253:PHE:CE1	3:EP1:341:VAL:HG11	2.47	0.49
4:FP1:65:LYS:HD2	4:FP1:65:LYS:N	2.27	0.49
4:FP1:419:ASP:OD2	4:FP1:420:GLY:N	2.45	0.49
4:CP1:421:ASP:O	4:CP1:424:LYS:N	2.43	0.49
3:EP1:13:ASP:OD2	3:EP1:16:SER:OG	2.25	0.49
4:FP1:671:ASN:OD1	4:FP1:672:ASN:N	2.45	0.49
2:AP1:302:ASP:OD2	2:AP1:302:ASP:N	2.46	0.49
3:BP1:725:LYS:O	3:BP1:729:GLY:N	2.44	0.49
4:CP1:574:ARG:HG3	4:CP1:599:GLU:HG3	1.93	0.49
3:EP1:268:LEU:HD13	3:EP1:422:VAL:HG11	1.95	0.49
3:EP1:494:THR:O	3:EP1:495:SER:OG	2.21	0.49
2:DP1:570:CYS:O	2:DP1:573:THR:OG1	2.26	0.49
4:CP1:398:ILE:HG21	4:CP1:406:ARG:HG2	1.95	0.49
4:CP1:692:ARG:NH1	4:CP1:710:GLU:OE2	2.43	0.49
3:EP1:156:THR:HG23	3:EP1:157:GLU:N	2.26	0.49
4:FP1:280:SER:O	4:FP1:441:ARG:NH2	2.40	0.49
3:BP1:692:PHE:HD2	3:BP1:710:ILE:HG23	1.78	0.49
2:DP1:352:GLU:OE1	3:EP1:374:LYS:HD2	2.13	0.49
3:EP1:270:GLU:N	3:EP1:270:GLU:OE1	2.45	0.49
4:CP1:349:GLY:HA2	4:CP1:371:GLU:HB2	1.94	0.49
4:CP1:483:ILE:N	4:CP1:483:ILE:HD12	2.28	0.49
2:AP1:186:LYS:O	3:BP1:173:ILE:HG21	2.12	0.49
4:CP1:179:ALA:O	4:CP1:726:ARG:NH2	2.46	0.49
3:BP1:503:VAL:HG13	3:BP1:503:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CP1:704:THR:OG1	4:CP1:705:SER:N	2.45	0.49
2:DP1:394:ASP:OD2	2:DP1:394:ASP:N	2.47	0.48
2:AP1:104:GLU:C	2:AP1:105:ILE:HD12	2.34	0.48
2:AP1:105:ILE:HD12	2:AP1:105:ILE:N	2.29	0.48
4:FP1:493:LEU:HB2	4:FP1:496:VAL:HG21	1.96	0.48
2:AP1:63:LEU:O	2:AP1:67:ARG:NH2	2.46	0.48
2:AP1:350:ILE:HB	3:BP1:368:VAL:HG22	1.96	0.48
4:FP1:98:SER:OG	4:FP1:99:ALA:N	2.47	0.48
4:FP1:334:THR:C	4:FP1:335:LEU:HD12	2.34	0.48
4:FP1:409:LEU:C	4:FP1:409:LEU:HD23	2.34	0.48
2:DP1:306:GLN:NE2	2:DP1:519:HIS:O	2.47	0.48
4:FP1:694:PRO:C	4:FP1:695:LEU:HD12	2.34	0.48
4:FP1:742:VAL:HG22	4:FP1:742:VAL:O	2.13	0.48
3:EP1:78:LEU:O	3:EP1:78:LEU:HD23	2.14	0.48
3:EP1:225:THR:HG22	3:EP1:226:ILE:N	2.28	0.48
3:EP1:409:LEU:N	3:EP1:409:LEU:HD12	2.29	0.48
2:AP1:592:ASN:OD1	4:CP1:142:PHE:CE2	2.66	0.47
2:DP1:608:LYS:CB	2:DP1:613:ILE:HD11	2.44	0.47
4:CP1:516:LEU:N	4:CP1:516:LEU:HD23	2.29	0.47
3:EP1:655:ALA:O	4:FP1:122:TYR:OH	2.23	0.47
3:EP1:303:ASN:ND2	3:EP1:490:LEU:O	2.47	0.47
2:AP1:16:GLU:OE1	4:CP1:764:ASN:HA	2.15	0.47
3:BP1:486:SER:OG	3:BP1:487:LEU:N	2.47	0.47
4:CP1:626:GLN:OE1	4:CP1:637:LEU:HD21	2.14	0.47
2:DP1:232:SER:O	2:DP1:235:LYS:NZ	2.47	0.47
4:FP1:429:THR:HG1	4:FP1:452:TRP:HE1	1.62	0.47
2:DP1:298:ILE:HG23	2:DP1:527:ALA:CB	2.44	0.47
4:FP1:275:LEU:O	4:FP1:275:LEU:HD23	2.14	0.47
4:FP1:700:GLU:OE1	4:FP1:700:GLU:N	2.40	0.47
3:BP1:180:GLU:C	3:BP1:181:ILE:HD12	2.35	0.47
4:CP1:264:ASN:OD1	4:CP1:265:ASP:N	2.47	0.47
4:FP1:444:PRO:O	4:FP1:448:VAL:HG23	2.15	0.47
3:BP1:584:ILE:HG22	3:BP1:585:GLU:N	2.30	0.47
3:EP1:50:SER:OG	3:EP1:68:PHE:HB3	2.14	0.47
3:EP1:623:ASN:HB2	4:FP1:112:VAL:O	2.14	0.47
3:BP1:625:VAL:O	3:BP1:659:THR:HG23	2.15	0.47
4:CP1:662:ASP:OD2	4:FP1:736:GLN:NE2	2.48	0.47
3:EP1:444:SER:OG	3:EP1:445:SER:N	2.47	0.47
2:AP1:201:LEU:HD22	3:BP1:71:CYS:SG	2.55	0.47
2:AP1:393:SER:HB3	2:AP1:430:ASN:OD1	2.15	0.47
4:CP1:117:VAL:HG11	4:CP1:205:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:FP1:292:ILE:O	4:FP1:295:THR:HG22	2.14	0.47
4:CP1:139:GLU:OE1	4:CP1:139:GLU:N	2.43	0.47
4:CP1:140:LEU:HD12	4:CP1:248:ILE:O	2.15	0.47
3:EP1:357:ILE:HG13	3:EP1:370:ILE:HD11	1.97	0.47
4:FP1:574:ARG:NE	4:FP1:599:GLU:OE2	2.43	0.47
1:IN1:35:C:O5'	1:IN1:35:C:H6	1.98	0.46
3:EP1:495:SER:HB2	3:EP1:506:LEU:HB3	1.96	0.46
2:AP1:330:VAL:HG12	2:AP1:331:ILE:N	2.30	0.46
2:AP1:580:THR:HG23	2:AP1:584:ARG:HH11	1.80	0.46
2:AP1:187:LYS:HB3	2:AP1:192:LEU:HD21	1.97	0.46
3:EP1:76:ASP:OD1	3:EP1:76:ASP:N	2.48	0.46
4:FP1:517:SER:OG	4:FP1:518:ASP:N	2.48	0.46
2:DP1:677:CYS:O	2:DP1:678:LEU:HD12	2.16	0.46
4:CP1:168:ASP:OD1	4:CP1:169:LEU:N	2.49	0.46
2:DP1:680:ASN:ND2	2:DP1:680:ASN:O	2.49	0.46
3:EP1:156:THR:OG1	3:EP1:157:GLU:OE2	2.30	0.46
4:FP1:61:ILE:O	4:FP1:97:ALA:N	2.49	0.46
3:BP1:181:ILE:HD12	3:BP1:181:ILE:N	2.31	0.46
2:DP1:320:ILE:HD11	2:DP1:489:VAL:HG21	1.97	0.46
2:DP1:377:SER:OG	2:DP1:378:PHE:N	2.49	0.46
3:EP1:253:PHE:CD1	3:EP1:341:VAL:HG11	2.50	0.46
3:EP1:337:ASP:OD1	3:EP1:338:LEU:N	2.48	0.46
3:BP1:115:THR:O	3:BP1:115:THR:HG22	2.16	0.46
4:CP1:524:ASP:OD1	4:CP1:524:ASP:N	2.48	0.46
2:DP1:604:TRP:CD2	2:DP1:612:LEU:HD23	2.51	0.46
4:FP1:112:VAL:CG1	4:FP1:113:ASN:N	2.79	0.46
4:CP1:447:TYR:O	4:CP1:451:ASN:OD1	2.32	0.46
2:DP1:501:MET:SD	2:DP1:557:SER:OG	2.74	0.46
3:EP1:181:ILE:HD12	3:EP1:181:ILE:N	2.31	0.46
4:FP1:545:GLN:OE1	4:FP1:545:GLN:N	2.48	0.46
4:CP1:656:ARG:HD2	4:CP1:664:PHE:CD1	2.51	0.45
3:EP1:151:ASP:OD1	3:EP1:152:ALA:N	2.49	0.45
4:FP1:298:ARG:NE	4:FP1:301:GLU:O	2.49	0.45
2:DP1:236:LEU:HD22	3:EP1:468:ASN:HD22	1.81	0.45
4:FP1:309:LEU:O	4:FP1:313:THR:HG22	2.16	0.45
4:FP1:458:ASP:OD2	4:FP1:459:ASN:ND2	2.49	0.45
3:BP1:306:GLY:HA3	3:BP1:448:PHE:CZ	2.52	0.45
2:AP1:147:GLU:OE2	4:CP1:751:LYS:NZ	2.34	0.45
3:BP1:47:TYR:O	3:BP1:66:ARG:NH2	2.45	0.45
2:DP1:388:TRP:CH2	2:DP1:430:ASN:HB3	2.51	0.45
2:AP1:131:VAL:HG23	2:AP1:131:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AP1:647:LYS:O	2:AP1:651:MET:HG2	2.17	0.45
4:CP1:514:LEU:HB2	4:CP1:523:PHE:O	2.16	0.45
2:DP1:305:LEU:HD21	2:DP1:526:GLU:OE2	2.17	0.45
3:EP1:164:THR:HG22	3:EP1:165:MET:N	2.32	0.45
3:EP1:281:LYS:HZ1	3:EP1:538:ASN:CB	2.29	0.45
3:BP1:241:ARG:O	3:BP1:241:ARG:NE	2.50	0.45
4:FP1:256:ILE:HD12	4:FP1:256:ILE:O	2.16	0.45
3:BP1:303:ASN:HD21	3:BP1:490:LEU:H	1.65	0.45
2:DP1:358:ASP:N	2:DP1:358:ASP:OD2	2.48	0.45
4:FP1:361:VAL:HG23	4:FP1:362:ARG:N	2.32	0.45
4:CP1:481:MET:HB2	4:CP1:498:ILE:HD11	1.98	0.45
2:DP1:330:VAL:HG12	2:DP1:331:ILE:N	2.32	0.45
3:EP1:232:ASP:HB3	3:EP1:240:ARG:HB2	1.99	0.45
3:EP1:429:ASP:OD2	3:EP1:466:ARG:NH2	2.49	0.45
3:EP1:487:LEU:HB3	3:EP1:488:PRO:CD	2.47	0.45
2:DP1:306:GLN:O	2:DP1:306:GLN:HG3	2.17	0.44
2:DP1:403:GLU:N	2:DP1:403:GLU:OE1	2.49	0.44
2:DP1:578:VAL:HG22	2:DP1:621:LEU:HD22	1.99	0.44
3:EP1:152:ALA:O	3:EP1:156:THR:HG22	2.17	0.44
4:FP1:551:HIS:O	4:FP1:554:LEU:HD23	2.17	0.44
3:EP1:133:ASP:OD1	3:EP1:134:TRP:N	2.50	0.44
4:FP1:343:LYS:NZ	4:FP1:506:PRO:O	2.50	0.44
4:CP1:155:GLN:HG2	4:CP1:219:ASN:O	2.18	0.44
4:FP1:341:LEU:C	4:FP1:341:LEU:HD23	2.37	0.44
4:FP1:706:LEU:N	4:FP1:706:LEU:HD22	2.31	0.44
3:BP1:519:ASN:O	3:BP1:523:ASP:OD1	2.36	0.44
4:CP1:453:ILE:HD12	4:CP1:460:LEU:HA	1.98	0.44
4:CP1:514:LEU:HD22	4:CP1:530:VAL:HG11	2.00	0.44
2:AP1:120:PHE:O	2:AP1:124:GLY:N	2.50	0.44
3:BP1:428:MET:SD	3:BP1:429:ASP:N	2.90	0.44
3:BP1:754:ARG:NH1	4:CP1:22:GLN:OE1	2.50	0.44
2:DP1:532:VAL:O	2:DP1:542:GLY:HA2	2.18	0.44
3:BP1:50:SER:HB3	3:BP1:68:PHE:HB3	2.00	0.44
3:BP1:341:VAL:O	3:BP1:344:VAL:HG22	2.18	0.44
3:BP1:249:ILE:O	3:BP1:249:ILE:HG22	2.18	0.44
4:CP1:334:THR:CG2	4:CP1:341:LEU:HD11	2.48	0.44
4:CP1:662:ASP:OD1	4:CP1:662:ASP:O	2.36	0.44
3:BP1:225:THR:HG22	3:BP1:226:ILE:N	2.34	0.43
3:EP1:16:SER:C	3:EP1:17:LEU:HD23	2.39	0.43
3:EP1:429:ASP:N	3:EP1:429:ASP:OD1	2.51	0.43
4:CP1:327:LEU:N	4:CP1:327:LEU:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DP1:477:VAL:HG13	2:DP1:478:PRO:HD2	1.99	0.43
3:EP1:623:ASN:OD1	3:EP1:624:ARG:N	2.51	0.43
4:CP1:381:SER:OG	4:CP1:405:ASP:OD2	2.36	0.43
3:EP1:70:ASN:N	3:EP1:85:VAL:O	2.49	0.43
4:FP1:691:ILE:HG22	4:FP1:692:ARG:N	2.34	0.43
2:AP1:554:THR:OG1	2:AP1:555:ALA:N	2.52	0.43
2:DP1:495:LEU:HA	2:DP1:500:GLY:HA2	2.00	0.43
3:EP1:606:HIS:NE2	4:FP1:238:LEU:HD21	2.33	0.43
4:FP1:235:ARG:HD2	4:FP1:235:ARG:N	2.33	0.43
4:FP1:633:SER:HA	4:FP1:700:GLU:O	2.18	0.43
4:CP1:536:LEU:HD12	4:CP1:536:LEU:O	2.19	0.43
2:DP1:417:HIS:NE2	2:DP1:595:GLU:OE2	2.44	0.43
3:EP1:58:SER:OG	3:EP1:59:LYS:N	2.52	0.43
3:EP1:166:LEU:HD22	3:EP1:166:LEU:N	2.33	0.43
2:AP1:47:MET:O	2:AP1:50:ASP:OD1	2.37	0.43
2:DP1:356:THR:CG2	2:DP1:357:GLN:H	2.28	0.43
2:DP1:694:LEU:CD1	3:EP1:10:LEU:HD21	2.48	0.43
4:FP1:418:ARG:CZ	4:FP1:446:GLN:OE1	2.66	0.43
4:FP1:574:ARG:HG3	4:FP1:582:ILE:HD12	2.01	0.43
4:FP1:585:LEU:HD13	4:FP1:593:SER:OG	2.18	0.43
3:BP1:137:GLU:OE2	3:BP1:222:ARG:CZ	2.66	0.43
3:BP1:561:ARG:NH2	4:CP1:56:SER:HB3	2.33	0.43
3:EP1:585:GLU:OE1	3:EP1:586:ASN:ND2	2.50	0.43
1:IN1:11:A:OP2	2:AP1:343:ILE:O	2.37	0.43
2:DP1:392:ASP:O	2:DP1:392:ASP:OD1	2.37	0.43
4:FP1:636:GLU:OE1	4:FP1:639:LYS:NZ	2.43	0.43
2:AP1:178:ASN:OD1	2:AP1:179:GLU:HG3	2.18	0.43
3:BP1:443:GLN:HG3	3:BP1:444:SER:O	2.19	0.43
4:CP1:498:ILE:HG22	4:CP1:499:GLN:N	2.33	0.43
2:DP1:350:ILE:HB	3:EP1:368:VAL:HG22	2.00	0.43
3:EP1:212:ASP:OD2	3:EP1:213:SER:N	2.51	0.43
3:EP1:658:SER:OG	3:EP1:659:THR:N	2.52	0.43
4:FP1:529:ILE:N	4:FP1:529:ILE:HD12	2.34	0.43
3:BP1:106:PHE:HB3	3:BP1:327:ILE:HG23	2.01	0.42
2:DP1:274:ILE:HD12	2:DP1:274:ILE:H	1.84	0.42
2:DP1:387:MET:SD	3:EP1:3:ILE:HD11	2.59	0.42
3:EP1:72:LEU:N	3:EP1:84:ASN:OD1	2.52	0.42
3:EP1:518:VAL:O	3:EP1:519:ASN:OD1	2.37	0.42
4:FP1:549:PHE:O	4:FP1:554:LEU:HD22	2.19	0.42
3:EP1:37:LYS:NZ	3:EP1:41:GLU:OE2	2.51	0.42
3:EP1:519:ASN:HB2	3:EP1:522:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AP1:396:THR:OG1	2:AP1:397:GLY:N	2.52	0.42
4:FP1:259:VAL:HG23	4:FP1:260:ASP:N	2.34	0.42
2:AP1:315:ASN:CB	2:AP1:336:HIS:CD2	3.03	0.42
3:EP1:250:VAL:O	3:EP1:250:VAL:HG22	2.19	0.42
4:FP1:307:GLU:N	4:FP1:307:GLU:OE1	2.53	0.42
4:FP1:671:ASN:ND2	4:FP1:673:VAL:HG22	2.35	0.42
4:CP1:384:ALA:HB2	4:CP1:409:LEU:HD21	2.02	0.42
3:EP1:51:ARG:HB2	3:EP1:72:LEU:HD12	2.02	0.42
3:EP1:489:GLU:OE2	4:FP1:486:SER:HB3	2.20	0.42
4:FP1:456:SER:OG	4:FP1:459:ASN:OD1	2.33	0.42
2:AP1:386:TRP:O	2:AP1:390:ILE:HG12	2.20	0.42
3:BP1:273:LEU:HD23	3:BP1:415:MET:HA	2.02	0.42
3:BP1:497:PHE:HB2	3:BP1:503:VAL:CG1	2.49	0.42
2:DP1:604:TRP:CE3	2:DP1:612:LEU:HD23	2.55	0.42
4:FP1:551:HIS:ND1	4:FP1:552:PRO:O	2.45	0.42
2:AP1:152:ARG:NH1	4:CP1:758:ALA:O	2.52	0.42
2:AP1:329:MET:SD	2:AP1:329:MET:N	2.93	0.42
2:AP1:495:LEU:HD13	2:AP1:558:LYS:HG3	2.02	0.42
2:AP1:683:MET:O	2:AP1:687:MET:HG2	2.20	0.42
4:CP1:592:LEU:HD23	4:CP1:592:LEU:C	2.40	0.42
2:DP1:226:LYS:NZ	3:EP1:88:SER:OG	2.53	0.42
4:FP1:516:LEU:HD12	4:FP1:516:LEU:N	2.35	0.42
2:DP1:328:THR:O	2:DP1:328:THR:HG23	2.20	0.42
4:FP1:347:GLY:O	4:FP1:348:SER:OG	2.30	0.42
2:AP1:615:GLN:HB2	2:AP1:616:PRO:HD2	2.02	0.41
2:AP1:4:THR:HG23	2:AP1:7:GLU:H	1.84	0.41
4:CP1:177:ASP:N	4:CP1:177:ASP:OD1	2.54	0.41
4:CP1:559:ASP:OD1	4:CP1:559:ASP:O	2.38	0.41
3:EP1:534:ASN:HB2	3:EP1:540:LEU:HD12	2.03	0.41
3:EP1:30:MET:HB3	3:EP1:32:HIS:CD2	2.55	0.41
3:EP1:47:TYR:OH	3:EP1:405:PRO:HD3	2.20	0.41
2:AP1:290:PHE:HD2	2:AP1:295:LEU:HD23	1.84	0.41
4:CP1:371:GLU:OE1	4:CP1:372:GLN:N	2.48	0.41
3:EP1:69:CYS:SG	3:EP1:87:ILE:HD11	2.61	0.41
3:EP1:278:ASN:OD1	3:EP1:278:ASN:N	2.54	0.41
4:CP1:616:SER:O	4:CP1:617:ARG:C	2.59	0.41
4:FP1:305:LYS:O	4:FP1:309:LEU:HD23	2.19	0.41
3:EP1:302:VAL:HG22	3:EP1:486:SER:O	2.21	0.41
4:FP1:556:VAL:HG13	4:FP1:557:LEU:N	2.35	0.41
4:FP1:714:VAL:HG22	4:FP1:715:CYS:N	2.35	0.41
4:CP1:352:VAL:HG21	4:CP1:370:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DP1:641:GLY:O	2:DP1:645:GLU:HG2	2.20	0.41
3:BP1:498:PHE:CE2	3:BP1:502:PHE:CD1	3.08	0.41
3:BP1:725:LYS:CB	3:BP1:731:ILE:HD12	2.50	0.41
4:CP1:335:LEU:HB2	4:CP1:342:LEU:HB2	2.02	0.41
4:CP1:343:LYS:HD2	4:CP1:506:PRO:HG2	2.02	0.41
4:CP1:582:ILE:N	4:CP1:583:PRO:CD	2.84	0.41
3:EP1:249:ILE:HD12	3:EP1:249:ILE:N	2.35	0.41
3:EP1:357:ILE:CG1	3:EP1:370:ILE:HD11	2.50	0.41
2:AP1:595:GLU:O	2:AP1:599:ASN:ND2	2.54	0.41
3:BP1:691:MET:HE2	4:CP1:14:LEU:HD23	2.03	0.41
4:CP1:224:PHE:CD1	4:CP1:507:GLU:OE1	2.74	0.41
2:DP1:660:LYS:O	2:DP1:662:SER:N	2.54	0.41
4:FP1:585:LEU:HD12	4:FP1:594:LEU:HD23	2.01	0.41
2:AP1:390:ILE:O	2:AP1:390:ILE:HG22	2.19	0.40
3:BP1:487:LEU:HD23	3:BP1:487:LEU:HA	1.95	0.40
2:DP1:629:PHE:O	2:DP1:632:CYS:N	2.55	0.40
3:EP1:498:PHE:CD2	3:EP1:503:VAL:HG22	2.55	0.40
4:FP1:552:PRO:O	4:FP1:553:ASP:HB2	2.21	0.40
2:DP1:646:GLN:NE2	3:EP1:21:THR:HB	2.36	0.40
3:EP1:231:LYS:HD2	3:EP1:232:ASP:N	2.36	0.40
3:EP1:519:ASN:OD1	3:EP1:662:PHE:N	2.45	0.40
4:FP1:430:ILE:N	4:FP1:430:ILE:HD12	2.36	0.40
4:FP1:529:ILE:HD12	4:FP1:529:ILE:H	1.86	0.40
2:AP1:36:ILE:O	2:AP1:37:GLN:C	2.59	0.40
2:AP1:76:GLN:OE1	2:AP1:91:LEU:HD12	2.21	0.40
2:AP1:604:TRP:CE3	2:AP1:614:ALA:HB2	2.56	0.40
4:CP1:228:PHE:CZ	4:CP1:243:GLY:HA3	2.57	0.40
2:DP1:267:GLU:OE1	2:DP1:519:HIS:CE1	2.74	0.40
2:DP1:298:ILE:CG2	2:DP1:527:ALA:HB1	2.51	0.40
2:DP1:367:GLN:HB2	3:EP1:382:MET:HA	2.03	0.40
2:DP1:583:LEU:O	2:DP1:587:ALA:N	2.54	0.40
1:IN1:38:U:O2'	1:IN1:39:G:OP1	2.32	0.40
3:BP1:164:THR:OG1	3:BP1:165:MET:N	2.55	0.40
4:CP1:358:ILE:HG22	4:CP1:359:GLN:HG3	2.02	0.40
4:CP1:421:ASP:O	4:CP1:425:ASP:N	2.49	0.40
4:FP1:496:VAL:HG12	4:FP1:497:THR:N	2.36	0.40
3:BP1:162:GLY:HA2	3:BP1:167:GLU:OE1	2.21	0.40
3:EP1:311:TRP:HZ3	3:EP1:476:ILE:HG23	1.87	0.40
3:EP1:509:GLU:O	3:EP1:534:ASN:ND2	2.54	0.40
4:FP1:141:ARG:NE	4:FP1:250:GLU:OE1	2.54	0.40
4:FP1:637:LEU:O	4:FP1:641:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
2	AP1	692/709 (98%)	661 (96%)	31 (4%)	0	100	100
2	DP1	523/709 (74%)	505 (97%)	18 (3%)	0	100	100
3	BP1	704/754 (93%)	661 (94%)	43 (6%)	0	100	100
3	EP1	609/754 (81%)	566 (93%)	43 (7%)	0	100	100
4	CP1	770/774 (100%)	729 (95%)	41 (5%)	0	100	100
4	FP1	593/774 (77%)	552 (93%)	41 (7%)	0	100	100
All	All	3891/4474 (87%)	3674 (94%)	217 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	
2	AP1	620/631 (98%)	617 (100%)	3 (0%)	88	94
2	DP1	468/631 (74%)	463 (99%)	5 (1%)	73	86
3	BP1	632/669 (94%)	626 (99%)	6 (1%)	78	90
3	EP1	547/669 (82%)	539 (98%)	8 (2%)	65	82
4	CP1	677/679 (100%)	671 (99%)	6 (1%)	78	90
4	FP1	521/679 (77%)	517 (99%)	4 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3465/3958 (88%)	3433 (99%)	32 (1%)	79 90

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AP1	62	VAL
2	AP1	122	LYS
2	AP1	329	MET
3	BP1	50	SER
3	BP1	68	PHE
3	BP1	70	ASN
3	BP1	241	ARG
3	BP1	741	ASP
3	BP1	745	ASP
4	CP1	43	LYS
4	CP1	51	MET
4	CP1	52	ARG
4	CP1	371	GLU
4	CP1	446	GLN
4	CP1	451	ASN
2	DP1	235	LYS
2	DP1	242	GLU
2	DP1	292	LYS
2	DP1	414	TYR
2	DP1	543	ARG
3	EP1	30	MET
3	EP1	70	ASN
3	EP1	231	LYS
3	EP1	240	ARG
3	EP1	245	THR
3	EP1	362	LYS
3	EP1	386	TYR
3	EP1	410	MET
4	FP1	118	ILE
4	FP1	261	GLN
4	FP1	388	ARG
4	FP1	549	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	IN1	18/47 (38%)	8 (44%)	1 (5%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	IN1	6	A
1	IN1	8	A
1	IN1	11	A
1	IN1	14	G
1	IN1	36	C
1	IN1	37	C
1	IN1	38	U
1	IN1	39	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	IN1	38	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10659. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.