



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:02 PM EDT

PDB ID : 3THW / pdb_00003thw
Title : Human MutSbeta complexed with an IDL of 4 bases (Loop4) and ADP
Authors : Yang, W.
Deposited on : 2011-08-19
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

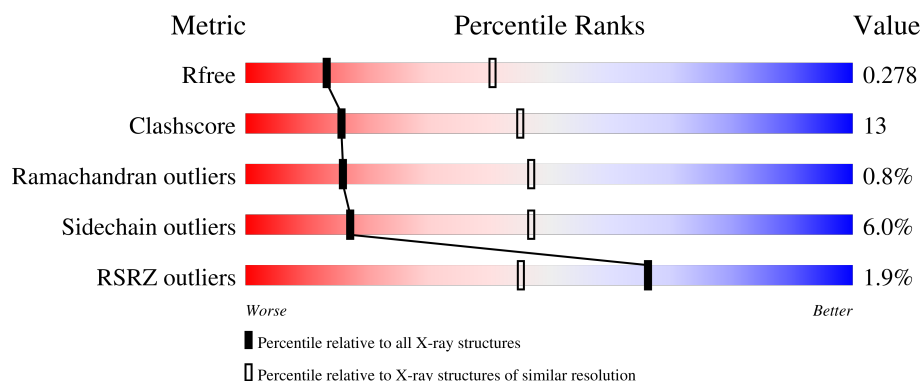
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	934	
2	B	918	
3	D	53	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14911 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	890	Total	C	N	O	S	0	0	0
			6939	4406	1178	1319	36			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	860	Total	C	N	O	S	0	2	0
			6825	4357	1169	1269	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	GLY	-	expression tag	GB 119616268
B	209	PRO	-	expression tag	GB 119616268

- Molecule 3 is a DNA chain called DNA Loop4 hairpin.

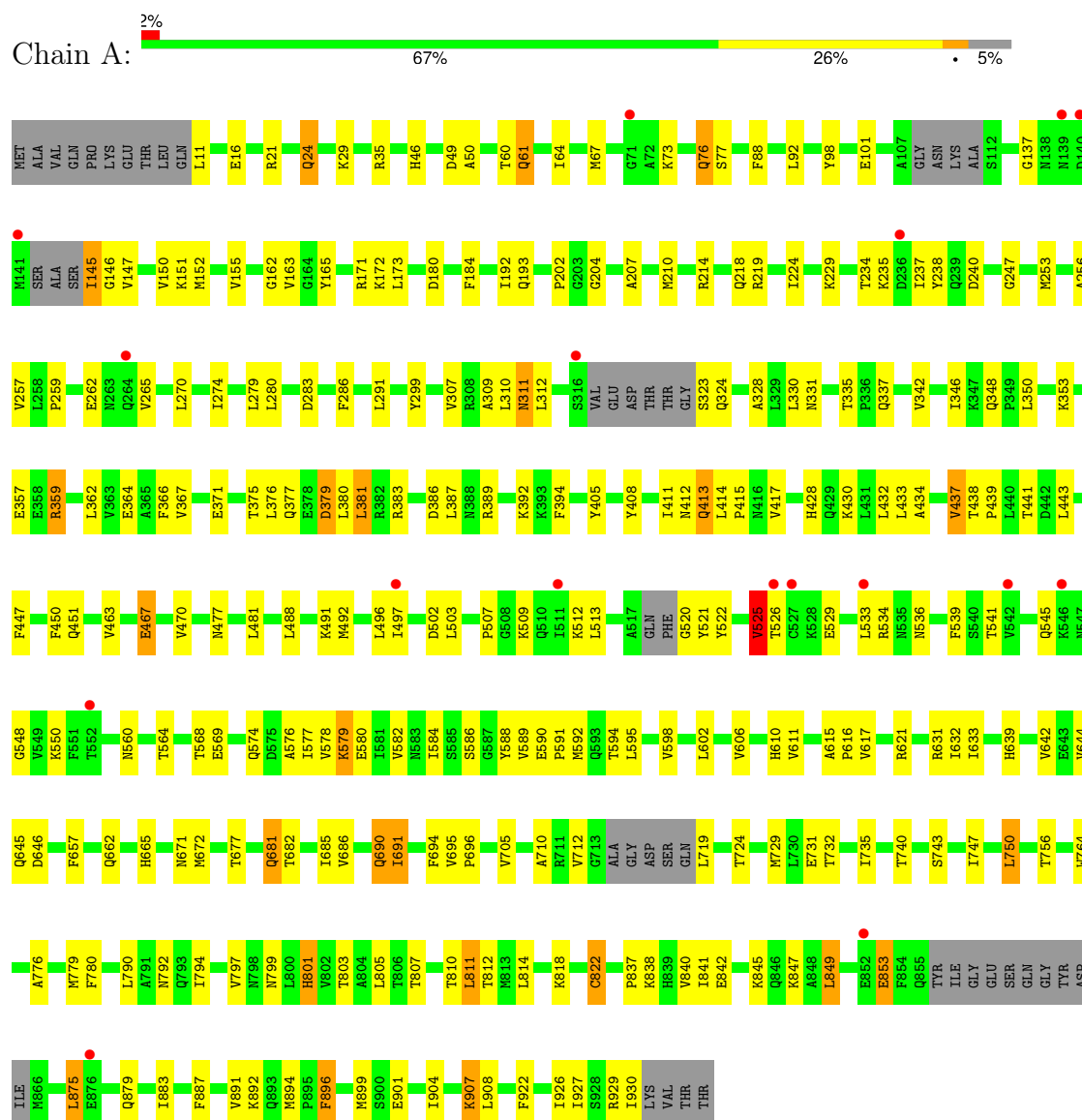
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	53	Total	C	N	O	P	0	2	0
			1116	531	209	322	54			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

3 Residue-property plots

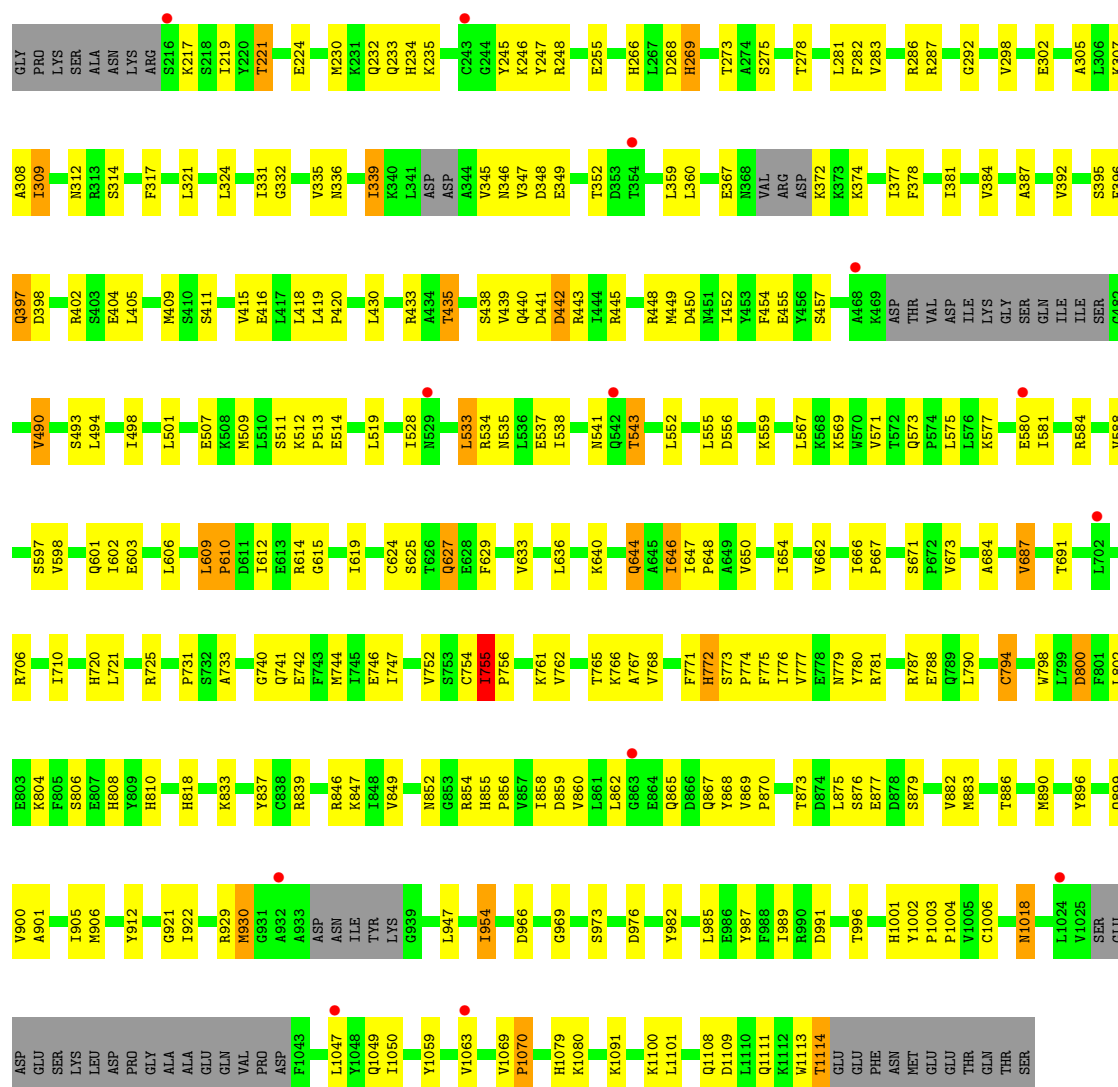
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA mismatch repair protein Msh2



• Molecule 2: DNA mismatch repair protein Msh3





● Molecule 3: DNA Loop4 hairpin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 116.13Å 180.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.53 – 3.09 32.53 – 3.09	Depositor EDS
% Data completeness (in resolution range)	92.8 (32.53-3.09) 91.5 (32.53-3.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.226 , 0.287 0.219 , 0.278	Depositor DCC
R_{free} test set	2065 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14911	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ADP

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	0.27	0/7046	0.70	0/9505
2	B	0.28	0/6954	0.70	2/9395 (0.0%)
3	D	0.10	0/1266	0.43	0/1952
All	All	0.27	0/15266	0.68	2/20852 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	755	ILE	CA-C-N	5.09	125.02	119.78
2	B	755	ILE	C-N-CA	5.09	125.02	119.78

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	6939	0	6911	179	0
2	B	6825	0	6896	186	0
3	D	1116	0	610	39	0
4	A	27	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14911	0	14429	390	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 13.

All (390) 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:D:24:DA:H8	3:D:26:DG:H1	1.15	0.94
1:A:413:GLN:HE21	1:A:413:GLN:HA	1.34	0.92
3:D:3:DT:H2''	3:D:4:DC:H5''	1.52	0.91
1:A:894:MET:HB3	1:A:896:PHE:HE2	1.37	0.88
2:B:969:GLY:HA3	2:B:1002:TYR:HE2	1.40	0.85
2:B:314:SER:HB2	3:D:28:DA:H2'	1.60	0.84
2:B:741:GLN:HE22	2:B:762:VAL:HB	1.44	0.82
2:B:248:ARG:HH11	2:B:273:THR:HG21	1.44	0.81
3:D:8:DC:H2''	3:D:9:DT:H5'	1.63	0.79
1:A:533:LEU:HD11	1:A:541:THR:HG21	1.65	0.79
3:D:12:DA:H2''	3:D:13:DG:C8	2.21	0.76
2:B:646:ILE:CG2	2:B:646:ILE:O	2.34	0.76
2:B:439:VAL:HG12	2:B:440:GLN:H	1.51	0.75
1:A:61:GLN:HG3	1:A:64:ILE:HD12	1.70	0.73
2:B:331:ILE:HD11	2:B:387:ALA:HA	1.71	0.73
2:B:746:GLU:HG3	2:B:768:VAL:HG21	1.69	0.72
1:A:375:THR:O	1:A:379:ASP:HB2	1.90	0.71
1:A:274:ILE:HG23	1:A:279:LEU:HD12	1.70	0.71
2:B:646:ILE:O	2:B:646:ILE:HG23	1.92	0.70
1:A:894:MET:HB3	1:A:896:PHE:CE2	2.25	0.70
3:D:26:DG:H2''	3:D:27:DC:OP2	1.93	0.68
3:D:39[A]:DA:H2'	3:D:40[A]:DG:O4'	1.94	0.68
3:D:50:DG:H2''	3:D:51:DA:OP2	1.94	0.67
2:B:969:GLY:HA3	2:B:1002:TYR:CE2	2.28	0.67
1:A:534:ARG:HG3	2:B:752:VAL:HB	1.76	0.67
3:D:10:DG:H1'	3:D:11:DA:H5'	1.75	0.67
1:A:283:ASP:HA	1:A:286:PHE:CD2	2.30	0.67
1:A:323:SER:HA	1:A:645:GLN:HE22	1.61	0.66
2:B:875:LEU:HD21	2:B:883:MET:HE3	1.78	0.66
1:A:807:THR:HB	1:A:810:THR:HB	1.77	0.66
2:B:706:ARG:HB3	2:B:790:LEU:HD12	1.77	0.65
2:B:559:LYS:HE3	2:B:603:GLU:HG3	1.77	0.65
2:B:230:MET:HE1	2:B:298:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HG21	1:A:750:LEU:HD23	1.79	0.64
1:A:408:TYR:HA	1:A:451:GLN:HE22	1.62	0.64
2:B:282:PHE:O	2:B:286:ARG:HG3	1.97	0.64
3:D:26:DG:H4'	3:D:27:DC:H5'	1.80	0.64
3:D:50:DG:H1'	3:D:51:DA:H5'	1.78	0.64
1:A:202:PRO:C	1:A:204:GLY:H	2.04	0.64
1:A:204:GLY:HA2	1:A:229:LYS:NZ	2.13	0.64
1:A:433:LEU:HD12	1:A:434:ALA:N	2.13	0.64
1:A:764:TRP:CE2	2:B:1080:LYS:HE3	2.33	0.63
2:B:217:LYS:HG2	2:B:219:ILE:HG22	1.80	0.63
3:D:22:DT:H4'	3:D:23:DG:OP1	1.99	0.63
2:B:494:LEU:O	2:B:498:ILE:HG13	1.99	0.62
2:B:535:ASN:HB3	2:B:930:MET:HE2	1.81	0.62
2:B:233:GLN:HG3	2:B:234:HIS:CD2	2.34	0.62
3:D:47:DA:H2''	3:D:48:DT:H5''	1.81	0.62
2:B:232:GLN:HA	2:B:235:LYS:HE3	1.80	0.62
1:A:16:GLU:HG3	1:A:67:MET:HE3	1.81	0.61
2:B:398:ASP:CG	2:B:404:GLU:HB2	2.26	0.61
1:A:162:GLY:HA3	1:A:265:VAL:HG12	1.83	0.61
2:B:612:ILE:HD12	2:B:612:ILE:H	1.65	0.60
1:A:447:PHE:HZ	1:A:592:MET:HB3	1.65	0.60
1:A:376:LEU:O	1:A:381:LEU:HB2	2.02	0.60
1:A:240:ASP:CG	1:A:280:LEU:HD11	2.27	0.59
1:A:76:GLN:H	1:A:76:GLN:HE21	1.48	0.59
1:A:150:VAL:HG22	1:A:163:VAL:HG22	1.83	0.59
1:A:346:ILE:HA	1:A:691:ILE:HD11	1.84	0.59
2:B:541:ASN:OD1	2:B:543:THR:HG23	2.03	0.59
3:D:22:DT:H2''	3:D:23:DG:O5'	2.03	0.58
3:D:38:DC:H2''	3:D:39[B]:DA:C8	2.38	0.58
1:A:522:TYR:CE1	1:A:550:LYS:HD3	2.39	0.58
1:A:521:TYR:H	1:A:560:ASN:ND2	2.02	0.58
2:B:747:ILE:O	2:B:768:VAL:HG23	2.03	0.58
3:D:37:DA:H1'	3:D:38:DC:H5''	1.85	0.58
1:A:534:ARG:H	1:A:534:ARG:HD3	1.69	0.57
1:A:430:LYS:O	1:A:433:LEU:HG	2.05	0.57
1:A:46:HIS:ND1	1:A:77:SER:HB3	2.19	0.57
1:A:503:LEU:HD21	1:A:539:PHE:HE2	1.70	0.57
2:B:741:GLN:NE2	2:B:762:VAL:HB	2.17	0.57
2:B:360:LEU:HD11	2:B:381:ILE:HB	1.87	0.57
3:D:2:DC:H2'	3:D:3:DT:C6	2.40	0.57
1:A:642:VAL:HA	1:A:645:GLN:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:VAL:HG12	2:B:440:GLN:N	2.20	0.56
1:A:270:LEU:O	1:A:274:ILE:HG13	2.06	0.56
1:A:801:HIS:HD2	1:A:822:CYS:HB2	1.70	0.56
1:A:896:PHE:N	1:A:896:PHE:CD2	2.69	0.56
2:B:612:ILE:HG21	2:B:636:LEU:HD21	1.86	0.56
2:B:862:LEU:HD13	2:B:865:GLN:NE2	2.20	0.56
3:D:51:DA:H2''	3:D:52:DG:O4'	2.06	0.56
1:A:376:LEU:HD21	1:A:602:LEU:HD21	1.87	0.56
1:A:896:PHE:N	1:A:896:PHE:HD2	2.02	0.55
1:A:639:HIS:CD2	1:A:642:VAL:HG23	2.41	0.55
3:D:24:DA:H2''	3:D:25:DA:C2	2.42	0.55
1:A:283:ASP:HA	1:A:286:PHE:CE2	2.41	0.55
1:A:337:GLN:OE1	1:A:386:ASP:HA	2.07	0.55
1:A:450:PHE:HB2	1:A:588:TYR:CE2	2.41	0.55
2:B:746:GLU:HG3	2:B:768:VAL:CG2	2.35	0.55
1:A:171:ARG:O	1:A:172:LYS:HD3	2.07	0.55
1:A:477:ASN:O	1:A:481:LEU:HD13	2.06	0.55
3:D:24:DA:H8	3:D:26:DG:N1	1.94	0.55
1:A:837:PRO:HB2	1:A:840:VAL:HG23	1.89	0.55
2:B:662:VAL:HG13	2:B:818:HIS:HB3	1.88	0.55
2:B:746:GLU:CG	2:B:768:VAL:HG21	2.35	0.55
2:B:1006:CYS:HB3	2:B:1018:ASN:HD21	1.72	0.55
1:A:588:TYR:C	1:A:591:PRO:HD2	2.32	0.55
1:A:926:ILE:O	1:A:930:ILE:HG13	2.07	0.55
2:B:307:LYS:C	2:B:309:ILE:H	2.15	0.55
2:B:392:VAL:HG11	2:B:519:LEU:HD13	1.87	0.55
2:B:575:LEU:HD13	2:B:580:GLU:HG3	1.89	0.55
1:A:180:ASP:OD2	1:A:184:PHE:HA	2.07	0.55
2:B:740:GLY:O	2:B:742:GLU:HG3	2.07	0.55
2:B:985:LEU:O	2:B:989:ILE:HG13	2.08	0.54
3:D:49:DA:H2'	3:D:50:DG:C8	2.43	0.54
1:A:780:PHE:C	1:A:780:PHE:HD1	2.16	0.54
2:B:305:ALA:HB3	2:B:788:GLU:CD	2.33	0.54
1:A:525:VAL:HG11	1:A:529:GLU:HB2	1.90	0.54
2:B:773:SER:O	2:B:777:VAL:HG23	2.08	0.54
3:D:46:DG:H2''	3:D:47:DA:OP2	2.08	0.54
1:A:307:VAL:HG13	1:A:312:LEU:HD12	1.89	0.54
1:A:470:VAL:HG11	1:A:577:ILE:HD11	1.89	0.53
2:B:377:ILE:HG12	2:B:378:PHE:H	1.72	0.53
2:B:584:ARG:O	2:B:588:VAL:HG23	2.07	0.53
1:A:568:THR:HG23	1:A:569:GLU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:GLU:CD	2:B:514:GLU:H	2.16	0.53
2:B:777:VAL:O	2:B:781:ARG:HG3	2.08	0.53
2:B:619:ILE:HG12	2:B:624:CYS:SG	2.48	0.53
2:B:755:ILE:HD12	2:B:756:PRO:O	2.08	0.53
1:A:875:LEU:O	1:A:879:GLN:HG2	2.08	0.53
1:A:247:GLY:HA2	1:A:253:MET:HE2	1.90	0.53
1:A:496:LEU:HD22	1:A:513:LEU:HB3	1.91	0.53
1:A:433:LEU:HA	1:A:437:VAL:HG12	1.91	0.53
1:A:579:LYS:NZ	1:A:579:LYS:HB3	2.24	0.53
2:B:528:ILE:HG21	2:B:533:LEU:HD13	1.90	0.53
1:A:411:ILE:O	1:A:414:LEU:HB2	2.09	0.52
2:B:1113:TRP:CE3	2:B:1114:THR:HG23	2.43	0.52
1:A:214:ARG:O	1:A:218:GLN:HB2	2.09	0.52
2:B:569:LYS:O	2:B:573:GLN:HG2	2.10	0.52
2:B:640:LYS:O	2:B:644:GLN:HB2	2.09	0.52
2:B:647:ILE:HB	2:B:648:PRO:HD3	1.91	0.52
1:A:729:MET:HA	1:A:729:MET:HE2	1.92	0.52
1:A:631:ARG:HH21	1:A:633:ILE:HD11	1.74	0.52
1:A:743:SER:O	1:A:776:ALA:HB1	2.09	0.52
1:A:794:ILE:HB	1:A:797:VAL:HG23	1.90	0.52
2:B:317:PHE:CD1	3:D:16:DG:H3'	2.45	0.52
2:B:398:ASP:OD2	2:B:402:ARG:HA	2.10	0.52
1:A:202:PRO:C	1:A:204:GLY:N	2.68	0.51
1:A:463:VAL:HA	1:A:467:GLU:O	2.09	0.51
1:A:586:SER:O	1:A:589:VAL:HG23	2.10	0.51
1:A:35:ARG:HG2	1:A:101:GLU:HB2	1.92	0.51
1:A:671:ASN:O	1:A:672:MET:HB2	2.10	0.51
2:B:246:LYS:HD3	2:B:275:SER:HB3	1.92	0.51
1:A:61:GLN:HB3	2:B:339:ILE:HD13	1.92	0.51
2:B:597:SER:O	2:B:601:GLN:HG3	2.11	0.51
2:B:773:SER:HB2	2:B:774:PRO:HD2	1.93	0.51
3:D:2:DC:H2''	3:D:3:DT:O5'	2.11	0.51
1:A:324:GLN:HG2	1:A:328:ALA:HB3	1.93	0.51
1:A:887:PHE:O	1:A:891:VAL:HG23	2.10	0.51
2:B:377:ILE:HG12	2:B:378:PHE:N	2.26	0.51
2:B:847:LYS:HG3	2:B:876:SER:HB3	1.93	0.51
3:D:8:DC:C2'	3:D:9:DT:H5'	2.37	0.51
1:A:849:LEU:HB3	1:A:929:ARG:NH2	2.26	0.50
1:A:780:PHE:C	1:A:780:PHE:CD1	2.87	0.50
3:D:2:DC:H4'	3:D:3:DT:OP1	2.11	0.50
1:A:46:HIS:HA	1:A:50:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:862:LEU:HD13	2:B:865:GLN:HE22	1.76	0.50
2:B:283:VAL:O	2:B:287:ARG:HG3	2.11	0.50
1:A:847:LYS:HE3	2:B:982:TYR:CZ	2.46	0.50
2:B:438:SER:OG	2:B:443:ARG:HA	2.12	0.50
1:A:76:GLN:H	1:A:76:GLN:NE2	2.10	0.50
2:B:741:GLN:HB3	2:B:744:MET:SD	2.52	0.50
2:B:765:THR:C	2:B:767:ALA:H	2.20	0.50
2:B:776:ILE:O	2:B:780:TYR:HB2	2.11	0.50
1:A:525:VAL:HG12	1:A:526:THR:H	1.77	0.50
1:A:413:GLN:HA	1:A:413:GLN:NE2	2.16	0.50
2:B:292:GLY:O	2:B:445:ARG:HD2	2.12	0.49
2:B:612:ILE:HD12	2:B:612:ILE:N	2.27	0.49
1:A:210:MET:O	1:A:214:ARG:HG3	2.11	0.49
2:B:602:ILE:O	2:B:606:LEU:HD13	2.11	0.49
2:B:268:ASP:O	2:B:269:HIS:HB2	2.12	0.49
1:A:67:MET:C	1:A:73:LYS:HB2	2.37	0.49
2:B:349:GLU:HA	2:B:614:ARG:HH12	1.77	0.49
2:B:846:ARG:HA	2:B:921:GLY:HA3	1.95	0.49
2:B:646:ILE:O	2:B:650:VAL:HG23	2.12	0.49
1:A:29:LYS:HB3	1:A:35:ARG:NH2	2.28	0.49
1:A:580:GLU:O	1:A:584:ILE:HG13	2.12	0.49
1:A:672:MET:HA	1:A:672:MET:HE2	1.95	0.49
2:B:1001:HIS:O	2:B:1003:PRO:HD3	2.11	0.49
1:A:387:LEU:HD11	1:A:595:LEU:HD23	1.95	0.49
2:B:747:ILE:O	2:B:747:ILE:HD12	2.13	0.49
2:B:837:TYR:HB3	2:B:912:TYR:HB3	1.95	0.48
1:A:764:TRP:NE1	2:B:1080:LYS:HE3	2.28	0.48
1:A:438:THR:HB	1:A:439:PRO:HD3	1.94	0.48
2:B:882:VAL:HG22	2:B:996:THR:HB	1.94	0.48
1:A:310:LEU:O	1:A:311:ASN:C	2.57	0.48
1:A:439:PRO:O	1:A:443:LEU:HD23	2.12	0.48
1:A:488:LEU:O	1:A:492:MET:HG3	2.13	0.48
1:A:60:THR:HB	2:B:286:ARG:HD3	1.95	0.48
1:A:238:TYR:CE1	1:A:256:ALA:HA	2.48	0.48
1:A:534:ARG:CG	2:B:752:VAL:HB	2.44	0.48
2:B:899:GLN:HG3	2:B:900:VAL:N	2.28	0.48
2:B:973:SER:HB2	2:B:976:ASP:HB2	1.95	0.48
1:A:67:MET:HA	1:A:73:LYS:HD2	1.95	0.48
1:A:632:ILE:HB	1:A:657:PHE:HB2	1.96	0.48
2:B:806:SER:C	2:B:808:HIS:H	2.21	0.48
2:B:987:TYR:O	2:B:991:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD21	1:A:359:ARG:NH1	2.28	0.48
2:B:552:LEU:O	2:B:556:ASP:HB2	2.13	0.48
1:A:731:GLU:O	1:A:735:ILE:HG13	2.14	0.47
2:B:455:GLU:OE1	2:B:457:SER:HB3	2.13	0.47
2:B:633:VAL:HG13	2:B:673:VAL:HG13	1.96	0.47
1:A:621:ARG:HB2	1:A:694:PHE:CE1	2.48	0.47
1:A:801:HIS:CE1	1:A:818:LYS:HB3	2.49	0.47
2:B:559:LYS:HE3	2:B:603:GLU:CG	2.43	0.47
2:B:849:VAL:HA	2:B:873:THR:O	2.14	0.47
2:B:854:ARG:HE	2:B:859:ASP:CG	2.22	0.47
3:D:33:DT:H2''	3:D:34:DC:H5'	1.96	0.47
2:B:856:PRO:O	2:B:860:VAL:HG23	2.14	0.47
2:B:896:TYR:O	2:B:899:GLN:HG2	2.13	0.47
1:A:259:PRO:O	1:A:262:GLU:HG2	2.13	0.47
1:A:380:LEU:HA	1:A:383:ARG:HD2	1.96	0.47
2:B:528:ILE:CG2	2:B:533:LEU:HD13	2.44	0.47
2:B:555:LEU:HD21	2:B:906:MET:HE3	1.97	0.47
2:B:775:PHE:O	2:B:779:ASN:HB2	2.14	0.47
2:B:865:GLN:HE21	2:B:868:TYR:H	1.63	0.47
2:B:1108:GLN:O	2:B:1111:GLN:HB3	2.15	0.47
3:D:3:DT:C2'	3:D:4:DC:H5''	2.34	0.47
1:A:588:TYR:O	1:A:592:MET:HG2	2.14	0.47
1:A:681:GLN:O	1:A:685:ILE:HG12	2.15	0.46
1:A:803:THR:OG1	1:A:814:LEU:HB2	2.16	0.46
2:B:372:LYS:C	2:B:374:LYS:H	2.22	0.46
2:B:537:GLU:HG2	2:B:541:ASN:HA	1.96	0.46
1:A:450:PHE:HD2	1:A:451:GLN:HE21	1.64	0.46
1:A:564:THR:O	1:A:568:THR:HG22	2.14	0.46
2:B:533:LEU:HD12	2:B:538:ILE:HG13	1.97	0.46
3:D:37:DA:H2''	3:D:38:DC:H5'	1.96	0.46
2:B:359:LEU:HD12	2:B:416:GLU:O	2.16	0.46
1:A:376:LEU:HD23	1:A:606:VAL:HG21	1.97	0.46
2:B:610:PRO:HD2	2:B:612:ILE:HD11	1.97	0.46
2:B:930:MET:CB	2:B:966:ASP:HB3	2.45	0.46
1:A:497:ILE:HA	1:A:507:PRO:HB3	1.98	0.46
1:A:677:THR:O	1:A:681:GLN:HB3	2.16	0.46
1:A:838:LYS:O	1:A:842:GLU:HG2	2.16	0.46
1:A:899:MET:HB2	1:A:904:ILE:HD11	1.98	0.46
2:B:221:THR:HG23	2:B:224:GLU:OE1	2.16	0.46
3:D:3:DT:H1'	3:D:4:DC:O4'	2.15	0.46
3:D:7:DT:H2''	3:D:8:DC:O5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD11	1:A:165:TYR:HB2	1.96	0.46
1:A:377:GLN:HE22	1:A:610:HIS:HB2	1.80	0.46
2:B:452:ILE:N	2:B:452:ILE:HD12	2.31	0.46
3:D:51:DA:H2'	3:D:52:DG:C8	2.51	0.46
1:A:204:GLY:HA2	1:A:229:LYS:HZ2	1.80	0.46
2:B:395:SER:HB3	2:B:490:VAL:CG1	2.46	0.46
2:B:450:ASP:HB3	2:B:452:ILE:HD13	1.97	0.46
2:B:575:LEU:HB2	2:B:581:ILE:HG12	1.98	0.46
1:A:219:ARG:HG2	1:A:719:LEU:HA	1.98	0.46
1:A:526:THR:HA	1:A:548:GLY:HA3	1.98	0.46
1:A:922:PHE:O	1:A:926:ILE:HD12	2.16	0.46
2:B:435:THR:CG2	2:B:435:THR:O	2.64	0.46
2:B:646:ILE:CG2	2:B:650:VAL:HG23	2.46	0.46
2:B:877:GLU:C	2:B:879:SER:H	2.24	0.46
1:A:496:LEU:HD11	1:A:512:LYS:HA	1.98	0.45
2:B:221:THR:CG2	2:B:269:HIS:HD2	2.29	0.45
2:B:302:GLU:CD	2:B:307:LYS:HE2	2.41	0.45
1:A:428:HIS:O	1:A:432:LEU:HB2	2.16	0.45
1:A:331:ASN:OD1	1:A:342:VAL:HB	2.16	0.45
2:B:405:LEU:HD23	2:B:430:LEU:HD23	1.97	0.45
2:B:1050:ILE:HG23	2:B:1050:ILE:O	2.17	0.45
2:B:1113:TRP:HE3	2:B:1114:THR:HG23	1.82	0.45
1:A:853:GLU:OE1	2:B:1091:LYS:HD3	2.16	0.45
1:A:810:THR:HG22	1:A:811:LEU:N	2.30	0.45
2:B:609:LEU:HD12	2:B:609:LEU:HA	1.82	0.45
1:A:899:MET:HB2	1:A:904:ILE:CD1	2.46	0.45
1:A:371:GLU:H	1:A:371:GLU:CD	2.25	0.45
2:B:221:THR:HG22	2:B:269:HIS:HD2	1.82	0.45
2:B:409:MET:HE2	2:B:409:MET:HB3	1.91	0.45
1:A:29:LYS:HB3	1:A:35:ARG:CZ	2.47	0.45
1:A:92:LEU:HD22	1:A:98:TYR:HD1	1.82	0.45
1:A:579:LYS:HD2	1:A:579:LYS:O	2.17	0.45
2:B:430:LEU:HA	2:B:433:ARG:NH1	2.31	0.45
1:A:145:ILE:HD13	1:A:146:GLY:N	2.31	0.44
1:A:657:PHE:CE2	1:A:779:MET:HE3	2.53	0.44
2:B:512:LYS:HG3	2:B:810:HIS:CE1	2.53	0.44
2:B:798:TRP:O	2:B:802:LEU:HG	2.17	0.44
2:B:752:VAL:C	2:B:754:CYS:H	2.24	0.44
2:B:335:VAL:HG22	2:B:335:VAL:O	2.18	0.44
1:A:394:PHE:HD1	1:A:582:VAL:HG13	1.83	0.44
2:B:396:PHE:CE1	2:B:404:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:511:SER:O	2:B:513:PRO:HD3	2.18	0.44
2:B:247:TYR:CZ	2:B:281:LEU:HD22	2.52	0.44
2:B:352:THR:HG21	2:B:415:VAL:HG11	2.00	0.44
2:B:800:ASP:O	2:B:804:LYS:HG3	2.18	0.44
1:A:24:GLN:HE21	1:A:24:GLN:HA	1.83	0.44
1:A:662:GLN:HB3	1:A:665:HIS:CE1	2.53	0.44
1:A:710:ALA:HB1	1:A:712:VAL:HG23	1.99	0.44
2:B:666:ILE:N	2:B:667:PRO:HD2	2.32	0.44
2:B:721:LEU:O	2:B:725:ARG:HG3	2.18	0.44
3:D:28:DA:H2''	3:D:29:DT:O5'	2.17	0.43
2:B:855:HIS:CG	2:B:858:ILE:HD13	2.54	0.43
1:A:330:LEU:HA	1:A:611:VAL:HG21	2.01	0.43
1:A:502:ASP:C	1:A:503:LEU:HD22	2.43	0.43
1:A:837:PRO:HG2	2:B:954:ILE:HG21	2.00	0.43
2:B:286:ARG:NH1	2:B:335:VAL:O	2.52	0.43
2:B:245:TYR:C	2:B:278:THR:HG23	2.43	0.43
2:B:625:SER:HB2	2:B:627:GLN:OE1	2.19	0.43
2:B:629:PHE:O	2:B:633:VAL:HG23	2.19	0.43
2:B:706:ARG:O	2:B:710:ILE:HG13	2.18	0.43
2:B:221:THR:CG2	2:B:269:HIS:CD2	3.01	0.43
2:B:321:LEU:HD21	2:B:324:LEU:HD21	2.01	0.43
1:A:594:THR:O	1:A:598:VAL:HG23	2.19	0.43
2:B:378:PHE:HA	2:B:397:GLN:HA	2.00	0.43
2:B:725:ARG:HG2	2:B:733:ALA:HB3	2.00	0.43
1:A:801:HIS:HE1	1:A:818:LYS:HB3	1.83	0.43
1:A:740:THR:O	1:A:776:ALA:HB2	2.18	0.43
2:B:419:LEU:O	2:B:448:ARG:HA	2.18	0.43
2:B:684:ALA:O	2:B:687:VAL:HG13	2.19	0.43
2:B:720:HIS:NE2	2:B:775:PHE:HB3	2.34	0.43
2:B:852:ASN:C	2:B:870:PRO:HB3	2.44	0.43
1:A:414:LEU:N	1:A:415:PRO:CD	2.82	0.43
1:A:695:VAL:HA	1:A:696:PRO:HD3	1.83	0.43
2:B:567:LEU:O	2:B:571:VAL:HG23	2.19	0.43
1:A:234:THR:O	1:A:237:ILE:HG22	2.18	0.42
1:A:682:THR:O	1:A:686:VAL:HG23	2.19	0.42
1:A:840:VAL:HG22	2:B:987:TYR:CD1	2.54	0.42
2:B:650:VAL:HG13	2:B:654:ILE:HD12	2.01	0.42
2:B:1003:PRO:HB2	2:B:1004:PRO:HD3	2.00	0.42
3:D:27:DC:H2'	3:D:28:DA:C8	2.54	0.42
1:A:299:TYR:CD1	1:A:348:GLN:HB3	2.54	0.42
2:B:575:LEU:CD1	2:B:580:GLU:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1069:VAL:O	2:B:1070:PRO:C	2.62	0.42
1:A:11:LEU:HD13	1:A:67:MET:HE1	2.01	0.42
1:A:525:VAL:HG21	1:A:529:GLU:HG2	1.99	0.42
2:B:755:ILE:HA	2:B:756:PRO:HD3	1.87	0.42
1:A:534:ARG:HD3	1:A:534:ARG:N	2.34	0.42
2:B:533:LEU:HD12	2:B:533:LEU:HA	1.76	0.42
2:B:865:GLN:NE2	2:B:867:GLN:HB2	2.35	0.42
1:A:362:LEU:O	1:A:366:PHE:HD2	2.03	0.42
1:A:892:LYS:C	1:A:894:MET:H	2.28	0.42
2:B:627:GLN:CD	2:B:627:GLN:H	2.28	0.42
1:A:283:ASP:HA	1:A:286:PHE:HD2	1.82	0.42
2:B:1047:LEU:C	2:B:1047:LEU:HD13	2.45	0.42
2:B:248:ARG:NH1	2:B:273:THR:HG21	2.23	0.42
2:B:1109:ASP:C	2:B:1111:GLN:H	2.28	0.42
3:D:48:DT:H2''	3:D:49:DA:H8	1.84	0.42
2:B:725:ARG:HD3	2:B:731:PRO:HA	2.02	0.42
2:B:441:ASP:OD2	2:B:442:ASP:N	2.53	0.41
2:B:452:ILE:HD12	2:B:452:ILE:H	1.85	0.41
1:A:411:ILE:HD13	1:A:447:PHE:CG	2.55	0.41
1:A:412:ASN:O	1:A:415:PRO:HD2	2.20	0.41
2:B:761:LYS:HD2	2:B:761:LYS:O	2.20	0.41
3:D:12:DA:H2''	3:D:13:DG:H8	1.76	0.41
1:A:488:LEU:HD12	1:A:491:LYS:HE2	2.02	0.41
1:A:690:GLN:HE21	1:A:690:GLN:HB3	1.66	0.41
2:B:418:LEU:HD11	2:B:449:MET:HE3	2.02	0.41
2:B:439:VAL:C	2:B:441:ASP:H	2.28	0.41
2:B:766:LYS:HE3	2:B:766:LYS:HB2	1.87	0.41
1:A:309:ALA:C	1:A:311:ASN:H	2.28	0.41
1:A:520:GLY:HA3	1:A:560:ASN:HD21	1.86	0.41
1:A:574:GLN:C	1:A:576:ALA:H	2.28	0.41
2:B:901:ALA:O	2:B:905:ILE:HG13	2.21	0.41
1:A:193:GLN:HB2	1:A:348:GLN:HG2	2.03	0.41
1:A:376:LEU:HD21	1:A:602:LEU:HD11	2.02	0.41
1:A:747:ILE:CG2	1:A:750:LEU:HD23	2.50	0.41
3:D:2:DC:H2''	3:D:3:DT:C5'	2.50	0.41
1:A:841:ILE:O	1:A:845:LYS:HG3	2.21	0.41
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.55	0.41
1:A:353:LYS:O	1:A:357:GLU:HG2	2.21	0.41
1:A:61:GLN:CB	2:B:339:ILE:HD13	2.50	0.41
2:B:615:GLY:O	2:B:619:ILE:HG13	2.20	0.41
1:A:173:LEU:O	1:A:291:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HA	1:A:367:VAL:HG22	2.03	0.41
1:A:376:LEU:HD11	1:A:417:VAL:HG13	2.03	0.41
1:A:907:LYS:HZ3	1:A:907:LYS:HB2	1.86	0.41
1:A:927:ILE:HA	1:A:930:ILE:HD12	2.03	0.41
2:B:266:HIS:H	2:B:266:HIS:CD2	2.38	0.41
2:B:747:ILE:HD11	2:B:771:PHE:HE2	1.86	0.41
2:B:762:VAL:HG11	2:B:772:HIS:CD2	2.56	0.41
2:B:930:MET:HB3	2:B:966:ASP:HB3	2.03	0.41
2:B:420:PRO:HG3	2:B:454:PHE:CZ	2.56	0.41
1:A:29:LYS:HE2	1:A:49:ASP:OD2	2.21	0.40
1:A:151:LYS:HG2	1:A:152:MET:N	2.37	0.40
1:A:389:ARG:O	1:A:392:LYS:HB3	2.21	0.40
1:A:405:TYR:CE1	1:A:463:VAL:HG21	2.56	0.40
2:B:332:GLY:O	2:B:336:ASN:HB2	2.21	0.40
2:B:346:ASN:CG	2:B:347:VAL:N	2.79	0.40
2:B:833:LYS:HE3	2:B:833:LYS:HB2	1.87	0.40
2:B:1100:LYS:HE2	2:B:1100:LYS:HB3	1.83	0.40
3:D:18:DT:H2''	3:D:19:DC:H5'	2.02	0.40
3:D:22:DT:H2'	3:D:23:DG:C8	2.56	0.40
1:A:578:VAL:O	1:A:582:VAL:HG23	2.22	0.40
1:A:590:GLU:HB3	1:A:591:PRO:HD3	2.03	0.40
1:A:615:ALA:O	1:A:616:PRO:C	2.65	0.40
1:A:794:ILE:HB	1:A:797:VAL:CG2	2.52	0.40
1:A:891:VAL:HG21	2:B:1101:LEU:HD21	2.02	0.40
2:B:246:LYS:HB3	2:B:246:LYS:HE2	1.83	0.40
2:B:575:LEU:HB2	2:B:581:ILE:CG1	2.51	0.40
2:B:691:THR:HA	2:B:794:CYS:SG	2.61	0.40
1:A:790:LEU:C	1:A:792:ASN:H	2.28	0.40
2:B:384:VAL:HB	2:B:509:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	876/934 (94%)	787 (90%)	81 (9%)	8 (1%)	14	44
2	B	850/918 (93%)	767 (90%)	77 (9%)	6 (1%)	18	49
All	All	1726/1852 (93%)	1554 (90%)	158 (9%)	14 (1%)	16	47

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	610	PRO
1	A	155	VAL
2	B	269	HIS
1	A	137	GLY
1	A	207	ALA
1	A	311	ASN
1	A	509	LYS
2	B	367	GLU
1	A	235	LYS
1	A	646	ASP
2	B	308	ALA
1	A	525	VAL
2	B	922	ILE
2	B	1070	PRO

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	746/808 (92%)	701 (94%)	45 (6%)	17	47
2	B	751/818 (92%)	706 (94%)	45 (6%)	17	47
All	All	1497/1626 (92%)	1407 (94%)	90 (6%)	17	47

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	61	GLN
1	A	76	GLN
1	A	145	ILE
1	A	147	VAL
1	A	192	ILE
1	A	224	ILE
1	A	257	VAL
1	A	335	THR
1	A	359	ARG
1	A	379	ASP
1	A	381	LEU
1	A	413	GLN
1	A	437	VAL
1	A	441	THR
1	A	467	GLU
1	A	525	VAL
1	A	536	ASN
1	A	545	GLN
1	A	579	LYS
1	A	617	VAL
1	A	644	VAL
1	A	681	GLN
1	A	690	GLN
1	A	691	ILE
1	A	705	VAL
1	A	724	THR
1	A	732	THR
1	A	750	LEU
1	A	756	THR
1	A	799	ASN
1	A	801	HIS
1	A	805	LEU
1	A	811	LEU
1	A	812	THR
1	A	822	CYS
1	A	849	LEU
1	A	853	GLU
1	A	875	LEU
1	A	883	ILE
1	A	896	PHE
1	A	901	GLU
1	A	907	LYS

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Mol	Chain	Res	Type
1	A	908	LEU
2	B	221	THR
2	B	255	GLU
2	B	309	ILE
2	B	312	ASN
2	B	339	ILE
2	B	345	VAL
2	B	348	ASP
2	B	397	GLN
2	B	411	SER
2	B	435	THR
2	B	442	ASP
2	B	490	VAL
2	B	493	SER
2	B	501	LEU
2	B	507	GLU
2	B	533	LEU
2	B	534	ARG
2	B	543	THR
2	B	577	LYS
2	B	598	VAL
2	B	609	LEU
2	B	627	GLN
2	B	644	GLN
2	B	646	ILE
2	B	671	SER
2	B	687	VAL
2	B	755	ILE
2	B	772	HIS
2	B	787	ARG
2	B	794	CYS
2	B	800	ASP
2	B	839	ARG
2	B	869	VAL
2	B	886	THR
2	B	890	MET
2	B	929	ARG
2	B	930	MET
2	B	947	LEU
2	B	954	ILE
2	B	1018	ASN
2	B	1049	GLN

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Mol	Chain	Res	Type
2	B	1059	TYR
2	B	1063	VAL
2	B	1079	HIS
2	B	1114	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	76	GLN
1	A	170	GLN
1	A	183	GLN
1	A	193	GLN
1	A	239	GLN
1	A	242	ASN
1	A	288	GLN
1	A	311	ASN
1	A	314	GLN
1	A	377	GLN
1	A	397	GLN
1	A	409	GLN
1	A	413	GLN
1	A	419	GLN
1	A	428	HIS
1	A	451	GLN
1	A	486	ASN
1	A	536	ASN
1	A	538	ASN
1	A	560	ASN
1	A	610	HIS
1	A	639	HIS
1	A	645	GLN
1	A	662	GLN
1	A	665	HIS
2	B	234	HIS
2	B	262	ASN
2	B	266	HIS
2	B	269	HIS
2	B	300	GLN
2	B	458	HIS
2	B	461	GLN
2	B	535	ASN

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Mol	Chain	Res	Type
2	B	557	HIS
2	B	621	HIS
2	B	734	GLN
2	B	741	GLN
2	B	772	HIS
2	B	779	ASN
2	B	784	ASN
2	B	785	GLN
2	B	808	HIS
2	B	810	HIS
2	B	865	GLN
2	B	867	GLN
2	B	1001	HIS
2	B	1018	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	935	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	935	-	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	935	ADP	C5-C4	4.74	1.47	1.39
4	A	935	ADP	C5-C6	2.67	1.48	1.41
4	A	935	ADP	C8-N7	2.30	1.36	1.31
4	A	935	ADP	C5-N7	-2.28	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	935	ADP	C5-C4-N3	-5.79	118.75	126.72
4	A	935	ADP	N3-C4-N9	4.72	135.20	127.17
4	A	935	ADP	C2-N3-C4	3.62	120.67	111.83
4	A	935	ADP	C4-C5-N7	-3.24	106.87	110.58
4	A	935	ADP	N3-C2-N1	-3.12	123.85	128.58
4	A	935	ADP	C4-N9-C8	2.75	108.62	105.74
4	A	935	ADP	C3'-C2'-C1'	2.43	106.06	101.46
4	A	935	ADP	C5-N7-C8	2.37	107.18	103.45

There are no chirality outliers.

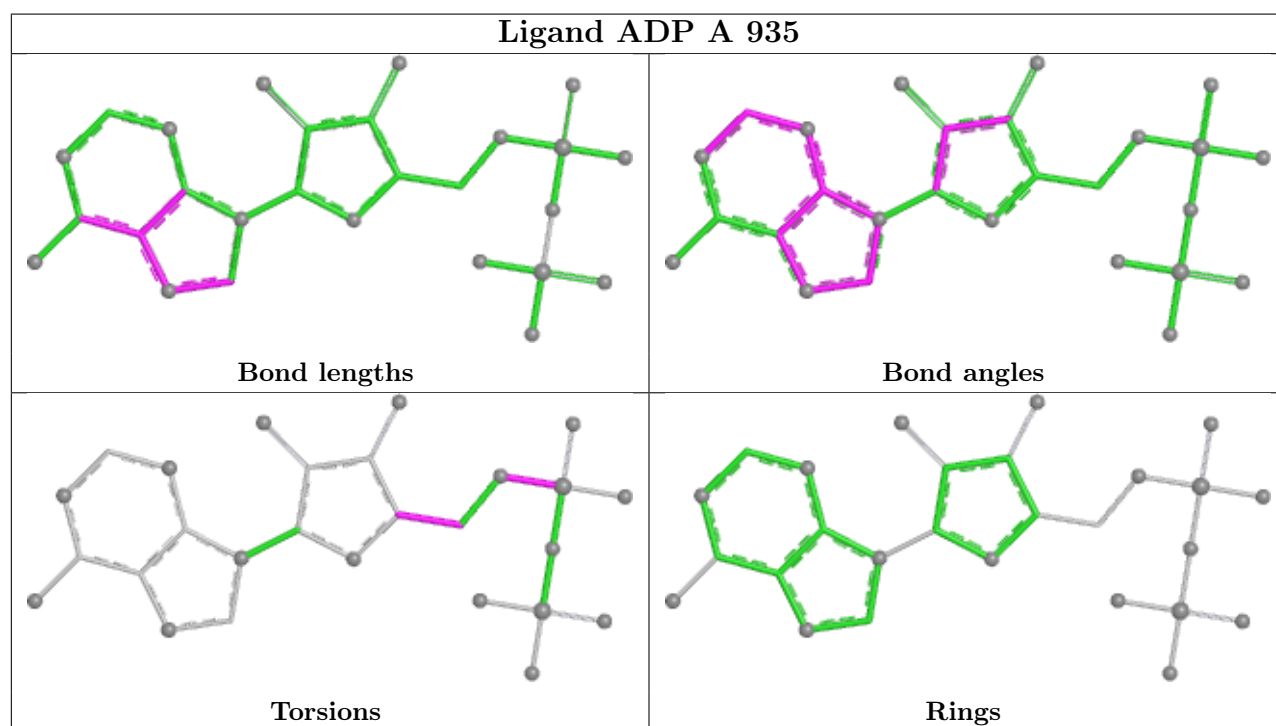
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	935	ADP	C5'-O5'-PA-O1A
4	A	935	ADP	C3'-C4'-C5'-O5'
4	A	935	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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, 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(Å ²)	Q < 0.9
1	A	890/934 (95%)	0.02	17 (1%)	66 45	14, 62, 172, 438	0
2	B	860/918 (93%)	-0.15	13 (1%)	72 52	11, 49, 123, 310	2 (0%)
3	D	53/53 (100%)	1.00	5 (9%)	14 8	25, 135, 221, 235	2 (3%)
All	All	1803/1905 (94%)	-0.03	35 (1%)	66 45	11, 56, 155, 438	4 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	354	THR	3.2
1	A	876	GLU	3.0
2	B	932	ALA	2.9
2	B	529	ASN	2.8
2	B	863	GLY	2.8
2	B	216	SER	2.6
1	A	140	ASP	2.6
1	A	139	ASN	2.6
1	A	552	THR	2.6
1	A	527	CYS	2.6
1	A	141	MET	2.5
2	B	1047	LEU	2.5
2	B	580	GLU	2.5
1	A	533	LEU	2.4
2	B	1063	VAL	2.4
1	A	316	SER	2.3
2	B	702	LEU	2.3
3	D	25	DA	2.3
1	A	542	VAL	2.3
3	D	48	DT	2.3
1	A	852	GLU	2.2
1	A	71	GLY	2.2
2	B	468	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	497	ILE	2.2
1	A	526	THR	2.1
2	B	1024	LEU	2.1
2	B	243	CYS	2.1
1	A	546	LYS	2.1
1	A	264	GLN	2.1
3	D	26	DG	2.1
3	D	50	DG	2.1
1	A	236	ASP	2.1
3	D	39[A]	DA	2.1
2	B	542	GLN	2.1
1	A	511	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](#)

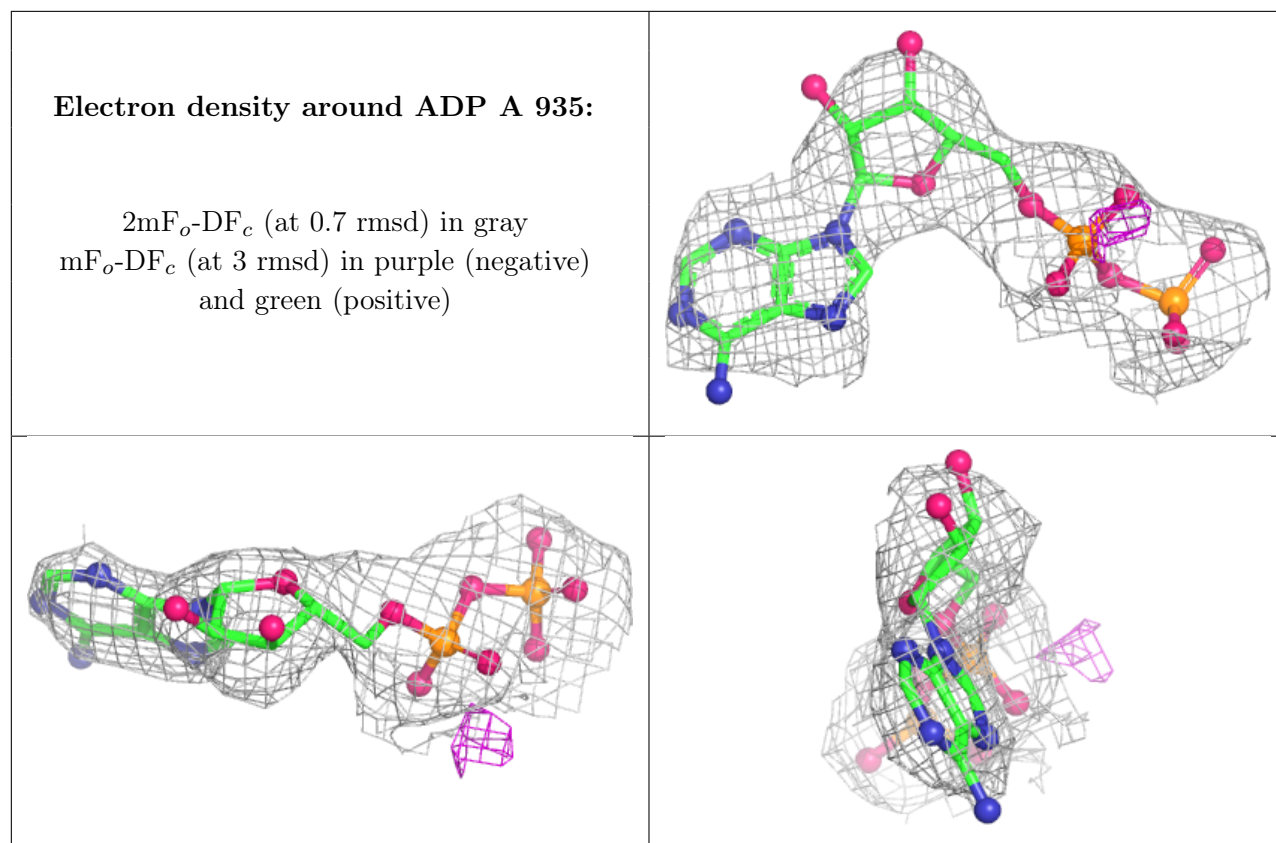
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	A	935	27/27	0.94	0.10	56,91,103,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.