



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:52 PM UTC

PDB ID : 5EAW / pdb_00005eaw
Title : Crystal structure of Dna2 nuclease-helicase
Authors : Zhou, C.; Pourmal, S.; Pavletich, N.P.
Deposited on : 2015-10-17
Resolution : 3.00 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

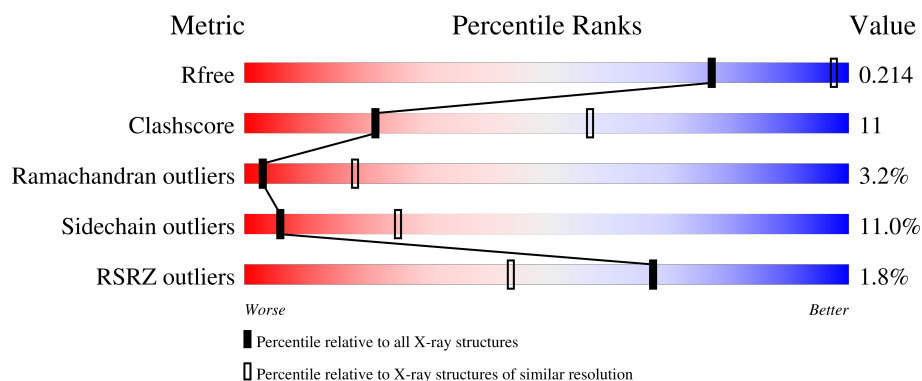
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1056	2% 68% 25% 5% ..
1	B	1056	2% 67% 27% 5% ..

2 Entry composition [i](#)

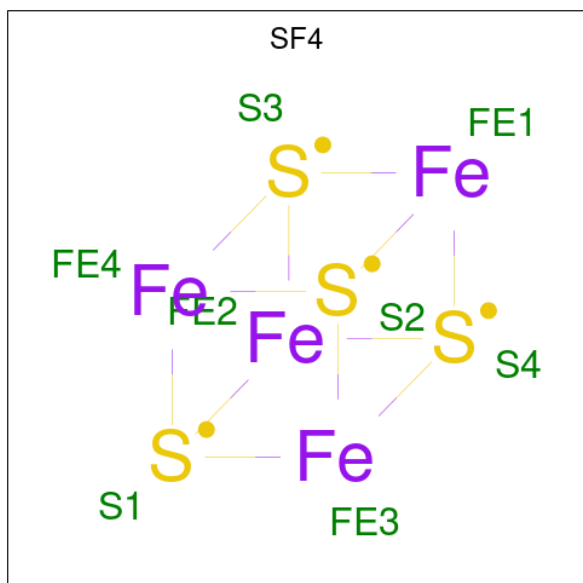
There are 3 unique types of molecules in this entry. The entry contains 16612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 replication ATP-dependent helicase/nuclease DNA2.

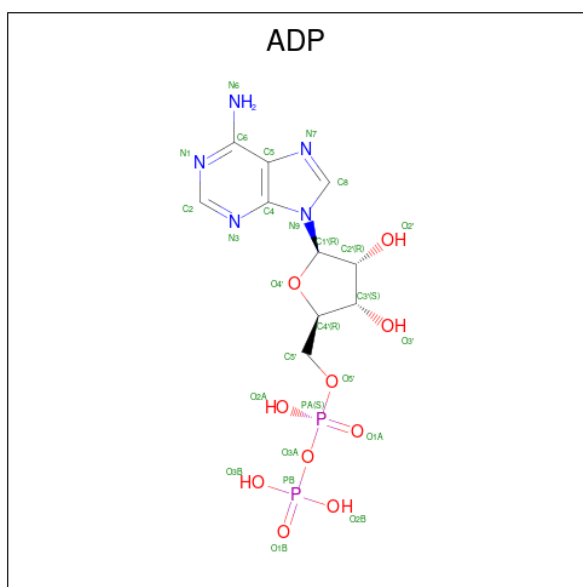
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1046	Total	C	N	O	S	0	0	0
			8271	5222	1456	1548	45			
1	B	1046	Total	C	N	O	S	0	0	0
			8271	5222	1456	1548	45			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

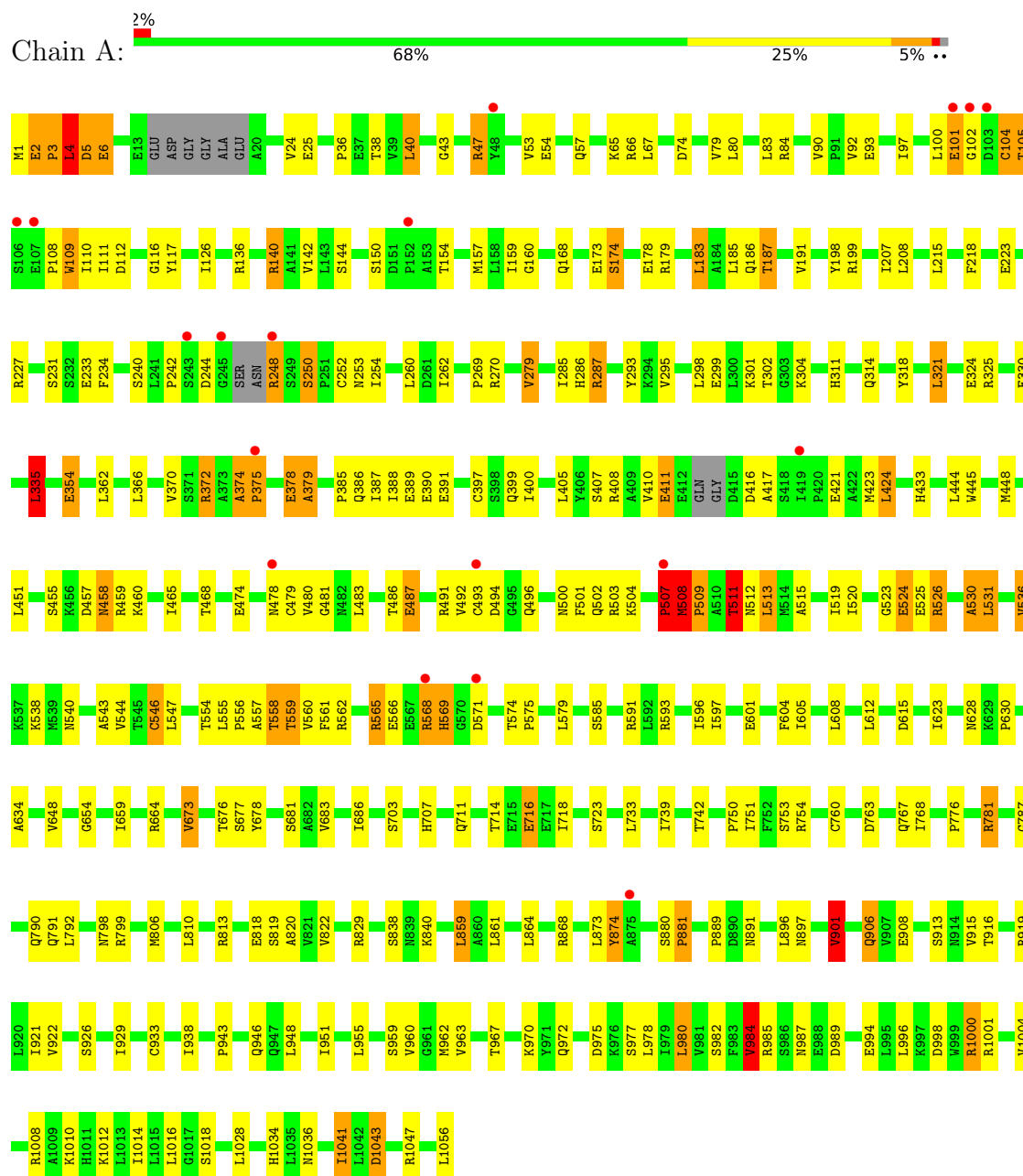


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

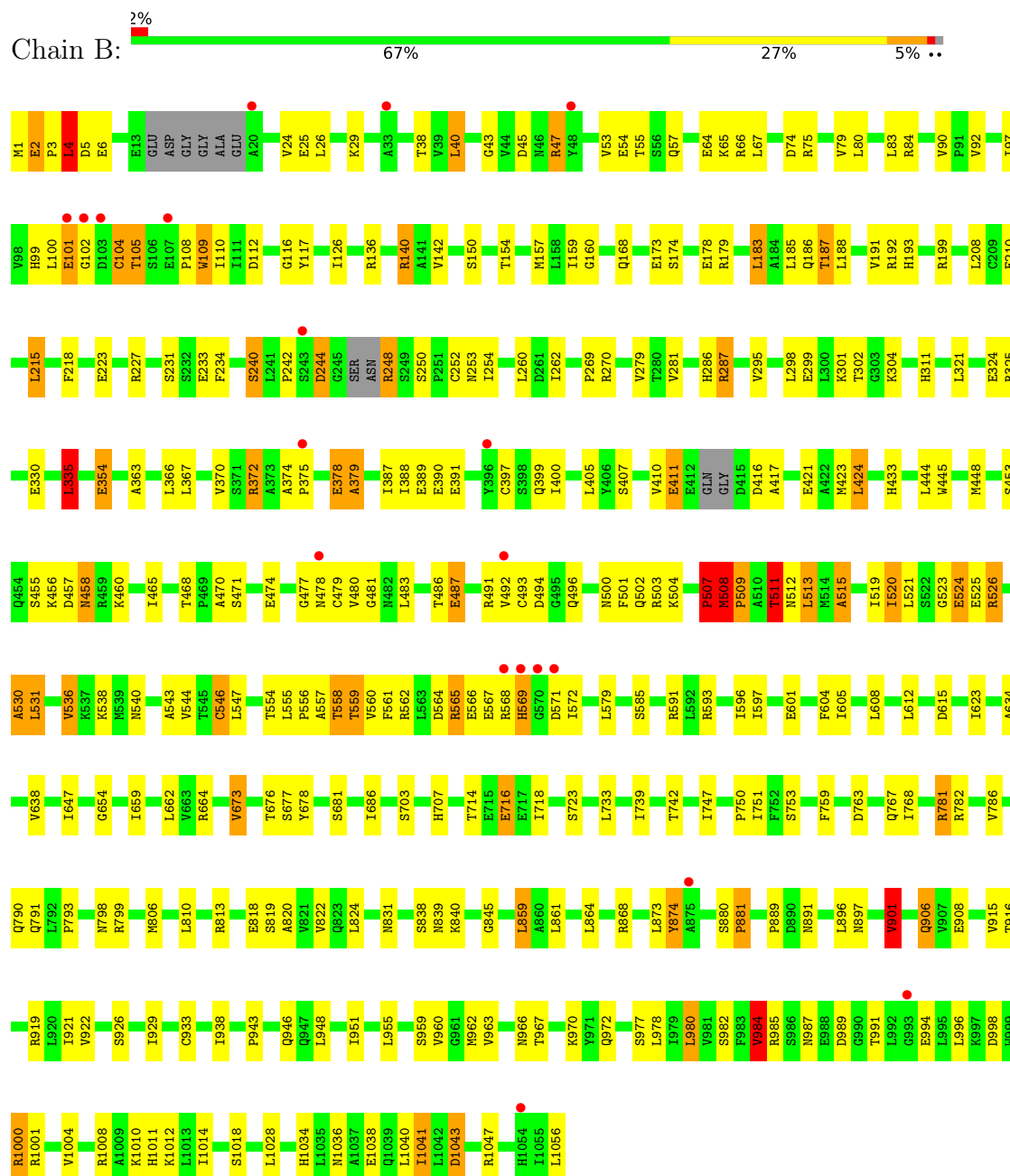
3 Residue-property plots

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 replication ATP-dependent helicase/nuclease DNA2



● Molecule 1: DNA replication ATP-dependent helicase/nuclease DNA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.90Å 148.60Å 170.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.2 (50.00-3.00) 89.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.209 , 0.247 (Not available) , 0.214	Depositor DCC
R_{free} test set	1555 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtrriage
Anisotropy	0.455	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16612	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1691e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SF4

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	0.76	0/8421	1.13	16/11387 (0.1%)
1	B	0.76	0/8421	1.13	17/11387 (0.1%)
All	All	0.76	0/16842	1.13	33/22774 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	707	HIS	CA-C-N	8.60	130.59	119.84
1	A	707	HIS	C-N-CA	8.60	130.59	119.84
1	A	5	ASP	N-CA-C	8.16	121.20	111.33
1	B	707	HIS	CA-C-N	8.11	129.97	119.84
1	B	707	HIS	C-N-CA	8.11	129.97	119.84
1	B	5	ASP	N-CA-C	7.38	120.26	111.33
1	B	335	LEU	N-CA-C	7.30	120.31	111.40
1	A	374	ALA	CA-C-N	7.13	128.75	119.84
1	A	374	ALA	C-N-CA	7.13	128.75	119.84
1	B	374	ALA	CA-C-N	6.59	128.08	119.84
1	B	374	ALA	C-N-CA	6.59	128.08	119.84
1	B	901	VAL	N-CA-C	-6.54	103.01	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	ALA	N-CA-C	6.52	120.12	110.48
1	A	901	VAL	N-CA-C	-6.49	103.05	108.63
1	A	411	GLU	N-CA-C	6.06	116.28	108.34
1	B	90	VAL	N-CA-CB	5.87	116.69	110.17
1	A	379	ALA	N-CA-C	5.83	118.72	110.50
1	A	378	GLU	N-CA-C	5.75	117.72	110.24
1	B	4	LEU	CA-C-N	5.72	128.22	120.38
1	B	4	LEU	C-N-CA	5.72	128.22	120.38
1	B	281	VAL	N-CA-C	5.62	116.57	108.48
1	A	90	VAL	N-CA-CB	5.54	116.32	110.17
1	B	215	LEU	N-CA-C	5.53	120.43	113.25
1	A	293	TYR	N-CA-C	5.52	117.73	108.73
1	B	470	ALA	N-CA-C	5.48	117.70	111.02
1	B	966	ASN	N-CA-C	5.44	116.80	108.42
1	A	408	ARG	N-CA-C	5.36	117.12	111.28
1	A	4	LEU	CA-C-N	5.29	127.62	120.38
1	A	4	LEU	C-N-CA	5.29	127.62	120.38
1	B	411	GLU	N-CA-C	5.25	115.32	108.07
1	B	378	GLU	N-CA-C	5.14	116.92	110.24
1	A	335	LEU	N-CA-C	5.12	119.42	112.04
1	A	566	GLU	N-CA-C	5.11	115.95	107.73

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	CYS	Peptide
1	A	507	PRO	Peptide
1	A	508	MET	Peptide
1	B	104	CYS	Peptide
1	B	507	PRO	Peptide
1	B	508	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8271	0	8411	182	0
1	B	8271	0	8411	181	0
2	A	8	0	0	0	0
2	B	8	0	0	1	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
All	All	16612	0	16846	361	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 11.

All (361) 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:458:ASN:HB2	1:B:569:HIS:HB3	1.53	0.90
1:A:511:THR:H	1:A:513:LEU:HD21	1.37	0.89
1:A:43:GLY:H	1:A:105:THR:HG21	1.41	0.86
1:B:511:THR:H	1:B:513:LEU:HD21	1.38	0.85
1:B:183:LEU:O	1:B:187:THR:HG23	1.77	0.85
1:B:43:GLY:H	1:B:105:THR:HG21	1.41	0.84
1:B:154:THR:HG22	1:B:157:MET:HG3	1.63	0.81
1:A:458:ASN:HB2	1:A:569:HIS:HB3	1.62	0.81
1:A:183:LEU:O	1:A:187:THR:HG23	1.80	0.79
1:A:298:LEU:HD11	1:A:335:LEU:HB2	1.68	0.75
1:B:799:ARG:HH22	1:B:994:GLU:HG3	1.51	0.75
1:A:154:THR:HG22	1:A:157:MET:HG3	1.69	0.75
1:B:298:LEU:HD11	1:B:335:LEU:HB2	1.69	0.74
1:B:493:CYS:O	1:B:496:GLN:HG2	1.89	0.72
1:A:593:ARG:HG2	1:A:597:ILE:HD12	1.72	0.72
1:B:596:ILE:O	1:B:813:ARG:NH1	2.23	0.72
1:A:493:CYS:O	1:A:496:GLN:HG2	1.89	0.72
1:B:508:MET:HB3	1:B:509:PRO:HD3	1.71	0.72
1:B:2:GLU:HB2	1:B:3:PRO:HD3	1.72	0.71
1:B:478:ASN:HB3	1:B:565:ARG:HG2	1.72	0.71
1:B:593:ARG:HG2	1:B:597:ILE:HD12	1.72	0.71
1:B:891:ASN:O	1:B:1012:LYS:NZ	2.24	0.71
1:B:433:HIS:CG	1:B:585:SER:HB3	2.27	0.70
1:A:596:ILE:O	1:A:813:ARG:NH1	2.24	0.70
1:A:714:THR:HG22	1:A:716:GLU:H	1.57	0.70
1:A:508:MET:HB3	1:A:509:PRO:HD3	1.73	0.70
1:B:526:ARG:HG2	1:B:526:ARG:HH11	1.58	0.69
1:B:444:LEU:HG	1:B:448:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASN:HB3	1:A:565:ARG:CG	2.23	0.68
1:A:511:THR:N	1:A:513:LEU:HD21	2.08	0.68
1:B:714:THR:HG22	1:B:716:GLU:H	1.58	0.68
1:B:84:ARG:HH21	1:B:110:ILE:HG21	1.59	0.67
1:A:487:GLU:HG3	1:A:500:ASN:HB3	1.75	0.67
1:A:799:ARG:HH22	1:A:994:GLU:HG3	1.60	0.66
1:A:503:ARG:HH11	1:A:503:ARG:HB2	1.61	0.66
1:B:503:ARG:HH11	1:B:503:ARG:HB2	1.60	0.66
1:A:2:GLU:HB2	1:A:3:PRO:HD3	1.79	0.65
1:A:109:TRP:HB3	1:A:110:ILE:HD12	1.77	0.65
1:A:901:VAL:HG23	1:A:1047:ARG:HB3	1.77	0.65
1:A:335:LEU:HD12	1:A:335:LEU:O	1.96	0.65
1:A:880:SER:N	1:A:881:PRO:HD2	2.13	0.64
1:B:102:GLY:HA3	1:B:116:GLY:HA2	1.80	0.64
1:B:511:THR:N	1:B:513:LEU:HD21	2.12	0.64
1:A:478:ASN:HB3	1:A:565:ARG:HG2	1.79	0.64
1:B:487:GLU:HG3	1:B:500:ASN:HB3	1.79	0.63
1:B:880:SER:N	1:B:881:PRO:HD2	2.13	0.63
1:A:526:ARG:HG2	1:A:526:ARG:HH11	1.62	0.63
1:A:102:GLY:CA	1:A:117:TYR:H	2.11	0.63
1:B:407:SER:O	1:B:411:GLU:HB3	1.99	0.63
1:B:102:GLY:CA	1:B:117:TYR:H	2.12	0.62
1:A:654:GLY:HA2	3:A:1102:ADP:O2B	1.98	0.62
1:A:84:ARG:HH21	1:A:110:ILE:HG21	1.65	0.62
1:A:767:GLN:OE1	1:A:972:GLN:NE2	2.32	0.62
1:B:53:VAL:HG22	1:B:67:LEU:HD22	1.82	0.61
1:A:178:GLU:HB3	1:B:608:LEU:HD21	1.82	0.61
1:A:102:GLY:HA3	1:A:116:GLY:HA2	1.83	0.61
1:B:372:ARG:HH21	1:B:379:ALA:HB2	1.66	0.61
1:B:511:THR:H	1:B:513:LEU:CD2	2.13	0.61
1:A:448:MET:HB3	1:A:806:MET:HG3	1.82	0.61
1:A:524:GLU:HG3	1:A:525:GLU:H	1.66	0.61
1:B:524:GLU:HB3	1:B:560:VAL:HB	1.82	0.61
1:B:901:VAL:HG23	1:B:1047:ARG:HB3	1.83	0.61
1:A:524:GLU:HB3	1:A:560:VAL:HB	1.81	0.60
1:B:465:ILE:HA	1:B:562:ARG:NH1	2.17	0.60
1:A:511:THR:H	1:A:513:LEU:CD2	2.11	0.60
1:B:455:SER:OG	1:B:798:ASN:HB2	2.01	0.60
1:B:526:ARG:HG2	1:B:526:ARG:NH1	2.17	0.60
1:B:335:LEU:O	1:B:335:LEU:HD12	2.02	0.60
1:A:444:LEU:HG	1:A:448:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:GLU:HG3	1:B:525:GLU:H	1.67	0.59
1:B:1000:ARG:HH11	1:B:1000:ARG:HB2	1.66	0.59
1:B:2:GLU:HB2	1:B:3:PRO:CD	2.32	0.59
1:B:433:HIS:CD2	1:B:585:SER:HB3	2.37	0.59
1:B:102:GLY:CA	1:B:116:GLY:HA2	2.33	0.59
1:B:388:ILE:HD12	1:B:390:GLU:HB3	1.84	0.58
1:A:840:LYS:HD2	1:A:1034:HIS:CD2	2.39	0.58
1:A:891:ASN:O	1:A:1012:LYS:NZ	2.35	0.58
1:B:301:LYS:HZ3	1:B:311:HIS:HD2	1.51	0.58
1:A:102:GLY:CA	1:A:116:GLY:HA2	2.33	0.58
1:A:227:ARG:HG2	1:A:234:PHE:CE1	2.39	0.58
1:A:526:ARG:HG2	1:A:526:ARG:NH1	2.19	0.58
1:B:227:ARG:HG2	1:B:234:PHE:CE1	2.39	0.57
1:A:240:SER:HA	1:A:248:ARG:HB3	1.86	0.57
1:B:109:TRP:HB3	1:B:110:ILE:HD12	1.85	0.57
1:B:503:ARG:HG2	1:B:504:LYS:O	2.04	0.57
1:A:465:ILE:HA	1:A:562:ARG:NH1	2.20	0.57
1:A:101:GLU:OE2	1:A:270:ARG:HD2	2.04	0.57
1:A:503:ARG:HG2	1:A:504:LYS:O	2.04	0.57
1:B:387:ILE:HG21	1:B:423:MET:HG2	1.86	0.56
1:B:520:ILE:HG23	1:B:564:ASP:HB2	1.87	0.56
1:B:767:GLN:OE1	1:B:972:GLN:NE2	2.39	0.56
1:A:524:GLU:CG	1:A:525:GLU:H	2.18	0.56
1:B:242:PRO:HG2	1:B:330:GLU:HG2	1.87	0.56
1:A:231:SER:HA	1:A:234:PHE:HD2	1.69	0.56
1:A:929:ILE:HA	1:A:933:CYS:O	2.06	0.56
1:A:1000:ARG:HH11	1:A:1000:ARG:HB2	1.70	0.56
1:A:372:ARG:HH21	1:A:379:ALA:HB2	1.71	0.56
1:A:407:SER:O	1:A:411:GLU:HB3	2.06	0.56
1:B:948:LEU:HD11	1:B:967:THR:HG23	1.88	0.56
1:B:673:VAL:HG13	1:B:739:ILE:HG12	1.86	0.56
1:B:354:GLU:OE2	1:B:354:GLU:HA	2.05	0.55
1:B:101:GLU:OE2	1:B:270:ARG:HD2	2.07	0.55
1:B:458:ASN:CB	1:B:569:HIS:HB3	2.33	0.55
1:A:301:LYS:HZ3	1:A:314:GLN:HE22	1.53	0.55
1:A:325:ARG:HH22	1:A:531:LEU:H	1.53	0.55
1:A:433:HIS:CG	1:A:585:SER:HB3	2.42	0.55
1:A:474:GLU:HB3	1:A:479:CYS:O	2.06	0.55
1:B:977:SER:HA	1:B:1010:LYS:HB2	1.89	0.54
1:A:591:ARG:NH1	1:A:781:ARG:O	2.41	0.54
1:B:154:THR:HG23	1:B:157:MET:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLU:HB3	1:B:479:CYS:O	2.08	0.54
1:A:53:VAL:HG22	1:A:67:LEU:HD22	1.90	0.54
1:B:231:SER:HA	1:B:234:PHE:HD2	1.71	0.54
1:A:555:LEU:O	1:A:559:THR:OG1	2.23	0.54
1:A:569:HIS:C	1:A:571:ASP:N	2.66	0.54
1:B:142:VAL:HG13	1:B:366:LEU:HD23	1.90	0.54
1:B:325:ARG:HH22	1:B:531:LEU:H	1.55	0.54
1:A:262:ILE:HG22	1:A:279:VAL:HG13	1.90	0.54
1:B:524:GLU:CG	1:B:525:GLU:H	2.20	0.54
1:A:530:ALA:O	1:A:531:LEU:HB2	2.07	0.54
1:A:714:THR:HG22	1:A:716:GLU:N	2.23	0.54
1:B:873:LEU:O	1:B:874:TYR:HB2	2.08	0.53
1:A:2:GLU:HB2	1:A:3:PRO:CD	2.38	0.53
1:A:676:THR:HA	1:A:742:THR:O	2.08	0.53
1:A:301:LYS:HZ3	1:A:314:GLN:NE2	2.06	0.53
1:A:478:ASN:HB3	1:A:565:ARG:HG3	1.90	0.53
1:A:387:ILE:HG21	1:A:423:MET:HG2	1.90	0.53
1:A:388:ILE:HD12	1:A:390:GLU:HB3	1.90	0.53
1:A:677:SER:HB3	1:A:763:ASP:HB3	1.91	0.53
1:A:242:PRO:HG2	1:A:330:GLU:HG2	1.90	0.53
1:A:906:GLN:OE1	1:A:915:VAL:HG23	2.08	0.53
1:B:262:ILE:HG22	1:B:279:VAL:HG13	1.90	0.53
1:B:508:MET:HB3	1:B:509:PRO:CD	2.38	0.53
1:B:906:GLN:OE1	1:B:915:VAL:HG23	2.08	0.53
1:B:638:VAL:HG11	1:B:662:LEU:HD11	1.91	0.52
1:B:922:VAL:HG22	1:B:955:LEU:HG	1.91	0.52
1:B:980:LEU:HD23	1:B:1014:ILE:HB	1.90	0.52
1:B:569:HIS:C	1:B:571:ASP:N	2.68	0.52
1:A:38:THR:HG21	1:A:97:ILE:HG21	1.92	0.52
1:B:718:ILE:HG21	1:B:733:LEU:HD13	1.91	0.52
1:A:455:SER:OG	1:A:798:ASN:HB2	2.10	0.51
1:A:767:GLN:CD	1:A:972:GLN:HE21	2.18	0.51
1:A:634:ALA:HA	1:A:822:VAL:HG11	1.92	0.51
1:A:569:HIS:C	1:A:571:ASP:H	2.16	0.51
1:B:998:ASP:CG	1:B:1001:ARG:HG3	2.35	0.51
1:A:354:GLU:OE2	1:A:354:GLU:HA	2.10	0.51
1:B:591:ARG:NH1	1:B:781:ARG:O	2.44	0.51
1:A:160:GLY:HA2	1:A:302:THR:HG21	1.92	0.51
1:A:948:LEU:HD11	1:A:967:THR:HG23	1.92	0.51
1:A:199:ARG:HG3	1:A:753:SER:OG	2.10	0.51
1:B:659:ILE:HG21	1:B:686:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG13	1:A:366:LEU:HD23	1.92	0.51
1:A:324:GLU:OE1	1:A:526:ARG:NH2	2.44	0.51
1:A:223:GLU:O	1:A:227:ARG:HB3	2.11	0.50
1:A:703:SER:HB3	1:A:714:THR:HG21	1.92	0.50
1:A:252:CYS:HB2	1:A:286:HIS:O	2.12	0.50
1:A:673:VAL:HG13	1:A:739:ILE:HG12	1.94	0.50
1:B:324:GLU:OE1	1:B:526:ARG:NH2	2.45	0.50
1:A:659:ILE:HG21	1:A:686:ILE:HD13	1.93	0.50
1:A:998:ASP:CG	1:A:1001:ARG:HG3	2.36	0.50
1:B:160:GLY:HA2	1:B:302:THR:HG21	1.93	0.50
1:A:301:LYS:NZ	1:A:311:HIS:HD2	2.10	0.49
1:A:718:ILE:HG21	1:A:733:LEU:HD13	1.93	0.49
1:B:791:GLN:O	1:B:1000:ARG:HG2	2.12	0.49
1:A:154:THR:HG23	1:A:157:MET:H	1.77	0.49
1:B:677:SER:HB3	1:B:763:ASP:HB3	1.93	0.49
1:A:43:GLY:N	1:A:105:THR:HG21	2.20	0.49
1:B:38:THR:HG21	1:B:97:ILE:HG21	1.94	0.49
1:B:634:ALA:HA	1:B:822:VAL:HG11	1.93	0.49
1:B:540:ASN:HB2	1:B:543:ALA:H	1.77	0.49
1:A:678:TYR:HB2	1:A:768:ILE:HG12	1.95	0.49
1:B:199:ARG:HB2	1:B:750:PRO:HB3	1.93	0.49
1:B:929:ILE:HA	1:B:933:CYS:O	2.13	0.49
1:A:301:LYS:HD2	1:A:311:HIS:CD2	2.47	0.49
1:A:861:LEU:HD12	1:A:889:PRO:HG3	1.95	0.49
1:B:569:HIS:C	1:B:571:ASP:H	2.20	0.49
1:A:921:ILE:HG23	1:A:1016:LEU:HD22	1.95	0.48
1:A:790:GLN:O	1:A:1000:ARG:HG3	2.13	0.48
1:B:938:ILE:HG12	1:B:978:LEU:HD23	1.94	0.48
1:B:593:ARG:HG2	1:B:597:ILE:CD1	2.43	0.48
1:B:604:PHE:CZ	1:B:820:ALA:HA	2.48	0.48
1:B:240:SER:HA	1:B:248:ARG:HB3	1.96	0.48
1:B:678:TYR:HB2	1:B:768:ILE:HG12	1.94	0.48
1:A:3:PRO:O	1:A:4:LEU:C	2.56	0.48
1:A:508:MET:HB3	1:A:509:PRO:CD	2.42	0.48
1:B:480:VAL:HG23	1:B:513:LEU:HD22	1.96	0.48
1:A:929:ILE:HD13	1:A:960:VAL:CG1	2.44	0.48
1:B:325:ARG:NH2	1:B:531:LEU:H	2.12	0.48
1:B:676:THR:HA	1:B:742:THR:O	2.13	0.48
1:A:524:GLU:HG3	1:A:525:GLU:N	2.28	0.48
1:A:604:PHE:CZ	1:A:820:ALA:HA	2.48	0.47
1:B:253:ASN:HB2	1:B:286:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:VAL:HG22	1:A:955:LEU:HG	1.95	0.47
1:A:199:ARG:HB2	1:A:750:PRO:HB3	1.97	0.47
1:A:445:TRP:HB3	1:A:579:LEU:HD11	1.96	0.47
1:B:174:SER:HB3	1:B:179:ARG:HH11	1.79	0.47
1:A:421:GLU:HA	1:A:424:LEU:HB2	1.95	0.47
1:B:301:LYS:HD2	1:B:311:HIS:CD2	2.50	0.47
1:B:1036:ASN:OD1	1:B:1041:ILE:HG12	2.15	0.47
1:A:215:LEU:O	1:A:218:PHE:HB2	2.14	0.47
1:B:215:LEU:O	1:B:218:PHE:HB2	2.14	0.47
1:A:628:ASN:OD1	1:A:630:PRO:HD2	2.14	0.47
1:A:859:LEU:HD12	1:A:1012:LYS:HD2	1.97	0.47
1:A:980:LEU:HD23	1:A:1014:ILE:HB	1.95	0.47
1:B:252:CYS:HB2	1:B:286:HIS:O	2.15	0.47
1:B:260:LEU:CD1	1:B:295:VAL:HG22	2.45	0.47
1:B:536:VAL:HA	1:B:546:CYS:HB3	1.96	0.47
1:A:260:LEU:CD1	1:A:295:VAL:HG22	2.45	0.47
1:B:301:LYS:NZ	1:B:311:HIS:HD2	2.12	0.47
1:B:919:ARG:HD2	1:B:1056:LEU:HD23	1.96	0.47
1:A:36:PRO:HD2	1:A:459:ARG:O	2.15	0.46
1:B:623:ILE:HD13	1:B:664:ARG:HB3	1.96	0.46
1:A:873:LEU:O	1:A:874:TYR:HB2	2.14	0.46
1:B:269:PRO:HD2	1:B:526:ARG:HH22	1.79	0.46
1:A:40:LEU:HA	1:A:47:ARG:O	2.16	0.46
1:B:168:GLN:HB3	1:B:262:ILE:HD13	1.97	0.46
1:A:269:PRO:HD2	1:A:526:ARG:HH22	1.80	0.46
1:A:325:ARG:NH2	1:A:531:LEU:H	2.14	0.46
1:B:880:SER:O	1:B:881:PRO:C	2.57	0.46
1:A:540:ASN:HB2	1:A:543:ALA:H	1.80	0.46
1:A:168:GLN:HB3	1:A:262:ILE:HD13	1.97	0.46
1:A:2:GLU:O	1:A:3:PRO:C	2.59	0.46
1:A:897:ASN:HB3	1:A:1043:ASP:HA	1.97	0.46
1:A:174:SER:HB3	1:A:179:ARG:HH11	1.81	0.45
1:B:523:GLY:HA2	1:B:561:PHE:HA	1.97	0.45
1:B:524:GLU:HG3	1:B:525:GLU:N	2.30	0.45
1:B:421:GLU:HA	1:B:424:LEU:HB2	1.98	0.45
1:A:503:ARG:HB2	1:A:503:ARG:NH1	2.30	0.45
1:A:703:SER:O	1:A:711:GLN:NE2	2.49	0.45
1:A:929:ILE:CD1	1:A:960:VAL:HG11	2.46	0.45
1:B:468:THR:O	1:B:562:ARG:NH2	2.49	0.45
1:B:793:PRO:HG3	1:B:1000:ARG:NH2	2.31	0.45
1:A:524:GLU:CG	1:A:525:GLU:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:TRP:HB3	1:B:579:LEU:HD11	1.97	0.45
1:A:253:ASN:HB2	1:A:286:HIS:HB2	1.99	0.45
1:A:919:ARG:HD2	1:A:1056:LEU:HD23	1.99	0.45
1:B:3:PRO:O	1:B:4:LEU:C	2.59	0.45
1:B:43:GLY:N	1:B:105:THR:HG21	2.20	0.45
1:B:861:LEU:HD12	1:B:889:PRO:HG3	1.98	0.45
1:B:943:PRO:HD3	1:B:982:SER:O	2.17	0.45
1:B:66:ARG:HH22	1:B:80:LEU:HD11	1.80	0.45
1:B:596:ILE:HG12	1:B:810:LEU:HD11	1.98	0.45
1:A:536:VAL:HA	1:A:546:CYS:HB3	1.97	0.45
1:A:880:SER:O	1:A:881:PRO:C	2.60	0.45
1:A:943:PRO:HD3	1:A:982:SER:O	2.17	0.45
1:A:299:GLU:OE2	1:A:301:LYS:HE3	2.17	0.45
1:B:2:GLU:O	1:B:3:PRO:C	2.58	0.45
1:A:507:PRO:HG2	1:A:508:MET:HG2	1.99	0.45
1:A:648:VAL:HA	1:A:787:GLY:O	2.17	0.45
1:B:487:GLU:H	1:B:487:GLU:HG2	1.55	0.45
1:A:556:PRO:O	1:A:558:THR:N	2.50	0.44
1:B:102:GLY:HA3	1:B:117:TYR:H	1.80	0.44
1:B:448:MET:HB3	1:B:806:MET:HG3	1.97	0.44
1:B:501:PHE:HB2	1:B:544:VAL:HG13	2.00	0.44
1:B:524:GLU:CG	1:B:525:GLU:N	2.81	0.44
1:B:839:ASN:OD1	1:B:845:GLY:HA2	2.17	0.44
1:A:1036:ASN:OD1	1:A:1041:ILE:HG12	2.18	0.44
1:B:154:THR:HG22	1:B:157:MET:CG	2.42	0.44
1:A:938:ILE:HG12	1:A:978:LEU:HD23	2.00	0.44
1:B:555:LEU:O	1:B:559:THR:OG1	2.26	0.44
1:A:433:HIS:CD2	1:A:585:SER:HB3	2.53	0.44
1:A:574:THR:HB	1:A:575:PRO:HD3	1.98	0.44
1:A:977:SER:HA	1:A:1010:LYS:HB2	1.99	0.44
1:B:79:VAL:HG11	1:B:108:PRO:HG2	1.98	0.44
1:A:84:ARG:HB2	1:A:112:ASP:HB3	2.00	0.44
1:A:677:SER:OG	1:A:683:VAL:HB	2.18	0.44
1:B:840:LYS:HD2	1:B:1034:HIS:CD2	2.52	0.44
1:B:897:ASN:HB3	1:B:1043:ASP:HA	2.00	0.44
1:B:248:ARG:HA	1:B:248:ARG:HD2	1.80	0.44
1:A:250:SER:O	1:A:287:ARG:NH2	2.51	0.43
1:B:556:PRO:O	1:B:558:THR:N	2.51	0.43
1:A:568:ARG:HH11	1:A:571:ASP:HB2	1.83	0.43
1:B:647:ILE:HB	1:B:786:VAL:HG22	2.00	0.43
1:A:501:PHE:HB2	1:A:544:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:LEU:HD12	1:A:1012:LYS:HB3	2.00	0.43
1:B:831:ASN:HD22	1:B:1011:HIS:HA	1.83	0.43
1:B:929:ILE:HD13	1:B:960:VAL:CG1	2.48	0.43
1:B:26:LEU:HA	1:B:29:LYS:HD2	2.00	0.43
1:B:299:GLU:OE2	1:B:301:LYS:HE3	2.19	0.43
1:B:287:ARG:NH1	1:B:287:ARG:HG3	2.34	0.43
1:B:478:ASN:HB2	1:B:565:ARG:NH1	2.34	0.43
1:B:231:SER:HA	1:B:234:PHE:CD2	2.53	0.43
1:B:477:GLY:C	1:B:565:ARG:HH11	2.26	0.43
1:A:159:ILE:HD13	1:A:207:ILE:HG23	2.00	0.43
1:A:523:GLY:HA2	1:A:561:PHE:HA	1.99	0.43
1:B:244:ASP:O	1:B:248:ARG:HD3	2.19	0.43
1:B:1000:ARG:HB2	1:B:1000:ARG:NH1	2.33	0.43
1:B:84:ARG:HB2	1:B:112:ASP:HB3	2.00	0.43
1:B:530:ALA:O	1:B:531:LEU:HB2	2.19	0.43
1:B:1004:VAL:O	1:B:1008:ARG:HG2	2.19	0.43
1:A:3:PRO:C	1:A:5:ASP:N	2.77	0.42
1:A:792:LEU:HD12	1:A:972:GLN:OE1	2.19	0.42
1:A:623:ILE:HD13	1:A:664:ARG:HB3	1.99	0.42
1:B:45:ASP:HA	1:B:99:HIS:HE1	1.85	0.42
1:B:471:SER:O	1:B:474:GLU:HG2	2.19	0.42
1:B:508:MET:HA	1:B:508:MET:HE2	2.00	0.42
1:A:198:TYR:O	1:A:754:ARG:HD3	2.18	0.42
1:A:231:SER:HA	1:A:234:PHE:CD2	2.51	0.42
1:A:493:CYS:HB3	1:A:496:GLN:HE21	1.85	0.42
1:B:173:GLU:HB3	1:B:174:SER:H	1.64	0.42
1:B:929:ILE:CD1	1:B:960:VAL:HG11	2.50	0.42
1:A:79:VAL:HG11	1:A:108:PRO:HG2	2.00	0.42
1:B:703:SER:HB3	1:B:714:THR:HG21	2.02	0.42
1:B:839:ASN:OD1	1:B:845:GLY:CA	2.68	0.42
1:A:102:GLY:HA3	1:A:116:GLY:CA	2.48	0.42
1:B:515:ALA:HA	1:B:536:VAL:HB	2.01	0.42
1:B:859:LEU:HD12	1:B:1012:LYS:HB3	2.00	0.42
1:A:47:ARG:HG2	1:A:97:ILE:CG2	2.50	0.42
1:A:173:GLU:HB3	1:A:174:SER:H	1.61	0.42
1:A:301:LYS:HZ3	1:A:311:HIS:HD2	1.66	0.42
1:A:508:MET:HE2	1:A:508:MET:HA	2.01	0.42
1:A:515:ALA:HA	1:A:536:VAL:HB	2.02	0.42
1:B:104:CYS:O	1:B:105:THR:CB	2.68	0.42
1:B:397:CYS:C	1:B:399:GLN:H	2.28	0.42
1:A:66:ARG:HH22	1:A:80:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLU:OE1	1:A:179:ARG:HD3	2.19	0.41
1:A:451:LEU:HB3	1:A:798:ASN:OD1	2.20	0.41
1:A:468:THR:O	1:A:562:ARG:NH2	2.53	0.41
1:B:55:THR:HA	1:B:64:GLU:O	2.19	0.41
1:B:192:ARG:NH2	1:B:193:HIS:CE1	2.87	0.41
1:B:1038:GLU:HB2	1:B:1040:LEU:HG	2.02	0.41
1:A:791:GLN:O	1:A:1000:ARG:HG2	2.20	0.41
1:B:943:PRO:HD2	1:B:984:VAL:HG13	2.02	0.41
1:A:287:ARG:NH1	1:A:287:ARG:HG3	2.35	0.41
1:B:453:SER:HB2	1:B:572:ILE:HG21	2.02	0.41
1:B:507:PRO:HG2	1:B:508:MET:HG2	2.02	0.41
1:B:40:LEU:HA	1:B:47:ARG:O	2.20	0.41
1:B:126:ILE:HD11	1:B:363:ALA:HA	2.02	0.41
1:B:102:GLY:HA3	1:B:116:GLY:CA	2.49	0.41
1:A:921:ILE:HD11	1:A:951:ILE:HD13	2.03	0.41
1:A:943:PRO:HD2	1:A:984:VAL:HG13	2.03	0.41
1:A:248:ARG:HA	1:A:248:ARG:HD2	1.78	0.41
1:A:397:CYS:C	1:A:399:GLN:H	2.29	0.41
1:B:242:PRO:HD2	1:B:330:GLU:HB3	2.03	0.41
1:B:747:ILE:H	1:B:747:ILE:HG13	1.68	0.41
1:B:790:GLN:O	1:B:1000:ARG:HG3	2.20	0.41
1:A:318:TYR:HD1	1:A:321:LEU:HD23	1.85	0.41
1:A:1004:VAL:O	1:A:1008:ARG:HG2	2.21	0.41
1:B:223:GLU:O	1:B:227:ARG:HB3	2.21	0.41
1:B:521:LEU:HD11	1:B:561:PHE:HB3	2.02	0.41
1:A:608:LEU:HD21	1:B:178:GLU:HB3	2.03	0.41
1:A:829:ARG:NE	1:A:975:ASP:HB3	2.36	0.41
1:A:929:ILE:HD13	1:A:960:VAL:HG11	2.03	0.41
1:B:183:LEU:O	1:B:187:THR:CG2	2.60	0.41
1:B:921:ILE:HD11	1:B:951:ILE:HD13	2.02	0.40
1:A:104:CYS:O	1:A:105:THR:CB	2.69	0.40
1:A:140:ARG:HG3	1:A:397:CYS:SG	2.61	0.40
1:A:760:CYS:SG	1:A:776:PRO:HB2	2.61	0.40
1:A:102:GLY:HA3	1:A:117:TYR:H	1.83	0.40
1:B:159:ILE:HD12	1:B:210:GLU:HG2	2.02	0.40
1:A:2:GLU:N	1:A:6:GLU:HG3	2.36	0.40
1:A:374:ALA:HA	1:A:375:PRO:HD2	1.96	0.40
1:A:480:VAL:HG23	1:A:513:LEU:HD22	2.02	0.40
1:B:199:ARG:HG3	1:B:753:SER:OG	2.21	0.40
1:B:654:GLY:HA2	3:B:1102:ADP:O2B	2.21	0.40
1:B:759:PHE:HA	1:B:782:ARG:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG21	1:A:362:LEU:HD23	2.04	0.40
1:A:596:ILE:HG12	1:A:810:LEU:HD11	2.02	0.40
1:B:140:ARG:HG3	1:B:397:CYS:SG	2.62	0.40
1:B:387:ILE:HG23	2:B:1101:SF4:S3	2.61	0.40
1:B:493:CYS:HB3	1:B:496:GLN:HE21	1.86	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 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	1038/1056 (98%)	916 (88%)	90 (9%)	32 (3%)	3	19
1	B	1038/1056 (98%)	919 (88%)	85 (8%)	34 (3%)	3	17
All	All	2076/2112 (98%)	1835 (88%)	175 (8%)	66 (3%)	3	18

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	105	THR
1	A	375	PRO
1	A	508	MET
1	A	524	GLU
1	A	874	TYR
1	A	989	ASP
1	B	2	GLU
1	B	105	THR
1	B	375	PRO
1	B	508	MET
1	B	524	GLU
1	B	554	THR

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Mol	Chain	Res	Type
1	B	565	ARG
1	B	566	GLU
1	B	567	GLU
1	B	874	TYR
1	B	989	ASP
1	A	4	LEU
1	A	554	THR
1	A	557	ALA
1	A	565	ARG
1	A	569	HIS
1	A	959	SER
1	B	4	LEU
1	B	417	ALA
1	B	530	ALA
1	B	557	ALA
1	B	569	HIS
1	B	959	SER
1	A	109	TRP
1	A	417	ALA
1	A	530	ALA
1	A	531	LEU
1	B	109	TRP
1	B	723	SER
1	B	984	VAL
1	A	40	LEU
1	A	244	ASP
1	A	492	VAL
1	A	511	THR
1	A	984	VAL
1	B	40	LEU
1	B	492	VAL
1	B	494	ASP
1	B	531	LEU
1	A	250	SER
1	A	416	ASP
1	A	494	ASP
1	A	507	PRO
1	A	723	SER
1	A	881	PRO
1	B	244	ASP
1	B	250	SER
1	B	416	ASP

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Mol	Chain	Res	Type
1	B	507	PRO
1	B	511	THR
1	B	515	ALA
1	B	881	PRO
1	B	75	ARG
1	A	509	PRO
1	A	481	GLY
1	B	509	PRO
1	A	3	PRO
1	A	385	PRO
1	B	481	GLY

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	931/937 (99%)	828 (89%)	103 (11%)	6	25
1	B	931/937 (99%)	830 (89%)	101 (11%)	6	26
All	All	1862/1874 (99%)	1658 (89%)	204 (11%)	6	25

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	GLU
1	A	24	VAL
1	A	25	GLU
1	A	47	ARG
1	A	54	GLU
1	A	57	GLN
1	A	65	LYS
1	A	74	ASP
1	A	83	LEU
1	A	92	VAL
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	100	LEU
1	A	101	GLU
1	A	111	ILE
1	A	136	ARG
1	A	140	ARG
1	A	144	SER
1	A	150	SER
1	A	174	SER
1	A	183	LEU
1	A	185	LEU
1	A	186	GLN
1	A	187	THR
1	A	191	VAL
1	A	208	LEU
1	A	233	GLU
1	A	248	ARG
1	A	254	ILE
1	A	279	VAL
1	A	285	ILE
1	A	287	ARG
1	A	304	LYS
1	A	321	LEU
1	A	335	LEU
1	A	354	GLU
1	A	370	VAL
1	A	372	ARG
1	A	378	GLU
1	A	386	GLN
1	A	389	GLU
1	A	391	GLU
1	A	400	ILE
1	A	405	LEU
1	A	410	VAL
1	A	424	LEU
1	A	457	ASP
1	A	458	ASN
1	A	460	LYS
1	A	483	LEU
1	A	486	THR
1	A	487	GLU
1	A	491	ARG
1	A	502	GLN

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Mol	Chain	Res	Type
1	A	511	THR
1	A	512	ASN
1	A	513	LEU
1	A	519	ILE
1	A	520	ILE
1	A	526	ARG
1	A	536	VAL
1	A	538	LYS
1	A	546	CYS
1	A	547	LEU
1	A	558	THR
1	A	559	THR
1	A	568	ARG
1	A	601	GLU
1	A	605	ILE
1	A	612	LEU
1	A	615	ASP
1	A	673	VAL
1	A	681	SER
1	A	716	GLU
1	A	751	ILE
1	A	781	ARG
1	A	818	GLU
1	A	819	SER
1	A	838	SER
1	A	859	LEU
1	A	864	LEU
1	A	868	ARG
1	A	896	LEU
1	A	901	VAL
1	A	906	GLN
1	A	908	GLU
1	A	913	SER
1	A	916	THR
1	A	926	SER
1	A	946	GLN
1	A	962	MET
1	A	963	VAL
1	A	970	LYS
1	A	980	LEU
1	A	984	VAL
1	A	985	ARG

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Mol	Chain	Res	Type
1	A	987	ASN
1	A	996	LEU
1	A	1000	ARG
1	A	1018	SER
1	A	1028	LEU
1	A	1041	ILE
1	A	1043	ASP
1	B	1	MET
1	B	6	GLU
1	B	24	VAL
1	B	25	GLU
1	B	47	ARG
1	B	54	GLU
1	B	57	GLN
1	B	65	LYS
1	B	74	ASP
1	B	83	LEU
1	B	92	VAL
1	B	100	LEU
1	B	101	GLU
1	B	136	ARG
1	B	140	ARG
1	B	150	SER
1	B	183	LEU
1	B	185	LEU
1	B	186	GLN
1	B	187	THR
1	B	188	LEU
1	B	191	VAL
1	B	208	LEU
1	B	233	GLU
1	B	240	SER
1	B	248	ARG
1	B	254	ILE
1	B	287	ARG
1	B	304	LYS
1	B	321	LEU
1	B	335	LEU
1	B	354	GLU
1	B	367	LEU
1	B	370	VAL
1	B	372	ARG

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Mol	Chain	Res	Type
1	B	378	GLU
1	B	389	GLU
1	B	391	GLU
1	B	400	ILE
1	B	405	LEU
1	B	410	VAL
1	B	424	LEU
1	B	456	LYS
1	B	457	ASP
1	B	458	ASN
1	B	460	LYS
1	B	483	LEU
1	B	486	THR
1	B	487	GLU
1	B	491	ARG
1	B	502	GLN
1	B	511	THR
1	B	512	ASN
1	B	513	LEU
1	B	519	ILE
1	B	520	ILE
1	B	526	ARG
1	B	536	VAL
1	B	538	LYS
1	B	546	CYS
1	B	547	LEU
1	B	558	THR
1	B	559	THR
1	B	568	ARG
1	B	601	GLU
1	B	605	ILE
1	B	612	LEU
1	B	615	ASP
1	B	673	VAL
1	B	681	SER
1	B	716	GLU
1	B	751	ILE
1	B	781	ARG
1	B	818	GLU
1	B	819	SER
1	B	824	LEU
1	B	838	SER

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Mol	Chain	Res	Type
1	B	859	LEU
1	B	864	LEU
1	B	868	ARG
1	B	896	LEU
1	B	901	VAL
1	B	906	GLN
1	B	908	GLU
1	B	916	THR
1	B	926	SER
1	B	946	GLN
1	B	962	MET
1	B	963	VAL
1	B	970	LYS
1	B	980	LEU
1	B	984	VAL
1	B	985	ARG
1	B	987	ASN
1	B	991	THR
1	B	996	LEU
1	B	1000	ARG
1	B	1018	SER
1	B	1028	LEU
1	B	1041	ILE
1	B	1043	ASP

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

Mol	Chain	Res	Type
1	A	68	HIS
1	A	164	HIS
1	A	238	GLN
1	A	311	HIS
1	A	314	GLN
1	A	323	GLN
1	A	399	GLN
1	A	402	ASN
1	A	458	ASN
1	A	482	ASN
1	A	502	GLN
1	A	505	ASN
1	A	704	HIS
1	A	711	GLN

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Mol	Chain	Res	Type
1	A	770	GLN
1	A	946	GLN
1	A	1003	ASN
1	A	1034	HIS
1	B	68	HIS
1	B	164	HIS
1	B	201	ASN
1	B	238	GLN
1	B	314	GLN
1	B	323	GLN
1	B	458	ASN
1	B	482	ASN
1	B	502	GLN
1	B	505	ASN
1	B	704	HIS
1	B	770	GLN
1	B	946	GLN
1	B	1034	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	$\# Z > 2$
2	SF4	B	1101	1	0,12,12	-	-	-		
3	ADP	B	1102	-	28,29,29	1.61	5 (17%)	43,45,45	1.78	8 (18%)
3	ADP	A	1102	-	28,29,29	1.62	5 (17%)	43,45,45	1.84	8 (18%)
2	SF4	A	1101	1	0,12,12	-	-	-		

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
2	SF4	B	1101	1	-	-	0/6/5/5
3	ADP	A	1102	-	-	6/16/32/32	0/3/3/3
3	ADP	B	1102	-	-	6/16/32/32	0/3/3/3
2	SF4	A	1101	1	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	ADP	C5-C4	5.35	1.48	1.39
3	A	1102	ADP	C5-C4	5.30	1.48	1.39
3	B	1102	ADP	C5-C6	3.38	1.50	1.41
3	A	1102	ADP	C5-C6	3.28	1.50	1.41
3	A	1102	ADP	C8-N7	2.54	1.36	1.31
3	B	1102	ADP	C8-N7	2.44	1.36	1.31
3	A	1102	ADP	PA-O3A	2.39	1.62	1.59
3	B	1102	ADP	C5-N7	-2.23	1.35	1.39
3	A	1102	ADP	C5-N7	-2.22	1.35	1.39
3	B	1102	ADP	C4-N9	-2.06	1.33	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	ADP	C5-C4-N3	-5.70	118.88	126.72
3	B	1102	ADP	C5-C4-N3	-5.57	119.04	126.72
3	A	1102	ADP	N3-C4-N9	4.22	134.34	127.17
3	B	1102	ADP	N3-C4-N9	4.06	134.06	127.17
3	A	1102	ADP	C2-N3-C4	3.87	121.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	ADP	C2-N3-C4	3.79	121.09	111.83
3	A	1102	ADP	C4-C5-N7	-3.71	106.34	110.58
3	A	1102	ADP	N3-C2-N1	-3.52	123.25	128.58
3	B	1102	ADP	C4-C5-N7	-3.48	106.61	110.58
3	B	1102	ADP	N3-C2-N1	-3.19	123.75	128.58
3	A	1102	ADP	C5-N7-C8	2.60	107.53	103.45
3	A	1102	ADP	C6-C5-N7	2.45	136.81	132.09
3	B	1102	ADP	C6-C5-N7	2.40	136.71	132.09
3	B	1102	ADP	C3'-C2'-C1'	2.28	105.77	101.46
3	B	1102	ADP	C5-N7-C8	2.12	106.78	103.45
3	A	1102	ADP	C2-N1-C6	2.08	122.15	118.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	ADP	PA-O3A-PB-O2B
3	B	1102	ADP	PA-O3A-PB-O2B
3	A	1102	ADP	O4'-C4'-C5'-O5'
3	B	1102	ADP	O4'-C4'-C5'-O5'
3	A	1102	ADP	C3'-C4'-C5'-O5'
3	B	1102	ADP	C3'-C4'-C5'-O5'
3	A	1102	ADP	C5'-O5'-PA-O1A
3	B	1102	ADP	C5'-O5'-PA-O1A
3	B	1102	ADP	C4'-C5'-O5'-PA
3	A	1102	ADP	C4'-C5'-O5'-PA
3	A	1102	ADP	PA-O3A-PB-O1B
3	B	1102	ADP	PA-O3A-PB-O1B

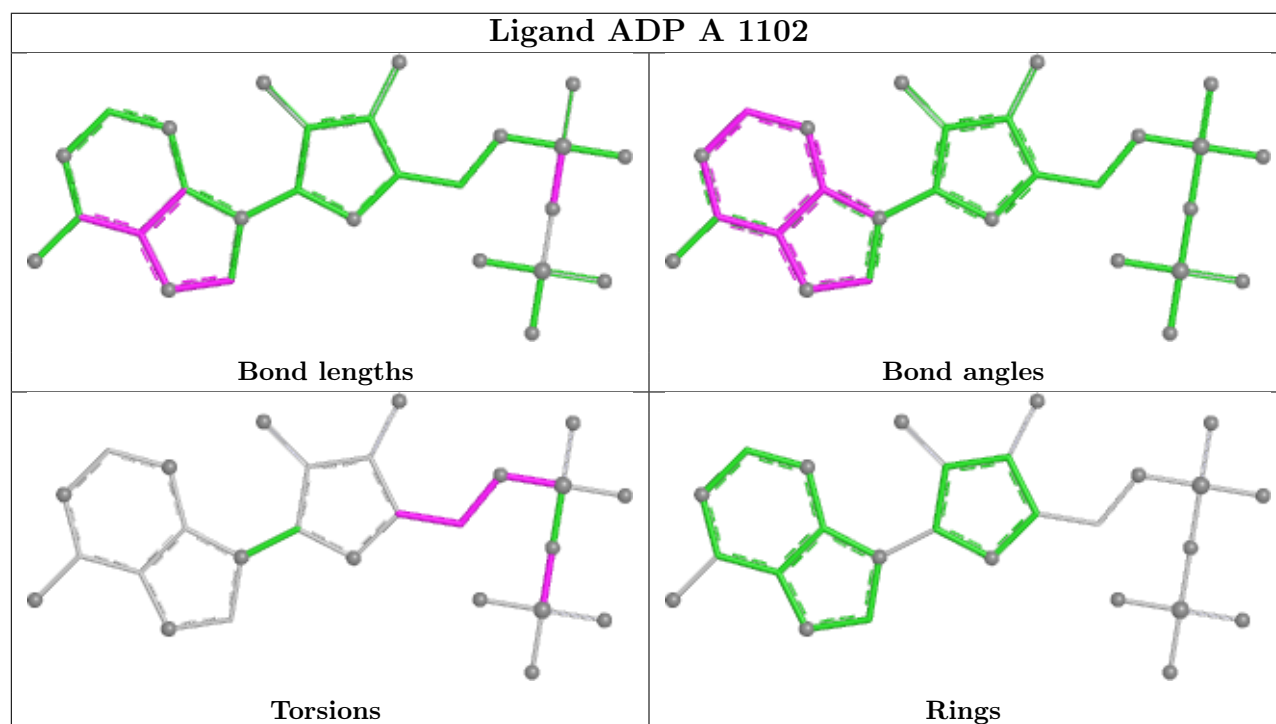
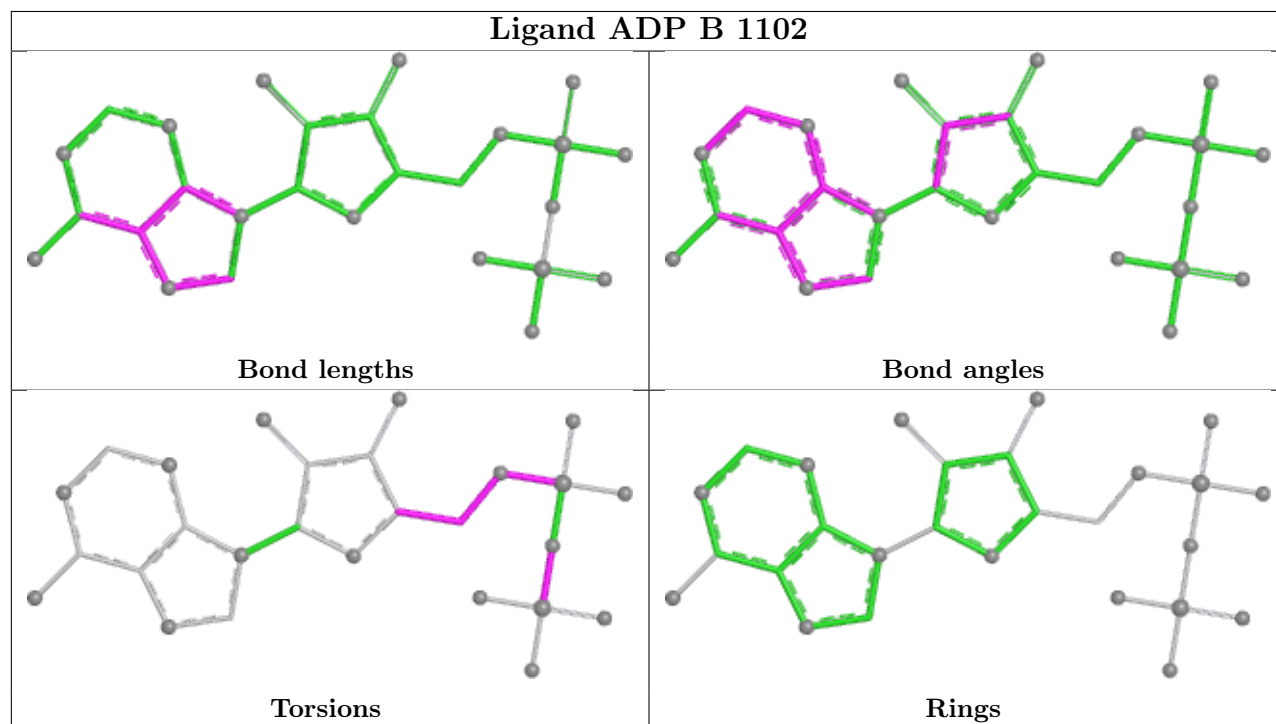
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	SF4	1	0
3	B	1102	ADP	1	0
3	A	1102	ADP	1	0

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	1046/1056 (99%)	-0.14	18 (1%) 69 45	24, 53, 119, 169	0
1	B	1046/1056 (99%)	-0.07	19 (1%) 67 44	23, 56, 126, 193	0
All	All	2092/2112 (99%)	-0.11	37 (1%) 67 44	23, 55, 123, 193	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ASP	3.5
1	A	875	ALA	3.5
1	B	101	GLU	3.4
1	A	101	GLU	3.3
1	B	243	SER	3.1
1	A	102	GLY	3.1
1	A	571	ASP	3.1
1	A	478	ASN	3.1
1	A	152	PRO	3.0
1	B	570	GLY	2.8
1	A	103	ASP	2.8
1	B	875	ALA	2.8
1	B	107	GLU	2.7
1	A	419	ILE	2.4
1	B	492	VAL	2.4
1	A	245	GLY	2.4
1	A	243	SER	2.4
1	B	569	HIS	2.3
1	B	375	PRO	2.3
1	A	48	TYR	2.3
1	B	1054	HIS	2.2
1	A	248	ARG	2.2
1	B	568	ARG	2.2
1	B	20	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	375	PRO	2.2
1	B	102	GLY	2.2
1	B	33	ALA	2.1
1	B	396	TYR	2.1
1	A	107	GLU	2.1
1	B	571	ASP	2.1
1	A	568	ARG	2.1
1	A	493	CYS	2.1
1	A	507	PRO	2.1
1	B	48	TYR	2.0
1	A	106	SER	2.0
1	B	478	ASN	2.0
1	B	993	GLY	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](#)

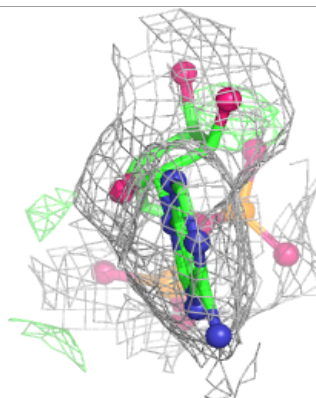
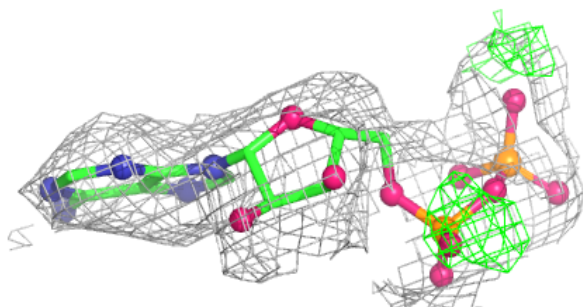
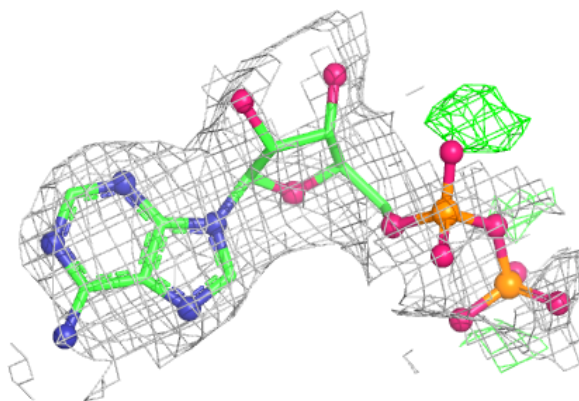
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ADP	A	1102	27/27	0.82	0.12	63,86,136,141	0
3	ADP	B	1102	27/27	0.83	0.13	62,99,131,140	0
2	SF4	A	1101	8/8	0.99	0.04	51,58,63,64	0
2	SF4	B	1101	8/8	0.99	0.03	57,63,71,72	0

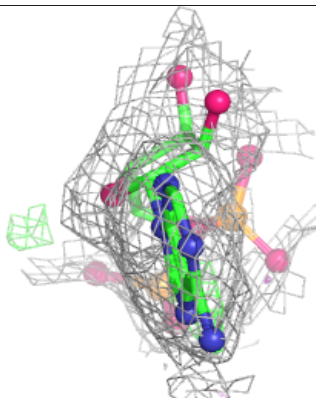
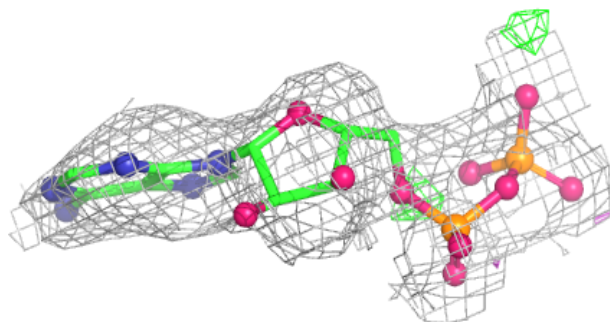
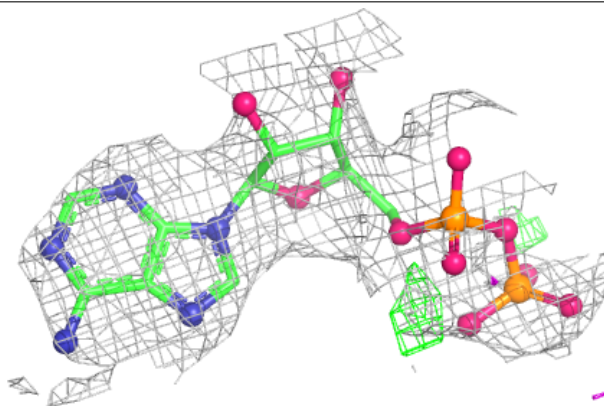
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 1102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.