



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 8TO4 / pdb_00008to4
Title : EGFR(T790M/V948R) in complex with the allosteric inhibitor FRF-06-057
Authors : Chitnis, S.P.; Deng, M.Q.; Pham, C.P.; Heppner, D.E.
Deposited on : 2023-08-02
Resolution : 2.99 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

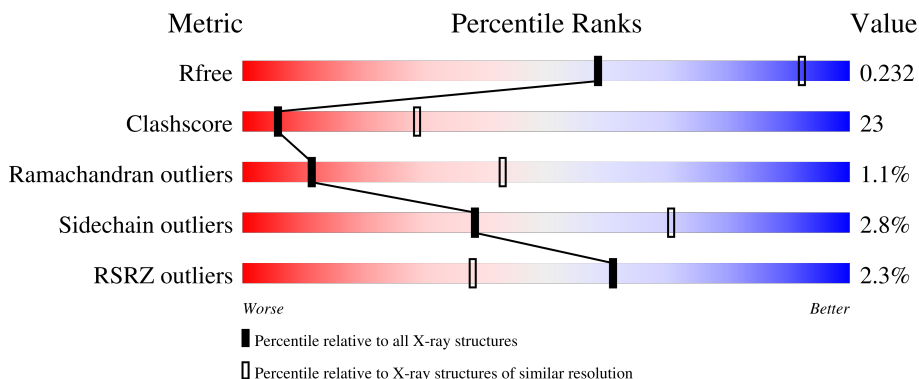
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	328	2% 53% 37% 9%
1	B	328	3% 53% 35% 12%
1	C	328	2% 54% 32% 12%
1	D	328	2% 53% 31% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9523 atoms, of which 52 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	283	Total	C	N	O	S	0	0	0
			2227	1439	370	400	18			
1	A	300	Total	C	N	O	S	0	0	0
			2390	1540	400	431	19			
1	B	290	Total	C	N	O	S	0	1	0
			2307	1486	386	417	18			
1	C	289	Total	C	N	O	S	0	1	0
			2297	1478	385	416	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

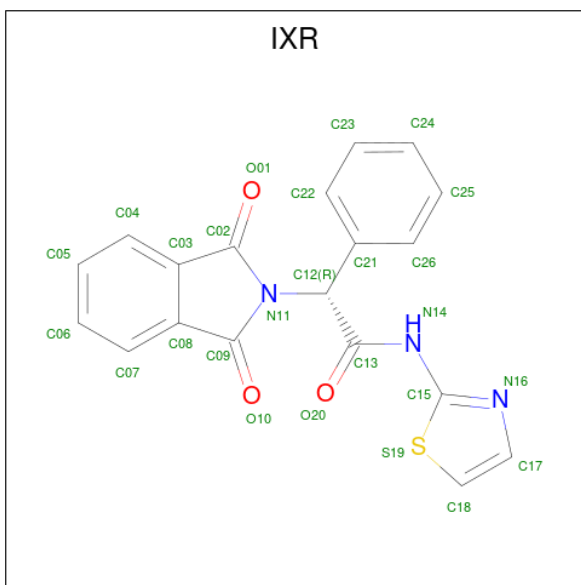
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	A	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		
3	C	1	Total	C	H	N	O	P	0	0
			44	10	13	6	12	3		

- Molecule 4 is (2R)-2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)-2-phenyl-N-(1,3-thiazol-2-yl)acetamide (CCD ID: IXR) (formula: $C_{19}H_{13}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 26	C 19	N 3	O 3	S 1	0	0
4	C	1	Total 26	C 19	N 3	O 3	S 1	0	0

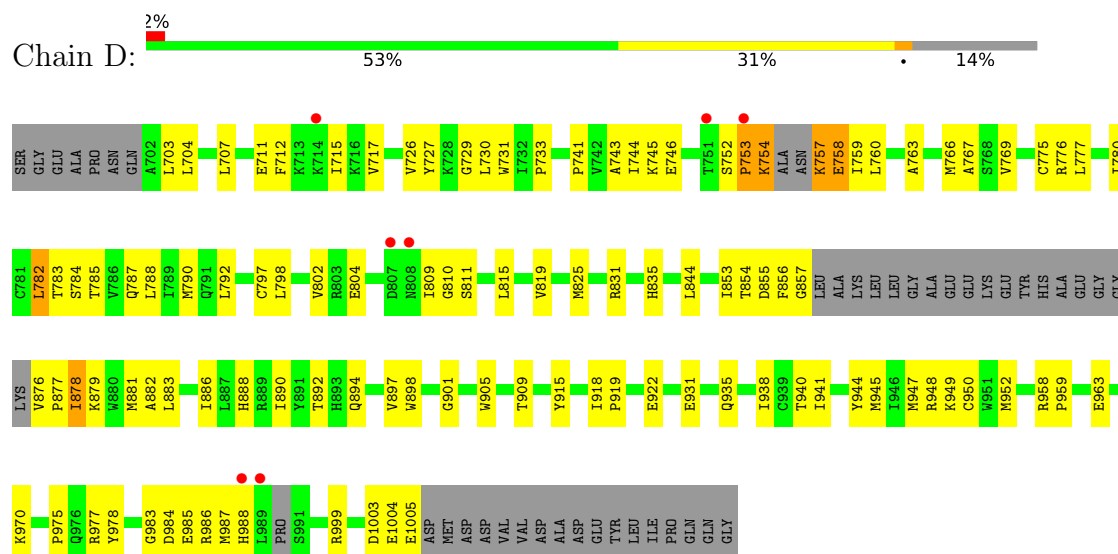
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	18	Total O 18 18	0	0
5	A	18	Total O 18 18	0	0
5	B	11	Total O 11 11	0	0
5	C	23	Total O 23 23	0	0

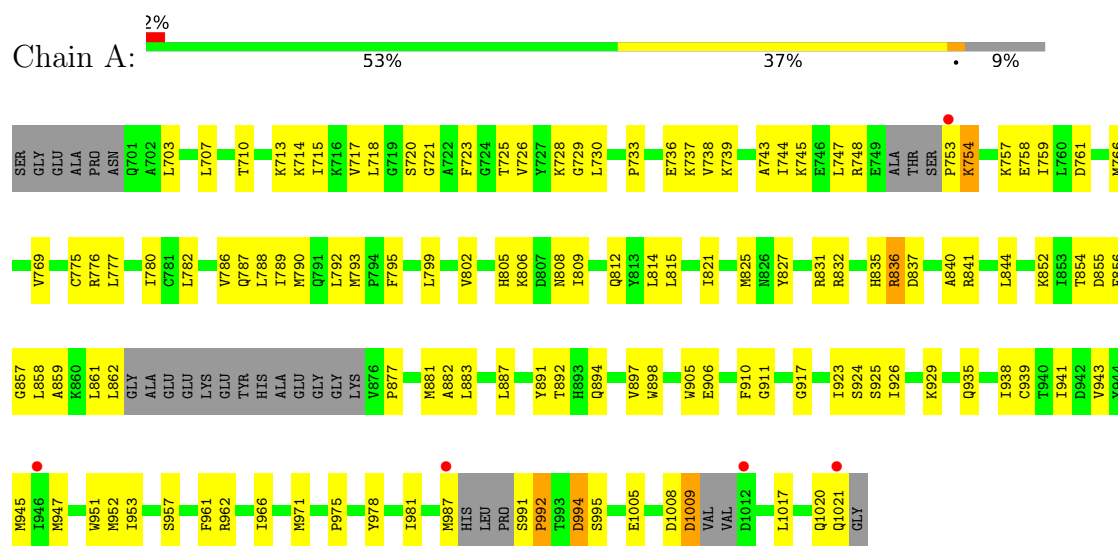
3 Residue-property plots

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: Epidermal growth factor receptor

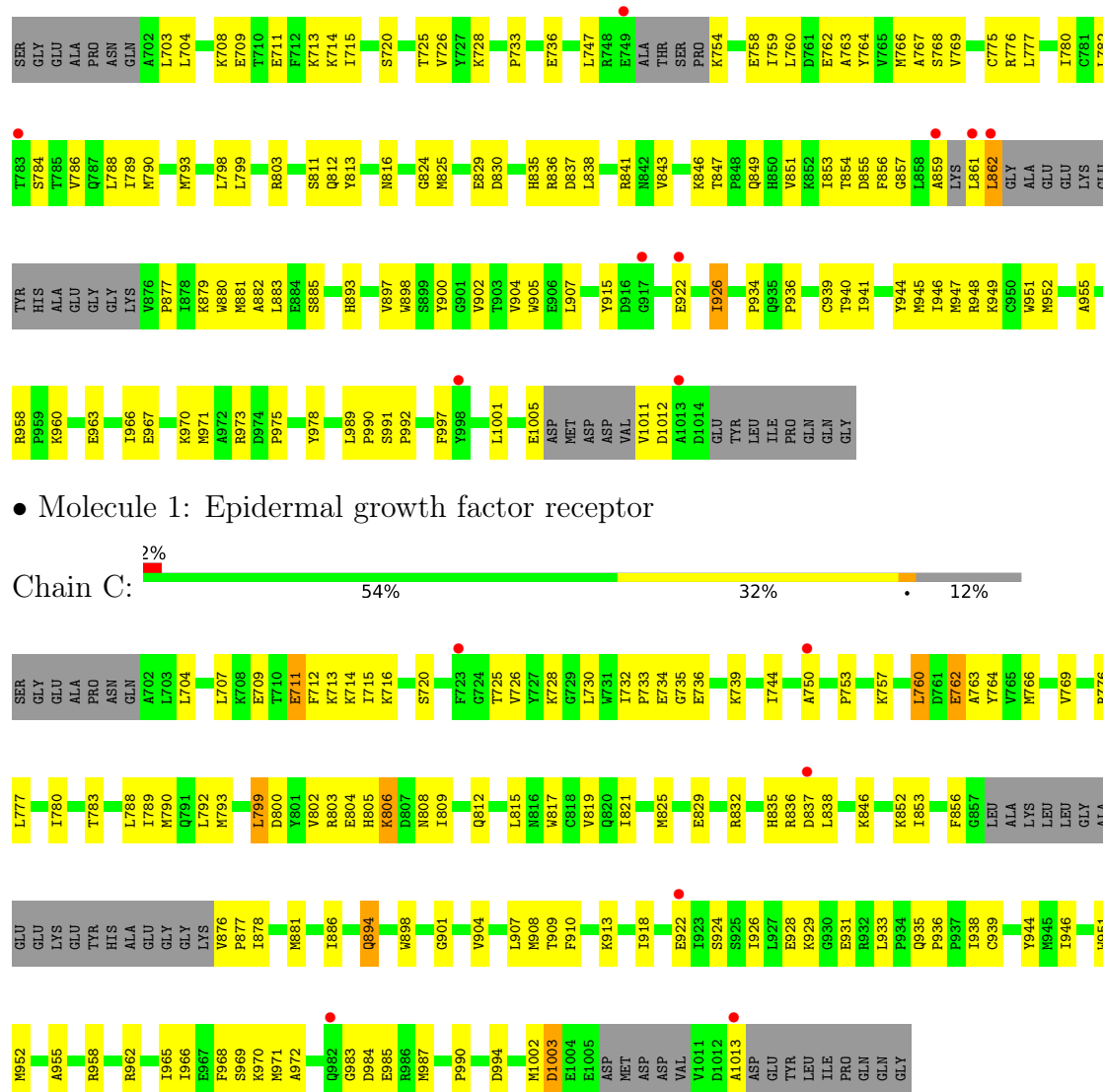


• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor





• Molecule 1: Epidermal growth factor receptor

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.35Å 103.11Å 86.87Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	70.96 – 2.99 70.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (70.96-2.99) 92.4 (70.96-2.99)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.171 , 0.231 0.172 , 0.232	Depositor DCC
R_{free} test set	1997 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9523	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% 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: ANP, IXR, MG

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	0.52	0/2439	0.74	1/3297 (0.0%)
1	B	0.43	0/2354	0.68	1/3184 (0.0%)
1	C	0.44	0/2347	0.67	0/3179
1	D	0.48	0/2275	0.71	0/3082
All	All	0.47	0/9415	0.70	2/12742 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	994	ASP	N-CA-C	-5.23	105.48	111.07
1	B	728	LYS	N-CA-C	-5.20	102.16	109.96

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	2390	0	2406	133	0
1	B	2307	0	2319	111	0
1	C	2297	0	2307	93	0
1	D	2227	0	2233	108	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	13	13	4	0
3	B	31	13	13	3	0
3	C	31	13	13	0	0
3	D	31	13	13	1	0
4	C	26	0	0	2	0
4	D	26	0	0	2	0
5	A	18	0	0	8	0
5	B	11	0	0	6	0
5	C	23	0	0	7	0
5	D	18	0	0	6	0
All	All	9471	52	9317	433	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 23.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:VAL:HG22	1:A:971:MET:HE1	1.43	1.01
1:A:941:ILE:HD13	1:C:922[B]:GLU:HG2	1.45	0.96
1:A:877:PRO:O	1:A:881:MET:HG3	1.74	0.87
1:B:816:ASN:HD21	1:B:1011:VAL:N	1.73	0.86
1:C:817:TRP:O	1:C:821:ILE:HG13	1.76	0.86
1:C:846:LYS:CG	1:C:1002:MET:HE1	2.06	0.86
1:B:708:LYS:O	1:B:711:GLU:HG2	1.77	0.84
1:A:723:PHE:HB2	3:A:1102:ANP:O1B	1.76	0.83
1:C:1002:MET:O	1:C:1003:ASP:HB2	1.76	0.83
1:A:766:MET:HE3	1:A:856:PHE:O	1.79	0.83
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.44	0.83
1:A:945:MET:HE3	5:C:1219:HOH:O	1.82	0.80
1:C:966:ILE:HG23	1:C:970:LYS:HE3	1.62	0.79
1:B:811:SER:OG	1:B:975:PRO:HB2	1.83	0.79
1:A:703:LEU:HB2	5:A:1214:HOH:O	1.84	0.77
1:C:803:ARG:HH22	1:C:913:LYS:NZ	1.83	0.77
1:D:854:THR:CG2	5:D:1209:HOH:O	2.31	0.77
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.20	0.76
1:D:999:ARG:HD2	1:D:1003:ASP:O	1.86	0.76
1:A:721:GLY:HA3	3:A:1102:ANP:N3B	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:LYS:HG3	1:C:1002:MET:HE1	1.67	0.76
1:B:989:LEU:HB3	1:B:990:PRO:HD2	1.68	0.75
1:D:707:LEU:HD12	1:D:711:GLU:CD	2.12	0.75
1:A:723:PHE:CD2	1:A:858:LEU:HD23	2.22	0.75
1:B:762:GLU:O	1:B:766:MET:HG2	1.87	0.74
1:D:1004:GLU:HG2	5:D:1211:HOH:O	1.87	0.74
1:C:715:ILE:HG13	1:C:716:LYS:H	1.53	0.73
1:C:966:ILE:CG2	1:C:970:LYS:HE3	2.17	0.73
1:D:854:THR:HG21	5:D:1209:HOH:O	1.87	0.73
1:D:811:SER:OG	1:D:975:PRO:HB2	1.88	0.72
1:C:715:ILE:HG12	1:C:728:LYS:O	1.90	0.72
1:D:922:GLU:HG2	1:B:941:ILE:HB	1.72	0.72
1:D:940:THR:HG23	1:D:978:TYR:O	1.88	0.72
1:A:747:LEU:HD12	1:A:786:VAL:HG11	1.69	0.72
1:A:861:LEU:HG	1:A:862:LEU:CD1	2.20	0.72
1:C:846:LYS:HG2	1:C:1002:MET:HE1	1.69	0.71
1:A:720:SER:HB3	1:A:725:THR:HG23	1.71	0.71
1:D:769:VAL:HG21	1:D:856:PHE:HZ	1.55	0.70
1:B:775:CYS:HA	5:B:1204:HOH:O	1.91	0.70
1:A:726:VAL:HG22	1:A:745:LYS:HE3	1.73	0.70
1:A:943:VAL:HG22	1:A:971:MET:CE	2.19	0.70
1:B:879:LYS:HD3	1:B:915:TYR:HB2	1.73	0.70
1:D:881:MET:HE2	1:D:886:ILE:CG1	2.21	0.70
1:A:883:LEU:HD22	1:A:953:ILE:HD12	1.74	0.70
1:D:775:CYS:HB3	1:D:790:MET:HE1	1.74	0.70
1:D:922:GLU:OE1	1:B:941:ILE:HD13	1.92	0.70
1:C:886:ILE:HG21	1:C:924:SER:HB3	1.73	0.69
1:D:726:VAL:CG2	1:D:745:LYS:HG3	2.21	0.69
1:C:962:ARG:HA	1:C:965:ILE:HD12	1.74	0.69
1:A:861:LEU:O	1:A:862:LEU:HD12	1.92	0.69
1:A:747:LEU:HD11	1:A:788:LEU:HD11	1.73	0.69
1:A:1008:ASP:O	1:A:1009:ASP:C	2.36	0.69
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.58	0.69
1:C:805:HIS:O	1:C:809:ILE:HG13	1.93	0.69
1:A:726:VAL:CG2	1:A:745:LYS:HE3	2.22	0.69
1:D:876:VAL:HG12	1:D:878:ILE:HG12	1.75	0.69
1:C:812:GLN:HE22	1:C:1013:ALA:H	1.38	0.68
1:A:790:MET:HE1	5:A:1213:HOH:O	1.91	0.68
1:C:757:LYS:HD2	1:C:757:LYS:N	2.07	0.68
1:D:810:GLY:HA2	1:D:987:MET:HE3	1.75	0.68
1:D:815:LEU:HD12	1:D:975:PRO:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:HIS:O	1:A:809:ILE:HG13	1.94	0.67
1:D:879:LYS:HG2	1:D:915:TYR:HD2	1.57	0.67
1:A:723:PHE:HZ	1:A:859:ALA:HB2	1.58	0.67
1:D:726:VAL:HG22	1:D:745:LYS:HG3	1.76	0.67
1:A:962:ARG:O	1:A:966:ILE:HD12	1.95	0.67
1:A:836:ARG:HG3	1:A:891:TYR:CD2	2.30	0.67
1:A:835:HIS:O	1:A:836:ARG:HB3	1.93	0.67
1:B:835:HIS:O	1:B:836:ARG:HB2	1.95	0.66
1:B:714:LYS:C	1:B:715:ILE:HD13	2.21	0.66
1:A:861:LEU:HG	1:A:862:LEU:HD12	1.78	0.66
1:A:733:PRO:HB2	1:A:736:GLU:HG3	1.78	0.66
1:C:918:ILE:HD11	5:C:1215:HOH:O	1.94	0.66
1:B:720:SER:HB3	1:B:725:THR:HG23	1.77	0.66
1:C:762:GLU:O	1:C:764:TYR:N	2.28	0.66
1:B:946:ILE:HD13	1:B:971:MET:HE1	1.78	0.66
1:A:747:LEU:HD12	1:A:786:VAL:CG1	2.24	0.66
1:B:966:ILE:HG22	1:B:970:LYS:HE3	1.78	0.66
1:C:735:GLY:O	1:C:736:GLU:HG2	1.96	0.66
1:C:825:MET:HE2	1:C:838:LEU:HD22	1.77	0.66
1:A:782:LEU:CD2	1:A:786:VAL:HG22	2.26	0.65
1:C:835:HIS:O	1:C:836:ARG:HB2	1.95	0.65
1:D:790:MET:HG2	4:D:1103:IXR:S19	2.36	0.65
1:C:829:GLU:O	1:C:832:ARG:N	2.27	0.64
1:A:757:LYS:NZ	1:A:761:ASP:OD1	2.21	0.64
1:D:881:MET:HE2	1:D:886:ILE:HG13	1.78	0.64
1:C:815:LEU:O	1:C:819:VAL:HG23	1.98	0.64
1:C:728:LYS:HG3	1:C:792:LEU:HD22	1.81	0.63
1:C:803:ARG:HH22	1:C:913:LYS:HZ1	1.46	0.63
1:D:775:CYS:HB3	1:D:790:MET:CE	2.29	0.63
1:D:769:VAL:HG21	1:D:856:PHE:CZ	2.33	0.63
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.34	0.62
1:D:746:GLU:HG3	1:D:787:GLN:HG3	1.81	0.62
1:A:941:ILE:HD13	1:C:922[B]:GLU:CG	2.27	0.62
1:B:946:ILE:CD1	1:B:971:MET:HE1	2.30	0.62
1:A:883:LEU:CD2	1:A:953:ILE:HD12	2.30	0.61
1:A:766:MET:HE1	1:A:858:LEU:CD1	2.31	0.61
1:C:966:ILE:O	1:C:970:LYS:HG3	2.01	0.61
1:B:788:LEU:HD11	5:B:1211:HOH:O	2.01	0.60
1:A:837:ASP:OD1	1:A:877:PRO:HG3	2.00	0.60
1:A:730:LEU:HD13	1:A:739:LYS:HB3	1.84	0.60
1:B:798:LEU:CD2	1:B:907:LEU:HD21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LYS:NZ	1:A:787:GLN:OE1	2.35	0.60
1:D:877:PRO:O	1:D:881:MET:HG3	2.01	0.59
1:C:983:GLY:C	1:C:985:GLU:H	2.10	0.59
1:B:905:TRP:HB2	1:B:947:MET:HE3	1.84	0.59
1:A:780:ILE:HG13	1:A:788:LEU:HD23	1.85	0.59
1:A:938:ILE:HG23	5:A:1205:HOH:O	2.02	0.59
1:A:802:VAL:HA	1:A:809:ILE:HD11	1.84	0.59
1:B:944:TYR:CZ	1:B:948:ARG:HD3	2.38	0.59
1:D:938:ILE:HG12	5:D:1204:HOH:O	2.03	0.58
1:A:723:PHE:HZ	1:A:859:ALA:CB	2.15	0.58
1:A:725:THR:OG1	1:B:830:ASP:OD2	2.22	0.58
1:A:947:MET:HE3	1:A:951:TRP:CH2	2.38	0.58
1:A:947:MET:HE3	1:A:951:TRP:HH2	1.69	0.58
1:D:767:ALA:O	1:D:776:ARG:NH1	2.29	0.58
1:C:790:MET:HG2	4:C:1103:IXR:C18	2.34	0.58
1:B:769:VAL:HG21	1:B:856:PHE:HZ	1.68	0.58
1:D:715:ILE:HG13	1:D:730:LEU:HG	1.85	0.57
1:A:898:TRP:CE3	1:A:951:TRP:HA	2.39	0.57
1:C:909:THR:HG22	1:C:936:PRO:HB3	1.86	0.57
1:D:881:MET:HE2	1:D:886:ILE:HG12	1.85	0.57
1:B:754:LYS:HG3	1:B:758:GLU:OE1	2.04	0.57
1:A:832:ARG:NH1	5:A:1202:HOH:O	2.38	0.57
1:C:715:ILE:HG13	1:C:716:LYS:N	2.18	0.57
1:A:941:ILE:HG12	1:C:926:ILE:HG22	1.87	0.56
1:A:806:LYS:HE3	1:A:910:PHE:O	2.06	0.56
1:C:1002:MET:HB3	5:C:1217:HOH:O	2.05	0.56
1:D:949:LYS:HB3	1:D:959:PRO:HD3	1.85	0.56
1:D:918:ILE:HG23	1:B:941:ILE:HD11	1.86	0.56
1:B:777:LEU:CD1	1:B:788:LEU:HB3	2.35	0.56
1:C:803:ARG:HH22	1:C:913:LYS:HZ2	1.54	0.56
1:C:799:LEU:O	1:C:802:VAL:HG22	2.06	0.56
1:C:1002:MET:O	1:C:1003:ASP:CB	2.52	0.56
1:C:846:LYS:HD2	1:C:852:LYS:HD2	1.86	0.56
1:C:715:ILE:CG1	1:C:716:LYS:H	2.17	0.55
1:B:922[A]:GLU:O	1:B:926:ILE:HG23	2.06	0.55
1:B:922[B]:GLU:O	1:B:926:ILE:HG23	2.07	0.55
1:B:1011:VAL:HG12	1:B:1012:ASP:H	1.71	0.55
1:B:936:PRO:HB2	1:B:939:CYS:SG	2.47	0.55
1:D:766:MET:HE1	1:D:857:GLY:CA	2.37	0.55
1:B:762:GLU:OE1	1:B:861:LEU:HB3	2.06	0.55
1:B:825:MET:HE3	1:B:825:MET:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:LYS:HB2	1:B:963:GLU:HG3	1.88	0.54
1:A:748:ARG:HG3	1:B:830:ASP:HA	1.89	0.54
1:C:931:GLU:HG3	5:C:1219:HOH:O	2.07	0.54
1:D:766:MET:O	1:D:769:VAL:HG22	2.08	0.54
1:A:858:LEU:HA	1:A:861:LEU:CD2	2.38	0.54
1:B:893:HIS:O	1:B:897:VAL:HG23	2.08	0.54
1:A:799:LEU:HB2	1:A:840:ALA:C	2.34	0.53
1:C:908:MET:HG3	1:C:939:CYS:SG	2.48	0.53
1:D:717:VAL:HG22	1:D:727:TYR:CE2	2.43	0.53
1:B:782:LEU:CD2	1:B:786:VAL:HG13	2.39	0.53
1:B:948:ARG:HG3	5:B:1207:HOH:O	2.07	0.53
1:B:877:PRO:HB2	1:B:880:TRP:HB2	1.90	0.53
1:B:997:PHE:CE2	1:B:1001:LEU:HD12	2.44	0.53
1:C:878:ILE:CD1	1:C:886:ILE:HG12	2.38	0.53
1:C:898:TRP:CE3	1:C:951:TRP:HA	2.44	0.53
1:A:782:LEU:HD23	1:A:786:VAL:HG22	1.89	0.53
1:C:762:GLU:O	1:C:763:ALA:HB3	2.09	0.53
1:D:754:LYS:HB2	1:D:757:LYS:HB3	1.91	0.53
1:D:757:LYS:O	1:D:758:GLU:C	2.52	0.53
1:D:752:SER:O	1:D:753:PRO:C	2.53	0.52
1:B:777:LEU:HD11	1:B:788:LEU:HB3	1.91	0.52
1:C:800:ASP:O	1:C:804:GLU:HG3	2.10	0.52
1:A:952:MET:HE1	1:A:957:SER:HB3	1.91	0.52
1:D:729:GLY:HA3	1:D:744:ILE:CD1	2.39	0.52
1:B:703:LEU:O	1:B:776:ARG:NH1	2.39	0.52
1:B:824:GLY:HA3	1:B:853:ILE:HD12	1.91	0.52
1:A:877:PRO:O	1:A:881:MET:CG	2.53	0.52
1:B:949:LYS:O	1:B:952:MET:HG3	2.09	0.52
1:D:743:ALA:HB2	1:D:792:LEU:HD12	1.92	0.52
1:A:906:GLU:O	1:A:911:GLY:N	2.36	0.52
1:D:888:HIS:O	1:D:890:ILE:HG13	2.09	0.51
1:B:788:LEU:C	1:B:789:ILE:HD12	2.35	0.51
1:D:760:LEU:HG	1:D:782:LEU:HD21	1.92	0.51
1:B:733:PRO:HB2	1:B:736:GLU:HB2	1.91	0.51
1:D:766:MET:CE	1:D:857:GLY:HA3	2.40	0.51
1:B:769:VAL:HG21	1:B:856:PHE:CZ	2.45	0.51
1:C:946:ILE:HD12	1:C:971:MET:HE1	1.91	0.51
1:D:952:MET:O	1:D:958:ARG:NH2	2.40	0.51
1:A:721:GLY:HA3	3:A:1102:ANP:PB	2.51	0.51
1:A:766:MET:HE1	1:A:858:LEU:HD13	1.92	0.51
1:D:810:GLY:CA	1:D:987:MET:HE3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:730:LEU:HD23	1:D:741:PRO:HA	1.93	0.51
1:D:879:LYS:HG2	1:D:915:TYR:CD2	2.43	0.51
1:B:798:LEU:HD21	1:B:907:LEU:HD21	1.92	0.51
1:A:992:PRO:C	1:A:994:ASP:H	2.18	0.51
1:B:714:LYS:O	1:B:715:ILE:HD13	2.11	0.51
1:C:776:ARG:HD3	5:C:1202:HOH:O	2.11	0.51
1:A:802:VAL:HA	1:A:809:ILE:CD1	2.41	0.51
1:C:728:LYS:HE2	1:C:792:LEU:CD2	2.40	0.51
1:A:723:PHE:CZ	1:A:859:ALA:HA	2.45	0.50
1:A:835:HIS:O	1:A:836:ARG:CB	2.59	0.50
1:A:723:PHE:CZ	1:A:859:ALA:HB2	2.43	0.50
1:A:703:LEU:O	1:A:776:ARG:NH1	2.41	0.50
1:A:713:LYS:HE2	1:A:730:LEU:HD12	1.92	0.50
1:A:808:ASN:C	1:A:987:MET:HG3	2.37	0.50
1:A:766:MET:HE1	1:A:858:LEU:HD12	1.94	0.50
1:B:747:LEU:HD12	1:B:786:VAL:HB	1.93	0.50
1:B:947:MET:HE2	1:B:951:TRP:HH2	1.76	0.50
1:C:910:PHE:CZ	1:C:938:ILE:HD13	2.46	0.50
1:D:783:THR:O	1:D:784:SER:C	2.54	0.50
1:A:737:LYS:HD3	5:A:1218:HOH:O	2.11	0.50
1:C:709:GLU:HA	1:C:712:PHE:CE1	2.47	0.50
1:A:707:LEU:HG	1:A:789:ILE:HG13	1.94	0.49
1:B:726:VAL:HB	3:B:1102:ANP:H5'1	1.94	0.49
1:C:762:GLU:HG3	1:C:766:MET:HG2	1.94	0.49
1:D:919:PRO:HD2	1:D:922:GLU:OE1	2.12	0.49
1:A:793:MET:HE1	1:A:852:LYS:HD3	1.94	0.49
1:B:947:MET:HE2	1:B:951:TRP:CH2	2.47	0.49
1:B:934:PRO:O	1:B:936:PRO:HD3	2.12	0.49
1:D:731:TRP:CH2	1:D:733:PRO:HG3	2.47	0.49
1:A:856:PHE:CG	1:A:857:GLY:N	2.80	0.49
1:B:812:GLN:O	1:B:816:ASN:HB2	2.13	0.49
1:A:844:LEU:HG	1:A:854:THR:HG21	1.94	0.49
1:D:854:THR:HG23	5:D:1209:HOH:O	2.03	0.49
1:A:935:GLN:NE2	1:A:939:CYS:O	2.34	0.49
1:A:775:CYS:SG	1:A:854:THR:HB	2.52	0.49
1:B:905:TRP:HB2	1:B:947:MET:CE	2.42	0.49
1:C:789:ILE:HD12	1:C:789:ILE:N	2.28	0.49
1:D:731:TRP:CZ3	1:D:733:PRO:HG3	2.48	0.49
1:D:931:GLU:HG2	1:B:945:MET:HE2	1.95	0.49
1:D:940:THR:HG21	1:D:978:TYR:HA	1.94	0.49
1:A:753:PRO:O	1:A:754:LYS:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:MET:O	1:A:769:VAL:HG22	2.13	0.49
1:A:941:ILE:O	1:A:945:MET:HG3	2.13	0.49
1:D:881:MET:CE	1:D:886:ILE:HG13	2.41	0.48
1:B:782:LEU:HD21	1:B:786:VAL:HG13	1.95	0.48
1:C:904:VAL:O	1:C:907:LEU:N	2.46	0.48
1:A:941:ILE:HG13	1:A:945:MET:HG3	1.95	0.48
1:D:949:LYS:O	1:D:958:ARG:HG2	2.13	0.48
1:B:760:LEU:HD13	1:B:782:LEU:CD1	2.43	0.48
1:B:944:TYR:O	1:B:948:ARG:HG2	2.13	0.48
1:D:815:LEU:O	1:D:819:VAL:HG23	2.12	0.48
1:A:861:LEU:HD23	1:A:861:LEU:H	1.79	0.48
1:A:882:ALA:HB2	1:A:898:TRP:CB	2.44	0.48
1:B:971:MET:HA	1:B:978:TYR:CE2	2.49	0.48
1:C:769:VAL:HG21	1:C:856:PHE:HZ	1.77	0.48
1:D:704:LEU:HD21	1:D:780:ILE:CG2	2.44	0.48
1:A:754:LYS:HA	1:A:758:GLU:OE1	2.13	0.48
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.48	0.48
1:B:898:TRP:CE3	1:B:951:TRP:HA	2.49	0.48
1:C:983:GLY:O	1:C:985:GLU:N	2.46	0.48
1:A:825:MET:HB3	1:A:961:PHE:CE1	2.48	0.47
1:A:854:THR:OG1	1:A:855:ASP:N	2.46	0.47
1:B:967:GLU:HG3	1:B:971:MET:HE2	1.96	0.47
1:A:744:ILE:HG12	1:A:789:ILE:CD1	2.44	0.47
1:D:717:VAL:HG22	1:D:727:TYR:CD2	2.50	0.47
1:D:905:TRP:CE2	1:D:909:THR:HG21	2.50	0.47
1:D:704:LEU:HD21	1:D:780:ILE:HG21	1.95	0.47
1:D:831:ARG:NE	5:D:1203:HOH:O	2.48	0.47
1:B:708:LYS:O	1:B:711:GLU:N	2.45	0.47
1:A:718:LEU:HD21	1:A:728:LYS:HB2	1.96	0.47
1:A:992:PRO:C	1:A:994:ASP:N	2.73	0.47
1:D:746:GLU:HG2	1:D:785:THR:CG2	2.45	0.46
1:A:923:ILE:HD13	1:A:926:ILE:HD11	1.97	0.46
1:D:945:MET:SD	1:A:929:LYS:NZ	2.87	0.46
1:A:766:MET:CE	1:A:856:PHE:O	2.59	0.46
1:B:793:MET:H	3:B:1102:ANP:H2	1.81	0.46
1:B:843:VAL:HG12	1:B:851:VAL:HB	1.96	0.46
1:B:847:THR:C	1:B:849:GLN:H	2.23	0.46
1:A:836:ARG:HG3	1:A:891:TYR:CE2	2.51	0.46
1:D:729:GLY:HA3	1:D:744:ILE:HD11	1.98	0.46
1:D:780:ILE:HD12	1:D:788:LEU:HD21	1.98	0.46
1:D:986:ARG:C	1:D:987:MET:HG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:LEU:HD11	1:A:788:LEU:HB3	1.97	0.46
1:C:935:GLN:HA	1:C:944:TYR:CD1	2.50	0.46
1:D:948:ARG:NH2	1:A:917:GLY:O	2.49	0.46
1:A:856:PHE:CD1	1:A:857:GLY:N	2.83	0.46
1:C:790:MET:HG2	4:C:1103:IXR:S19	2.55	0.46
1:C:878:ILE:HD12	1:C:886:ILE:HG12	1.98	0.46
1:D:726:VAL:HG23	1:D:745:LYS:HG3	1.98	0.46
1:D:1004:GLU:O	1:D:1005:GLU:C	2.59	0.46
1:B:704:LEU:HD23	1:B:764:TYR:CE1	2.51	0.46
1:C:793:MET:HE1	1:C:852:LYS:HD3	1.97	0.46
1:A:753:PRO:O	1:A:754:LYS:C	2.59	0.45
1:D:905:TRP:CZ2	1:D:909:THR:HG21	2.52	0.45
1:A:841:ARG:HG2	1:A:841:ARG:HH11	1.82	0.45
1:B:973:ARG:CG	1:B:1011:VAL:HG11	2.47	0.45
1:D:941:ILE:CD1	5:A:1209:HOH:O	2.65	0.45
1:C:968:PHE:CD1	1:C:971:MET:HE3	2.51	0.45
1:D:810:GLY:HA2	1:D:987:MET:CE	2.45	0.45
1:C:769:VAL:HG23	1:C:769:VAL:O	2.16	0.45
1:C:735:GLY:C	1:C:736:GLU:HG2	2.41	0.45
1:C:987:MET:HB2	1:C:987:MET:HE3	1.56	0.45
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.15	0.45
1:B:881:MET:HB3	1:B:885:SER:HB2	1.99	0.45
1:D:825:MET:HE1	1:D:835:HIS:HB2	1.99	0.45
1:B:793:MET:H	3:B:1102:ANP:C2	2.29	0.45
1:A:861:LEU:HG	1:A:862:LEU:HD13	1.96	0.45
1:B:713:LYS:HG3	1:B:715:ILE:HD11	1.99	0.45
1:B:714:LYS:HE2	1:B:714:LYS:HB2	1.72	0.45
1:C:766:MET:HE2	1:C:766:MET:HA	1.98	0.45
1:C:924:SER:O	1:C:928:GLU:HG3	2.17	0.45
1:D:746:GLU:HG2	1:D:785:THR:HG22	1.99	0.44
1:D:775:CYS:CB	1:D:790:MET:HE1	2.46	0.44
1:A:723:PHE:CZ	1:A:859:ALA:CA	3.00	0.44
1:A:815:LEU:HD12	1:A:975:PRO:HB3	1.99	0.44
1:B:837:ASP:HA	5:B:1206:HOH:O	2.17	0.44
1:D:877:PRO:O	1:D:878:ILE:C	2.59	0.44
1:D:983:GLY:C	1:D:985:GLU:N	2.75	0.44
1:A:714:LYS:C	1:A:715:ILE:HG12	2.43	0.44
1:A:882:ALA:HA	1:A:898:TRP:CG	2.52	0.44
1:A:994:ASP:O	1:A:995:SER:C	2.61	0.44
1:D:941:ILE:HD11	5:A:1209:HOH:O	2.18	0.44
1:A:799:LEU:O	1:A:802:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:GLY:O	1:B:861:LEU:HB2	2.18	0.44
1:B:1011:VAL:HG12	1:B:1012:ASP:N	2.32	0.44
1:C:898:TRP:O	1:C:901:GLY:N	2.50	0.44
1:A:723:PHE:HZ	1:A:859:ALA:CA	2.31	0.44
1:B:812:GLN:HG2	1:B:975:PRO:HG3	1.99	0.44
1:B:846:LYS:NZ	1:B:1005:GLU:OE2	2.50	0.44
1:D:898:TRP:O	1:D:901:GLY:N	2.51	0.44
1:D:986:ARG:O	1:D:987:MET:HG2	2.18	0.44
1:B:788:LEU:CD1	5:B:1211:HOH:O	2.64	0.44
1:B:789:ILE:C	1:B:790:MET:HG3	2.42	0.44
1:B:989:LEU:HB3	1:B:990:PRO:CD	2.44	0.44
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.82	0.43
1:B:945:MET:O	1:B:949:LYS:HG3	2.18	0.43
1:B:991:SER:HB2	1:B:992:PRO:HD2	2.00	0.43
1:C:894:GLN:HB3	1:C:955:ALA:HB1	1.99	0.43
1:A:844:LEU:HG	1:A:854:THR:CG2	2.48	0.43
1:B:709:GLU:OE2	1:B:784:SER:OG	2.29	0.43
1:B:829:GLU:HA	1:B:893:HIS:NE2	2.33	0.43
1:B:955:ALA:HA	1:B:958:ARG:NH1	2.33	0.43
1:B:760:LEU:HD13	1:B:782:LEU:HD12	2.00	0.43
1:C:805:HIS:O	1:C:806:LYS:C	2.61	0.43
1:A:806:LYS:HG3	1:A:910:PHE:HB3	2.00	0.43
1:B:838:LEU:HD12	1:B:838:LEU:HA	1.75	0.43
1:D:922:GLU:CG	1:B:941:ILE:HB	2.46	0.43
1:A:858:LEU:HA	1:A:861:LEU:HD21	2.01	0.43
1:B:766:MET:HB2	1:B:777:LEU:CB	2.49	0.43
1:B:788:LEU:HD21	5:B:1211:HOH:O	2.18	0.43
1:C:969:SER:O	1:C:972:ALA:HB3	2.18	0.43
1:D:757:LYS:HB2	1:D:757:LYS:HE3	1.45	0.43
1:A:861:LEU:C	1:A:862:LEU:HD12	2.44	0.43
1:B:767:ALA:O	1:B:776:ARG:HD2	2.18	0.43
1:D:984:ASP:HA	1:D:987:MET:HE2	2.00	0.43
1:D:783:THR:HG22	1:D:784:SER:N	2.32	0.43
1:D:815:LEU:HD23	1:D:815:LEU:HA	1.79	0.43
1:D:753:PRO:O	1:D:754:LYS:C	2.61	0.43
1:D:798:LEU:O	1:D:802:VAL:HG22	2.19	0.43
1:A:894:GLN:O	1:A:897:VAL:HB	2.18	0.43
1:B:859:ALA:O	1:B:861:LEU:N	2.52	0.43
1:D:759:ILE:HG23	4:D:1103:IXR:C05	2.49	0.43
1:B:760:LEU:HD12	1:B:760:LEU:HA	1.84	0.43
1:C:990:PRO:HB2	1:C:994:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:MET:HG2	1:B:766:MET:H	1.58	0.42
1:A:991:SER:O	1:A:992:PRO:O	2.37	0.42
1:C:707:LEU:HA	1:C:711:GLU:OE2	2.19	0.42
1:C:776:ARG:NH1	5:C:1202:HOH:O	2.29	0.42
1:A:952:MET:CE	1:A:957:SER:HB3	2.49	0.42
1:B:900:TYR:O	1:B:904:VAL:HG23	2.19	0.42
1:C:733:PRO:O	1:C:734:GLU:C	2.60	0.42
1:C:780:ILE:O	1:C:780:ILE:HG23	2.18	0.42
1:D:703:LEU:HD23	1:D:703:LEU:HA	1.56	0.42
1:D:890:ILE:HG22	1:D:892:THR:HG23	2.00	0.42
1:A:808:ASN:HB2	5:A:1211:HOH:O	2.19	0.42
1:A:814:LEU:HD12	1:A:981:ILE:HD11	2.00	0.42
1:D:986:ARG:C	1:D:987:MET:CG	2.92	0.42
1:B:759:ILE:HG21	1:B:782:LEU:HD21	2.02	0.42
1:C:983:GLY:C	1:C:985:GLU:N	2.77	0.42
1:D:712:PHE:HA	1:D:730:LEU:O	2.19	0.42
1:D:948:ARG:HA	1:D:948:ARG:HD2	1.83	0.42
1:A:743:ALA:HB2	1:A:792:LEU:HA	2.01	0.42
1:A:821:ILE:O	1:A:825:MET:HG2	2.19	0.42
1:A:827:TYR:OH	1:A:831:ARG:NH1	2.50	0.42
1:D:935:GLN:HB2	1:D:944:TYR:CD2	2.54	0.42
1:B:841:ARG:HH22	1:B:877:PRO:HB3	1.84	0.42
1:C:725:THR:HG22	1:C:726:VAL:N	2.35	0.42
1:C:825:MET:SD	1:C:853:ILE:HD13	2.59	0.42
1:C:876:VAL:HA	1:C:877:PRO:HD3	1.92	0.42
1:D:882:ALA:O	1:D:883:LEU:C	2.62	0.42
1:D:970:LYS:HB3	1:D:970:LYS:HE2	1.83	0.42
1:A:729:GLY:HA3	1:A:744:ILE:HD12	2.02	0.42
1:A:733:PRO:HD2	1:A:738:VAL:HG23	2.02	0.42
1:A:808:ASN:O	1:A:987:MET:HG3	2.20	0.42
1:A:887:LEU:HD21	1:A:924:SER:HB2	2.02	0.42
1:A:858:LEU:O	1:A:861:LEU:HD23	2.20	0.41
1:A:891:TYR:C	1:A:892:THR:HG23	2.45	0.41
1:B:955:ALA:O	1:B:958:ARG:HB2	2.20	0.41
1:A:710:THR:H	1:A:710:THR:HG23	1.61	0.41
1:A:793:MET:O	1:A:795:PHE:N	2.53	0.41
3:A:1102:ANP:N3B	3:A:1102:ANP:O2A	2.53	0.41
1:B:799:LEU:HD21	1:B:803:ARG:NH2	2.34	0.41
1:B:825:MET:HE3	1:B:825:MET:CA	2.50	0.41
1:C:713:LYS:HE3	1:C:732:ILE:HD11	2.03	0.41
1:C:946:ILE:HD12	1:C:971:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:ALA:HA	1:D:777:LEU:O	2.20	0.41
1:B:763:ALA:HB2	1:B:780:ILE:HD12	2.02	0.41
1:A:802:VAL:O	1:A:806:LYS:N	2.54	0.41
1:A:952:MET:HE3	1:A:957:SER:HB2	2.03	0.41
1:B:837:ASP:OD1	1:B:877:PRO:HG3	2.21	0.41
1:D:797:CYS:HA	1:D:844:LEU:HA	2.02	0.41
1:A:759:ILE:HG21	1:A:782:LEU:HD21	2.02	0.41
1:B:854:THR:HG23	1:B:855:ASP:OD2	2.20	0.41
1:C:744:ILE:HA	1:C:788:LEU:O	2.21	0.41
1:C:933:LEU:HD12	1:C:951:TRP:CZ2	2.55	0.41
1:A:883:LEU:HD23	1:A:953:ILE:HG23	2.02	0.41
1:C:728:LYS:HG3	1:C:792:LEU:CD2	2.48	0.41
1:D:949:LYS:HA	1:D:952:MET:HG3	2.02	0.41
1:B:883:LEU:HA	1:B:883:LEU:HD12	1.86	0.41
1:B:940:THR:OG1	1:B:978:TYR:HA	2.21	0.41
1:B:861:LEU:O	1:B:862:LEU:C	2.62	0.41
1:D:879:LYS:HE2	1:D:915:TYR:HB2	2.03	0.41
1:B:847:THR:C	1:B:849:GLN:N	2.79	0.41
1:C:704:LEU:HD13	1:C:777:LEU:HD23	2.02	0.41
1:D:815:LEU:HD12	1:D:975:PRO:CB	2.49	0.41
1:A:733:PRO:O	1:A:736:GLU:HB2	2.20	0.41
1:C:715:ILE:CG1	1:C:716:LYS:N	2.79	0.41
1:C:878:ILE:HD13	1:C:886:ILE:HG12	2.02	0.41
1:D:745:LYS:HE3	3:D:1102:ANP:O1A	2.21	0.40
1:D:854:THR:O	1:D:855:ASP:HB2	2.21	0.40
1:D:876:VAL:CG1	1:D:878:ILE:HG12	2.49	0.40
1:A:757:LYS:HA	1:A:757:LYS:HD2	1.83	0.40
1:A:808:ASN:HA	1:A:987:MET:SD	2.61	0.40
1:C:730:LEU:HD13	1:C:739:LYS:HB3	2.01	0.40
1:C:952:MET:O	1:C:958:ARG:NH2	2.48	0.40
1:D:783:THR:CG2	1:D:784:SER:N	2.84	0.40
1:A:971:MET:HE3	1:A:978:TYR:HB3	2.03	0.40
1:A:1020:GLN:O	1:A:1021:GLN:C	2.65	0.40
1:B:902:VAL:HG23	1:B:951:TRP:HE1	1.86	0.40
1:C:881:MET:HE2	1:C:886:ILE:HG13	2.03	0.40
1:C:757:LYS:HA	1:C:757:LYS:HE3	2.03	0.40
1:C:760:LEU:HD23	1:C:760:LEU:HA	1.86	0.40
1:D:897:VAL:O	1:D:950:CYS:HB3	2.21	0.40
1:C:709:GLU:HG2	5:C:1213:HOH:O	2.19	0.40
1:D:763:ALA:HB1	1:D:777:LEU:CD2	2.52	0.40
1:D:766:MET:CE	1:D:857:GLY:CA	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:ILE:CG1	1:C:926:ILE:HG22	2.50	0.40
1:B:703:LEU:HD13	1:B:768:SER:HA	2.03	0.40
1:C:966:ILE:HG22	1:C:970:LYS:HE3	2.00	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	290/328 (88%)	265 (91%)	22 (8%)	3 (1%)	12	45
1	B	281/328 (86%)	263 (94%)	18 (6%)	0	100	100
1	C	284/328 (87%)	249 (88%)	28 (10%)	7 (2%)	4	23
1	D	275/328 (84%)	239 (87%)	34 (12%)	2 (1%)	18	53
All	All	1130/1312 (86%)	1016 (90%)	102 (9%)	12 (1%)	11	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	753	PRO
1	A	754	LYS
1	C	806	LYS
1	C	984	ASP
1	C	1003	ASP
1	A	992	PRO
1	C	750	ALA
1	A	836	ARG
1	C	808	ASN
1	C	837	ASP
1	D	758	GLU
1	C	799	LEU

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	260/288 (90%)	254 (98%)	6 (2%)	44	74
1	B	251/288 (87%)	249 (99%)	2 (1%)	73	86
1	C	250/288 (87%)	241 (96%)	9 (4%)	31	65
1	D	241/288 (84%)	230 (95%)	11 (5%)	24	58
All	All	1002/1152 (87%)	974 (97%)	28 (3%)	38	70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	754	LYS
1	D	757	LYS
1	D	782	LEU
1	D	804	GLU
1	D	809	ILE
1	D	853	ILE
1	D	878	ILE
1	D	894	GLN
1	D	963	GLU
1	D	977	ARG
1	D	988	HIS
1	A	717	VAL
1	A	812	GLN
1	A	925	SER
1	A	1005	GLU
1	A	1009	ASP
1	A	1017	LEU
1	B	862	LEU
1	B	926	ILE
1	C	711	GLU
1	C	714	LYS
1	C	720	SER
1	C	753	PRO
1	C	760	LEU

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Mol	Chain	Res	Type
1	C	762	GLU
1	C	783	THR
1	C	894	GLN
1	C	929	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	773	HIS
1	D	787	GLN
1	A	893	HIS
1	B	791	GLN
1	B	935	GLN
1	C	816	ASN
1	C	893	HIS
1	C	894	GLN
1	C	976	GLN

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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	IXR	C	1103	-	29,29,29	2.86	12 (41%)	38,41,41	2.05	9 (23%)
3	ANP	D	1102	2	33,33,33	1.02	4 (12%)	45,52,52	1.25	6 (13%)
3	ANP	B	1102	2	33,33,33	1.11	4 (12%)	45,52,52	1.07	2 (4%)
4	IXR	D	1103	-	29,29,29	2.78	12 (41%)	38,41,41	2.02	10 (26%)
3	ANP	C	1102	2	33,33,33	0.90	3 (9%)	45,52,52	0.95	3 (6%)
3	ANP	A	1102	2	33,33,33	0.96	3 (9%)	45,52,52	1.05	5 (11%)

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	IXR	C	1103	-	-	3/16/32/32	0/4/4/4
3	ANP	D	1102	2	-	3/18/38/38	0/3/3/3
3	ANP	B	1102	2	-	6/18/38/38	0/3/3/3
4	IXR	D	1103	-	-	4/16/32/32	0/4/4/4
3	ANP	C	1102	2	-	8/18/38/38	0/3/3/3
3	ANP	A	1102	2	-	7/18/38/38	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1103	IXR	C15-S19	-7.20	1.64	1.74
4	D	1103	IXR	C15-S19	-7.07	1.64	1.74
4	C	1103	IXR	C15-N14	5.64	1.46	1.38
4	C	1103	IXR	C15-N16	5.20	1.39	1.31
4	C	1103	IXR	C13-N14	5.20	1.46	1.36
4	D	1103	IXR	C17-N16	5.05	1.47	1.38
4	D	1103	IXR	C15-N16	4.80	1.39	1.31
4	D	1103	IXR	C08-C09	4.71	1.56	1.48
4	C	1103	IXR	C17-N16	4.70	1.46	1.38
4	D	1103	IXR	C13-N14	4.57	1.44	1.36
4	D	1103	IXR	C15-N14	4.32	1.44	1.38
4	C	1103	IXR	C09-N11	3.79	1.47	1.40
3	B	1102	ANP	PG-O1G	3.78	1.51	1.46
4	C	1103	IXR	C03-C02	3.76	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1103	IXR	C02-N11	3.61	1.47	1.40
4	D	1103	IXR	C17-C18	3.50	1.42	1.34
4	C	1103	IXR	C08-C09	3.46	1.54	1.48
4	D	1103	IXR	C03-C02	3.39	1.54	1.48
3	A	1102	ANP	PG-O1G	3.36	1.51	1.46
4	C	1103	IXR	C17-C18	3.25	1.41	1.34
3	C	1102	ANP	PG-O1G	3.11	1.50	1.46
3	B	1102	ANP	PG-N3B	3.00	1.71	1.63
3	D	1102	ANP	PA-O3A	2.82	1.62	1.59
3	D	1102	ANP	PG-N3B	2.74	1.70	1.63
3	A	1102	ANP	PG-N3B	2.62	1.70	1.63
4	C	1103	IXR	C02-N11	2.59	1.45	1.40
3	A	1102	ANP	PB-N3B	2.55	1.70	1.63
4	D	1103	IXR	C09-N11	2.52	1.45	1.40
3	B	1102	ANP	PB-O1B	2.39	1.49	1.46
3	C	1102	ANP	PB-O1B	2.35	1.49	1.46
3	D	1102	ANP	PB-O1B	2.32	1.49	1.46
3	B	1102	ANP	PB-N3B	2.32	1.69	1.63
3	C	1102	ANP	PG-N3B	2.30	1.69	1.63
3	D	1102	ANP	PG-O1G	2.28	1.49	1.46
4	D	1103	IXR	C18-S19	-2.25	1.60	1.70
4	C	1103	IXR	C18-S19	-2.21	1.60	1.70
4	C	1103	IXR	O20-C13	-2.13	1.19	1.23
4	D	1103	IXR	O01-C02	-2.07	1.18	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1103	IXR	C18-S19-C15	7.12	98.22	90.07
4	C	1103	IXR	C18-S19-C15	6.88	97.95	90.07
3	B	1102	ANP	O1G-PG-N3B	-4.60	105.00	111.77
4	C	1103	IXR	C18-C17-N16	-4.36	109.83	116.12
3	D	1102	ANP	O2A-PA-O3A	4.02	118.14	107.27
4	D	1103	IXR	C13-N14-C15	-4.01	119.66	124.54
4	C	1103	IXR	C13-N14-C15	-3.98	119.70	124.54
4	D	1103	IXR	C09-N11-C02	-3.82	107.21	111.55
3	A	1102	ANP	O1B-PB-N3B	-3.82	106.15	111.77
4	C	1103	IXR	C21-C12-N11	-3.73	108.33	112.82
4	C	1103	IXR	C09-N11-C02	-3.60	107.46	111.55
3	D	1102	ANP	O1G-PG-N3B	-3.56	106.52	111.77
4	D	1103	IXR	C18-C17-N16	-3.43	111.18	116.12
3	D	1102	ANP	O2G-PG-O1G	-3.37	104.99	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	ANP	O2B-PB-O3A	3.04	114.78	104.64
4	D	1103	IXR	O01-C02-C03	-2.97	122.90	128.66
3	D	1102	ANP	O2G-PG-O3G	2.91	115.41	107.59
3	C	1102	ANP	O2B-PB-O1B	-2.76	103.94	109.87
3	A	1102	ANP	O2G-PG-O1G	-2.74	106.57	113.45
4	C	1103	IXR	O10-C09-N11	2.72	128.82	124.99
3	C	1102	ANP	O3G-PG-O1G	-2.70	106.69	113.45
4	D	1103	IXR	O01-C02-N11	2.66	128.73	124.99
4	C	1103	IXR	O10-C09-C08	-2.64	123.55	128.66
3	D	1102	ANP	O3G-PG-O1G	-2.62	106.88	113.45
3	B	1102	ANP	O2B-PB-O3A	2.45	112.83	104.64
4	C	1103	IXR	S19-C15-N16	-2.35	110.16	114.59
4	D	1103	IXR	O20-C13-N14	-2.35	118.76	122.61
3	D	1102	ANP	O1B-PB-N3B	-2.31	108.37	111.77
3	A	1102	ANP	O1G-PG-N3B	-2.23	108.49	111.77
4	D	1103	IXR	C08-C09-N11	2.19	108.38	105.96
4	D	1103	IXR	C03-C02-N11	2.18	108.37	105.96
3	A	1102	ANP	O2B-PB-O1B	-2.09	105.38	109.87
3	A	1102	ANP	O3A-PB-N3B	2.08	112.36	106.59
4	C	1103	IXR	C03-C02-N11	2.02	108.20	105.96
4	D	1103	IXR	C07-C08-C09	2.02	132.97	129.59

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	ANP	PB-N3B-PG-O1G
3	A	1102	ANP	C5'-O5'-PA-O1A
3	A	1102	ANP	C5'-O5'-PA-O2A
3	A	1102	ANP	C5'-O5'-PA-O3A
3	B	1102	ANP	PB-N3B-PG-O1G
3	B	1102	ANP	PG-N3B-PB-O1B
3	C	1102	ANP	PB-N3B-PG-O1G
3	C	1102	ANP	PG-N3B-PB-O1B
3	C	1102	ANP	PG-N3B-PB-O3A
3	C	1102	ANP	PB-O3A-PA-O5'
4	D	1103	IXR	N16-C15-N14-C13
4	D	1103	IXR	S19-C15-N14-C13
3	B	1102	ANP	O4'-C4'-C5'-O5'
3	B	1102	ANP	C3'-C4'-C5'-O5'
3	C	1102	ANP	O4'-C4'-C5'-O5'
4	C	1103	IXR	N16-C15-N14-C13

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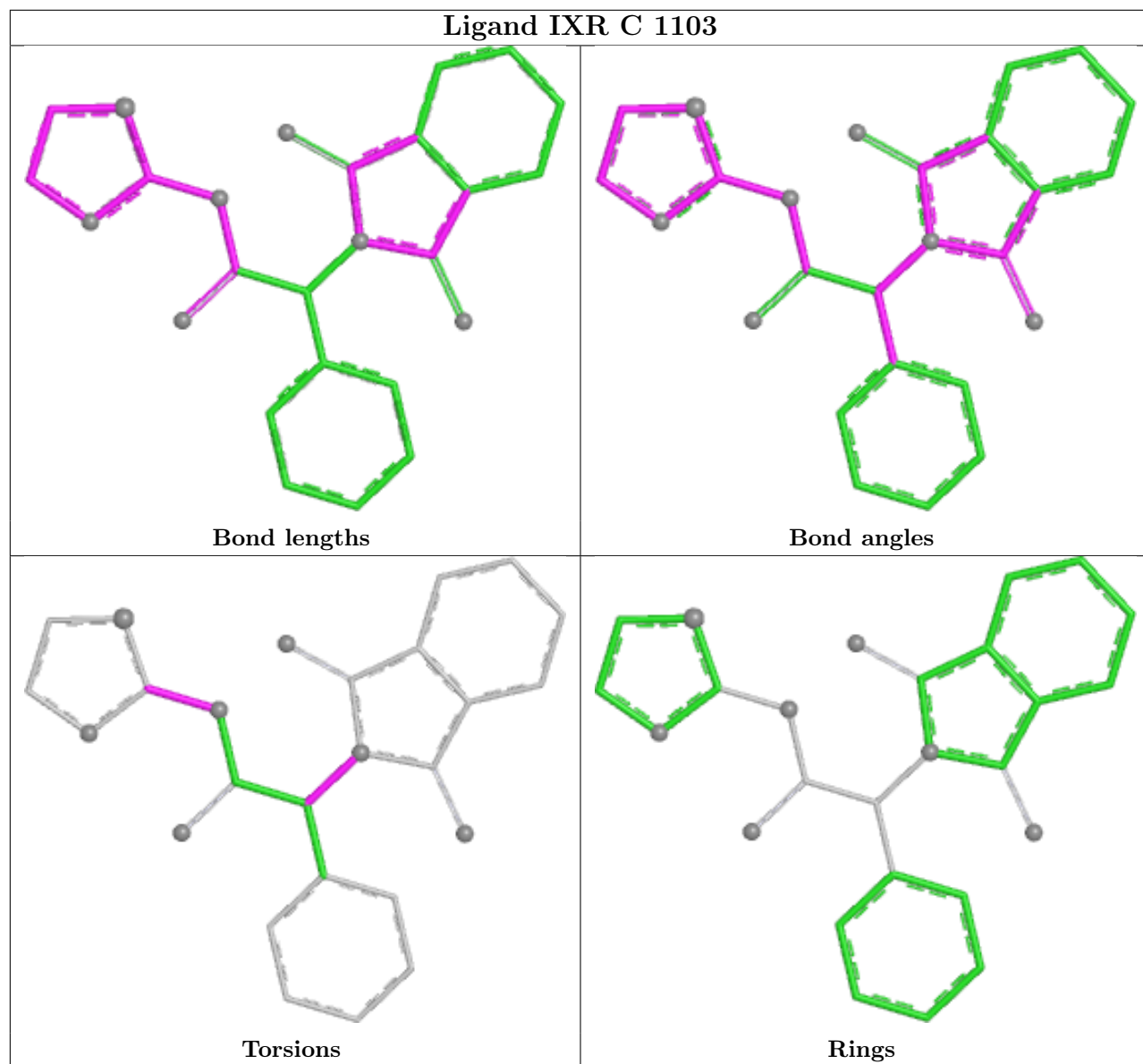
Mol	Chain	Res	Type	Atoms
4	C	1103	IXR	S19-C15-N14-C13
3	B	1102	ANP	PB-O3A-PA-O5'
3	C	1102	ANP	C3'-C4'-C5'-O5'
4	D	1103	IXR	C21-C12-N11-C02
4	D	1103	IXR	C21-C12-N11-C09
4	C	1103	IXR	C21-C12-N11-C09
3	B	1102	ANP	C5'-O5'-PA-O1A
3	C	1102	ANP	C5'-O5'-PA-O1A
3	A	1102	ANP	C4'-C5'-O5'-PA
3	A	1102	ANP	PG-N3B-PB-O1B
3	D	1102	ANP	PB-O3A-PA-O1A
3	D	1102	ANP	PB-O3A-PA-O2A
3	C	1102	ANP	PB-O3A-PA-O2A
3	D	1102	ANP	PB-N3B-PG-O1G
3	A	1102	ANP	PB-O3A-PA-O1A

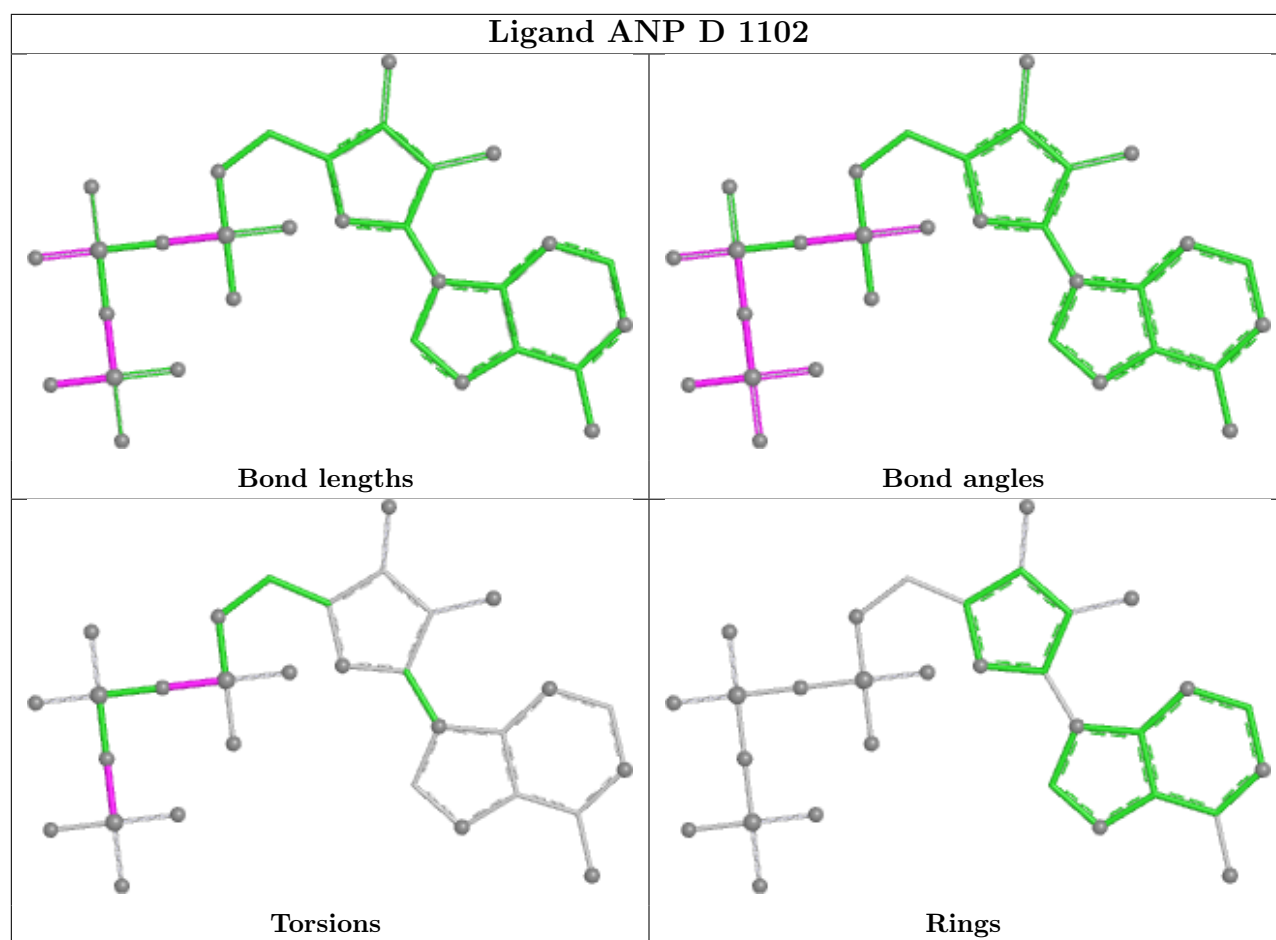
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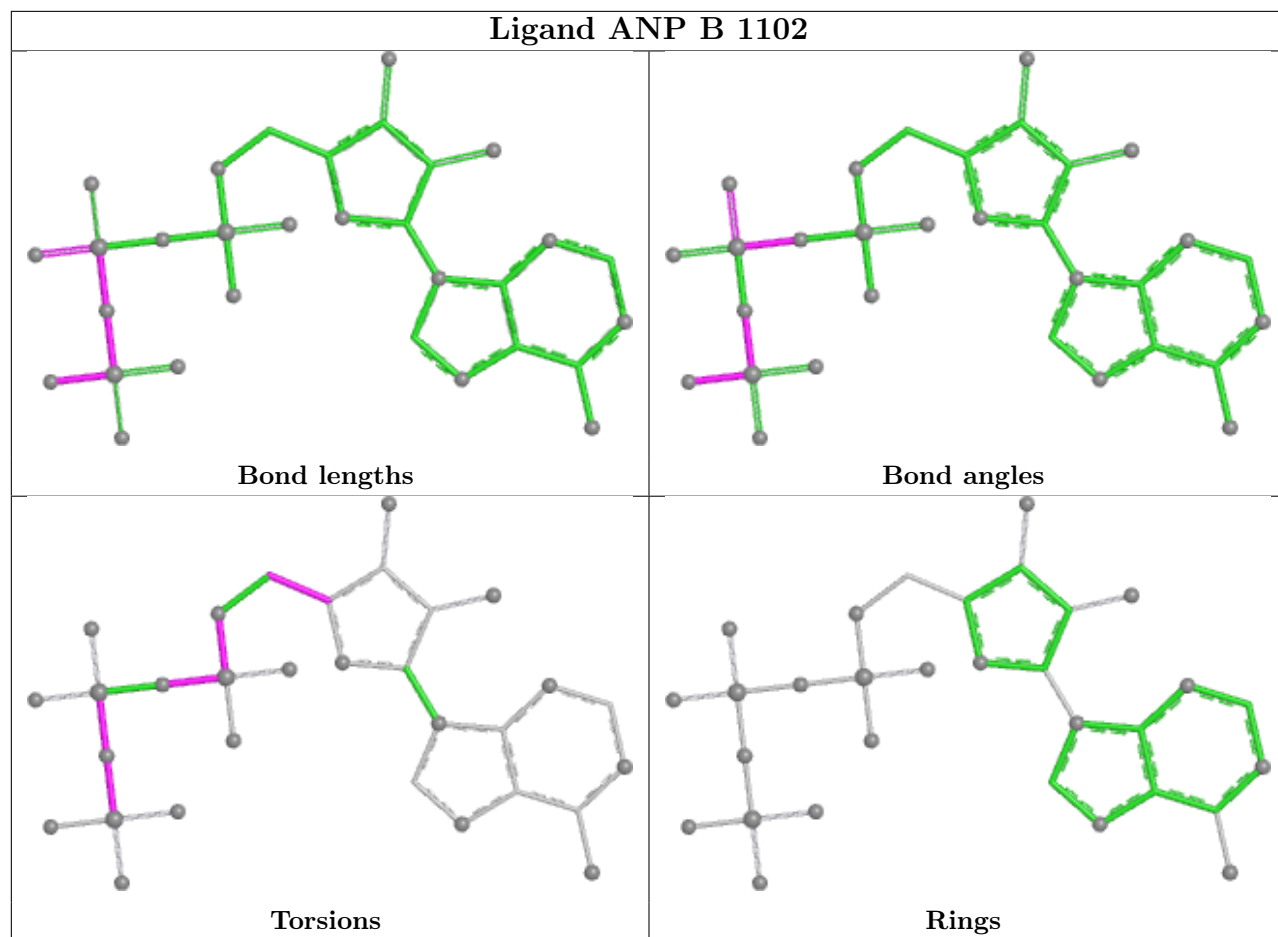
5 monomers are involved in 12 short contacts:

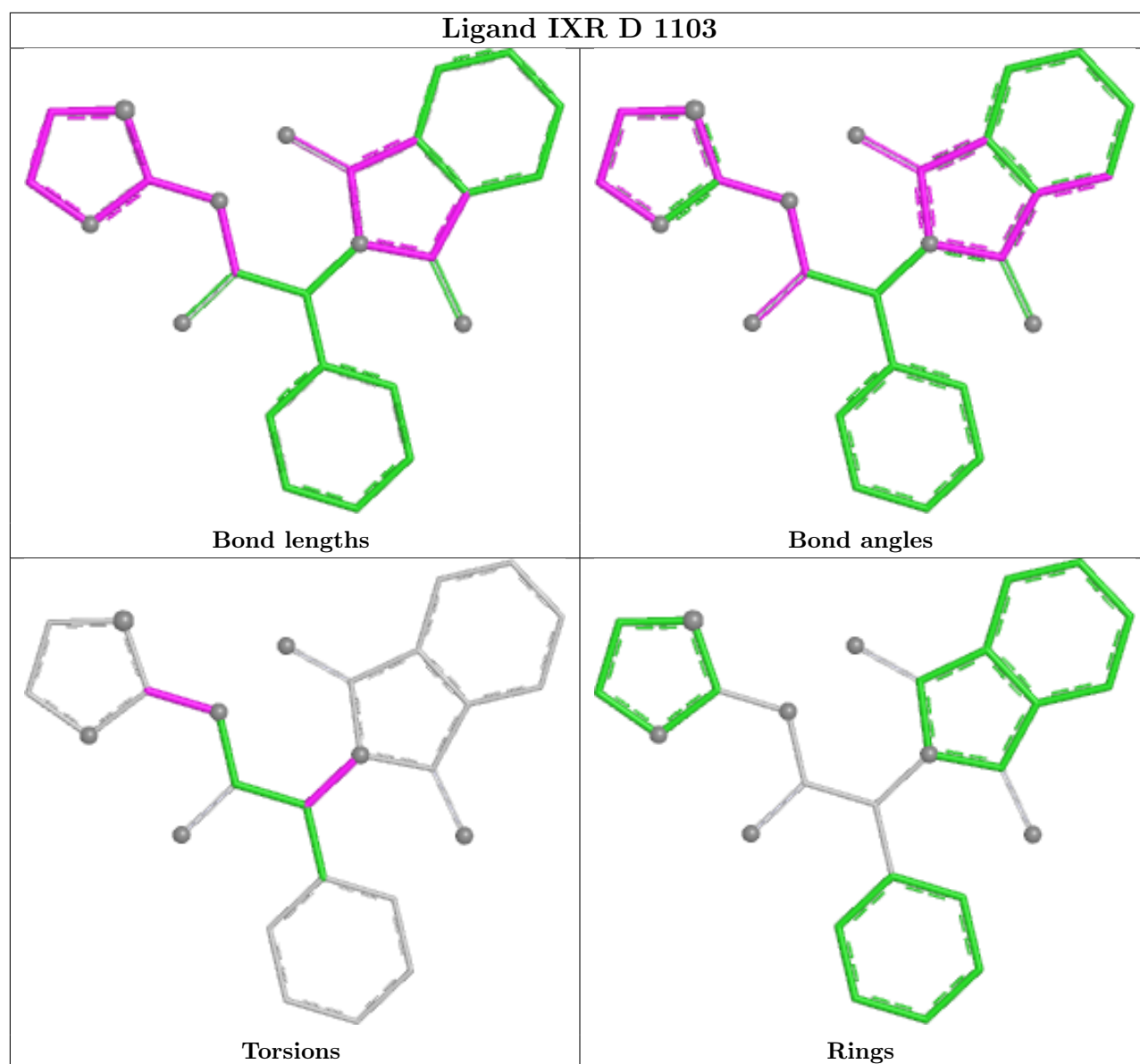
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1103	IXR	2	0
3	D	1102	ANP	1	0
3	B	1102	ANP	3	0
4	D	1103	IXR	2	0
3	A	1102	ANP	4	0

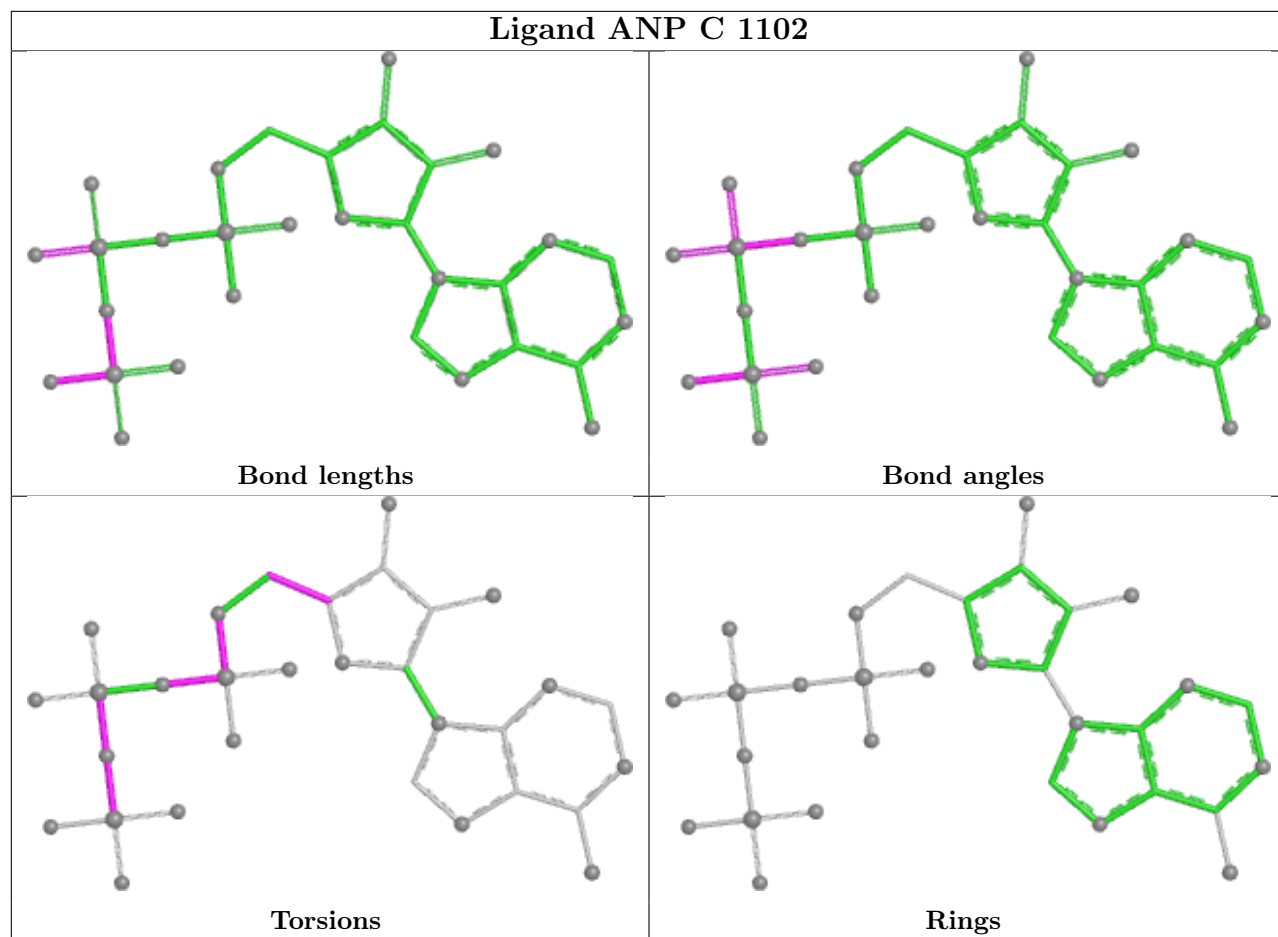
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

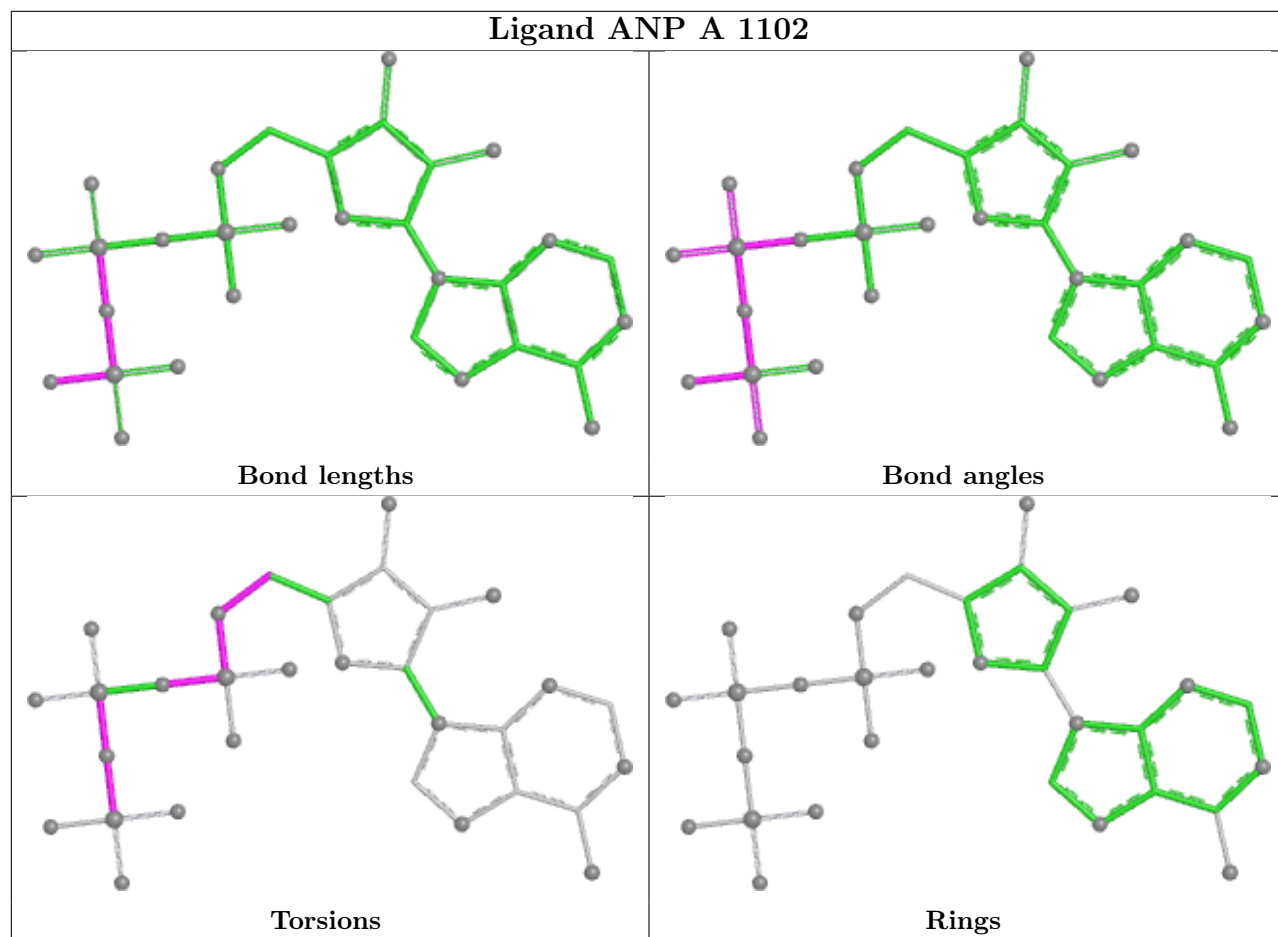












5.7 Other polymers [i](#)

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	300/328 (91%)	0.17	5 (1%) 69 45	19, 38, 59, 84	0
1	B	290/328 (88%)	0.35	9 (3%) 51 30	24, 43, 67, 85	1 (0%)
1	C	289/328 (88%)	0.32	6 (2%) 63 40	24, 40, 64, 92	1 (0%)
1	D	283/328 (86%)	0.26	7 (2%) 58 35	19, 38, 72, 98	0
All	All	1162/1312 (88%)	0.27	27 (2%) 61 38	19, 40, 65, 98	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1012	ASP	4.6
1	B	917	GLY	3.8
1	B	862	LEU	3.6
1	C	982	GLN	3.2
1	C	723	PHE	3.0
1	D	989	LEU	3.0
1	D	751	THR	2.8
1	A	987	MET	2.7
1	B	783	THR	2.7
1	B	1013	ALA	2.6
1	B	859	ALA	2.5
1	D	807	ASP	2.5
1	A	946	ILE	2.5
1	B	922[A]	GLU	2.4
1	D	988	HIS	2.4
1	B	749	GLU	2.4
1	B	998	TYR	2.4
1	C	922[A]	GLU	2.4
1	A	753	PRO	2.4
1	C	837	ASP	2.3
1	C	750	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1013	ALA	2.2
1	A	1021	GLN	2.1
1	D	714	LYS	2.1
1	B	861	LEU	2.0
1	D	753	PRO	2.0
1	D	808	ASN	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](#)

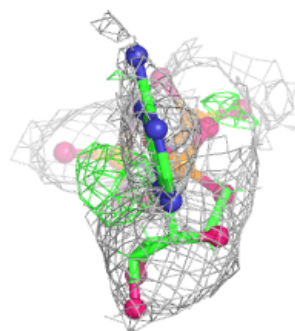
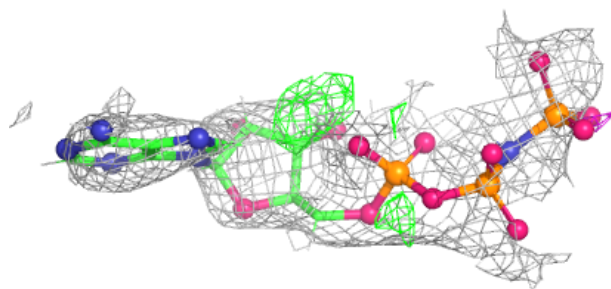
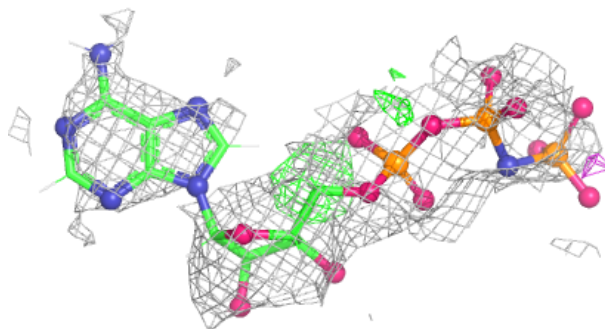
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	1101	1/1	0.76	0.17	46,46,46,46	0
3	ANP	A	1102	31/31	0.79	0.18	32,49,65,72	44
3	ANP	B	1102	31/31	0.86	0.12	34,60,72,76	0
3	ANP	C	1102	31/31	0.87	0.10	31,61,77,87	0
4	IXR	D	1103	26/26	0.89	0.12	37,46,54,64	0
4	IXR	C	1103	26/26	0.90	0.13	31,52,64,66	0
2	MG	B	1101	1/1	0.91	0.12	40,40,40,40	0
3	ANP	D	1102	31/31	0.92	0.10	27,43,59,69	0
2	MG	D	1101	1/1	0.94	0.18	22,22,22,22	0
2	MG	C	1101	1/1	0.99	0.05	39,39,39,39	0

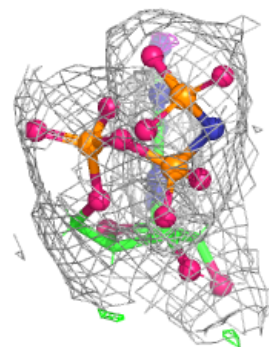
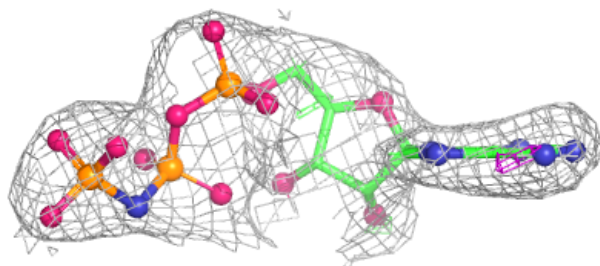
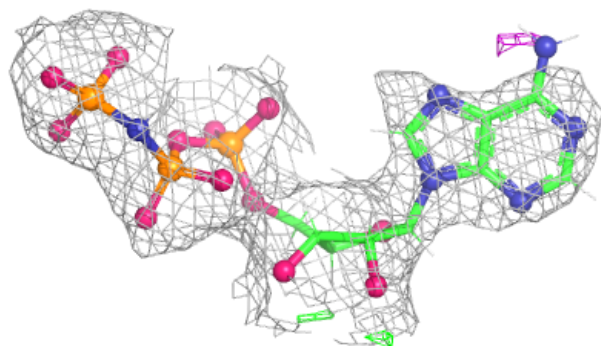
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

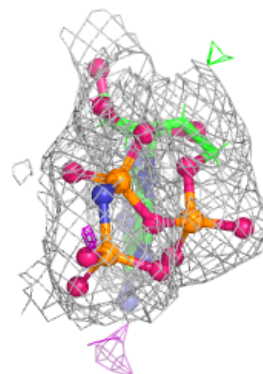
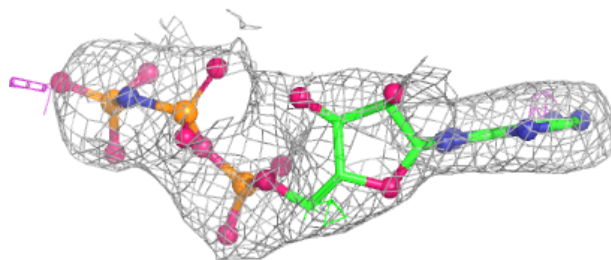
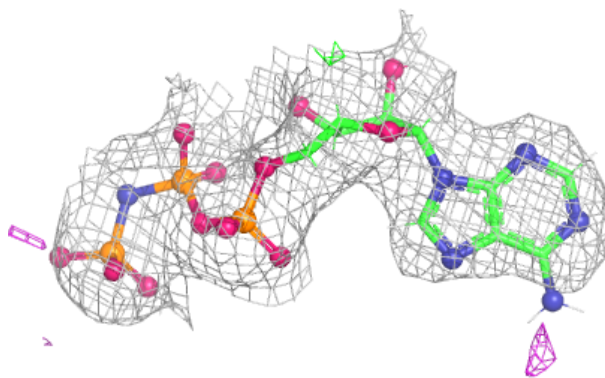
**Electron density around ANP B 1102:**

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



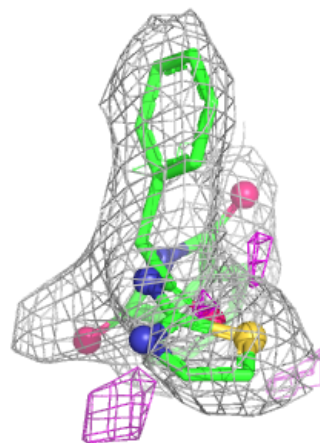
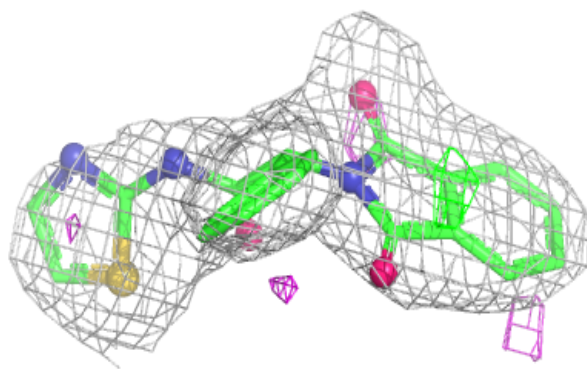
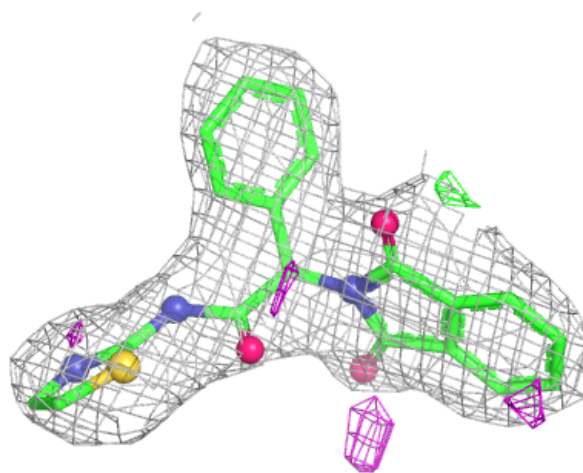
Electron density around ANP C 1102:

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



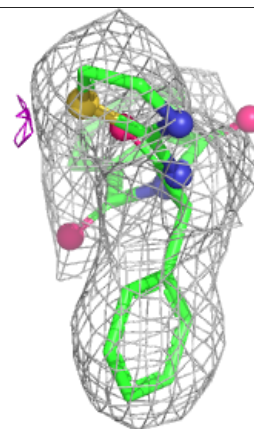
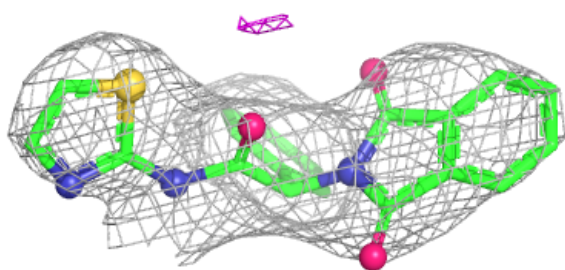
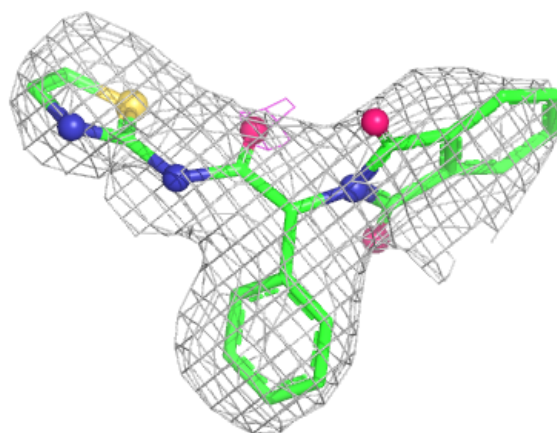
Electron density around IXR D 1103:

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

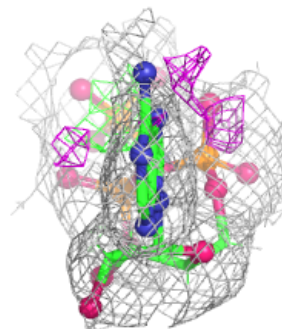
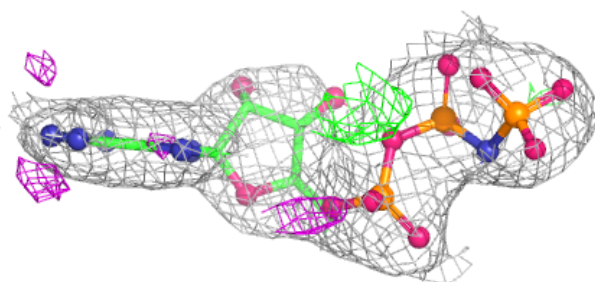
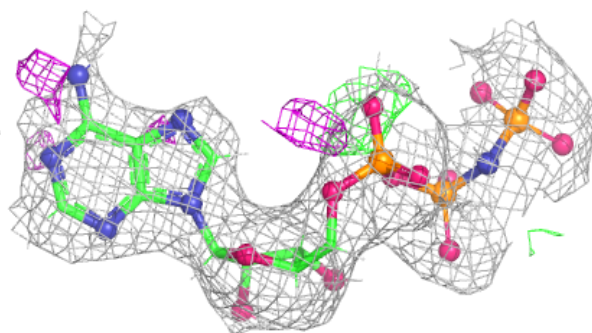


Electron density around IXR C 1103:

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

**Electron density around ANP D 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.