



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:23 AM UTC

PDB ID : 3FUP / pdb_00003fup
Title : Crystal structures of JAK1 and JAK2 inhibitor complexes
Authors : Williams, N.K.; Bamert, R.S.; Patel, O.; Fantino, E.; Rossjohn, J.; Lucet, I.S.
Deposited on : 2009-01-14
Resolution : 2.40 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)
Xtrriage (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

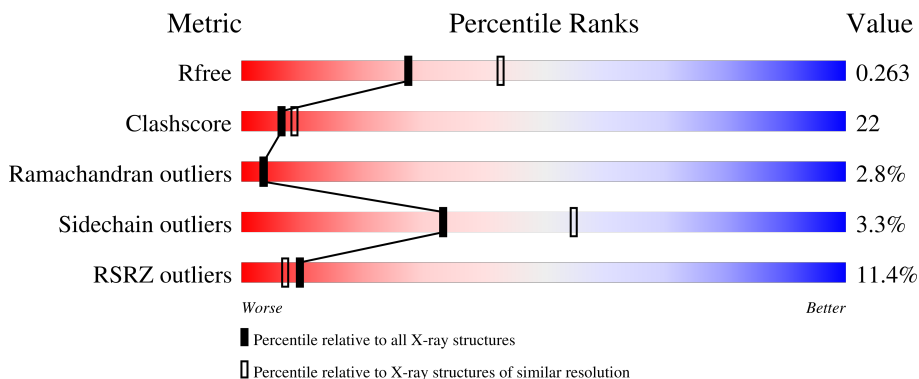
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	293	 9% 66% 27%
1	B	293	 13% 58% 32% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4938 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.

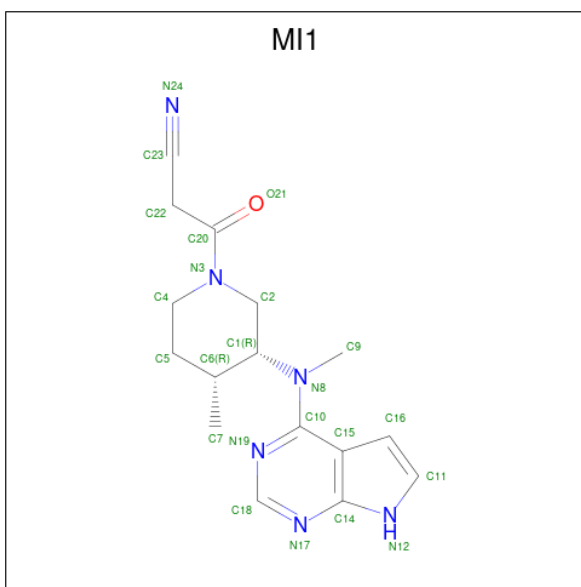
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	286	Total 2370	C 1504	N 407	O 443	P 2	S 14	0	0	0
1	B	289	Total 2387	C 1515	N 410	O 446	P 2	S 14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1129	GLN	ASN	engineered mutation	UNP O60674
B	1129	GLN	ASN	engineered mutation	UNP O60674

- Molecule 2 is 3-{(3R,4R)-4-methyl-3-[methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]piperidin-1-yl}-3-oxopropanenitrile (CCD ID: MI1) (formula: C₁₆H₂₀N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 23	C 16	N 6	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	23	16	6	1	0	0

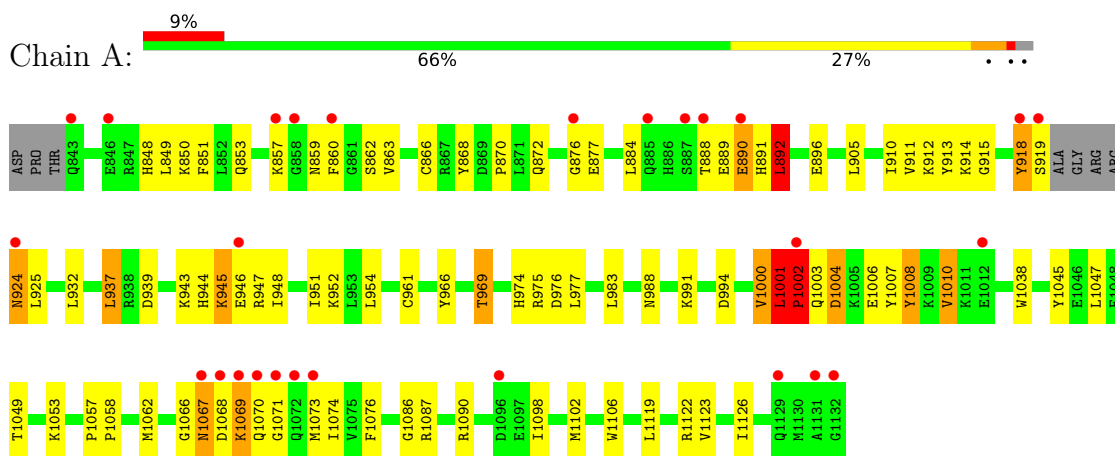
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	69	Total	O	0	0
			69	69		

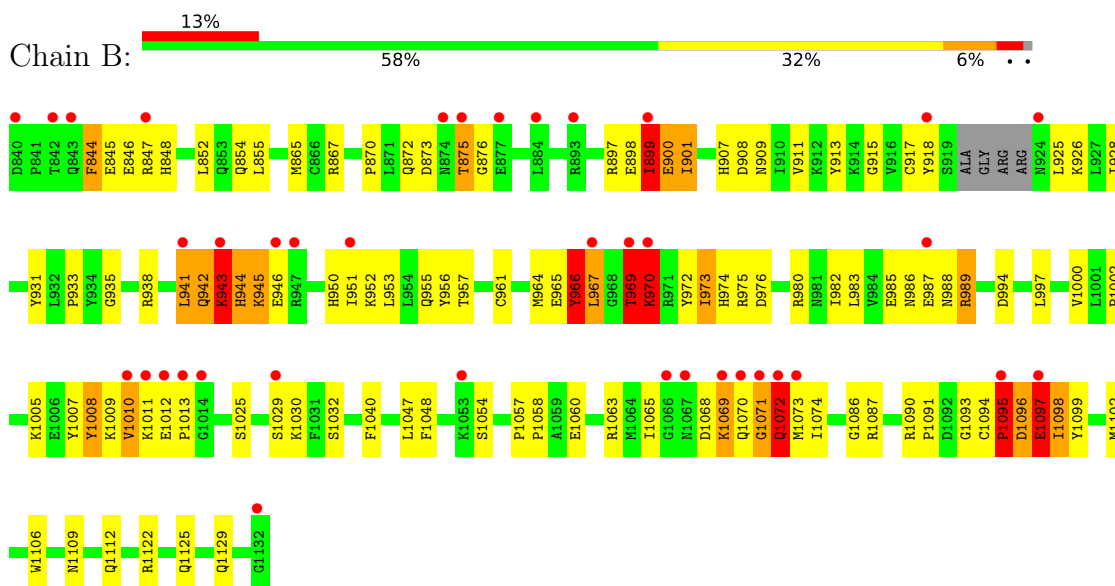
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Tyrosine-protein kinase JAK2



- Molecule 1: Tyrosine-protein kinase JAK2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	110.49Å 110.49Å 70.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.43 – 2.40 110.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (110.43-2.40) 94.4 (110.43-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.40Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.250 0.215 , 0.263	Depositor DCC
R_{free} test set	1601 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4938	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: PTR, MI1

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	0.90	0/2386	1.07	4/3208 (0.1%)
1	B	0.78	2/2404 (0.1%)	0.88	1/3234 (0.0%)
All	All	0.84	2/4790 (0.0%)	0.98	5/6442 (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	6
1	B	0	16
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	989	ARG	C-N	-5.50	1.25	1.33
1	B	911	VAL	CA-CB	5.33	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	924	ASN	O-C-N	-9.00	108.60	123.00
1	A	924	ASN	CA-C-N	7.84	132.72	121.50
1	A	924	ASN	C-N-CA	7.84	132.72	121.50
1	A	961	CYS	N-CA-C	5.60	117.39	111.28
1	B	989	ARG	O-C-N	-5.31	116.88	123.36

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	VAL	Peptide
1	A	1001	LEU	Peptide
1	A	1002	PRO	Peptide
1	A	892	LEU	Peptide
1	A	918	TYR	Peptide
1	A	945	LYS	Peptide
1	B	1010	VAL	Peptide
1	B	1071	GLY	Peptide
1	B	1072	GLN	Peptide
1	B	1095	PRO	Peptide
1	B	1096	ASP	Peptide
1	B	1097	GLU	Peptide
1	B	844	PHE	Peptide
1	B	899	ILE	Peptide
1	B	900	GLU	Peptide
1	B	941	LEU	Peptide
1	B	942	GLN	Peptide
1	B	943	LYS	Peptide
1	B	966	TYR	Peptide
1	B	967	LEU	Peptide
1	B	969	THR	Peptide
1	B	970	LYS	Peptide

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	2370	0	2334	72	2
1	B	2387	0	2345	127	1
2	A	23	0	18	7	0
2	B	23	0	20	5	0
3	A	66	0	0	3	0
3	B	69	0	0	8	0
All	All	4938	0	4717	206	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (206) 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:944:HIS:HA	1:A:946:GLU:OE1	1.39	1.18
1:B:867:ARG:NH1	1:B:876:GLY:O	1.86	1.09
1:A:919:SER:C	1:A:924:ASN:HB2	1.84	1.02
1:B:969:THR:O	1:B:969:THR:HG22	1.59	1.01
1:B:1071:GLY:O	1:B:1072:GLN:HG3	1.58	1.01
1:A:1002:PRO:HD3	1:A:1008:PTR:HD2	1.48	0.94
1:B:1071:GLY:HA3	1:B:1073:MET:H	1.35	0.92
1:A:944:HIS:C	1:A:946:GLU:HB2	1.97	0.89
1:B:1068:ASP:O	1:B:1070:GLN:HG3	1.73	0.89
1:B:942:GLN:O	1:B:942:GLN:HG2	1.71	0.87
1:B:1093:GLY:O	1:B:1095:PRO:HD3	1.75	0.85
1:A:892:LEU:C	1:A:892:LEU:HD23	2.01	0.84
1:B:1122:ARG:HD2	3:B:113:HOH:O	1.77	0.84
1:A:1008:PTR:HE1	1:A:1010:VAL:HB	1.60	0.83
1:B:969:THR:O	1:B:970:LYS:HB2	1.78	0.82
1:B:897:ARG:O	1:B:901:ILE:HG12	1.80	0.81
1:B:1012:GLU:CG	3:B:82:HOH:O	2.29	0.80
2:A:1:MI1:H1	2:A:1:MI1:H16	1.63	0.80
1:B:1012:GLU:HG2	3:B:82:HOH:O	1.81	0.80
1:B:942:GLN:O	1:B:942:GLN:CG	2.31	0.78
1:B:985:GLU:OE1	1:B:989:ARG:HD2	1.83	0.78
1:B:969:THR:O	1:B:969:THR:CG2	2.30	0.78
1:B:1010:VAL:HG12	1:B:1011:LYS:H	1.48	0.77
1:B:1102:MET:HE3	1:B:1106:TRP:CH2	2.19	0.77
1:B:873:ASP:OD1	1:B:875:THR:OG1	2.02	0.77
1:B:1071:GLY:C	1:B:1072:GLN:HG3	2.11	0.76
1:A:1062:MET:HB3	1:A:1067:ASN:OD1	1.86	0.75
1:A:974:HIS:O	1:A:975:ARG:HB2	1.86	0.74
1:A:945:LYS:N	1:A:946:GLU:HB2	2.03	0.74
1:A:943:LYS:HD2	3:A:73:HOH:O	1.90	0.72
1:B:967:LEU:HD23	1:B:967:LEU:O	1.90	0.72
2:A:1:MI1:H1	2:A:1:MI1:C16	2.16	0.71
1:B:973:ILE:HG23	1:B:1032:SER:O	1.89	0.71
1:B:1097:GLU:H	1:B:1099:TYR:H	1.38	0.71
1:A:939:ASP:HB3	1:A:943:LYS:NZ	2.06	0.71
1:A:892:LEU:HD23	1:A:892:LEU:O	1.91	0.70
1:B:974:HIS:O	1:B:975:ARG:HB2	1.91	0.70
1:B:1057:PRO:HB2	1:B:1058:PRO:HD3	1.74	0.70
1:A:888:THR:HB	1:A:891:HIS:HB2	1.74	0.69
1:A:913:TYR:CZ	1:A:915:GLY:HA2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MI1:H1	2:B:1:MI1:H16	1.76	0.67
1:B:1008:PTR:HE1	1:B:1008:PTR:O3P	1.94	0.67
1:B:1010:VAL:CG1	1:B:1011:LYS:H	2.07	0.67
1:B:1095:PRO:HB2	1:B:1098:ILE:HG12	1.75	0.66
1:B:972:TYR:CE1	1:B:1000:VAL:HG22	2.31	0.66
1:A:966:TYR:O	1:A:969:THR:HB	1.96	0.65
1:A:1086:GLY:O	1:A:1087:ARG:HG3	1.97	0.65
1:B:973:ILE:HD12	1:B:1032:SER:C	2.22	0.65
1:B:1010:VAL:HG12	1:B:1011:LYS:N	2.08	0.65
1:A:892:LEU:O	1:A:896:GLU:HG3	1.97	0.64
1:B:965:GLU:O	1:B:967:LEU:N	2.31	0.64
1:B:899:ILE:CD1	1:B:925:LEU:HD21	2.29	0.63
1:B:1096:ASP:O	1:B:1096:ASP:CG	2.40	0.63
1:B:973:ILE:CG2	1:B:1032:SER:O	2.47	0.63
1:B:1012:GLU:HG3	3:B:82:HOH:O	1.95	0.63
1:B:898:GLU:O	1:B:900:GLU:N	2.30	0.62
1:A:918:TYR:HB3	1:A:919:SER:O	1.98	0.62
1:A:1045:TYR:HB2	1:A:1102:MET:HE3	1.81	0.62
1:B:899:ILE:O	1:B:899:ILE:CG2	2.48	0.62
1:B:1060:GLU:CD	1:B:1063:ARG:HH21	2.07	0.62
1:B:1068:ASP:O	1:B:1070:GLN:N	2.32	0.62
1:A:918:TYR:HB3	1:A:919:SER:C	2.25	0.62
1:B:845:GLU:HG2	1:B:848:HIS:CE1	2.35	0.61
1:B:1068:ASP:O	1:B:1069:LYS:C	2.43	0.61
1:A:952:LYS:HE2	1:A:988:ASN:OD1	2.01	0.61
1:B:944:HIS:C	1:B:946:GLU:H	2.09	0.60
1:A:1057:PRO:HB2	1:A:1058:PRO:HD3	1.83	0.60
1:B:1102:MET:HE3	1:B:1106:TRP:HH2	1.63	0.60
1:B:852:LEU:HB2	1:B:865:MET:O	2.02	0.60
1:A:868:TYR:O	1:A:876:GLY:HA3	2.02	0.60
1:A:944:HIS:O	1:A:948:ILE:HD12	2.00	0.60
2:A:1:MI1:C16	2:A:1:MI1:C1	2.79	0.60
1:B:967:LEU:HD23	1:B:967:LEU:C	2.27	0.60
1:B:1086:GLY:O	1:B:1087:ARG:HD3	2.01	0.60
1:A:892:LEU:C	1:A:892:LEU:CD2	2.73	0.59
2:B:1:MI1:H1	2:B:1:MI1:C16	2.32	0.59
1:B:943:LYS:H	1:B:945:LYS:H	1.48	0.59
1:B:974:HIS:HD2	1:B:976:ASP:H	1.50	0.59
1:B:913:TYR:CZ	1:B:915:GLY:HA2	2.38	0.59
1:B:983:LEU:HD21	2:B:1:MI1:H6	1.85	0.58
1:B:1125:GLN:O	1:B:1129:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:VAL:CG1	1:B:1011:LYS:N	2.66	0.57
1:B:1109:ASN:HD22	1:B:1112:GLN:HE21	1.52	0.57
1:B:950:HIS:C	1:B:952:LYS:H	2.12	0.57
2:A:1:MI1:H16	2:A:1:MI1:C1	2.35	0.56
1:B:845:GLU:O	1:B:846:GLU:C	2.47	0.56
1:B:845:GLU:O	1:B:847:ARG:N	2.38	0.56
1:B:1098:ILE:N	1:B:1098:ILE:HD13	2.19	0.56
1:B:941:LEU:HD21	1:B:1047:LEU:HA	1.86	0.56
1:B:908:ASP:HB3	1:B:989:ARG:NH1	2.19	0.56
1:B:965:GLU:C	1:B:967:LEU:H	2.13	0.55
1:A:1004:ASP:N	1:A:1004:ASP:OD1	2.36	0.55
1:B:938:ARG:HD3	1:B:980:ARG:HB3	1.89	0.55
1:A:937:LEU:HD13	1:A:1047:LEU:HD21	1.89	0.54
2:A:1:MI1:C16	2:A:1:MI1:H6	2.38	0.54
1:B:950:HIS:CE1	1:B:1095:PRO:HD3	2.42	0.54
1:A:939:ASP:HB3	1:A:943:LYS:HZ1	1.72	0.54
1:A:1069:LYS:O	1:A:1070:GLN:NE2	2.40	0.53
1:A:954:LEU:HD21	1:A:1098:ILE:HD12	1.90	0.53
1:B:1068:ASP:OD1	1:B:1069:LYS:N	2.41	0.53
1:B:1090:ARG:HG2	1:B:1094:CYS:HB3	1.91	0.53
1:A:932:LEU:HD11	1:A:991:LYS:HD2	1.90	0.53
1:B:967:LEU:CD2	1:B:972:TYR:HB2	2.38	0.53
1:A:1066:GLY:C	1:A:1068:ASP:H	2.17	0.52
1:B:898:GLU:C	1:B:900:GLU:N	2.66	0.52
1:B:1068:ASP:O	1:B:1070:GLN:CG	2.53	0.52
1:A:1001:LEU:C	1:A:1002:PRO:O	2.52	0.52
1:B:966:TYR:O	1:B:966:TYR:CG	2.63	0.51
1:A:1102:MET:HE3	1:A:1106:TRP:CH2	2.46	0.51
1:B:974:HIS:HE1	1:B:994:ASP:O	1.93	0.51
1:A:905:LEU:HD13	1:A:910:ILE:HD13	1.93	0.51
1:A:944:HIS:HA	1:A:946:GLU:CD	2.28	0.51
1:A:863:VAL:CG2	2:A:1:MI1:O21	2.59	0.51
1:A:1102:MET:HE3	1:A:1106:TRP:HH2	1.75	0.50
1:B:844:PHE:CD2	1:B:928:ILE:HG13	2.46	0.50
1:B:965:GLU:C	1:B:967:LEU:N	2.67	0.50
1:B:852:LEU:HD12	1:B:865:MET:HG2	1.94	0.50
1:A:848:HIS:CG	1:A:870:PRO:HA	2.47	0.50
1:B:974:HIS:O	1:B:975:ARG:CB	2.60	0.50
1:B:941:LEU:HD11	1:B:953:LEU:HD21	1.93	0.49
1:B:1099:TYR:CD1	1:B:1102:MET:HE2	2.48	0.49
1:B:972:TYR:HE1	1:B:1000:VAL:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:PHE:CE2	1:B:1098:ILE:HG21	2.47	0.49
1:A:945:LYS:N	1:A:946:GLU:CB	2.74	0.49
1:B:899:ILE:HD12	1:B:925:LEU:HD21	1.94	0.48
1:A:1053:LYS:HB2	3:A:108:HOH:O	2.12	0.48
1:B:854:GLN:HG3	1:B:855:LEU:N	2.28	0.48
1:B:961:CYS:SG	1:B:1040:PHE:CZ	3.07	0.48
1:A:877:GLU:OE2	1:A:914:LYS:HE3	2.13	0.48
1:B:846:GLU:OE1	1:B:926:LYS:NZ	2.47	0.48
1:A:860:PHE:O	1:A:884:LEU:HD23	2.14	0.48
1:A:850:LYS:O	1:A:866:CYS:HA	2.14	0.47
1:B:1002:PRO:HG2	1:B:1005:LYS:HB2	1.96	0.47
1:A:974:HIS:HD2	1:A:976:ASP:H	1.62	0.47
1:B:944:HIS:C	1:B:946:GLU:N	2.66	0.47
1:B:974:HIS:CE1	1:B:994:ASP:O	2.67	0.47
1:A:888:THR:HG22	1:A:890:GLU:H	1.80	0.47
1:B:975:ARG:HD3	1:B:997:LEU:O	2.14	0.47
1:A:1008:PTR:O2P	1:A:1008:PTR:HE2	2.13	0.46
1:A:974:HIS:HE1	1:A:994:ASP:O	1.98	0.46
1:A:1122:ARG:O	1:A:1126:ILE:HG13	2.15	0.46
1:A:1071:GLY:HA2	1:A:1074:ILE:HD12	1.97	0.46
1:B:898:GLU:C	1:B:900:GLU:H	2.21	0.46
1:B:907:HIS:HE1	1:B:909:ASN:HD22	1.62	0.46
1:B:1008:PTR:O3P	1:B:1008:PTR:CE1	2.64	0.45
1:A:1003:GLN:O	1:A:1003:GLN:HG2	2.16	0.45
1:A:1090:ARG:HH22	1:B:1122:ARG:NH1	2.14	0.45
1:B:1091:PRO:HB2	1:B:1094:CYS:HB2	1.97	0.45
1:B:952:LYS:NZ	1:B:988:ASN:OD1	2.49	0.45
2:B:1:MI1:C16	2:B:1:MI1:C1	2.94	0.45
1:A:1073:MET:HE3	1:A:1076:PHE:CD2	2.52	0.45
1:A:1008:PTR:CD1	1:A:1008:PTR:C	2.94	0.45
1:B:967:LEU:HD23	1:B:972:TYR:HB2	1.99	0.45
1:B:899:ILE:O	1:B:899:ILE:HG22	2.16	0.45
1:A:888:THR:HG22	1:A:889:GLU:N	2.31	0.45
1:A:857:LYS:HG2	1:A:862:SER:HB2	1.99	0.45
1:B:1093:GLY:O	1:B:1095:PRO:CD	2.55	0.45
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.52	0.44
1:B:964:MET:O	1:B:967:LEU:HB3	2.17	0.44
1:B:986:ASN:O	1:B:987:GLU:C	2.61	0.44
1:A:919:SER:HB3	1:A:924:ASN:HA	1.99	0.44
1:B:956:TYR:O	1:B:957:THR:C	2.61	0.44
1:A:983:LEU:HD13	2:A:1:MI1:H7A	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:GLY:C	1:A:1068:ASP:N	2.75	0.43
1:B:1070:GLN:O	1:B:1071:GLY:C	2.61	0.43
1:A:974:HIS:CE1	1:A:994:ASP:O	2.71	0.43
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.18	0.43
1:B:1065:ILE:HG22	1:B:1065:ILE:O	2.19	0.43
1:B:848:HIS:HD2	1:B:872:GLN:NE2	2.17	0.43
1:B:941:LEU:CD2	1:B:1047:LEU:HA	2.49	0.43
1:B:950:HIS:C	1:B:952:LYS:N	2.71	0.43
1:B:955:GLN:NE2	3:B:107:HOH:O	2.51	0.43
1:A:849:LEU:HD12	1:A:849:LEU:HA	1.86	0.43
1:A:1119:LEU:O	1:A:1123:VAL:HG23	2.19	0.43
1:B:1071:GLY:CA	1:B:1073:MET:H	2.19	0.42
1:A:851:PHE:CZ	1:A:853:GLN:HA	2.54	0.42
1:B:1099:TYR:CD1	1:B:1102:MET:CE	3.02	0.42
1:B:1025:SER:HA	1:B:1030:LYS:H	1.84	0.42
1:B:918:TYR:CE1	1:B:925:LEU:HD13	2.54	0.42
1:B:1090:ARG:CG	1:B:1094:CYS:HB3	2.50	0.42
1:A:911:VAL:HG22	1:A:912:LYS:H	1.85	0.42
1:B:950:HIS:O	1:B:952:LYS:N	2.53	0.42
1:B:972:TYR:CD1	1:B:1000:VAL:HG22	2.54	0.42
1:B:846:GLU:CD	1:B:926:LYS:NZ	2.78	0.42
1:A:913:TYR:CZ	1:A:915:GLY:CA	3.02	0.42
1:B:1094:CYS:HA	1:B:1095:PRO:HD2	1.88	0.41
1:A:943:LYS:O	1:A:946:GLU:CD	2.63	0.41
1:B:974:HIS:CD2	1:B:976:ASP:C	2.98	0.41
1:B:899:ILE:O	1:B:899:ILE:HG23	2.20	0.41
1:B:935:GLY:HA2	3:B:16:HOH:O	2.21	0.41
1:B:848:HIS:CD2	1:B:870:PRO:HA	2.56	0.41
1:A:913:TYR:OH	1:A:915:GLY:HA2	2.20	0.41
1:B:917:CYS:SG	1:B:926:LYS:HE3	2.61	0.41
1:B:951:ILE:HG22	3:B:2:HOH:O	2.21	0.41
1:B:966:TYR:O	1:B:966:TYR:CD1	2.74	0.41
1:B:983:LEU:HD21	2:B:1:MI1:C6	2.51	0.41
1:B:1009:LYS:HA	1:B:1029:SER:O	2.21	0.41
1:B:1032:SER:HB2	3:B:13:HOH:O	2.20	0.41
1:A:1006:GLU:OE1	3:A:59:HOH:O	2.22	0.41
1:B:970:LYS:O	1:B:972:TYR:N	2.54	0.41
1:B:1057:PRO:CB	1:B:1058:PRO:HD3	2.47	0.41
1:A:977:LEU:HD23	1:A:977:LEU:HA	1.90	0.40
1:A:1001:LEU:HA	1:A:1002:PRO:HD2	1.14	0.40
1:B:931:TYR:CZ	1:B:933:PRO:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:LYS:O	1:B:1074:ILE:CG1	2.69	0.40
1:B:1099:TYR:HD1	1:B:1102:MET:CE	2.34	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:NH2	1:B:989:ARG:NH2[4_454]	1.66	0.54
1:A:872:GLN:O	1:A:1073:MET:SD[2_454]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/293 (96%)	263 (94%)	12 (4%)	5 (2%)	6	9
1	B	283/293 (97%)	251 (89%)	21 (7%)	11 (4%)	2	2
All	All	563/586 (96%)	514 (91%)	33 (6%)	16 (3%)	4	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1002	PRO
1	A	1069	LYS
1	B	901	ILE
1	B	943	LYS
1	B	970	LYS
1	B	1013	PRO
1	B	1069	LYS
1	B	945	LYS
1	B	1097	GLU
1	B	899	ILE

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Mol	Chain	Res	Type
1	B	966	TYR
1	B	1072	GLN
1	B	1095	PRO
1	A	1067	ASN
1	A	859	ASN
1	A	1001	LEU

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	259/265 (98%)	250 (96%)	9 (4%)	32	53
1	B	260/265 (98%)	252 (97%)	8 (3%)	35	57
All	All	519/530 (98%)	502 (97%)	17 (3%)	33	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	890	GLU
1	A	892	LEU
1	A	925	LEU
1	A	937	LEU
1	A	951	ILE
1	A	969	THR
1	A	1000	VAL
1	A	1004	ASP
1	A	1010	VAL
1	B	875	THR
1	B	899	ILE
1	B	944	HIS
1	B	969	THR
1	B	973	ILE
1	B	982	ILE
1	B	1054	SER
1	B	1098	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	848	HIS
1	A	885	GLN
1	A	909	ASN
1	A	942	GLN
1	A	955	GLN
1	A	974	HIS
1	A	1070	GLN
1	B	843	GLN
1	B	848	HIS
1	B	909	ASN
1	B	944	HIS
1	B	955	GLN
1	B	974	HIS
1	B	1067	ASN
1	B	1085	ASN
1	B	1112	GLN
1	B	1129	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](#)

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	A	1007	1	15,16,17	2.01	1 (6%)	17,22,24	0.61	0
1	PTR	B	1008	1	15,16,17	2.02	1 (6%)	17,22,24	0.61	0
1	PTR	B	1007	1	15,16,17	2.02	1 (6%)	17,22,24	0.60	0
1	PTR	A	1008	1	15,16,17	2.03	1 (6%)	17,22,24	0.60	0

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
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	2/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	PTR	OH-CZ	-7.67	1.23	1.40
1	B	1007	PTR	OH-CZ	-7.66	1.23	1.40
1	B	1008	PTR	OH-CZ	-7.62	1.23	1.40
1	A	1007	PTR	OH-CZ	-7.61	1.23	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1008	PTR	N-CA-CB-CG
1	B	1008	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1008	PTR	2	0
1	A	1008	PTR	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	MI1	A	1	-	23,25,25	2.57	4 (17%)	25,35,35	3.47	15 (60%)
2	MI1	B	1	-	23,25,25	2.27	2 (8%)	25,35,35	3.72	16 (64%)

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	MI1	A	1	-	-	0/15/28/28	0/3/3/3
2	MI1	B	1	-	-	0/15/28/28	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	MI1	C22-C23	-9.97	1.27	1.45
2	B	1	MI1	C22-C23	-8.39	1.30	1.45
2	A	1	MI1	C15-C14	4.93	1.47	1.41
2	B	1	MI1	C15-C14	4.75	1.46	1.41
2	A	1	MI1	C20-N3	-2.69	1.30	1.35
2	A	1	MI1	C11-C16	2.30	1.40	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	MI1	C22-C23-N24	-9.11	153.04	177.87
2	B	1	MI1	C15-C14-N17	-8.94	119.41	126.40
2	A	1	MI1	C15-C14-N17	-8.14	120.03	126.40
2	A	1	MI1	C14-C15-C16	5.89	109.31	106.40
2	A	1	MI1	N19-C18-N17	-5.16	120.77	128.58
2	B	1	MI1	C4-N3-C2	4.90	122.52	113.07
2	A	1	MI1	C15-C14-N12	-4.88	105.56	108.33
2	A	1	MI1	C18-N19-C10	4.76	123.46	111.83
2	A	1	MI1	N12-C14-N17	4.73	134.36	126.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	MI1	N12-C14-N17	4.72	134.34	126.69
2	A	1	MI1	C15-C16-C11	-4.42	102.07	106.64
2	B	1	MI1	C18-N19-C10	4.07	121.77	111.83
2	A	1	MI1	C4-N3-C2	3.99	120.77	113.07
2	A	1	MI1	C22-C23-N24	-3.87	167.33	177.87
2	A	1	MI1	C14-N12-C11	3.80	110.31	108.11
2	B	1	MI1	N19-C18-N17	-3.72	122.95	128.58
2	B	1	MI1	C15-C14-N12	-3.65	106.25	108.33
2	B	1	MI1	C2-C1-N8	-3.48	108.07	116.01
2	B	1	MI1	C14-N12-C11	3.48	110.12	108.11
2	B	1	MI1	C14-C15-C16	3.44	108.10	106.40
2	B	1	MI1	C7-C6-C1	3.42	118.93	113.31
2	B	1	MI1	C15-C16-C11	-2.97	103.56	106.64
2	A	1	MI1	C2-C1-N8	-2.94	109.31	116.01
2	B	1	MI1	O21-C20-N3	-2.72	117.27	122.12
2	B	1	MI1	C15-C10-N19	-2.49	118.08	122.53
2	B	1	MI1	C2-N3-C20	-2.49	114.19	122.11
2	A	1	MI1	N19-C10-N8	2.32	119.52	116.82
2	B	1	MI1	C7-C6-C5	-2.28	106.81	111.06
2	A	1	MI1	C2-C1-C6	2.19	113.39	109.16
2	A	1	MI1	C15-C10-N19	-2.17	118.67	122.53
2	A	1	MI1	C16-C11-N12	2.15	112.73	110.25

There are no chirality outliers.

There are no torsion outliers.

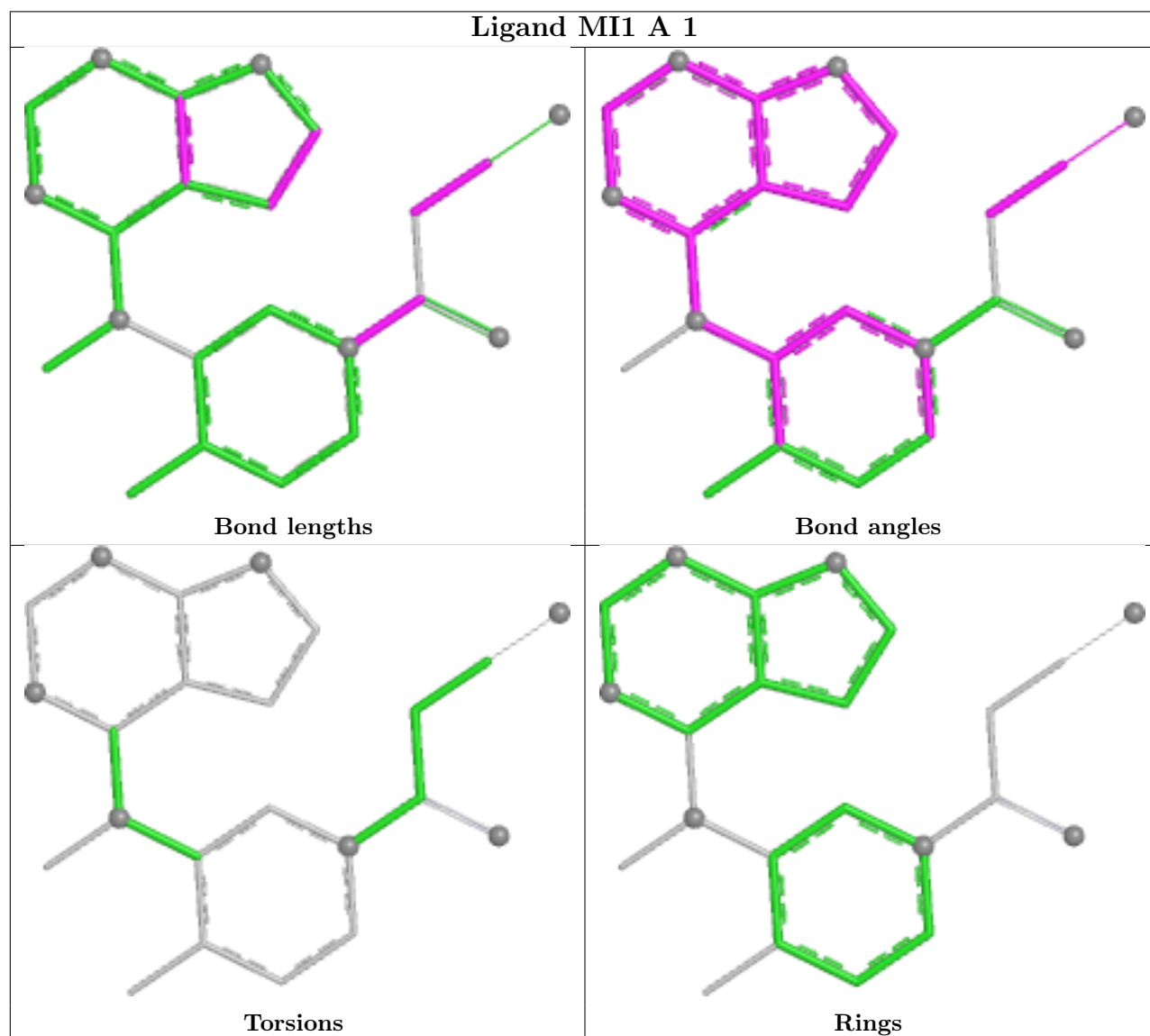
There are no ring outliers.

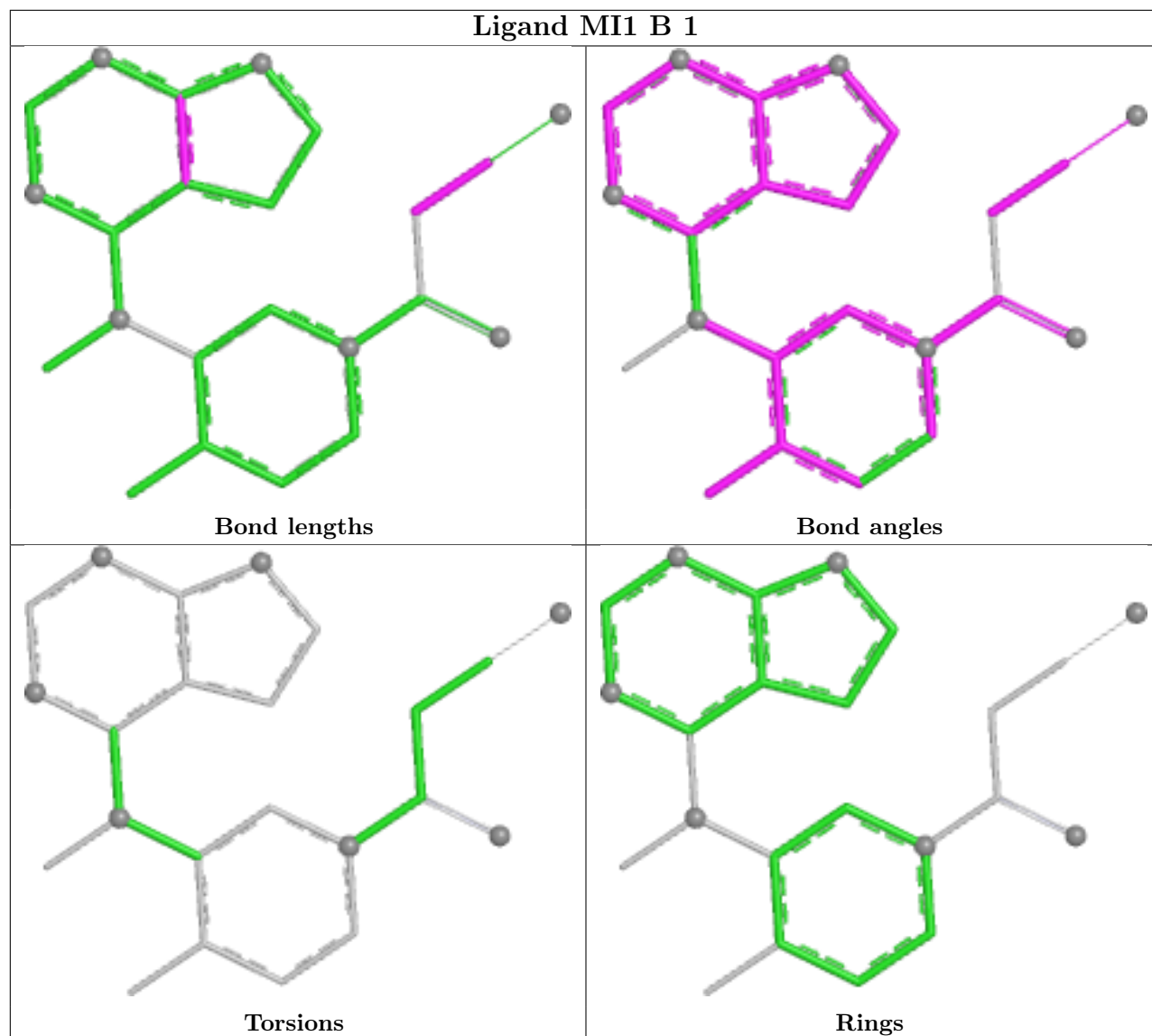
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MI1	7	0
2	B	1	MI1	5	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	284/293 (96%)	0.38	27 (9%) 14 11	24, 39, 73, 106	0
1	B	287/293 (97%)	0.70	38 (13%) 7 5	30, 41, 71, 116	0
All	All	571/586 (97%)	0.54	65 (11%) 10 7	24, 40, 72, 116	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	842	THR	5.3
1	A	919	SER	5.1
1	B	877	GLU	4.7
1	A	1131	ALA	4.3
1	A	1068	ASP	4.2
1	A	1069	LYS	4.2
1	A	1073	MET	3.9
1	A	860	PHE	3.9
1	B	1013	PRO	3.9
1	A	924	ASN	3.8
1	B	1066	GLY	3.8
1	B	941	LEU	3.8
1	A	1070	GLN	3.8
1	A	858	GLY	3.7
1	A	887	SER	3.6
1	B	918	TYR	3.5
1	B	1073	MET	3.5
1	B	1095	PRO	3.5
1	B	840	ASP	3.4
1	B	893	ARG	3.4
1	B	1067	ASN	3.4
1	A	1002	PRO	3.3
1	A	888	THR	3.3
1	B	1053	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	918	TYR	3.2
1	A	1067	ASN	3.2
1	B	1011	LYS	3.1
1	B	969	THR	3.1
1	B	1069	LYS	3.1
1	B	847	ARG	3.1
1	A	946	GLU	3.0
1	B	924	ASN	3.0
1	A	1072	GLN	2.9
1	A	1132	GLY	2.9
1	B	1132	GLY	2.9
1	B	1071	GLY	2.9
1	A	1071	GLY	2.8
1	B	1012	GLU	2.8
1	B	884	LEU	2.7
1	B	967	LEU	2.6
1	B	970	LYS	2.6
1	B	987	GLU	2.6
1	A	843	GLN	2.6
1	A	1129	GLN	2.6
1	A	1012	GLU	2.5
1	B	1070	GLN	2.5
1	B	899	ILE	2.4
1	A	885	GLN	2.4
1	B	1097	GLU	2.4
1	B	1010	VAL	2.3
1	B	1072	GLN	2.3
1	A	890	GLU	2.3
1	A	1096	ASP	2.2
1	B	874	ASN	2.2
1	B	951	ILE	2.2
1	B	1029	SER	2.2
1	B	943	LYS	2.1
1	A	876	GLY	2.1
1	B	947	ARG	2.1
1	B	1014	GLY	2.1
1	A	846	GLU	2.1
1	B	946	GLU	2.1
1	A	857	LYS	2.1
1	B	843	GLN	2.0
1	B	875	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	B	1007	16/17	0.89	0.12	43,58,77,82	0
1	PTR	B	1008	16/17	0.91	0.14	42,59,78,81	0
1	PTR	A	1008	16/17	0.92	0.12	28,56,67,67	0
1	PTR	A	1007	16/17	0.94	0.08	32,43,64,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

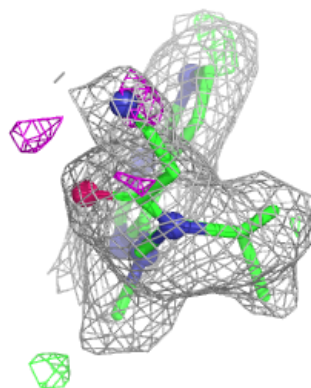
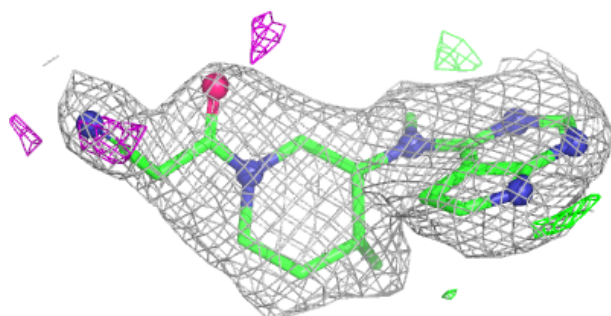
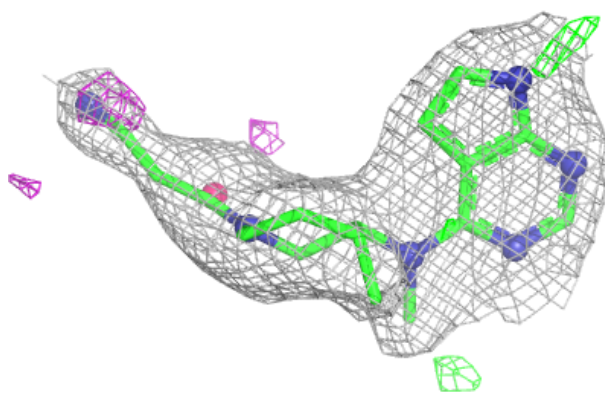
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MI1	A	1	23/23	0.91	0.11	26,40,44,50	0
2	MI1	B	1	23/23	0.92	0.12	28,35,48,55	0

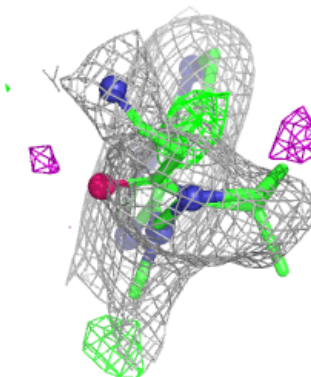
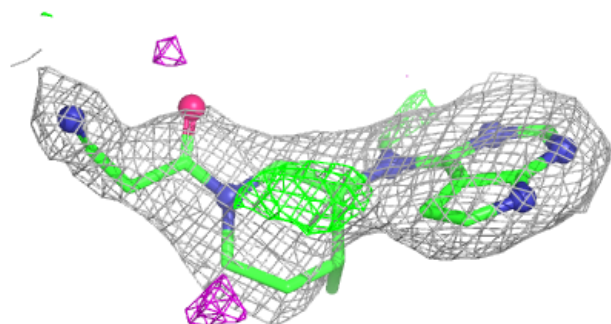
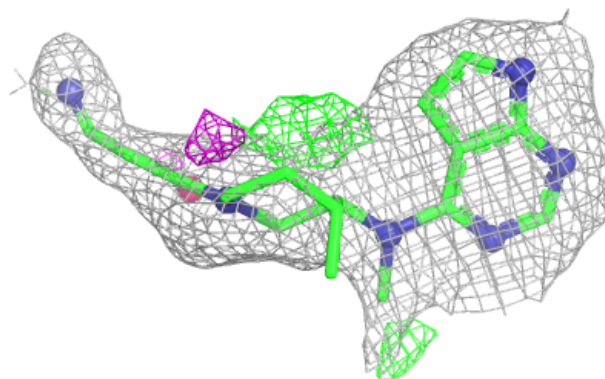
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MI1 A 1:

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

**Electron density around MI1 B 1:**

$2mF_o-DF_c$ (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.