



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:40 PM UTC

PDB ID : 3FCO / pdb_00003fco
Title : Crystal Structure of 11beta-Hydroxysteroid Dehydrogenase 1 (11b-HSD1) in Complex with Benzamide Inhibitor
Authors : Wang, Z.; Sudom, A.; Walker, N.P.
Deposited on : 2008-11-21
Resolution : 2.65 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

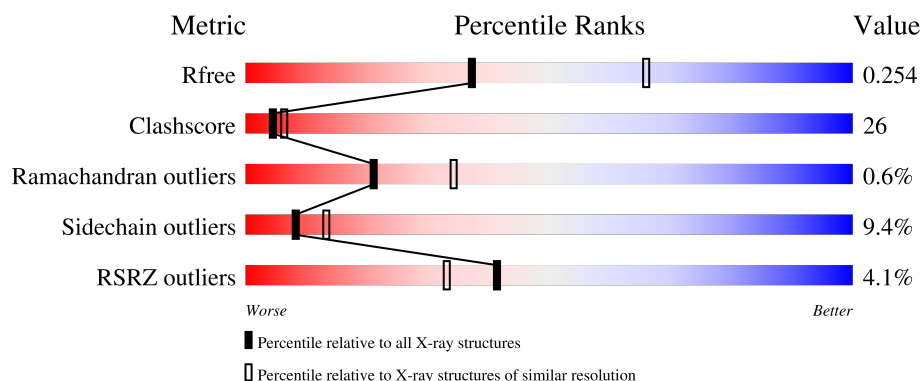
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	286	
1	B	286	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4328 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	10	0
			2060	1312	349	383	16			
1	B	266	Total	C	N	O	S	0	12	0
			2063	1315	348	384	16			

There are 36 discrepancies between the modelled and reference sequences:

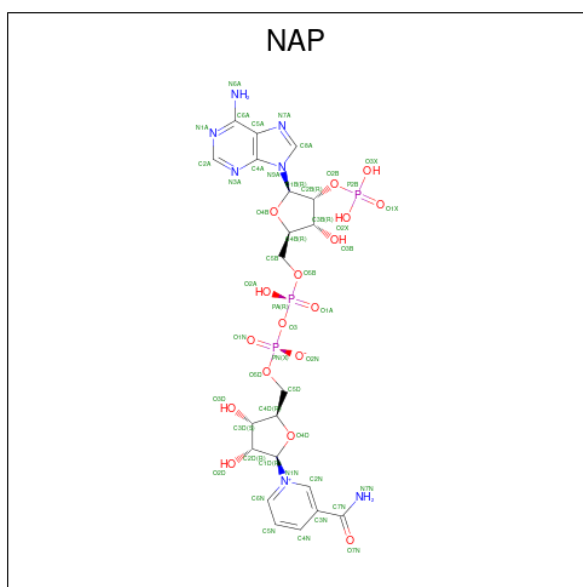
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845

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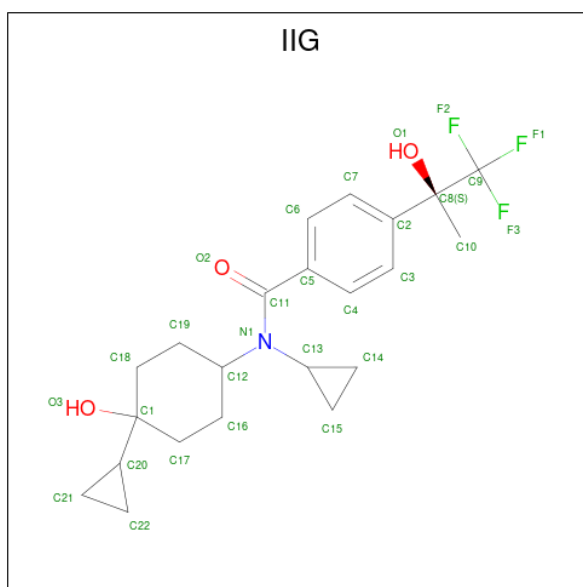
Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 is N-cyclopropyl-N-(cis-4-cyclopropyl-4-hydroxycyclohexyl)-4-[(1S)-2,2,2-trifluoro-1-hydroxy-1-methylethyl]benzamide (CCD ID: IIG) (formula: $C_{22}H_{28}F_3NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			29	22	3	1	3		
3	B	1	Total	C	F	N	O	0	0
			29	22	3	1	3		

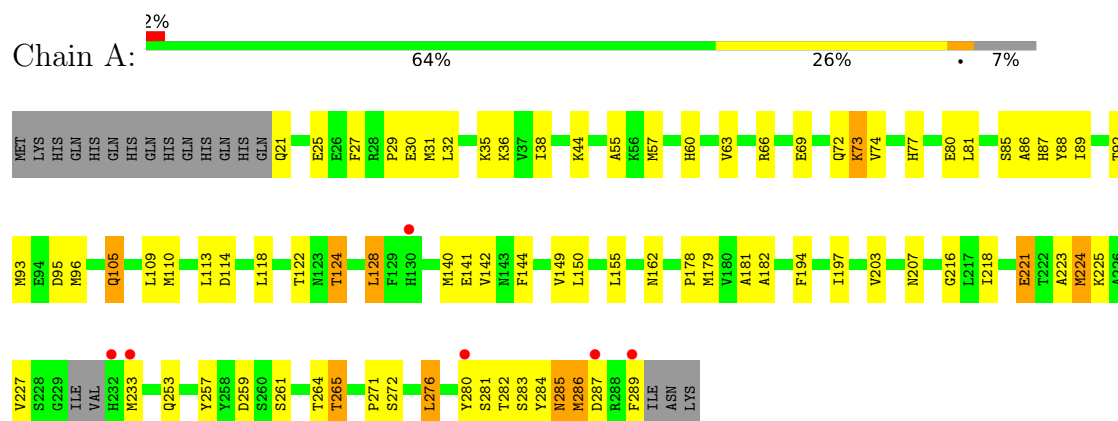
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	18	Total	O	0	0
			18	18		

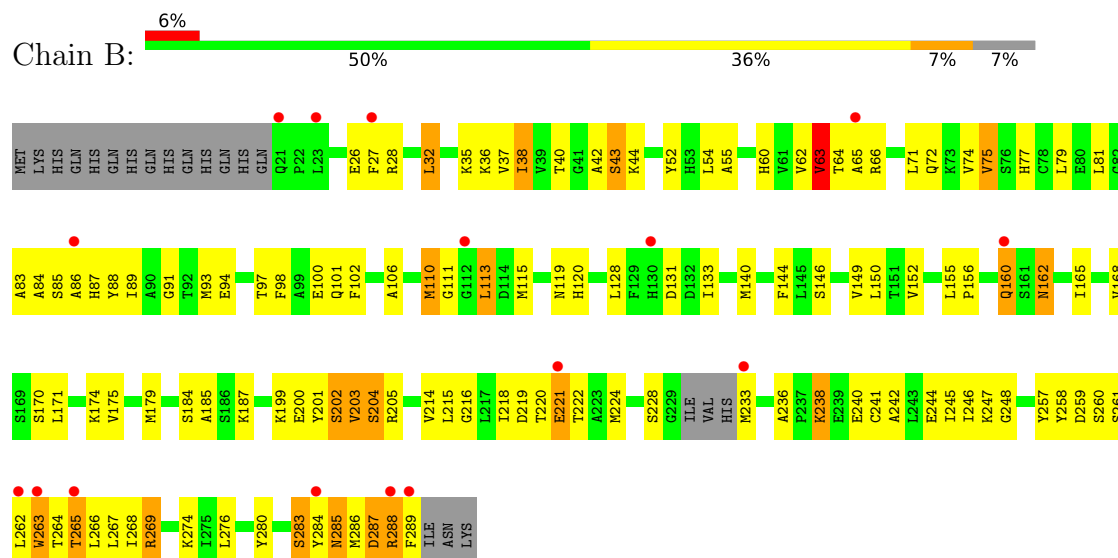
3 Residue-property plots [i](#)

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: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.19Å 109.19Å 135.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	94.49 – 2.65 94.49 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (94.49-2.65) 98.9 (94.49-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.254 0.219 , 0.254	Depositor DCC
R_{free} test set	1378 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4328	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: NAP, IIG

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	0.95	0/2098	1.25	10/2830 (0.4%)
1	B	0.95	2/2107 (0.1%)	1.22	9/2842 (0.3%)
All	All	0.95	2/4205 (0.0%)	1.23	19/5672 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	ILE	CA-CB	-5.56	1.47	1.54
1	B	63	VAL	CA-CB	-5.33	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLN	CA-C-N	8.88	128.83	120.03
1	A	21	GLN	C-N-CA	8.88	128.83	120.03
1	B	75	VAL	CB-CA-C	-7.52	102.25	111.88
1	B	89	ILE	N-CA-C	-6.98	98.12	108.45
1	A	155	LEU	CA-C-N	-6.81	111.50	119.05
1	A	155	LEU	C-N-CA	-6.81	111.50	119.05
1	B	38	ILE	CB-CA-C	-6.02	100.06	110.65
1	B	106	ALA	N-CA-C	-5.93	105.89	113.01
1	A	74	VAL	N-CA-C	5.80	115.99	110.42
1	A	285	ASN	N-CA-C	5.75	118.27	108.90
1	A	128	LEU	N-CA-C	-5.54	102.81	110.35
1	A	142	VAL	CB-CA-C	-5.38	105.03	112.24
1	B	152	VAL	CB-CA-C	-5.28	103.98	112.16
1	B	44	LYS	N-CA-C	5.20	115.25	108.07
1	A	93	MET	N-CA-C	-5.18	106.80	113.02
1	A	194	PHE	N-CA-C	5.11	118.29	111.75
1	B	285	ASN	N-CA-C	-5.06	103.66	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLU	N-CA-C	-5.05	106.38	112.54
1	B	201	TYR	N-CA-C	-5.02	106.00	111.82

There are no chirality outliers.

There are no planarity outliers.

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	2060	0	2077	80	0
1	B	2063	0	2083	147	0
2	A	48	0	25	1	0
2	B	48	0	25	4	0
3	A	29	0	28	2	0
3	B	29	0	28	4	0
4	A	33	0	0	0	0
4	B	18	0	0	1	0
All	All	4328	0	4266	226	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 26.

All (226) 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:128:LEU:HD21	1:B:179:MET:HE1	1.26	1.16
1:A:224:MET:HA	1:A:224:MET:HE2	1.27	1.11
1:B:263:TRP:HE3	1:B:263:TRP:N	1.49	1.09
1:B:286:MET:HE1	1:B:288:ARG:HH11	1.22	1.03
1:B:65:ALA:HB3	1:B:71:LEU:HD21	1.36	1.02
1:B:263:TRP:N	1:B:263:TRP:CE3	2.29	1.00
1:B:288:ARG:HH11	1:B:288:ARG:HG2	1.28	0.97
1:B:286:MET:HE1	1:B:288:ARG:NH1	1.80	0.96
1:B:43:SER:HB3	1:B:65:ALA:CB	1.97	0.95
1:B:128:LEU:CD2	1:B:179:MET:HE1	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:HE3	1:B:224:MET:HA	1.51	0.91
3:A:293:IIG:H21	1:B:280:TYR:OH	1.71	0.90
1:B:220:THR:HA	1:B:221[A]:GLU:OE2	1.72	0.90
1:A:77:HIS:CE1	1:A:81:LEU:HD11	2.06	0.88
1:A:285:ASN:ND2	1:A:287:ASP:H	1.72	0.88
1:B:203:VAL:O	1:B:203:VAL:HG23	1.75	0.87
1:B:220:THR:O	1:B:224:MET:HG2	1.75	0.87
1:A:162:ASN:HD22	1:A:207[A]:ASN:HB3	1.39	0.86
1:B:257:TYR:CD2	1:B:268:ILE:HG21	2.11	0.85
1:A:224:MET:HA	1:A:224:MET:CE	2.09	0.82
1:B:221[A]:GLU:CD	1:B:221[A]:GLU:H	1.86	0.81
1:B:288:ARG:HG2	1:B:288:ARG:NH1	1.89	0.80
1:B:262:LEU:C	1:B:263:TRP:HE3	1.89	0.79
1:A:261:SER:O	1:A:265:THR:HG23	1.82	0.79
1:B:62:VAL:HG12	1:B:62:VAL:O	1.81	0.79
1:A:162:ASN:ND2	1:A:207[A]:ASN:HB3	2.00	0.77
1:B:262:LEU:HB2	1:B:263:TRP:HZ3	1.48	0.77
1:A:221:GLU:CD	1:A:221:GLU:H	1.90	0.77
1:B:286:MET:HE3	1:B:286:MET:HA	1.68	0.76
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.69	0.74
1:A:286:MET:CE	1:A:289:PHE:CD1	2.70	0.74
1:B:63:VAL:HG13	1:B:64:THR:N	2.01	0.74
3:B:293:IIG:H19	3:B:293:IIG:H15A	1.69	0.73
1:B:40:THR:HA	1:B:64:THR:CG2	2.18	0.73
1:A:224:MET:HE2	1:A:224:MET:CA	2.13	0.73
1:B:242:ALA:O	1:B:246:ILE:HD12	1.87	0.72
1:B:63:VAL:CG1	1:B:64:THR:N	2.52	0.72
1:B:43:SER:HB3	1:B:65:ALA:HB1	1.68	0.72
1:A:128:LEU:HD23	1:A:179:MET:HE1	1.72	0.72
1:B:36:LYS:O	1:B:113:LEU:HD12	1.90	0.71
1:B:220:THR:CA	1:B:221[A]:GLU:OE2	2.39	0.71
1:A:29:PRO:HA	1:A:57:MET:HE2	1.73	0.70
1:A:286:MET:CE	1:A:289:PHE:HD1	2.03	0.70
1:B:288:ARG:HH11	1:B:288:ARG:CG	2.03	0.70
1:B:262:LEU:HB2	1:B:263:TRP:CZ3	2.25	0.70
1:B:119:ASN:ND2	2:B:1:NAP:H4D	2.07	0.69
1:B:37:VAL:HG21	1:B:54:LEU:HD22	1.73	0.69
1:B:100:GLU:HB2	4:B:308:HOH:O	1.93	0.69
1:B:37:VAL:HG12	1:B:38:ILE:N	2.07	0.69
1:A:286:MET:HE3	1:A:289:PHE:CD1	2.29	0.68
1:B:263:TRP:O	1:B:267:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:HZ	1:A:57:MET:CE	2.07	0.66
1:A:27:PHE:HZ	1:A:57:MET:HE1	1.59	0.66
3:B:293:IIG:H15A	3:B:293:IIG:C19	2.26	0.66
1:A:285:ASN:HD21	1:A:287:ASP:CB	2.08	0.66
1:B:128:LEU:CD2	1:B:179:MET:CE	2.71	0.66
1:A:122:THR:O	1:A:124[A]:THR:HG22	1.96	0.66
1:A:286:MET:HE3	1:A:289:PHE:HD1	1.62	0.65
1:A:223:ALA:O	1:A:227:VAL:HG22	1.97	0.64
1:A:285:ASN:HD21	1:A:287:ASP:HB2	1.61	0.64
1:B:40:THR:HA	1:B:64:THR:HG23	1.79	0.64
1:B:257:TYR:CD2	1:B:268:ILE:CG2	2.81	0.63
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.33	0.62
1:B:37:VAL:HG12	1:B:38:ILE:H	1.63	0.62
1:B:286:MET:HE3	1:B:286:MET:CA	2.30	0.62
1:A:128:LEU:CD2	1:A:179:MET:HE1	2.29	0.62
1:A:140:MET:HE1	1:A:144:PHE:CD2	2.35	0.62
1:B:288:ARG:O	1:B:289:PHE:CB	2.47	0.62
1:A:128:LEU:HD23	1:A:179:MET:CE	2.30	0.61
1:B:128:LEU:HD23	1:B:179:MET:SD	2.40	0.61
1:A:283:SER:O	1:A:284:TYR:CG	2.53	0.61
1:A:55:ALA:C	1:A:57:MET:H	2.09	0.60
1:B:88:TYR:CD1	1:B:88:TYR:C	2.78	0.60
1:A:276:LEU:O	1:A:280:TYR:HD1	1.83	0.59
1:A:77:HIS:ND1	1:A:81:LEU:HD11	2.17	0.59
1:A:140:MET:CE	1:A:144:PHE:CD2	2.87	0.58
1:B:65:ALA:CB	1:B:71:LEU:HD21	2.24	0.58
1:B:42:ALA:CB	1:B:63:VAL:HG22	2.34	0.58
1:B:146:SER:O	1:B:150:LEU:HG	2.04	0.58
1:A:96:MET:HE3	1:A:141:GLU:OE2	2.05	0.56
1:B:60:HIS:O	1:B:110:MET:SD	2.63	0.56
1:B:86:ALA:C	1:B:87:HIS:CD2	2.83	0.56
1:B:283:SER:OG	1:B:284[A]:TYR:CD2	2.59	0.56
1:A:27:PHE:CZ	1:A:57:MET:HE1	2.40	0.56
3:B:293:IIG:H19	3:B:293:IIG:C15	2.34	0.56
1:A:286:MET:HE2	1:A:289:PHE:CD1	2.41	0.56
1:A:69:GLU:OE2	1:A:69:GLU:N	2.34	0.55
1:B:42:ALA:HB3	1:B:63:VAL:HG13	1.89	0.55
1:A:286:MET:CE	1:A:289:PHE:CE1	2.91	0.54
1:B:286:MET:C	1:B:288:ARG:H	2.14	0.54
1:B:200:GLU:O	1:B:204[A]:SER:HB2	2.08	0.54
1:B:221[A]:GLU:HG2	1:B:222:THR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ARG:HD3	1:B:289:PHE:N	2.23	0.53
1:B:63:VAL:HG13	1:B:64:THR:H	1.73	0.53
1:A:88:TYR:CD1	1:A:88:TYR:C	2.87	0.53
1:B:97:THR:O	1:B:98:PHE:C	2.50	0.53
1:B:140:MET:HE3	1:B:144:PHE:HB3	1.90	0.53
1:A:55:ALA:C	1:A:57:MET:N	2.62	0.53
1:B:40:THR:HA	1:B:64:THR:HG22	1.91	0.53
1:A:261:SER:O	1:A:265:THR:CG2	2.57	0.52
1:B:244:GLU:O	1:B:245:ILE:C	2.51	0.52
1:B:286:MET:HA	1:B:286:MET:CE	2.30	0.52
1:A:276:LEU:HD21	1:B:267:LEU:HB3	1.92	0.52
1:A:36:LYS:NZ	1:A:110:MET:O	2.29	0.52
1:A:72:GLN:O	1:A:73:LYS:C	2.52	0.52
1:A:285:ASN:HD21	1:A:287:ASP:H	1.56	0.52
1:B:32:LEU:O	1:B:35:LYS:HB2	2.10	0.52
1:B:219:ASP:HA	1:B:224:MET:SD	2.50	0.52
1:A:224:MET:HE2	1:A:227:VAL:CG2	2.40	0.52
1:B:38:ILE:HG13	1:B:113:LEU:HD13	1.92	0.52
1:A:55:ALA:O	1:A:57:MET:N	2.42	0.52
1:B:162:ASN:N	1:B:162:ASN:HD22	2.08	0.52
1:A:27:PHE:CZ	1:A:57:MET:CE	2.93	0.51
1:A:60:HIS:ND1	1:A:85:SER:OG	2.42	0.51
1:A:36:LYS:HG3	1:A:114:ASP:OD2	2.09	0.51
1:A:224:MET:CE	1:A:224:MET:CA	2.82	0.51
3:B:293:IIG:C19	3:B:293:IIG:C15	2.89	0.51
1:B:91:GLY:HA3	1:B:98:PHE:CE2	2.45	0.50
1:A:63:VAL:O	1:A:88:TYR:HA	2.10	0.50
1:A:216:GLY:O	1:A:218:ILE:HG12	2.12	0.50
1:B:240:GLU:O	1:B:241:CYS:C	2.54	0.50
1:A:271:PRO:HD2	1:A:272:SER:H	1.77	0.49
1:A:95:ASP:OD1	1:A:95:ASP:C	2.55	0.49
1:B:60:HIS:CD2	1:B:84:ALA:HB3	2.47	0.49
1:B:171:LEU:HD23	1:B:214:VAL:HG12	1.95	0.49
1:B:155:LEU:HB3	1:B:156:PRO:CD	2.40	0.49
1:B:170:SER:O	1:B:171:LEU:C	2.55	0.49
1:B:259:ASP:OD1	1:B:261:SER:HB3	2.12	0.49
1:B:264:THR:OG1	1:B:265:THR:N	2.45	0.49
1:B:264:THR:C	1:B:266:LEU:N	2.70	0.49
1:B:128:LEU:HD23	1:B:179:MET:CE	2.42	0.48
1:B:101:GLN:O	1:B:102:PHE:C	2.56	0.48
1:B:263:TRP:O	1:B:267:LEU:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:HG3	1:B:258:TYR:CD2	2.49	0.48
1:B:265:THR:O	1:B:269:ARG:NH1	2.45	0.48
1:A:66:ARG:HB2	2:A:1:NAP:O2X	2.14	0.48
1:B:286:MET:C	1:B:288:ARG:N	2.72	0.48
1:B:60:HIS:CD2	1:B:84:ALA:CB	2.97	0.48
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.29	0.48
1:B:37:VAL:CG1	1:B:38:ILE:N	2.76	0.47
1:B:288:ARG:HD3	1:B:288:ARG:C	2.40	0.47
1:B:257:TYR:CE2	1:B:268:ILE:HG23	2.49	0.47
1:B:87:HIS:CD2	1:B:87:HIS:N	2.83	0.47
1:B:224:MET:HA	1:B:224:MET:CE	2.35	0.47
1:A:86:ALA:C	1:A:87:HIS:CD2	2.93	0.47
1:A:140:MET:CE	1:A:144:PHE:HD2	2.28	0.47
1:A:178:PRO:C	1:A:179:MET:HG2	2.40	0.47
1:B:52:TYR:O	1:B:55:ALA:HB3	2.14	0.47
1:B:262:LEU:N	1:B:263:TRP:CE3	2.83	0.47
1:A:286:MET:HG3	1:B:179:MET:HE3	1.97	0.47
1:A:257:TYR:CD1	1:A:257:TYR:N	2.82	0.47
1:B:236:ALA:HB2	1:B:260:SER:HB3	1.96	0.46
1:B:286:MET:CE	1:B:288:ARG:HH11	2.10	0.46
1:B:287:ASP:OD1	1:B:287:ASP:O	2.33	0.46
1:B:27:PHE:CD2	1:B:247:LYS:HG2	2.51	0.46
1:B:216:GLY:O	1:B:218:ILE:HG12	2.16	0.46
1:B:36:LYS:HB2	1:B:113:LEU:HA	1.97	0.45
1:A:181:ALA:O	1:A:182:ALA:C	2.58	0.45
1:A:233:MET:HB3	1:A:233:MET:HE2	1.71	0.45
1:B:27:PHE:CG	1:B:247:LYS:HG2	2.52	0.45
1:B:42:ALA:HB1	1:B:63:VAL:HG22	1.97	0.45
1:A:286:MET:HE2	1:A:289:PHE:HD1	1.73	0.45
1:A:140:MET:HE3	1:A:140:MET:HA	1.99	0.44
1:A:285:ASN:HD21	1:A:287:ASP:CG	2.25	0.44
1:B:257:TYR:CE2	1:B:268:ILE:CG2	3.01	0.44
1:A:88:TYR:C	1:A:89:ILE:HG13	2.42	0.44
1:A:221:GLU:OE1	1:A:221:GLU:N	2.40	0.44
1:B:37:VAL:HG21	1:B:54:LEU:CD2	2.44	0.44
1:B:269:ARG:HE	1:B:269:ARG:HB2	1.36	0.44
1:B:287:ASP:O	1:B:287:ASP:CG	2.60	0.44
1:A:118:LEU:HD22	1:A:150:LEU:HD13	1.99	0.44
1:B:149:VAL:O	1:B:150:LEU:C	2.60	0.44
1:B:264:THR:O	1:B:268:ILE:N	2.48	0.44
1:B:43:SER:HB3	1:B:65:ALA:HB3	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:HE2	1:B:179:MET:HG3	1.99	0.44
1:A:32:LEU:HA	1:A:35:LYS:HG3	2.00	0.43
1:A:149:VAL:HG22	1:B:133:ILE:HD13	2.00	0.43
3:A:293:IIG:C21	1:B:280:TYR:OH	2.56	0.43
1:B:36:LYS:NZ	1:B:111:GLY:O	2.49	0.43
1:A:140:MET:HE3	1:A:140:MET:CA	2.47	0.43
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.18	0.43
1:B:140:MET:HE3	1:B:140:MET:HA	1.99	0.43
1:A:178:PRO:O	1:A:179:MET:HB2	2.19	0.43
1:B:247:LYS:O	1:B:248:GLY:C	2.61	0.43
1:B:119:ASN:HD21	2:B:1:NAP:H4D	1.83	0.43
1:B:66:ARG:N	2:B:1:NAP:O2X	2.34	0.43
1:B:77:HIS:CD2	1:B:77:HIS:O	2.72	0.43
1:B:160:GLN:H	1:B:160:GLN:HE21	1.67	0.43
1:A:38:ILE:HG13	1:A:113:LEU:HD11	2.01	0.42
1:B:66:ARG:HB2	2:B:1:NAP:O2X	2.18	0.42
1:B:283:SER:OG	1:B:284[A]:TYR:CE2	2.72	0.42
1:A:280:TYR:HA	1:A:283:SER:HB3	2.00	0.42
1:B:93:MET:HG3	1:B:120:HIS:CE1	2.54	0.42
1:A:281:SER:OG	1:A:282:THR:N	2.52	0.42
1:B:262:LEU:CA	1:B:263:TRP:HE3	2.31	0.42
1:B:27:PHE:CD2	1:B:247:LYS:HD3	2.54	0.42
1:B:140:MET:CE	1:B:144:PHE:CD2	3.02	0.42
1:B:288:ARG:O	1:B:289:PHE:HB2	2.20	0.42
1:B:79:LEU:HD23	1:B:83:ALA:HB3	2.01	0.42
1:B:174:LYS:C	1:B:175:VAL:CG1	2.93	0.42
1:B:199:LYS:O	1:B:203:VAL:HG13	2.19	0.42
1:B:37:VAL:CG1	1:B:38:ILE:H	2.32	0.42
1:B:219:ASP:OD2	1:B:238:LYS:HD3	2.20	0.42
1:B:286:MET:O	1:B:288:ARG:HG3	2.19	0.42
1:B:288:ARG:O	1:B:289:PHE:HB3	2.17	0.41
1:B:32:LEU:HD13	1:B:32:LEU:HA	1.74	0.41
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.81	0.41
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.83	0.41
1:B:74:VAL:O	1:B:75:VAL:C	2.64	0.41
1:B:244:GLU:HG3	1:B:258:TYR:HD2	1.85	0.41
1:B:38:ILE:HG21	1:B:38:ILE:HD13	1.76	0.40
1:A:178:PRO:O	1:A:179:MET:CB	2.70	0.40
1:A:27:PHE:HZ	1:A:57:MET:HE2	1.84	0.40
1:B:170:SER:HA	1:B:215:LEU:H	1.86	0.40
1:A:264:THR:HA	1:B:276:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:ND2	1:A:287:ASP:OD1	2.54	0.40
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.68	0.40
1:A:89:ILE:HD13	1:A:105:GLN:HB3	2.04	0.40
1:B:168:VAL:O	1:B:187:LYS:NZ	2.55	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	264/286 (92%)	240 (91%)	23 (9%)	1 (0%)	30	45
1	B	265/286 (93%)	227 (86%)	36 (14%)	2 (1%)	16	27
All	All	529/572 (92%)	467 (88%)	59 (11%)	3 (1%)	21	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ASP
1	A	31	MET
1	B	131	ASP

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	225/243 (93%)	208 (92%)	17 (8%)	12	21
1	B	226/243 (93%)	200 (88%)	26 (12%)	5	8
All	All	451/486 (93%)	408 (90%)	43 (10%)	8	13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	30	GLU
1	A	44	LYS
1	A	73	LYS
1	A	92	THR
1	A	105	GLN
1	A	109	LEU
1	A	124[A]	THR
1	A	197	ILE
1	A	203	VAL
1	A	221	GLU
1	A	224	MET
1	A	225	LYS
1	A	253	GLN
1	A	265	THR
1	A	276	LEU
1	A	286	MET
1	B	26	GLU
1	B	28	ARG
1	B	32	LEU
1	B	43	SER
1	B	63	VAL
1	B	72	GLN
1	B	110	MET
1	B	113	LEU
1	B	115	MET
1	B	160	GLN
1	B	162	ASN
1	B	184[A]	SER
1	B	202	SER
1	B	203	VAL
1	B	204[A]	SER
1	B	221[A]	GLU
1	B	221[B]	GLU
1	B	228	SER

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Mol	Chain	Res	Type
1	B	233	MET
1	B	238	LYS
1	B	263	TRP
1	B	265	THR
1	B	269	ARG
1	B	274	LYS
1	B	283	SER
1	B	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	72	GLN
1	A	87	HIS
1	A	105	GLN
1	A	127	ASN
1	A	162	ASN
1	A	285	ASN
1	B	77	HIS
1	B	87	HIS
1	B	119	ASN
1	B	127	ASN
1	B	135	HIS
1	B	160	GLN
1	B	253	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	NAP	A	1	-	50,52,52	1.68	6 (12%)	71,80,80	1.86	18 (25%)
3	IIG	B	293	-	32,32,32	1.45	4 (12%)	47,51,51	4.89	17 (36%)
2	NAP	B	1	-	50,52,52	1.73	5 (10%)	71,80,80	1.84	12 (16%)
3	IIG	A	293	-	32,32,32	1.31	3 (9%)	47,51,51	5.12	22 (46%)

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	NAP	A	1	-	-	5/35/67/67	0/5/5/5
3	IIG	B	293	-	-	3/35/53/53	0/4/4/4
2	NAP	B	1	-	-	5/35/67/67	0/5/5/5
3	IIG	A	293	-	-	6/35/53/53	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAP	O7N-C7N	9.50	1.41	1.24
2	A	1	NAP	O7N-C7N	8.80	1.40	1.24
3	B	293	IIG	C12-N1	-3.63	1.43	1.48
3	A	293	IIG	C17-C1	3.48	1.57	1.53
2	B	1	NAP	C8A-N7A	3.45	1.38	1.31
3	B	293	IIG	O3-C1	-3.18	1.39	1.44
3	B	293	IIG	C17-C1	2.97	1.57	1.53
2	A	1	NAP	C2A-N1A	2.81	1.38	1.33
2	A	1	NAP	C8A-N7A	2.69	1.36	1.31
2	B	1	NAP	PA-O3	2.66	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	C2A-N3A	2.49	1.38	1.33
2	A	1	NAP	P2B-O2B	2.49	1.63	1.59
3	A	293	IIG	C14-C13	2.43	1.54	1.48
2	A	1	NAP	O4D-C4D	-2.30	1.39	1.45
3	A	293	IIG	C21-C20	2.27	1.55	1.50
2	B	1	NAP	PN-O3	2.14	1.61	1.59
2	B	1	NAP	O3D-C3D	-2.07	1.37	1.43
3	B	293	IIG	C14-C13	2.04	1.53	1.48

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	IIG	C18-C1-C17	-22.95	91.52	109.70
3	B	293	IIG	C18-C1-C17	-18.70	94.88	109.70
3	B	293	IIG	C17-C1-C20	-17.54	82.97	111.94
3	A	293	IIG	C17-C1-C20	-15.98	85.55	111.94
3	B	293	IIG	C18-C1-C20	8.40	125.81	111.94
3	B	293	IIG	O3-C1-C17	-7.88	91.34	108.20
3	B	293	IIG	F2-C9-C8	-7.81	101.36	112.40
2	B	1	NAP	N3A-C2A-N1A	-7.60	117.08	128.58
3	A	293	IIG	O3-C1-C20	7.49	119.62	108.81
3	A	293	IIG	O3-C1-C17	-6.92	93.40	108.20
3	B	293	IIG	C21-C20-C1	-6.89	112.26	122.01
3	B	293	IIG	C18-C19-C12	-6.67	101.74	110.99
3	A	293	IIG	F2-C9-C8	-6.66	102.99	112.40
3	A	293	IIG	C17-C16-C12	-6.50	101.96	110.99
3	B	293	IIG	O3-C1-C20	6.45	118.12	108.81
3	A	293	IIG	C18-C1-C20	6.19	122.15	111.94
2	A	1	NAP	N3A-C2A-N1A	-5.84	119.75	128.58
3	A	293	IIG	C18-C19-C12	-5.65	103.16	110.99
3	B	293	IIG	C22-C20-C1	-5.58	114.11	122.01
3	A	293	IIG	C16-C12-C19	-5.52	98.70	111.17
2	A	1	NAP	N9A-C8A-N7A	-4.81	107.11	113.94
3	A	293	IIG	C21-C20-C1	-4.69	115.37	122.01
3	A	293	IIG	O3-C1-C18	4.69	118.22	108.20
2	B	1	NAP	C5A-C4A-N3A	-4.61	120.37	126.72
3	A	293	IIG	C22-C20-C1	-4.52	115.62	122.01
2	B	1	NAP	C2A-N3A-C4A	4.31	122.35	111.83
2	A	1	NAP	C4D-O4D-C1D	-4.22	106.06	109.92
3	B	293	IIG	C16-C12-C19	-4.22	101.64	111.17
2	A	1	NAP	C5A-C4A-N3A	-4.14	121.01	126.72
2	B	1	NAP	N9A-C8A-N7A	-4.07	108.16	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAP	O4B-C1B-N9A	4.05	115.86	108.09
2	A	1	NAP	C3N-C7N-N7N	3.84	122.47	117.74
3	B	293	IIG	O3-C1-C18	3.67	116.05	108.20
2	A	1	NAP	C2A-N3A-C4A	3.47	120.31	111.83
2	B	1	NAP	O2N-PN-O1N	3.27	127.64	112.44
2	A	1	NAP	C5A-N7A-C8A	3.16	108.41	103.45
2	A	1	NAP	O2X-P2B-O2B	3.11	117.98	105.85
2	A	1	NAP	C4A-N9A-C8A	3.07	108.97	105.74
3	B	293	IIG	C17-C16-C12	-3.06	106.74	110.99
3	A	293	IIG	C3-C2-C8	-3.02	118.11	121.43
3	A	293	IIG	C3-C2-C7	2.97	122.46	118.03
2	B	1	NAP	O2B-P2B-O1X	-2.93	98.88	109.33
3	B	293	IIG	C16-C12-N1	-2.93	107.72	112.75
2	A	1	NAP	N3A-C4A-N9A	2.85	132.01	127.17
2	A	1	NAP	O2B-P2B-O1X	-2.84	99.20	109.33
3	A	293	IIG	C10-C8-C9	-2.83	105.28	109.04
3	A	293	IIG	C16-C12-N1	-2.82	107.90	112.75
2	B	1	NAP	C5A-N7A-C8A	2.79	107.83	103.45
2	B	1	NAP	C4D-O4D-C1D	-2.71	107.44	109.92
3	A	293	IIG	C16-C17-C1	2.67	116.29	112.32
3	A	293	IIG	O1-C8-C10	2.64	115.38	108.56
3	A	293	IIG	C19-C12-N1	2.58	117.19	112.75
2	B	1	NAP	N3A-C4A-N9A	2.58	131.56	127.17
3	A	293	IIG	C4-C3-C2	-2.57	117.61	121.17
3	A	293	IIG	C7-C6-C5	-2.40	118.23	120.80
2	A	1	NAP	O3X-P2B-O2X	-2.39	98.83	107.80
3	B	293	IIG	O1-C8-C9	2.36	109.54	105.94
2	A	1	NAP	O3X-P2B-O1X	2.33	119.93	110.83
2	A	1	NAP	O7N-C7N-C3N	-2.28	116.81	119.60
3	B	293	IIG	C3-C4-C5	-2.26	118.38	120.80
2	A	1	NAP	C2B-C1B-N9A	-2.21	110.12	113.75
2	B	1	NAP	C2B-C1B-N9A	-2.19	110.14	113.75
2	A	1	NAP	O2D-C2D-C3D	2.18	118.80	111.82
2	A	1	NAP	O2N-PN-O1N	2.11	122.26	112.44
3	B	293	IIG	O2-C11-C5	-2.10	116.12	120.29
2	B	1	NAP	C5A-C4A-N9A	2.07	108.07	105.81
2	A	1	NAP	O5B-C5B-C4B	-2.06	101.99	108.99
3	A	293	IIG	C6-C5-C4	2.04	121.16	118.57
3	B	293	IIG	C3-C2-C7	2.02	121.04	118.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

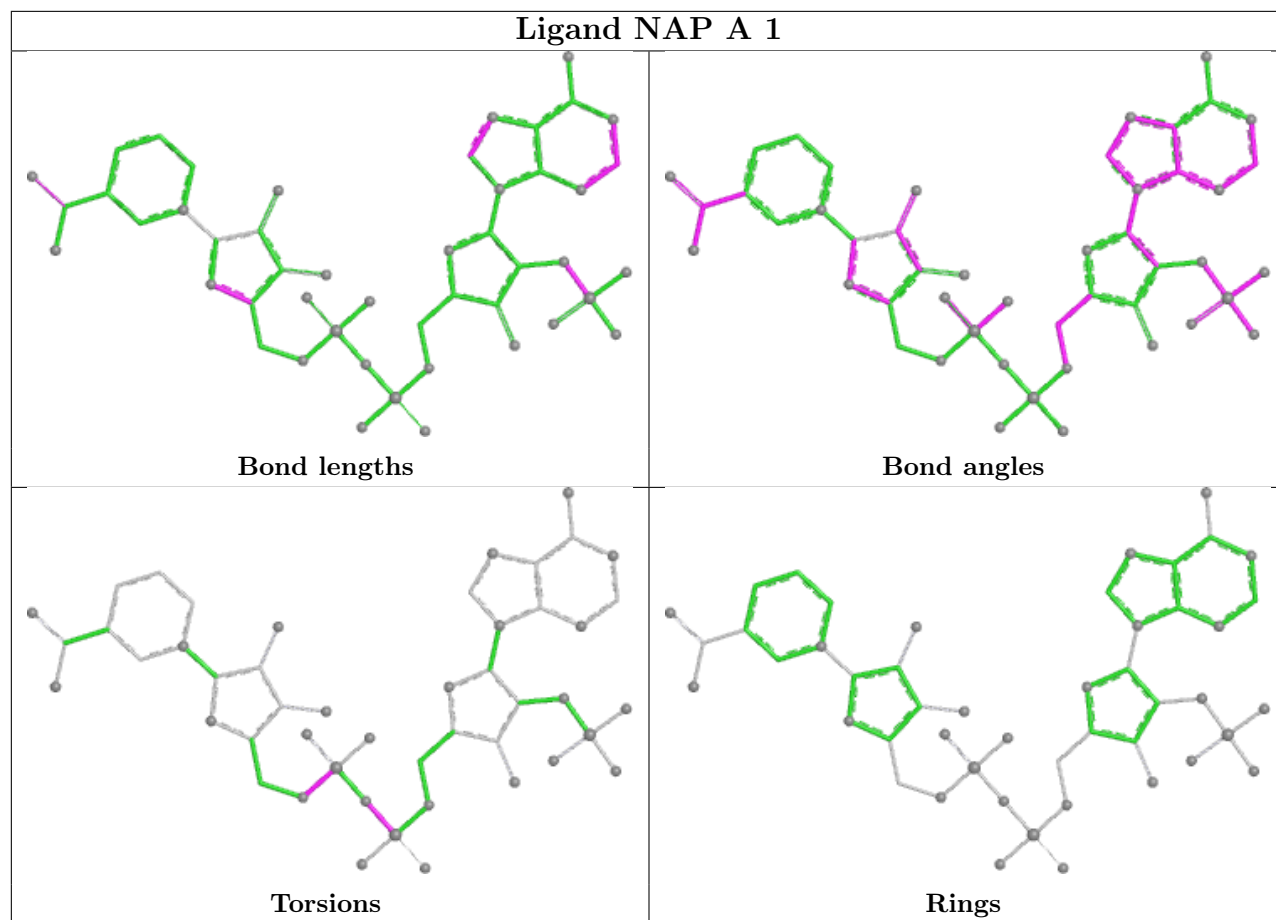
Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C5D-O5D-PN-O3
2	A	1	NAP	C5D-O5D-PN-O1N
2	B	1	NAP	C5D-O5D-PN-O1N
3	B	293	IIG	C18-C1-C20-C22
3	A	293	IIG	C16-C12-N1-C13
3	B	293	IIG	C14-C13-N1-C11
2	B	1	NAP	C3B-C2B-O2B-P2B
2	A	1	NAP	C5D-O5D-PN-O2N
2	B	1	NAP	C5D-O5D-PN-O3
2	A	1	NAP	PN-O3-PA-O1A
3	A	293	IIG	C18-C1-C20-C21
3	A	293	IIG	C15-C13-N1-C12
2	A	1	NAP	PN-O3-PA-O2A
3	A	293	IIG	C15-C13-N1-C11
3	A	293	IIG	C14-C13-N1-C11
3	B	293	IIG	C15-C13-N1-C11
2	B	1	NAP	C1B-C2B-O2B-P2B
3	A	293	IIG	C10-C8-C9-F2
2	B	1	NAP	PN-O3-PA-O2A

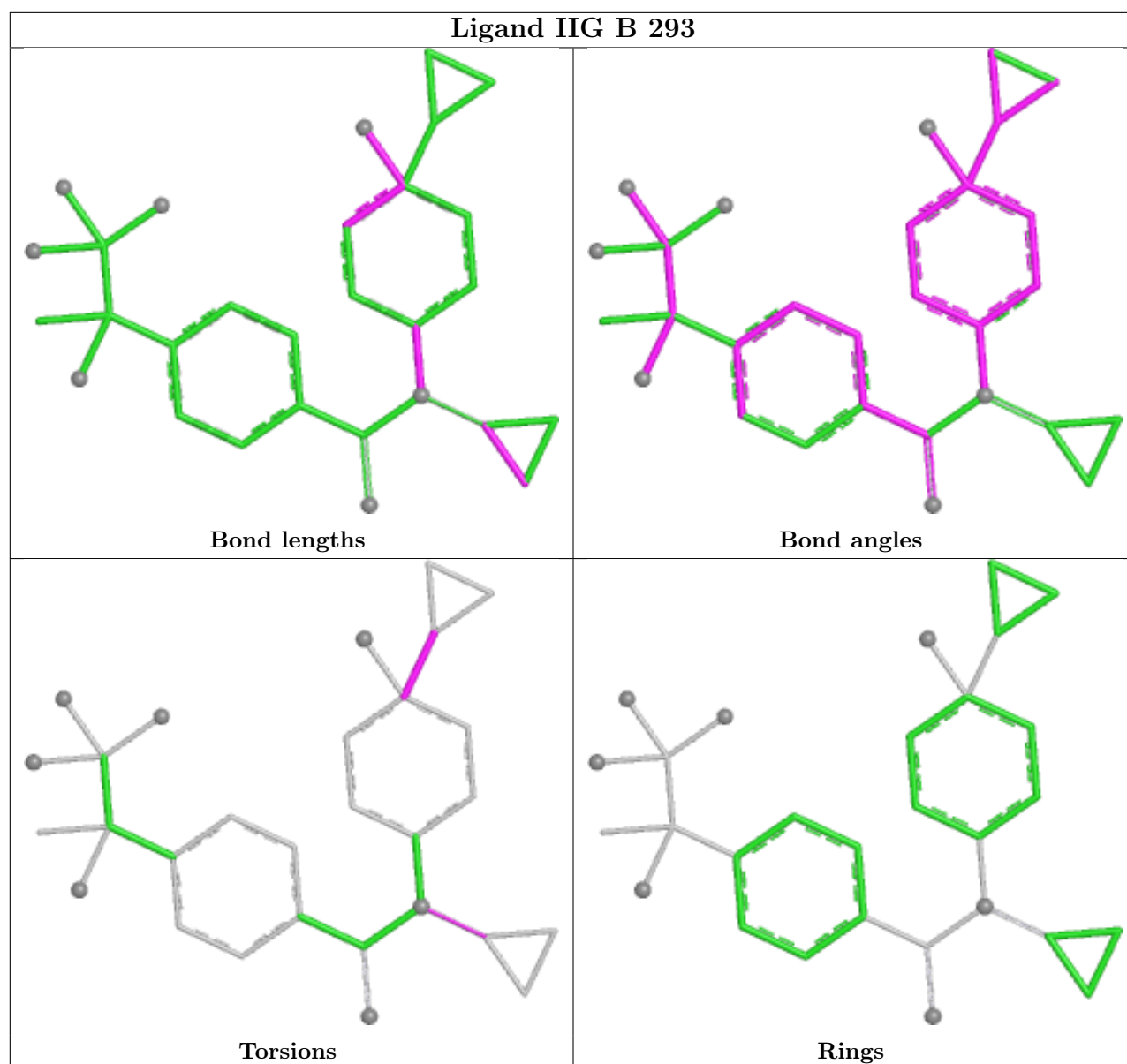
There are no ring outliers.

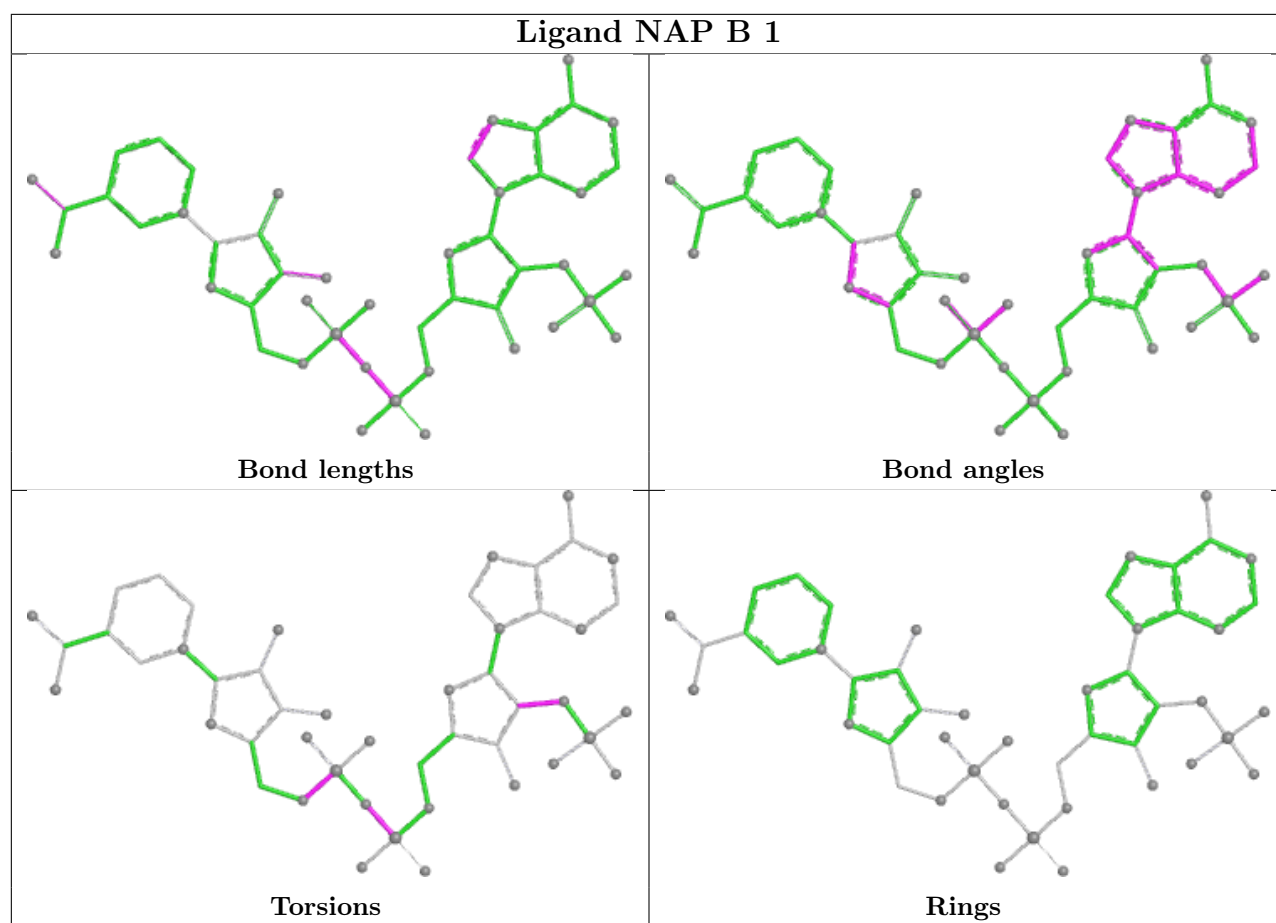
4 monomers are involved in 11 short contacts:

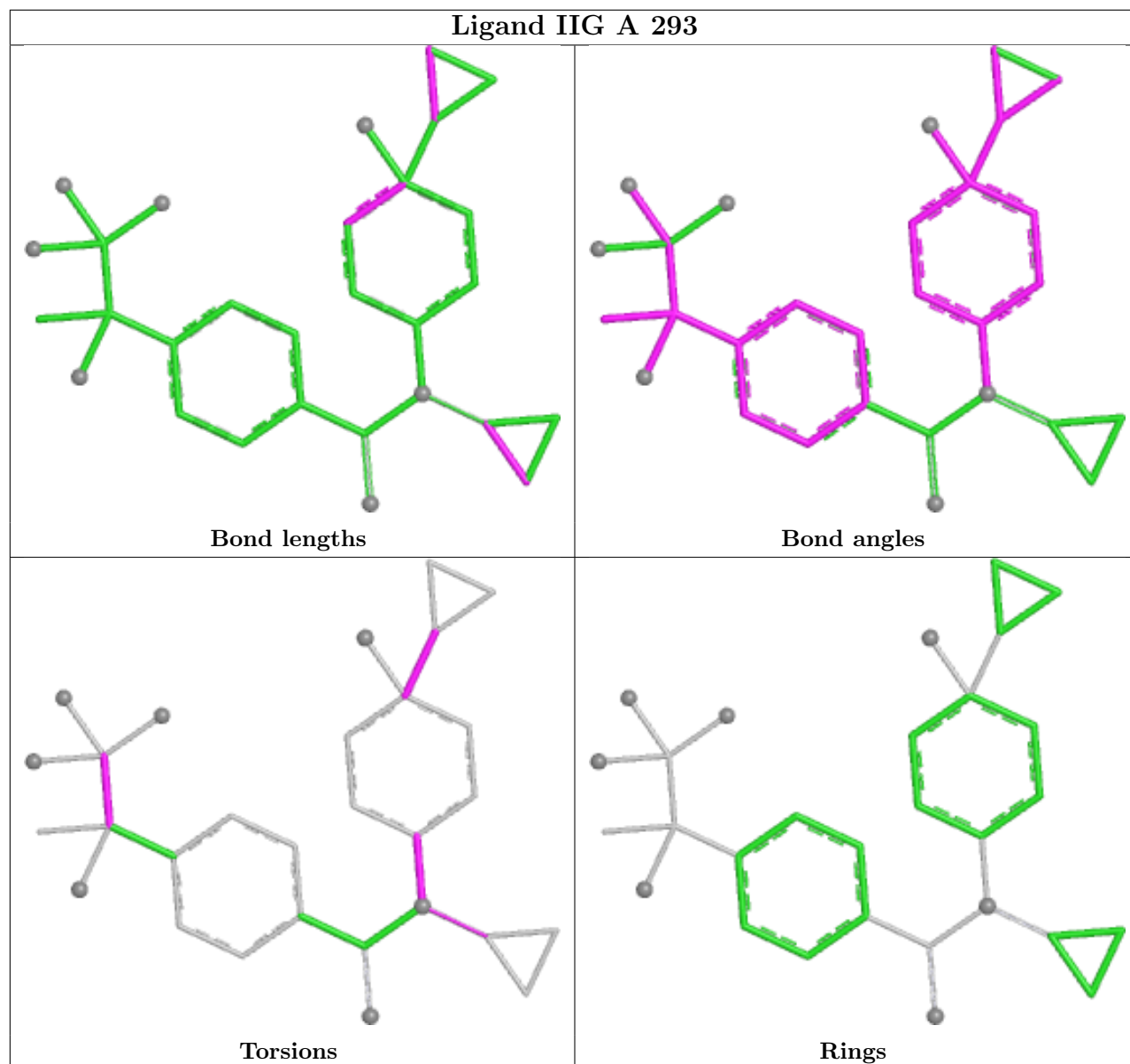
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAP	1	0
3	B	293	IIG	4	0
2	B	1	NAP	4	0
3	A	293	IIG	2	0

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	267/286 (93%)	0.11	6 (2%) 62 56	33, 60, 94, 131	10 (3%)
1	B	266/286 (93%)	0.29	16 (6%) 27 21	31, 65, 97, 124	12 (4%)
All	All	533/572 (93%)	0.20	22 (4%) 41 33	31, 62, 97, 131	22 (4%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	PHE	5.2
1	B	262	LEU	4.7
1	B	284[A]	TYR	3.3
1	A	130	HIS	3.3
1	B	65	ALA	3.2
1	B	130[A]	HIS	3.1
1	A	233	MET	3.0
1	A	232	HIS	2.9
1	A	280	TYR	2.9
1	B	263	TRP	2.9
1	B	160	GLN	2.7
1	B	221[A]	GLU	2.6
1	A	289	PHE	2.5
1	B	23	LEU	2.4
1	B	21	GLN	2.3
1	B	86	ALA	2.3
1	A	287	ASP	2.3
1	B	288	ARG	2.3
1	B	265	THR	2.2
1	B	233	MET	2.1
1	B	112	GLY	2.1
1	B	27	PHE	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](#)

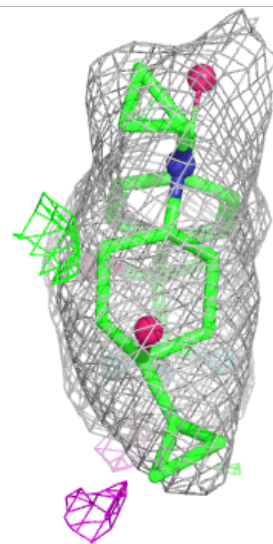
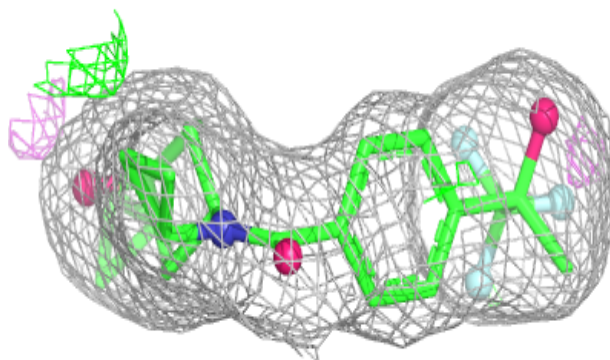
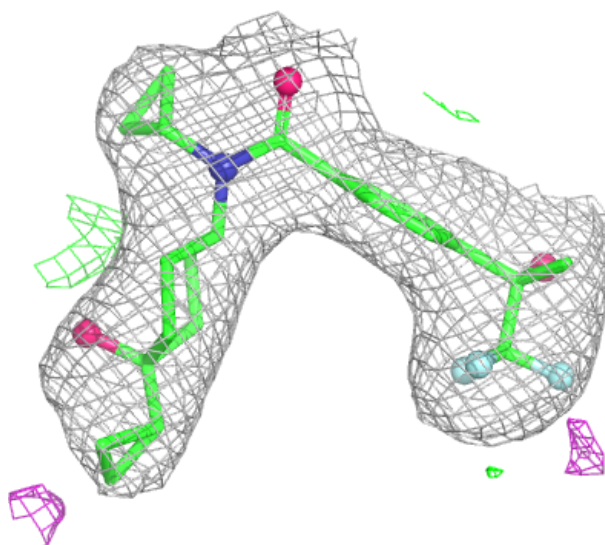
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IIG	B	293	29/29	0.93	0.10	46,56,62,63	0
3	IIG	A	293	29/29	0.95	0.08	39,48,57,59	0
2	NAP	A	1	48/48	0.96	0.07	43,51,57,60	0
2	NAP	B	1	48/48	0.96	0.06	38,54,59,62	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.

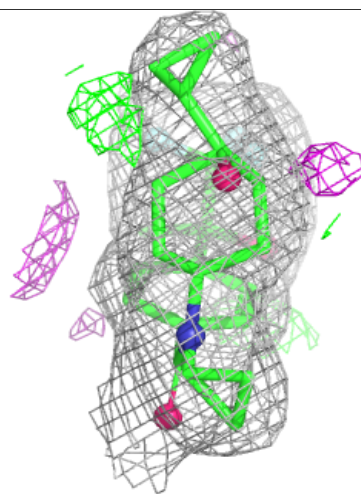
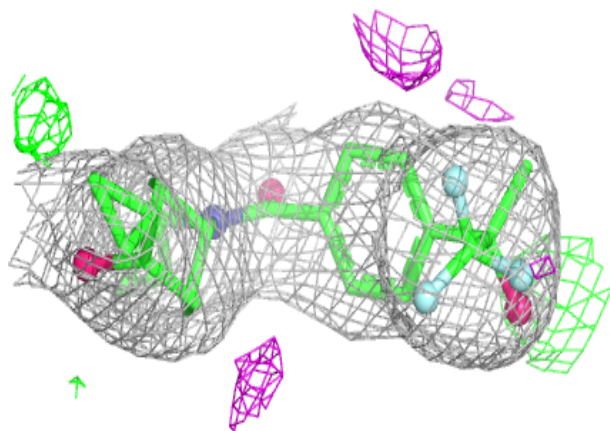
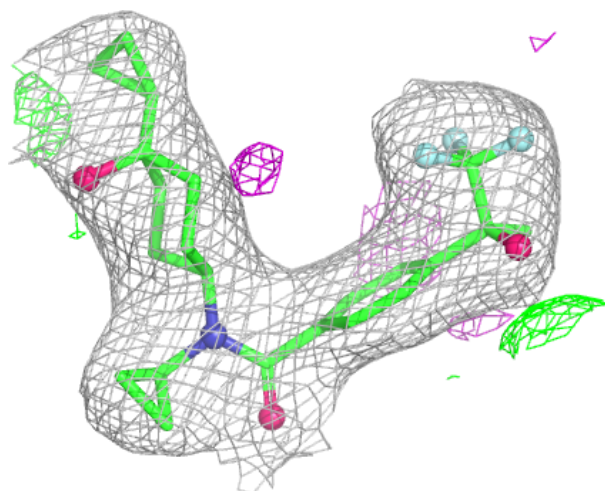
Electron density around IIG B 293:

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



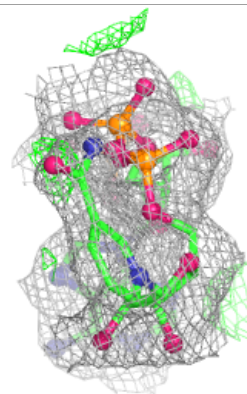
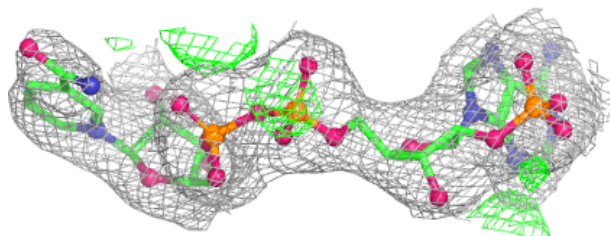
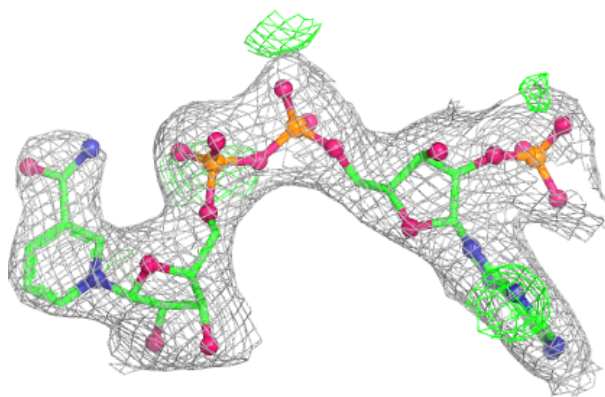
Electron density around IIG A 293:

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

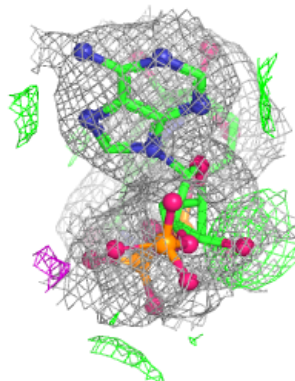
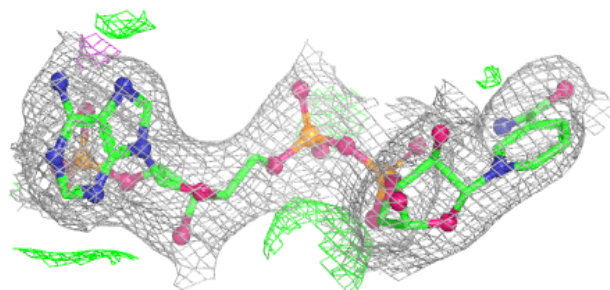
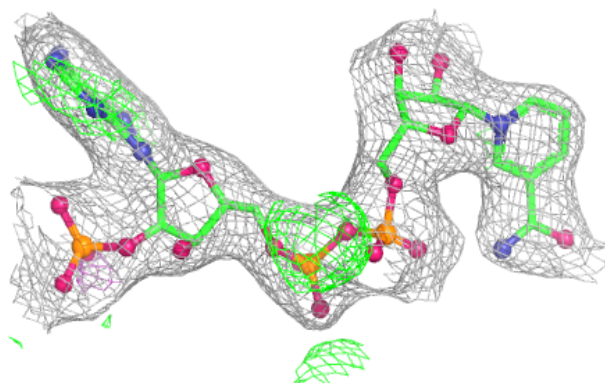


Electron density around NAP A 1:

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

**Electron density around NAP 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.