



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:50 PM UTC

PDB ID : 1W3C / pdb_00001w3c
Title : Crystal structure of the Hepatitis C Virus NS3 Protease in complex with a peptidomimetic inhibitor
Authors : Di Marco, S.; Volpari, C.
Deposited on : 2004-07-14
Resolution : 2.30 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

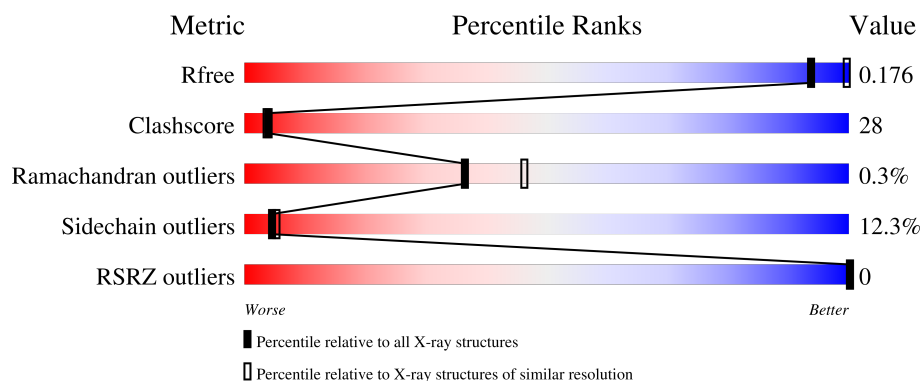
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

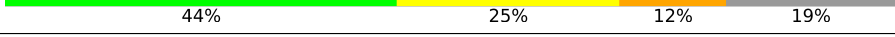
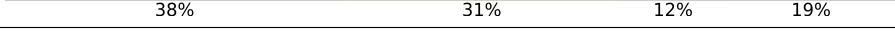
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	187	
1	B	187	
2	C	16	
2	D	16	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DN1	A	1176	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2988 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 PROTEASE/HELICASE NS3 (P70).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	1
			1272	793	230	239	10			
1	B	174	Total	C	N	O	S	0	0	1
			1272	793	230	239	10			

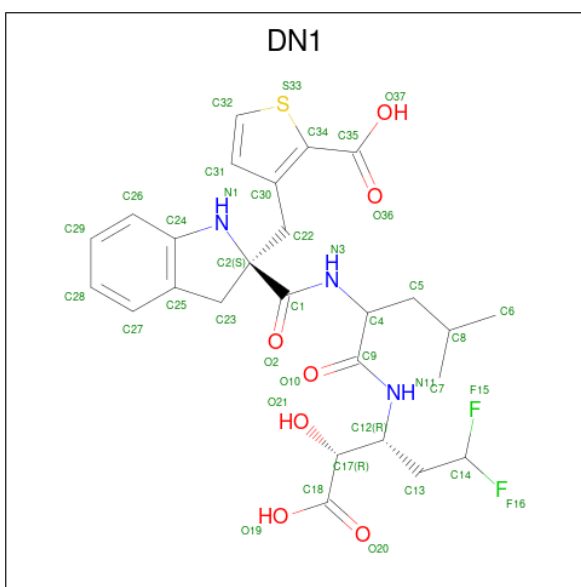
- Molecule 2 is a protein called NONSTRUCTURAL PROTEIN NS4A (P4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	1
			85	55	16	14			
2	D	13	Total	C	N	O	0	0	1
			85	55	16	14			

There are 4 discrepancies between the modelled and reference sequences:

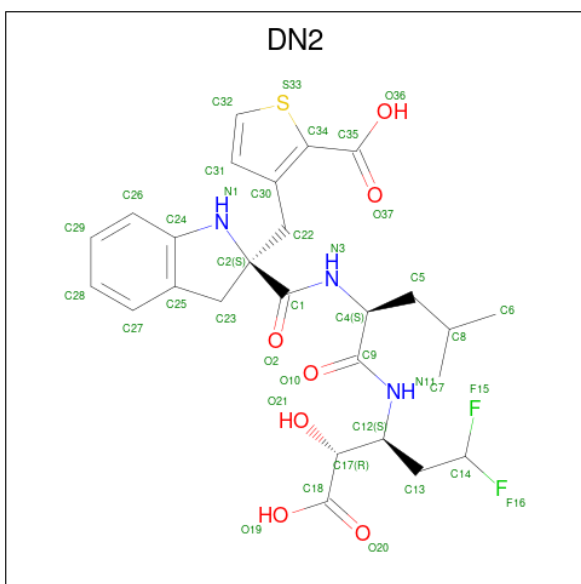
Chain	Residue	Modelled	Actual	Comment	Reference
C	220	LYS	THR	engineered mutation	UNP Q81755
C	235	LYS	PRO	engineered mutation	UNP Q81755
D	220	LYS	THR	engineered mutation	UNP Q81755
D	235	LYS	PRO	engineered mutation	UNP Q81755

- Molecule 3 is 3-({(2S)-2-[(1R)-1-[(1R)-1-[(R)-CARBOXY(HYDROXY)METHYL]-3,3-DIFLUOROPROPYL}AMINO)CARBONYL]-3-METHYLBUTYL}AMINO)CARB ON YL]-2,3-DIHYDRO-1H-INDOL-2-YL}METHYL)THIOPHENE-2-CARBOXYLIC ACID (CCD ID: DN1) (formula: C₂₆H₃₁F₂N₃O₇S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			39	26	2	3	7	1		

- Molecule 4 is 3-({(2S)-2-[(1S)-1-[(1S)-1-[(R)-CARBOXY(HYDROXY)METHYL]-3,3-DIFLUOROPROPYL}AMINO)CARBONYL]-3-METHYLBUTYL}AMINO)CARBONYL]-2,3-DIHYDRO-1H-INDOL-2-YL}METHYL)THIOPHENE-2-CARBOXYLIC ACID (CCD ID: DN2) (formula: C₂₆H₃₁F₂N₃O₇S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	0	0
			39	26	2	3	7	1		

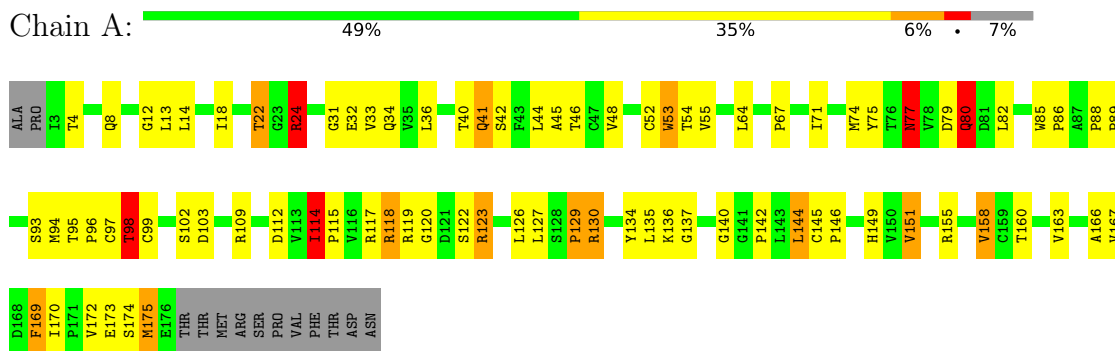
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total 89	O 89	0	0
5	B	96	Total 96	O 96	0	0
5	C	4	Total 4	O 4	0	0
5	D	7	Total 7	O 7	0	0

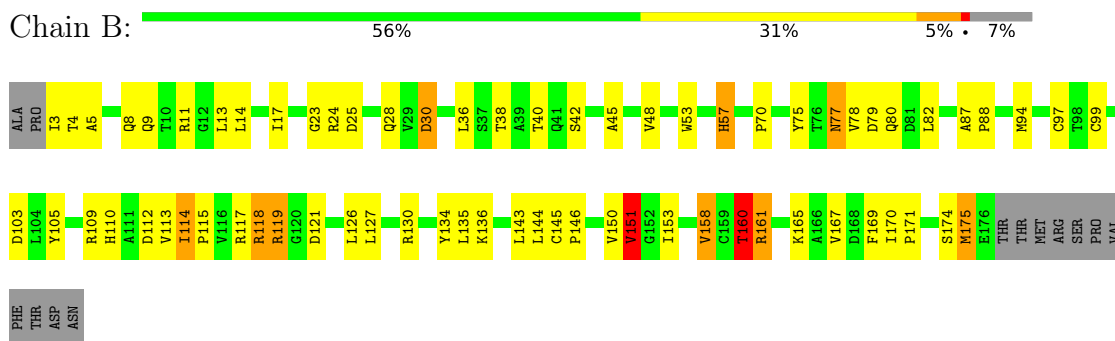
3 Residue-property plots

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.

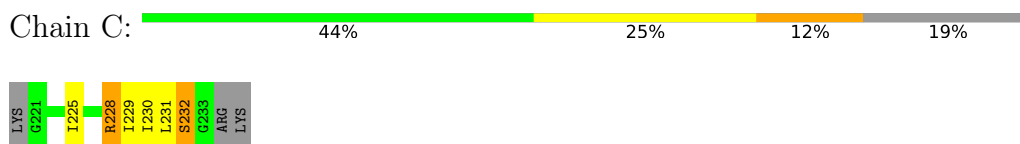
• Molecule 1: PROTEASE/HELICASE NS3 (P70)



• Molecule 1: PROTEASE/HELICASE NS3 (P70)

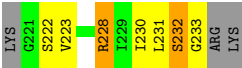


• Molecule 2: NONSTRUCTURAL PROTEIN NS4A (P4)



• Molecule 2: NONSTRUCTURAL PROTEIN NS4A (P4)





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.41 Å 92.41 Å 80.01 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-2.30) 89.6 (20.00-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.177 , 0.240 0.169 , 0.176	Depositor DCC
R_{free} test set	800 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.224 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2988	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DN2, DN1

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	0.62	1/1298 (0.1%)	1.66	15/1769 (0.8%)
1	B	0.63	1/1298 (0.1%)	1.60	14/1769 (0.8%)
2	C	0.79	1/84 (1.2%)	1.37	0/113
2	D	0.84	1/84 (1.2%)	1.73	1/113 (0.9%)
All	All	0.64	4/2764 (0.1%)	1.63	30/3764 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	232	SER	C-N	-5.62	1.25	1.33
2	C	232	SER	C-N	-5.62	1.25	1.33
1	A	175	MET	C-N	-5.62	1.25	1.33
1	B	175	MET	C-N	-5.33	1.25	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	HIS	CA-CB-CG	10.58	124.38	113.80
1	A	173	GLU	CB-CG-CD	10.24	130.01	112.60
1	B	119	ARG	CD-NE-CZ	8.78	136.69	124.40
1	A	80	GLN	CA-CB-CG	7.29	128.69	114.10
1	B	161	ARG	CD-NE-CZ	7.15	134.41	124.40
1	B	119	ARG	CG-CD-NE	6.55	126.41	112.00
1	A	24	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	A	130	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	A	169	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	52	CYS	N-CA-CB	5.86	119.53	110.21
1	A	22	THR	CA-C-O	-5.86	112.74	119.60
1	B	30	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	173	GLU	CA-C-N	5.74	128.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLU	C-N-CA	5.74	128.54	120.28
1	B	158	VAL	CB-CA-C	5.73	118.83	110.98
1	A	41	GLN	N-CA-C	5.62	117.51	109.14
1	B	161	ARG	N-CA-C	-5.61	105.06	112.24
1	A	77	ASN	CB-CA-C	-5.52	101.96	111.23
1	A	114	ILE	N-CA-C	5.50	114.54	108.05
1	B	151	VAL	N-CA-C	-5.38	107.57	113.43
2	D	222	SER	N-CA-CB	-5.37	101.53	110.23
1	A	24	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	48	VAL	CB-CA-C	-5.32	104.34	110.41
1	B	160	THR	CA-C-O	5.31	127.07	120.54
1	A	53	TRP	N-CA-C	5.29	118.69	110.17
1	B	25	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	169	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	11	ARG	CA-C-O	-5.18	115.55	121.40
1	B	30	ASP	CA-C-O	-5.11	115.98	121.45
1	B	9	GLN	CA-C-O	-5.09	116.15	121.55

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	1272	0	1281	75	1
1	B	1272	0	1281	73	1
2	C	85	0	99	7	0
2	D	85	0	99	13	0
3	A	39	0	27	6	0
4	B	39	0	28	5	0
5	A	89	0	0	12	0
5	B	96	0	0	6	0
5	C	4	0	0	0	0
5	D	7	0	0	1	0
All	All	2988	0	2815	155	1

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 28.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1176:DN1:H13D	3:A:1176:DN1:O19	1.52	1.02
1:A:32:GLU:HB3	1:A:94:MET:HE2	1.39	1.00
4:B:1176:DN2:H222	4:B:1176:DN2:O36	1.63	0.96
1:A:80:GLN:OE1	1:A:174:SER:HB3	1.67	0.95
1:B:160:THR:HG22	1:B:161:ARG:HG2	1.50	0.93
1:A:42:SER:OG	1:A:109:ARG:NH2	2.03	0.91
3:A:1176:DN1:H222	3:A:1176:DN1:O37	1.71	0.89
1:B:97:CYS:HG	1:B:99:CYS:HG	1.21	0.85
1:B:42:SER:OG	1:B:109:ARG:NH2	2.09	0.84
1:A:122:SER:HB2	1:A:169:PHE:O	1.82	0.80
1:B:4:THR:H	2:D:233:GLY:N	1.79	0.80
1:B:126:LEU:HD21	1:B:167:VAL:HG13	1.64	0.80
1:A:77:ASN:OD1	1:A:80:GLN:NE2	2.14	0.79
1:A:112:ASP:HB2	1:A:134:TYR:OH	1.82	0.79
1:B:160:THR:HB	1:B:165:LYS:NZ	1.98	0.77
1:A:77:ASN:CG	1:A:80:GLN:HE21	1.94	0.76
1:A:77:ASN:CB	1:A:80:GLN:HE21	1.99	0.74
1:B:4:THR:OG1	2:D:232:SER:HB3	1.88	0.74
1:A:89:PRO:HD2	5:A:2058:HOH:O	1.88	0.73
1:B:8:GLN:NE2	2:D:228:ARG:HH21	1.87	0.72
1:B:160:THR:CG2	1:B:161:ARG:HG2	2.20	0.72
1:A:158:VAL:HG13	1:A:166:ALA:HB3	1.72	0.71
1:B:77:ASN:C	1:B:77:ASN:HD22	1.99	0.71
1:A:46:THR:HG23	1:A:94:MET:HE3	1.72	0.71
1:B:77:ASN:CB	1:B:80:GLN:HE21	2.05	0.70
1:A:117:ARG:HD2	1:B:127:LEU:HD11	1.74	0.70
1:A:8:GLN:HE21	2:C:228:ARG:HE	1.39	0.70
1:A:97:CYS:HG	1:A:145:CYS:HG	1.37	0.70
2:D:232:SER:HB2	5:D:2007:HOH:O	1.92	0.70
1:B:75:TYR:OH	1:B:80:GLN:NE2	2.25	0.69
1:B:8:GLN:HE21	2:D:228:ARG:HE	1.41	0.67
1:A:123:ARG:HH11	1:A:123:ARG:HB2	1.59	0.66
1:A:88:PRO:HB3	5:A:2058:HOH:O	1.96	0.64
1:A:96:PRO:HB3	1:A:172:VAL:HG21	1.79	0.64
1:B:121:ASP:HB2	5:B:2079:HOH:O	1.99	0.63
1:B:97:CYS:HB3	1:B:151:VAL:HG12	1.80	0.62
1:B:160:THR:HG23	5:B:2092:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2005:HOH:O	2:D:230:ILE:HD13	2.00	0.62
1:B:160:THR:HB	1:B:165:LYS:HZ1	1.65	0.61
1:B:94:MET:HE3	1:B:150:VAL:CG2	2.31	0.60
1:A:4:THR:OG1	2:C:232:SER:HB3	2.02	0.60
3:A:1176:DN1:H232	3:A:1176:DN1:C34	2.32	0.60
1:B:160:THR:HB	1:B:165:LYS:HZ2	1.65	0.59
1:A:97:CYS:O	1:A:98:THR:HG23	2.03	0.59
1:A:114:ILE:HG22	1:A:130:ARG:NH2	2.17	0.59
1:A:112:ASP:HB2	1:A:134:TYR:HH	1.67	0.59
1:A:74:MET:SD	1:A:75:TYR:HB2	2.43	0.58
1:B:103:ASP:O	1:B:146:PRO:HD3	2.04	0.58
1:B:77:ASN:OD1	1:B:80:GLN:NE2	2.38	0.57
1:A:80:GLN:HG2	1:A:82:LEU:CB	2.35	0.57
1:A:155:ARG:HG3	1:A:170:ILE:HG13	1.87	0.56
1:B:97:CYS:CB	1:B:151:VAL:HG12	2.34	0.56
1:A:96:PRO:HB3	1:A:172:VAL:CG2	2.36	0.56
1:A:129:PRO:HB3	1:A:163:VAL:HG11	1.88	0.55
1:B:36:LEU:HD11	1:B:45:ALA:HB2	1.88	0.55
1:A:80:GLN:HG2	1:A:82:LEU:HB2	1.87	0.55
1:B:136:LYS:HE2	4:B:1176:DN2:H32	1.88	0.55
1:B:77:ASN:ND2	1:B:79:ASP:H	2.06	0.54
1:A:115:PRO:HB2	1:A:127:LEU:HD12	1.89	0.54
1:A:36:LEU:HD11	1:A:45:ALA:HB2	1.90	0.54
1:A:40:THR:OG1	1:A:41:GLN:HG2	2.08	0.53
1:B:77:ASN:HB3	1:B:80:GLN:HG2	1.91	0.52
1:A:40:THR:HG21	5:A:2032:HOH:O	2.08	0.52
1:A:34:GLN:HE21	2:C:225:ILE:HD13	1.75	0.52
1:A:136:LYS:HD3	3:A:1176:DN1:O19	2.10	0.51
1:B:77:ASN:HD22	1:B:79:ASP:H	1.58	0.51
1:B:53:TRP:HZ3	1:B:75:TYR:CD2	2.29	0.51
1:B:136:LYS:CE	4:B:1176:DN2:H32	2.40	0.51
1:A:129:PRO:HB3	1:A:163:VAL:CG1	2.41	0.51
1:B:8:GLN:HE22	2:D:228:ARG:HH21	1.57	0.51
1:B:126:LEU:CD2	1:B:167:VAL:HG13	2.37	0.51
1:A:18:ILE:O	1:A:22:THR:HG23	2.12	0.50
1:B:77:ASN:C	1:B:77:ASN:ND2	2.65	0.50
1:B:112:ASP:OD2	1:B:134:TYR:OH	2.28	0.50
1:B:118:ARG:NH1	1:B:121:ASP:HA	2.27	0.49
1:B:23:GLY:HA3	1:B:70:PRO:HG3	1.92	0.49
1:A:97:CYS:HB2	1:A:149:HIS:HB2	1.94	0.49
1:A:42:SER:O	1:A:137:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:CD2	1:B:113:VAL:HG12	2.47	0.48
1:A:119:ARG:HH11	1:B:117:ARG:NH2	2.11	0.48
1:B:80:GLN:OE1	1:B:174:SER:HB3	2.13	0.48
1:A:44:LEU:O	1:A:140:GLY:HA3	2.14	0.48
1:B:97:CYS:SG	1:B:145:CYS:HB3	2.54	0.48
1:B:75:TYR:HB2	5:B:2057:HOH:O	2.13	0.47
1:A:103:ASP:HB2	5:A:2072:HOH:O	2.13	0.47
1:A:155:ARG:HG3	1:A:170:ILE:CD1	2.45	0.47
1:A:112:ASP:CB	1:A:134:TYR:OH	2.59	0.47
1:A:170:ILE:HG12	5:A:2056:HOH:O	2.14	0.47
1:B:112:ASP:HB2	1:B:134:TYR:OH	2.15	0.47
1:A:158:VAL:CG1	1:A:166:ALA:HB3	2.40	0.47
3:A:1176:DN1:N3	3:A:1176:DN1:H6C2	2.30	0.47
1:B:114:ILE:HD11	1:B:126:LEU:HD11	1.96	0.46
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.30	0.46
1:B:121:ASP:HB3	5:B:2077:HOH:O	2.15	0.46
1:B:3:ILE:HA	2:D:233:GLY:N	2.30	0.46
1:B:99:CYS:SG	1:B:145:CYS:SG	3.12	0.46
1:A:118:ARG:HD2	1:A:120:GLY:O	2.15	0.46
1:B:105:TYR:O	1:B:143:LEU:HA	2.16	0.46
1:B:80:GLN:HG3	1:B:82:LEU:HB3	1.97	0.45
1:A:79:ASP:HB2	5:A:2051:HOH:O	2.16	0.45
4:B:1176:DN2:O36	4:B:1176:DN2:C22	2.44	0.45
1:A:67:PRO:CD	5:A:2058:HOH:O	2.65	0.45
1:B:5:ALA:HA	2:D:230:ILE:O	2.16	0.45
1:B:53:TRP:CD1	1:B:175:MET:HE3	2.51	0.45
1:B:13:LEU:O	1:B:17:ILE:HG13	2.17	0.45
1:A:85:TRP:O	1:A:86:PRO:C	2.60	0.45
2:D:228:ARG:N	2:D:228:ARG:HD3	2.32	0.45
1:B:38:THR:HG22	2:D:223:VAL:HG22	1.99	0.45
1:B:130:ARG:HA	1:B:130:ARG:HD2	1.84	0.44
1:B:57:HIS:CE1	4:B:1176:DN2:H5C1	2.52	0.44
1:B:77:ASN:HD22	1:B:78:VAL:N	2.15	0.44
1:B:110:HIS:HA	5:B:2071:HOH:O	2.17	0.44
1:A:88:PRO:HA	5:A:2058:HOH:O	2.18	0.44
1:A:34:GLN:NE2	2:C:225:ILE:HD13	2.32	0.44
1:A:136:LYS:HD2	5:A:2085:HOH:O	2.17	0.44
1:B:75:TYR:HE2	1:B:82:LEU:HD23	1.83	0.44
1:B:48:VAL:HG21	1:B:175:MET:HE1	2.00	0.43
1:B:80:GLN:HG3	1:B:82:LEU:CB	2.48	0.43
1:A:33:VAL:HB	2:C:229:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:HA	1:A:53:TRP:O	2.19	0.43
1:A:142:PRO:HB2	1:A:144:LEU:CD1	2.48	0.43
1:A:142:PRO:HB2	1:A:144:LEU:HD13	1.99	0.43
3:A:1176:DN1:O19	3:A:1176:DN1:C13	2.43	0.43
1:A:80:GLN:HG2	1:A:82:LEU:HB3	2.01	0.43
1:B:94:MET:HE3	1:B:150:VAL:HG21	1.99	0.43
1:A:97:CYS:HB3	1:A:151:VAL:HG12	2.01	0.43
1:A:112:ASP:CB	1:A:134:TYR:HH	2.30	0.43
1:B:77:ASN:HB3	1:B:80:GLN:HE21	1.84	0.43
1:B:75:TYR:CE2	1:B:82:LEU:HD23	2.54	0.42
1:A:31:GLY:CA	2:C:230:ILE:HD13	2.48	0.42
1:A:115:PRO:HG2	5:A:2074:HOH:O	2.18	0.42
1:A:75:TYR:HE2	1:A:77:ASN:HB2	1.84	0.42
1:A:119:ARG:NH1	1:B:117:ARG:NH2	2.67	0.42
1:B:30:ASP:O	2:D:228:ARG:HG3	2.20	0.42
1:A:64:LEU:HD23	1:A:71:ILE:HD12	2.00	0.42
1:A:126:LEU:CD1	1:A:167:VAL:HG13	2.49	0.42
1:B:77:ASN:CG	1:B:80:GLN:HG2	2.45	0.42
1:A:32:GLU:CB	1:A:94:MET:HE2	2.28	0.42
1:A:112:ASP:CG	1:A:134:TYR:HH	2.28	0.42
1:A:158:VAL:HG13	1:A:166:ALA:CB	2.47	0.41
1:A:114:ILE:CD1	1:A:134:TYR:HE2	2.33	0.41
1:A:97:CYS:HB2	1:A:149:HIS:CB	2.49	0.41
1:B:4:THR:N	2:D:233:GLY:N	2.58	0.41
1:A:4:THR:HG1	2:C:232:SER:HB3	1.85	0.41
5:A:2076:HOH:O	1:B:117:ARG:HD2	2.19	0.41
1:B:77:ASN:CG	1:B:80:GLN:HE21	2.29	0.41
1:A:54:THR:OG1	1:A:55:VAL:N	2.54	0.40
1:B:112:ASP:CG	1:B:134:TYR:HH	2.26	0.40
1:B:87:ALA:HA	1:B:88:PRO:HD3	1.87	0.40
1:B:114:ILE:HA	1:B:115:PRO:HD3	1.88	0.40
1:A:12:GLY:HA2	5:A:2011:HOH:O	2.22	0.40
1:A:75:TYR:CE2	1:A:77:ASN:HB2	2.57	0.40
1:A:172:VAL:HA	1:A:175:MET:HE3	2.03	0.40
1:B:53:TRP:NE1	1:B:175:MET:HE3	2.37	0.40
1:B:170:ILE:HA	1:B:171:PRO:HD3	1.85	0.40

All (1) 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:24:ARG:NH2	1:B:24:ARG:NH2[4_654]	1.84	0.36

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	172/187 (92%)	162 (94%)	9 (5%)	1 (1%)	21	27
1	B	172/187 (92%)	167 (97%)	5 (3%)	0	100	100
2	C	11/16 (69%)	11 (100%)	0	0	100	100
2	D	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
All	All	366/406 (90%)	350 (96%)	15 (4%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	THR

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	141/154 (92%)	121 (86%)	20 (14%)	3	3
1	B	141/154 (92%)	128 (91%)	13 (9%)	8	11
2	C	10/13 (77%)	8 (80%)	2 (20%)	1	1
2	D	10/13 (77%)	8 (80%)	2 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	302/334 (90%)	265 (88%)	37 (12%)	4 5

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	LEU
1	A	24	ARG
1	A	77	ASN
1	A	80	GLN
1	A	93	SER
1	A	95	THR
1	A	98	THR
1	A	99	CYS
1	A	102	SER
1	A	114	ILE
1	A	118	ARG
1	A	123	ARG
1	A	129	PRO
1	A	135	LEU
1	A	144	LEU
1	A	146	PRO
1	A	151	VAL
1	A	158	VAL
1	A	160	THR
1	B	14	LEU
1	B	28	GLN
1	B	40	THR
1	B	77	ASN
1	B	114	ILE
1	B	118	ARG
1	B	119	ARG
1	B	135	LEU
1	B	144	LEU
1	B	151	VAL
1	B	153	ILE
1	B	158	VAL
1	B	160	THR
2	C	228	ARG
2	C	231	LEU
2	D	228	ARG
2	D	231	LEU

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	8	GLN
1	A	27	ASN
1	A	34	GLN
1	A	41	GLN
1	A	77	ASN
1	A	80	GLN
1	A	110	HIS
1	B	8	GLN
1	B	27	ASN
1	B	28	GLN
1	B	77	ASN
1	B	80	GLN
1	B	110	HIS
1	B	149	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	DN2	B	1176	1	41,41,41	2.32	10 (24%)	49,59,59	2.28	17 (34%)
3	DN1	A	1176	1	41,41,41	2.09	9 (21%)	49,59,59	2.36	16 (32%)

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	DN2	B	1176	1	-	10/43/53/53	0/3/3/3
3	DN1	A	1176	1	1/1/10/13	24/43/53/53	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1176	DN2	C17-C12	8.26	1.63	1.54
3	A	1176	DN1	C17-C12	7.21	1.62	1.54
4	B	1176	DN2	C17-C18	6.91	1.62	1.52
4	B	1176	DN2	C2-N1	6.00	1.53	1.46
3	A	1176	DN1	C17-C18	5.07	1.59	1.52
3	A	1176	DN1	C2-N1	5.06	1.52	1.46
3	A	1176	DN1	C9-N11	3.45	1.41	1.34
4	B	1176	DN2	C22-C30	2.92	1.53	1.50
4	B	1176	DN2	C9-N11	2.87	1.40	1.34
3	A	1176	DN1	C22-C30	2.68	1.53	1.50
3	A	1176	DN1	F15-C14	-2.65	1.22	1.35
3	A	1176	DN1	C12-N11	2.63	1.50	1.46
4	B	1176	DN2	F16-C14	-2.56	1.23	1.35
4	B	1176	DN2	F15-C14	-2.48	1.23	1.35
3	A	1176	DN1	F16-C14	-2.33	1.24	1.35
4	B	1176	DN2	O21-C17	2.21	1.46	1.42
3	A	1176	DN1	C22-C2	2.11	1.57	1.55
4	B	1176	DN2	C22-C2	2.07	1.57	1.55
4	B	1176	DN2	C34-S33	-2.04	1.69	1.72

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1176	DN2	C23-C2-N1	7.10	106.93	102.07
3	A	1176	DN1	C23-C2-N1	6.98	106.85	102.07
4	B	1176	DN2	C13-C12-N11	6.85	118.98	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1176	DN1	C12-N11-C9	-5.39	113.87	123.25
3	A	1176	DN1	O10-C9-N11	-5.17	113.71	122.96
3	A	1176	DN1	C9-C4-N3	4.82	124.15	111.11
3	A	1176	DN1	C5-C4-C9	4.07	120.22	110.59
4	B	1176	DN2	O21-C17-C18	-3.97	102.21	110.69
3	A	1176	DN1	C25-C24-N1	3.89	114.92	110.74
4	B	1176	DN2	C27-C25-C24	3.75	121.56	119.67
3	A	1176	DN1	C35-C34-S33	3.45	126.20	119.02
4	B	1176	DN2	C22-C30-C34	-3.43	119.10	125.12
4	B	1176	DN2	C25-C24-N1	3.38	114.37	110.74
4	B	1176	DN2	O2-C1-C2	-3.28	116.08	120.99
3	A	1176	DN1	O37-C35-O36	3.23	131.58	123.90
4	B	1176	DN2	C2-C1-N3	3.17	121.99	116.55
4	B	1176	DN2	C30-C34-S33	3.09	113.95	111.38
3	A	1176	DN1	O10-C9-C4	3.01	126.78	120.48
4	B	1176	DN2	C35-C34-S33	3.01	125.29	119.02
3	A	1176	DN1	C27-C25-C24	3.00	121.18	119.67
4	B	1176	DN2	O19-C18-O20	3.00	130.89	124.08
3	A	1176	DN1	O19-C18-C17	3.00	121.65	113.31
3	A	1176	DN1	C30-C34-S33	2.99	113.87	111.38
3	A	1176	DN1	C26-C24-N1	-2.91	123.73	128.14
4	B	1176	DN2	C31-C30-C34	-2.85	108.64	111.64
4	B	1176	DN2	O20-C18-C17	-2.83	114.08	121.62
3	A	1176	DN1	O36-C35-C34	-2.64	112.87	121.02
4	B	1176	DN2	C23-C2-C1	2.58	118.50	111.53
4	B	1176	DN2	C26-C24-N1	-2.39	124.53	128.14
4	B	1176	DN2	C4-C9-N11	-2.30	111.72	116.63
3	A	1176	DN1	C8-C5-C4	-2.11	109.73	115.40
3	A	1176	DN1	C31-C30-C34	-2.10	109.42	111.64
4	B	1176	DN2	C17-C12-N11	2.10	113.83	109.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1176	DN1	C4

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1176	DN1	O2-C1-C2-N1
3	A	1176	DN1	N3-C1-C2-N1
3	A	1176	DN1	O2-C1-C2-C23

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Mol	Chain	Res	Type	Atoms
3	A	1176	DN1	N3-C1-C2-C23
3	A	1176	DN1	N1-C2-C22-C30
3	A	1176	DN1	C1-C2-C22-C30
3	A	1176	DN1	C23-C2-C22-C30
3	A	1176	DN1	C9-C4-N3-C1
3	A	1176	DN1	N3-C4-C5-C8
3	A	1176	DN1	C13-C12-N11-C9
3	A	1176	DN1	N11-C12-C13-C14
3	A	1176	DN1	C13-C12-C17-C18
3	A	1176	DN1	C13-C12-C17-O21
3	A	1176	DN1	C12-C13-C14-F15
3	A	1176	DN1	C12-C13-C14-F16
3	A	1176	DN1	O21-C17-C18-O19
3	A	1176	DN1	O21-C17-C18-O20
4	B	1176	DN2	O2-C1-C2-N1
4	B	1176	DN2	N3-C1-C2-N1
4	B	1176	DN2	O2-C1-C2-C23
4	B	1176	DN2	N3-C1-C2-C23
4	B	1176	DN2	C1-C2-C22-C30
3	A	1176	DN1	O2-C1-N3-C4
3	A	1176	DN1	C2-C1-N3-C4
4	B	1176	DN2	O21-C17-C18-O19
4	B	1176	DN2	O21-C17-C18-O20
4	B	1176	DN2	O10-C9-N11-C12
3	A	1176	DN1	N11-C12-C17-C18
3	A	1176	DN1	N11-C12-C17-O21
3	A	1176	DN1	C17-C12-C13-C14
4	B	1176	DN2	N1-C2-C22-C30
3	A	1176	DN1	N3-C4-C9-N11
3	A	1176	DN1	N3-C4-C9-O10
4	B	1176	DN2	C2-C22-C30-C31

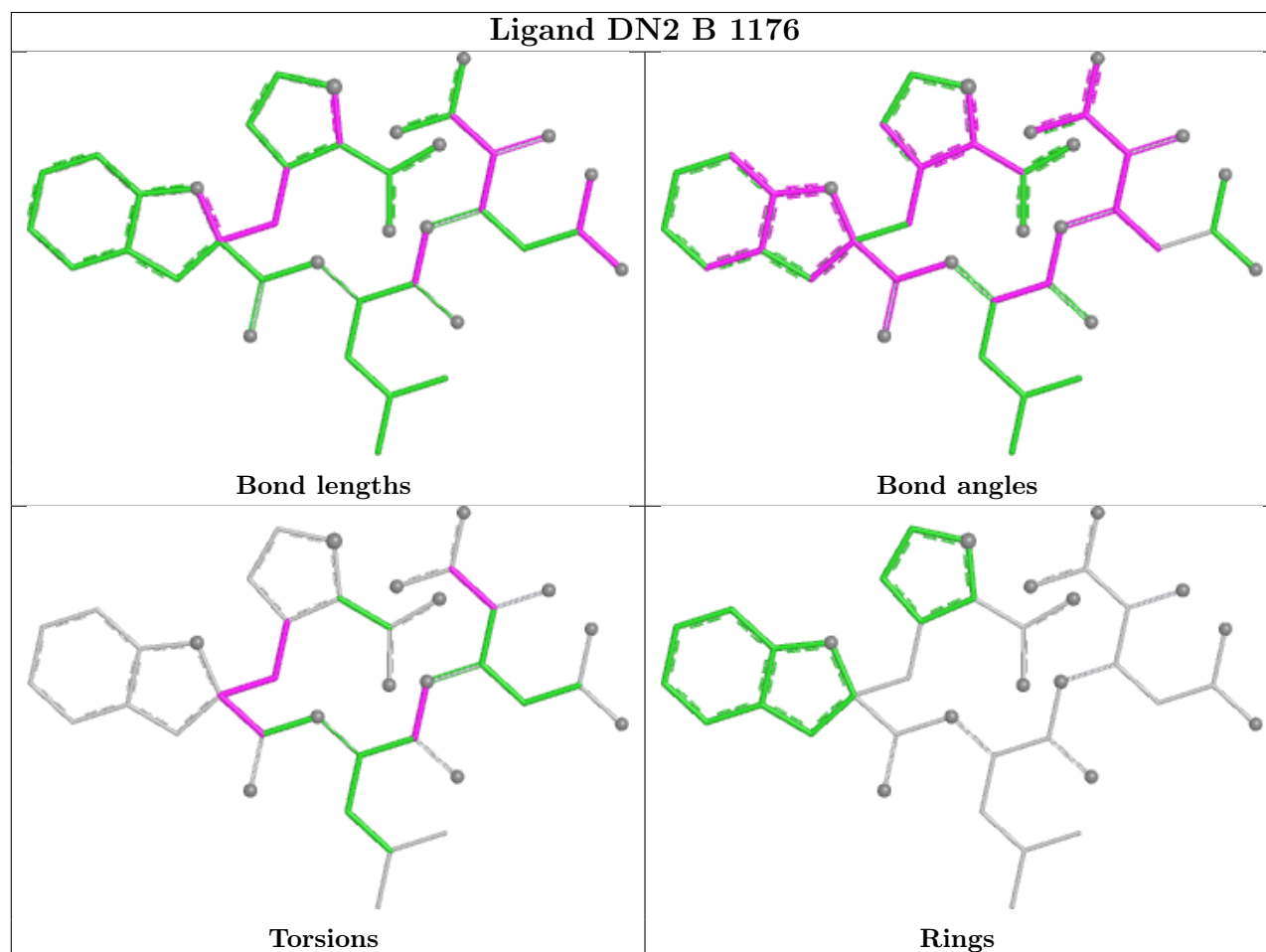
There are no ring outliers.

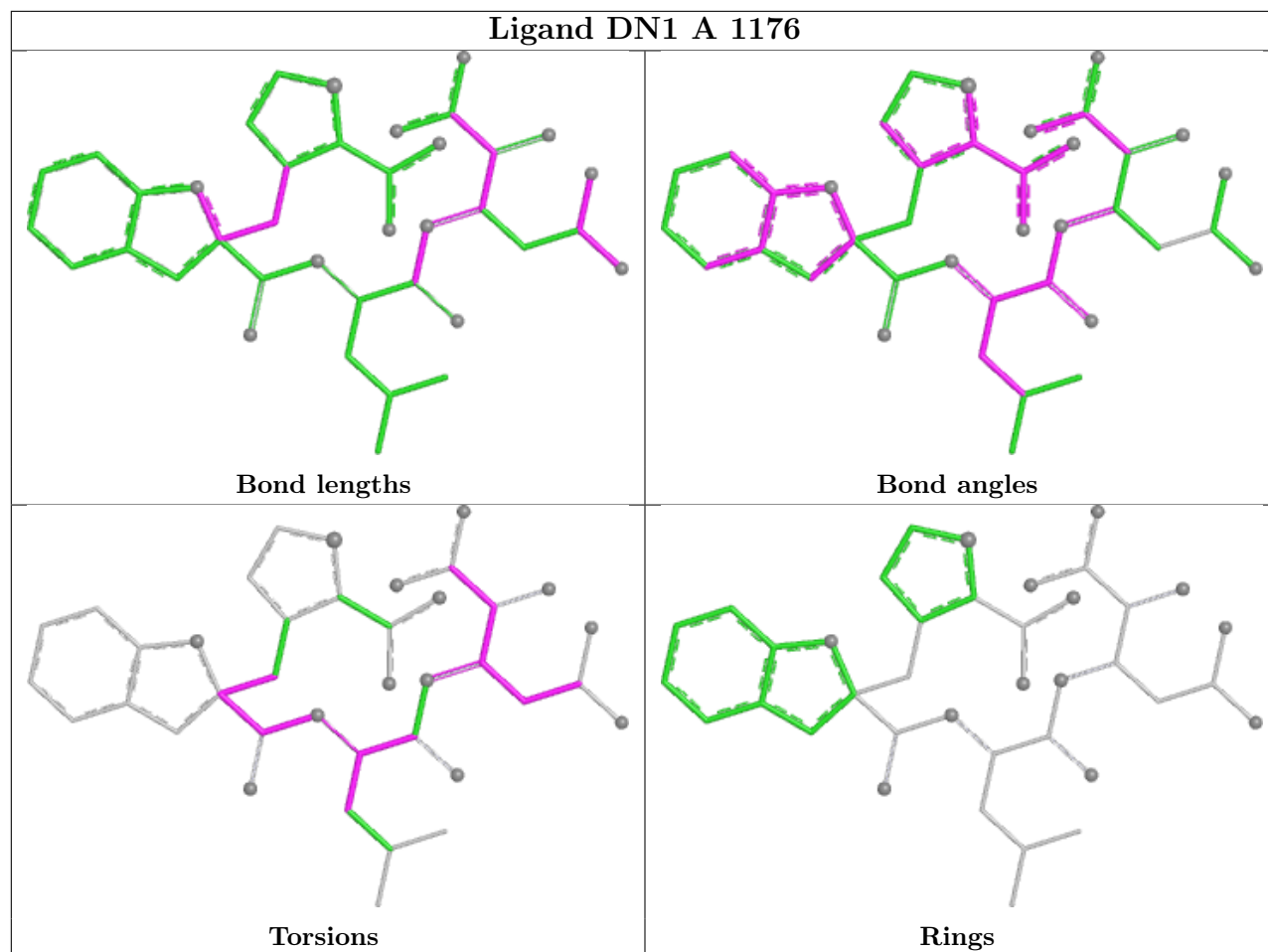
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1176	DN2	5	0
3	A	1176	DN1	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	174/187 (93%)	-1.35	0 100 100	30, 49, 73, 86	0
1	B	174/187 (93%)	-1.35	0 100 100	30, 47, 73, 87	0
2	C	13/16 (81%)	-1.29	0 100 100	33, 39, 75, 94	0
2	D	13/16 (81%)	-1.43	0 100 100	35, 39, 49, 67	0
All	All	374/406 (92%)	-1.35	0 100 100	30, 47, 73, 94	0

There are no RSRZ outliers to report.

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.

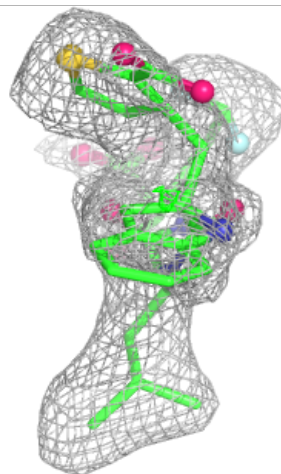
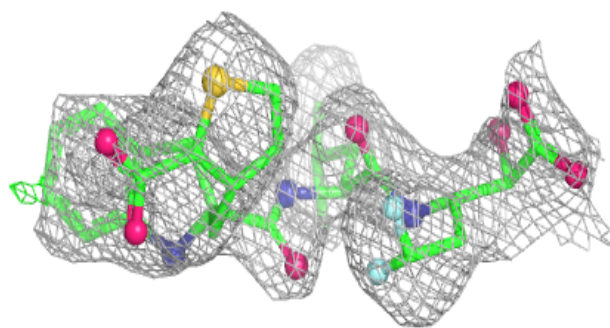
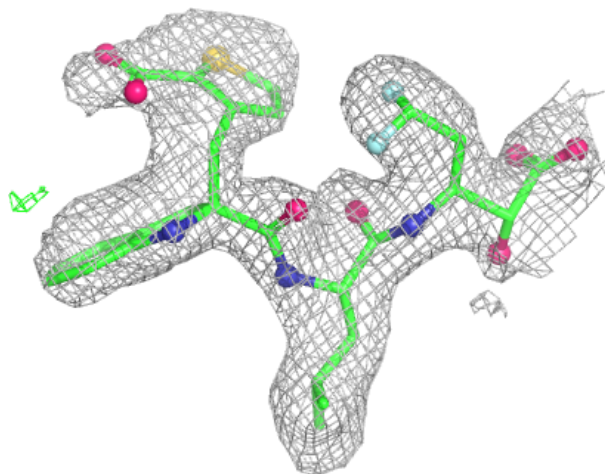
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DN2	B	1176	39/39	0.98	0.04	46,56,79,82	0
3	DN1	A	1176	39/39	0.99	0.04	47,58,84,85	0

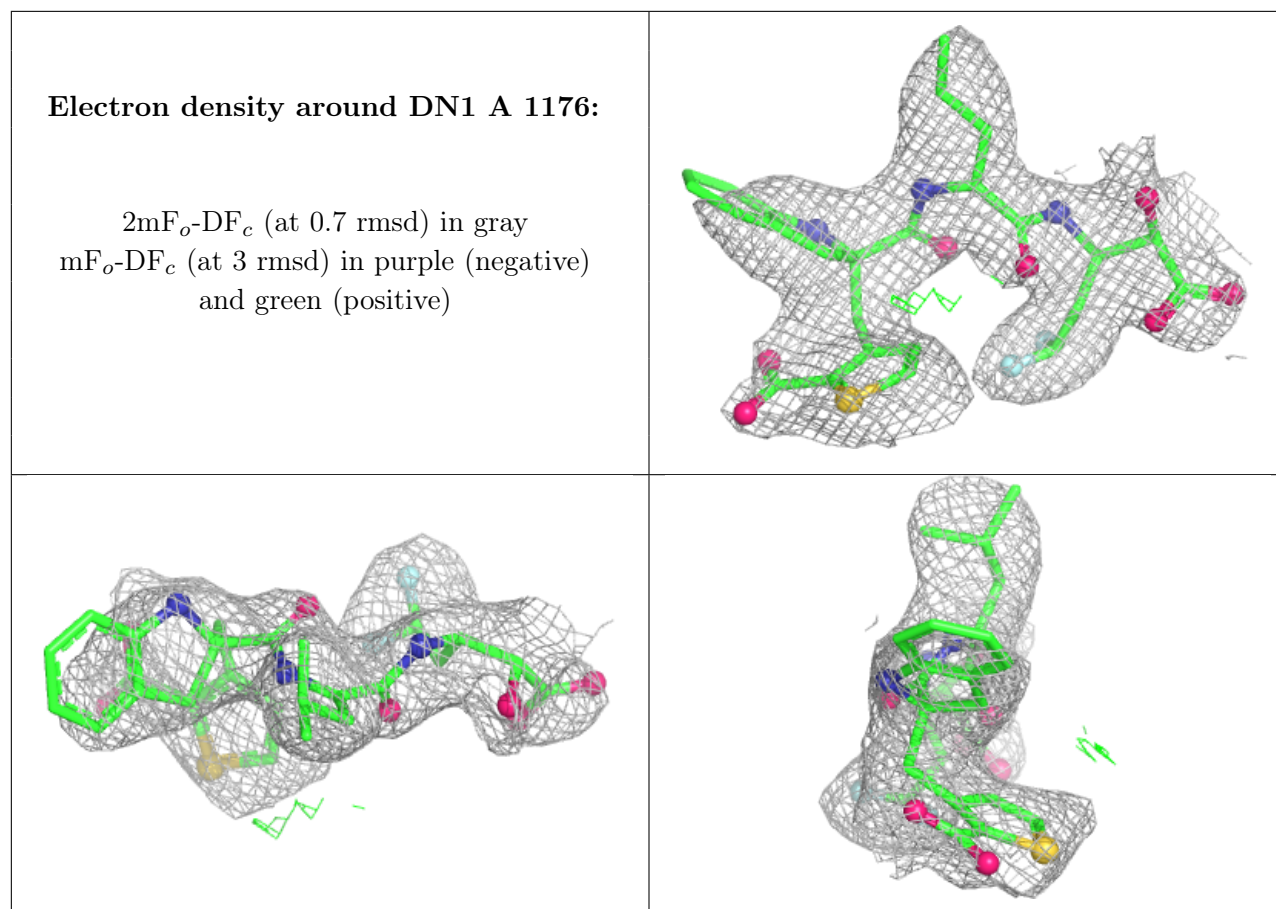
The following is a graphical depiction of the model fit to experimental electron density of all

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 DN2 B 1176:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.