



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:56 AM GMT

PDB ID : 1W3C
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

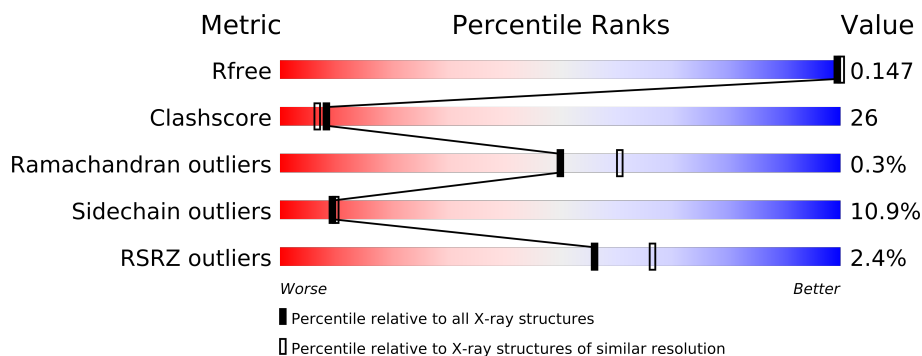
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	187	
1	B	187	
2	C	16	
2	D	16	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2988 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

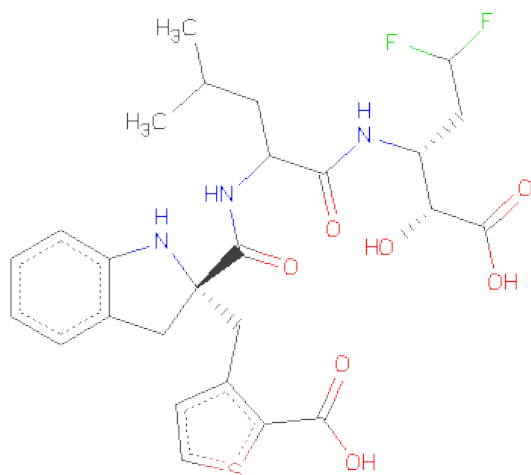
- Molecule 2 is a protein called NONSTRUCTURAL PROTEIN NS4A (P4).

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:

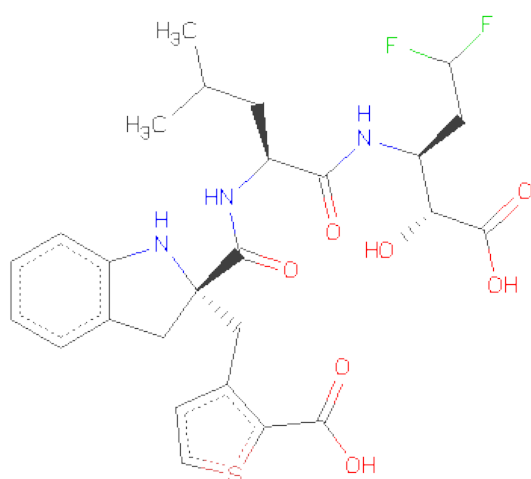
Chain	Residue	Modelled	Actual	Comment	Reference
C	220	LYS	THR	ENGINEERED MUTATION	UNP Q81755
C	235	LYS	PRO	ENGINEERED MUTATION	UNP Q81755
D	220	LYS	THR	ENGINEERED MUTATION	UNP Q81755
D	235	LYS	PRO	ENGINEERED MUTATION	UNP Q81755

- Molecule 3 is 3-({(2S)-2-[({(1R)-1-[({(1R)-1-[(R)-CARBOXY(HYDROXY)METHYL]-3,3-DIFLUOROPROPYL}AMINO)CARBONYL]-3-METHYLBUTYL}AMINO)CARBO NYL]-2,3-DIHYDRO-1H-INDOL-2-YL}METHYL)THIOPHENE-2-CARBOXYLICACID (three-letter code: 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-CARBOXYLICACID (three-letter code: 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.

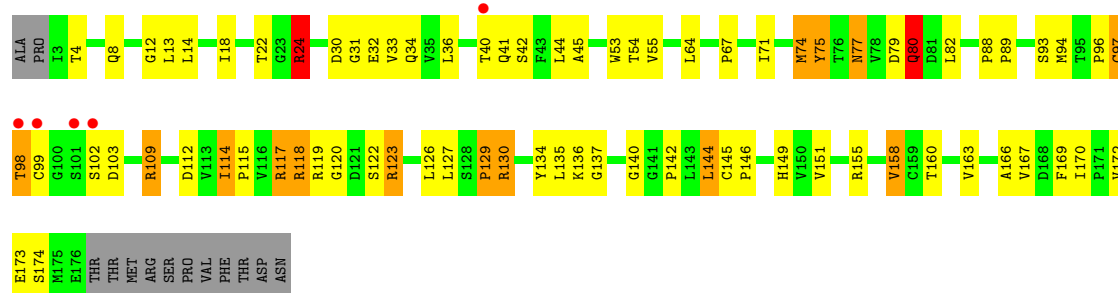
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total 89	O 89	0	0
5	B	96	Total 96	O 96	0	0
5	C	4	Total 4	O 4	0	0
5	D	7	Total 7	O 7	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

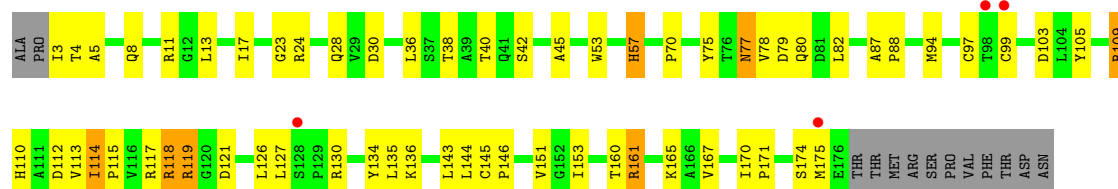
• Molecule 1: PROTEASE/HELICASE NS3 (P70)

Chain A: 



• Molecule 1: PROTEASE/HELICASE NS3 (P70)

Chain B: 



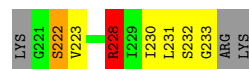
• Molecule 2: NONSTRUCTURAL PROTEIN NS4A (P4)

Chain C: 



• Molecule 2: NONSTRUCTURAL PROTEIN NS4A (P4)

Chain D: 



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 26.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (20.00-2.30) 89.5 (26.68-2.30)	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 0.149 , 0.147	Depositor DCC
R_{free} test set	800 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 69.5	EDS
Estimated twinning fraction	0.224 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 15517 reflections	Xtriage
F_o, F_c correlation	0.96	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.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1298	1.40	12/1769 (0.7%)
1	B	0.48	0/1298	1.26	8/1769 (0.5%)
2	C	0.65	0/84	1.33	1/113 (0.9%)
2	D	0.65	0/84	1.61	3/113 (2.7%)
All	All	0.49	0/2764	1.34	24/3764 (0.6%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	A	24	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	A	109	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	119	ARG	CD-NE-CZ	9.35	136.69	123.60
1	B	109	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	30	ASP	CB-CG-OD1	8.63	126.07	118.30
1	A	117	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	B	109	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	C	228	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	161	ARG	CD-NE-CZ	7.72	134.41	123.60
1	B	119	ARG	CG-CD-NE	6.96	126.41	111.80
1	A	80	GLN	CA-CB-CG	6.95	128.69	113.40
2	D	228	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	D	228	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	57	HIS	CA-CB-CG	6.34	124.38	113.60
1	A	109	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	30	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	D	222	SER	N-CA-CB	-5.98	101.53	110.50
1	A	173	GLU	CB-CG-CD	5.86	130.01	114.20
1	B	11	ARG	NE-CZ-NH2	5.75	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	CD-NE-CZ	-5.56	115.82	123.60
1	A	173	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	118	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	119	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1272	0	1281	71	1
1	B	1272	0	1281	67	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	145	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (145) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1176:DN1:O19	3:A:1176:DN1:H13D	1.52	1.02
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:SER:OG	1:B:109:ARG:NH2	2.09	0.84
1:B:97:CYS:HG	1:B:99:CYS:HG	1.28	0.81
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: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:A:77:ASN:CG	1:A:80:GLN:HE21	1.94	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:A:32:GLU:HB3	1:A:94:MET:HE2	1.76	0.67
1:B:8:GLN:HE21	2:D:228:ARG:HE	1.41	0.67
1:B:77:ASN:C	1:B:77:ASN:HD22	1.99	0.66
1:A:123:ARG:HB2	1:A:123:ARG:HH11	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
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:A:4:THR:OG1	2:C:232:SER:HB3	2.02	0.60
3:A:1176:DN1:C34	3:A:1176:DN1:H232	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	1.68	0.59
1:A:32:GLU:HB3	1:A:94:MET:CE	2.32	0.58
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:136:LYS:CE	4:B:1176:DN2:H32	2.40	0.51
1:B:53:TRP:HZ3	1:B:75:TYR:CD2	2.29	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: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
1:B:105:TYR:CD2	1:B:113:VAL:HG12	2.47	0.48
1:B:80:GLN:OE1	1:B:174:SER:HB3	2.13	0.48
1:A:119:ARG:HH11	1:B:117:ARG:NH2	2.11	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:B:77:ASN:ND2	1:B:77:ASN:C	2.65	0.47
1:A:94:MET:HE2	2:C:231:LEU:CD2	2.44	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1176:DN1:H6C2	3:A:1176:DN1:N3	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:99:CYS:SG	1:B:145:CYS:SG	3.12	0.46
1:B:3:ILE:HA	2:D:233:GLY:N	2.30	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:C22	4:B:1176:DN2:O36	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:13:LEU:O	1:B:17:ILE:HG13	2.17	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:94:MET:HB2	1:B:94:MET:HE3	1.91	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: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:A:34:GLN:NE2	2:C:225:ILE:HD13	2.32	0.44
1:B:80:GLN:HG3	1:B:82:LEU:CB	2.48	0.43
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:33:VAL:HB	2:C:229:ILE:HB	2.01	0.43
3:A:1176:DN1:O19	3:A:1176:DN1:C13	2.43	0.43
1:A:142:PRO:HB2	1:A:144:LEU:HD13	1.99	0.43
1:A:80:GLN:HG2	1:A:82:LEU:HB3	2.01	0.43
1:B:77:ASN:HB3	1:B:80:GLN:HE21	1.84	0.43
1:A:97:CYS:HB3	1:A:151:VAL:HG12	2.01	0.43
1:B:75:TYR:CE2	1:B:82:LEU:HD23	2.54	0.42
1:A:115:PRO:HG2	5:A:2074:HOH:O	2.18	0.42
1:A:31:GLY:CA	2:C:230:ILE:HD13	2.48	0.42
1:A:75:TYR:HE2	1:A:77:ASN:HB2	1.84	0.42
1:B:30:ASP:O	2:D:228:ARG:HG3	2.20	0.42
1:A:119:ARG:NH1	1:B:117:ARG:NH2	2.67	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
5:A:2076:HOH:O	1:B:117:ARG:HD2	2.19	0.41
1:B:175:MET:HB3	1:B:175:MET:HE3	1.81	0.41
1:A:54:THR:OG1	1:A:55:VAL:N	2.54	0.40
1:B:114:ILE:HA	1:B:115:PRO:HD3	1.88	0.40
1:B:87:ALA:HA	1:B:88:PRO:HD3	1.87	0.40
1:A:112:ASP:CB	1:A:134:TYR:HH	2.33	0.40
1:A:75:TYR:CE2	1:A:77:ASN:HB2	2.57	0.40
1:A:12:GLY:HA2	5:A:2011:HOH:O	2.22	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	Distance(Å)	Clash(Å)
1:A:24:ARG:NH2	1:B:24:ARG:NH2[4.654]	1.84	0.36

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	33	39
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%)	50	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/154 (92%)	122 (86%)	19 (14%)	6	5
1	B	141/154 (92%)	132 (94%)	9 (6%)	25	31
2	C	10/13 (77%)	8 (80%)	2 (20%)	2	1
2	D	10/13 (77%)	7 (70%)	3 (30%)	0	0
All	All	302/334 (90%)	269 (89%)	33 (11%)	9	10

All (33) 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	74	MET
1	A	75	TYR
1	A	77	ASN
1	A	80	GLN
1	A	93	SER
1	A	97	CYS
1	A	99	CYS
1	A	102	SER
1	A	114	ILE
1	A	123	ARG
1	A	129	PRO
1	A	135	LEU
1	A	144	LEU
1	A	146	PRO
1	A	158	VAL
1	A	160	THR
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

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	153	ILE
2	C	228	ARG
2	C	231	LEU
2	D	222	SER
2	D	228	ARG
2	D	231	LEU

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

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

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
3	DN1	A	1176	1	41,41,41	2.48	8 (19%)	58,59,59	2.26	19 (32%)
4	DN2	B	1176	1	41,41,41	2.70	8 (19%)	58,59,59	2.17	16 (27%)

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
3	DN1	A	1176	1	1/1/10/13	1/41/53/53	0/1/3/3
4	DN2	B	1176	1	-	0/41/53/53	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1176	DN2	C17-C12	8.22	1.63	1.54
3	A	1176	DN1	F15-C14	-7.70	1.22	1.35
4	B	1176	DN2	F16-C14	-7.42	1.23	1.35
4	B	1176	DN2	C17-C18	7.19	1.62	1.52
3	A	1176	DN1	C17-C12	7.17	1.62	1.54
4	B	1176	DN2	F15-C14	-7.16	1.23	1.35
3	A	1176	DN1	F16-C14	-6.70	1.24	1.35
4	B	1176	DN2	C2-N1	5.66	1.53	1.46
3	A	1176	DN1	C17-C18	5.25	1.59	1.52
3	A	1176	DN1	C2-N1	4.74	1.52	1.46
3	A	1176	DN1	C9-N11	3.15	1.41	1.34
4	B	1176	DN2	C9-N11	2.63	1.40	1.34
4	B	1176	DN2	C31-C30	2.29	1.44	1.40
3	A	1176	DN1	C12-N11	2.29	1.50	1.46
3	A	1176	DN1	C31-C30	2.20	1.44	1.40
4	B	1176	DN2	O21-C17	2.16	1.46	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1176	DN2	C22-C2-N1	-7.28	101.64	111.05
4	B	1176	DN2	C13-C12-N11	6.53	118.98	110.19
3	A	1176	DN1	O36-C35-C34	-5.58	112.87	123.11
3	A	1176	DN1	C12-N11-C9	-4.98	113.87	123.24
3	A	1176	DN1	C14-C13-C12	4.79	121.81	114.69
3	A	1176	DN1	O10-C9-N11	-4.79	113.71	122.93
3	A	1176	DN1	C9-C4-N3	4.58	124.15	111.28
4	B	1176	DN2	C12-C17-C18	-4.50	99.20	111.03
3	A	1176	DN1	C22-C2-N1	-4.42	105.35	111.05
4	B	1176	DN2	C22-C30-C34	-4.26	119.10	126.89
4	B	1176	DN2	O21-C17-C18	-3.97	102.21	110.73
3	A	1176	DN1	F15-C14-C13	3.95	120.41	109.46
3	A	1176	DN1	C25-C24-N1	3.88	114.92	110.99
3	A	1176	DN1	C2-C22-C30	-3.69	109.88	115.15
4	B	1176	DN2	C23-C2-C1	3.68	118.50	110.71
3	A	1176	DN1	C5-C4-C9	3.66	120.22	110.57
3	A	1176	DN1	O37-C35-O36	3.63	131.58	123.35
4	B	1176	DN2	C25-C24-N1	3.33	114.37	110.99
4	B	1176	DN2	O2-C1-C2	-3.13	116.08	120.98
4	B	1176	DN2	O19-C18-O20	3.02	130.89	124.07
3	A	1176	DN1	O10-C9-C4	2.94	126.78	120.31
4	B	1176	DN2	C2-C1-N3	2.89	121.99	116.52
3	A	1176	DN1	O19-C18-C17	2.66	121.65	113.89
4	B	1176	DN2	C30-C34-S33	2.47	113.95	111.00
3	A	1176	DN1	C22-C30-C34	-2.46	122.39	126.89
4	B	1176	DN2	O20-C18-C17	-2.41	114.08	121.15
4	B	1176	DN2	C27-C25-C24	2.40	121.56	119.82
3	A	1176	DN1	C30-C34-S33	2.40	113.87	111.00
3	A	1176	DN1	C23-C2-C1	2.25	115.47	110.71
4	B	1176	DN2	C4-C9-N11	-2.19	111.72	116.81
4	B	1176	DN2	O37-C35-C34	-2.17	119.13	123.11
3	A	1176	DN1	C26-C24-N1	-2.06	123.73	128.24
3	A	1176	DN1	C2-N1-C24	-2.04	105.34	109.39
3	A	1176	DN1	C22-C2-C23	-2.03	108.94	112.28
4	B	1176	DN2	C2-N1-C24	-2.03	105.36	109.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1176	DN1	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1176	DN1	C13-C12-N11-C9

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	174/187 (93%)	0.09	5 (2%) 49 59	30, 49, 73, 86	0
1	B	174/187 (93%)	0.01	4 (2%) 57 67	30, 47, 73, 87	0
2	C	13/16 (81%)	-0.01	0 100 100	33, 39, 75, 94	0
2	D	13/16 (81%)	-0.17	0 100 100	35, 39, 49, 67	0
All	All	374/406 (92%)	0.04	9 (2%) 56 66	30, 47, 73, 94	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	CYS	4.5
1	A	40	THR	3.4
1	B	175	MET	3.0
1	A	99	CYS	2.9
1	A	101	SER	2.6
1	B	128	SER	2.5
1	B	98	THR	2.3
1	A	98	THR	2.2
1	A	102	SER	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DN1	A	1176	39/39	0.16	1.76	47,58,84,85	0
4	DN2	B	1176	39/39	0.15	0.97	46,56,79,82	0

6.5 Other polymers

There are no such residues in this entry.