



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:53 AM UTC

PDB ID : 1DXP / pdb_00001dxp
Title : Inhibition of the Hepatitis C Virus NS3/4A Protease. The Crystal Structures of Two Protease-Inhibitor Complexes (apo structure)
Authors : Di Marco, S.; Rizzi, M.; Volpari, C.; Walsh, M.; Narjes, F.; Colarusso, S.; De Francesco, R.; Matassa, V.G.; Sollazzo, M.
Deposited on : 2000-01-13
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

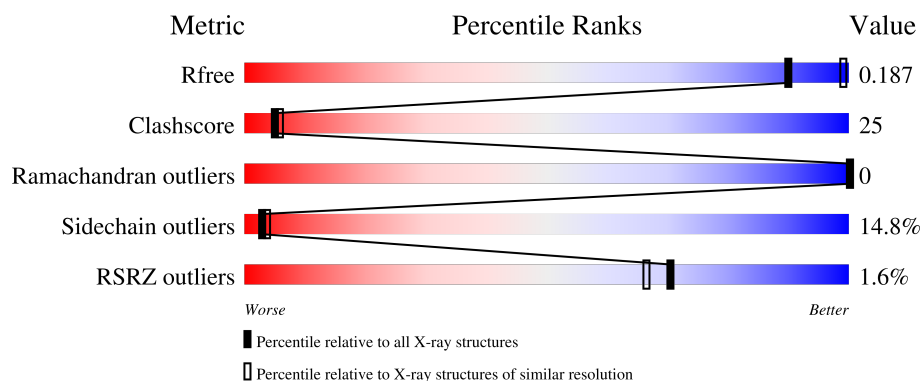
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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
4	GOL	B	202	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2951 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	175	Total	C	N	O	S	0	0	0
			1283	801	231	241	10			
1	B	175	Total	C	N	O	S	0	0	0
			1283	801	231	241	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			84	55	15	14			
2	D	12	Total	C	N	O	0	0	0
			84	55	15	14			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

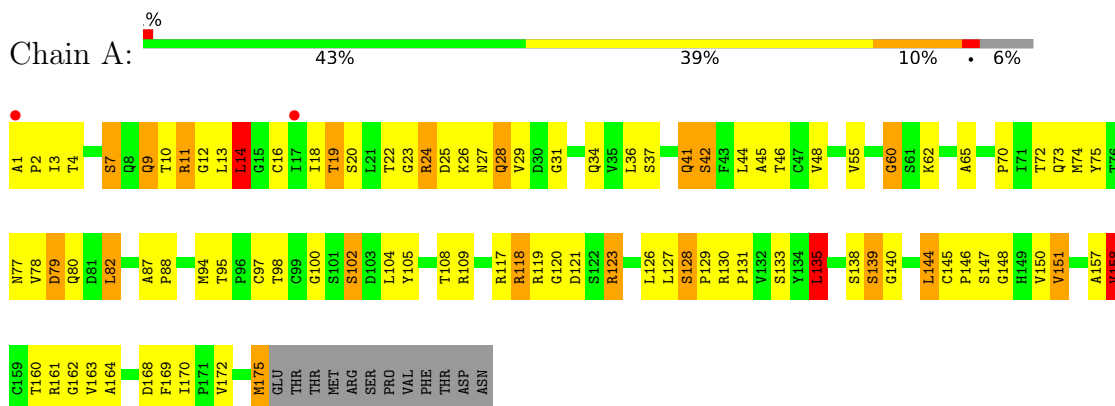
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	106	Total	O	0	0
			106	106		
5	C	11	Total	O	0	0
			11	11		
5	D	2	Total	O	0	0
			2	2		

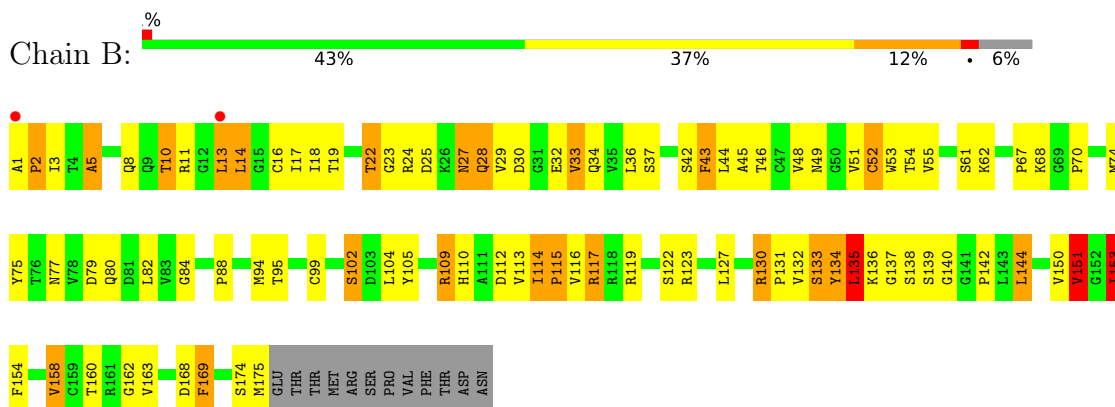
3 Residue-property plots

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.

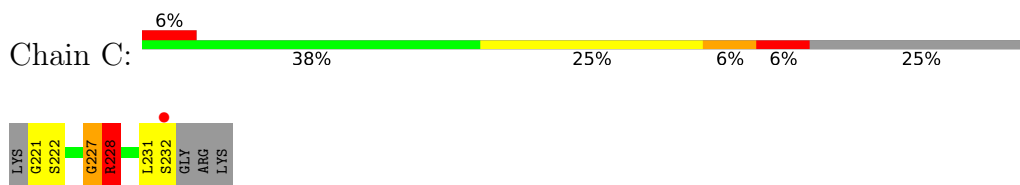
• Molecule 1: PROTEASE/HELICASE NS3 (P70)



• 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	92.98Å 92.98Å 81.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.40) 99.8 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.298 0.181 , 0.187	Depositor DCC
R_{free} test set	789 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2951	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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: GOL, ZN

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	0.73	0/1310	2.10	46/1786 (2.6%)
1	B	0.72	0/1310	2.03	45/1786 (2.5%)
2	C	0.78	0/83	1.94	3/111 (2.7%)
2	D	0.76	0/83	1.86	0/111
All	All	0.73	0/2786	2.05	94/3794 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ARG	CA-C-O	-10.88	109.80	121.45
1	B	133	SER	CA-C-O	10.10	131.58	119.97
1	B	109	ARG	CD-NE-CZ	-10.06	110.32	124.40
1	B	5	ALA	CA-C-O	-9.63	110.30	120.89
1	B	119	ARG	CD-NE-CZ	9.29	137.41	124.40
1	A	121	ASP	CA-CB-CG	9.17	121.77	112.60
1	B	110	HIS	CA-CB-CG	-8.65	105.15	113.80
1	A	158	VAL	CB-CA-C	8.55	123.44	110.96
1	A	108	THR	CA-C-N	8.12	137.04	121.54
1	A	108	THR	C-N-CA	8.12	137.04	121.54
1	B	109	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	B	28	GLN	N-CA-CB	7.69	121.67	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ILE	CA-C-O	7.66	123.67	119.15
1	B	158	VAL	N-CA-CB	7.58	120.08	111.21
1	A	157	ALA	CA-C-N	-7.47	113.41	123.12
1	A	157	ALA	C-N-CA	-7.47	113.41	123.12
1	A	117	ARG	CA-C-O	-7.26	112.81	120.58
1	B	134	TYR	CA-CB-CG	-7.17	100.98	113.90
1	A	79	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	169	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	34	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	B	114	ILE	CA-C-O	6.94	123.81	119.51
1	A	135	LEU	N-CA-C	-6.88	104.78	113.72
2	C	228	ARG	NE-CZ-NH2	-6.81	113.07	119.20
1	A	78	VAL	N-CA-C	6.79	118.36	110.62
1	A	31	GLY	CA-C-O	-6.72	117.61	122.45
1	A	14	LEU	N-CA-CB	6.62	119.86	110.12
1	A	133	SER	CA-C-O	6.42	127.27	119.49
1	A	130	ARG	CD-NE-CZ	-6.40	115.44	124.40
1	A	130	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	9	GLN	CB-CA-C	6.39	120.43	109.51
1	B	139	SER	CA-C-O	-6.38	114.17	121.19
1	B	113	VAL	O-C-N	6.34	130.40	122.66
1	B	151	VAL	CA-C-O	6.31	125.26	119.20
2	C	228	ARG	CD-NE-CZ	6.28	133.20	124.40
1	A	131	PRO	CA-C-O	-6.22	114.25	121.34
1	B	117	ARG	CA-CB-CG	-6.19	101.72	114.10
1	B	150	VAL	CA-C-O	-6.19	113.71	120.71
1	B	135	LEU	N-CA-C	-6.18	105.78	113.38
1	B	30	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	79	ASP	O-C-N	6.14	128.42	122.03
1	B	116	VAL	CA-C-N	-6.10	114.65	122.77
1	B	116	VAL	C-N-CA	-6.10	114.65	122.77
1	A	162	GLY	CA-C-N	-6.10	115.23	123.10
1	A	162	GLY	C-N-CA	-6.10	115.23	123.10
1	A	168	ASP	CA-CB-CG	-6.08	106.52	112.60
1	B	153	ILE	CB-CA-C	6.08	119.86	110.50
1	A	170	ILE	CA-C-N	6.03	125.79	119.76
1	A	170	ILE	C-N-CA	6.03	125.79	119.76
1	A	12	GLY	CA-C-O	-6.01	115.95	121.72
1	B	33	VAL	CA-C-O	-5.92	114.03	120.67
1	A	24	ARG	CA-CB-CG	5.91	125.93	114.10
1	B	168	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	29	VAL	CA-C-N	-5.68	113.01	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	C-N-CA	-5.68	113.01	122.21
1	B	2	PRO	N-CA-C	-5.68	107.41	114.68
1	B	49	ASN	CA-CB-CG	-5.62	106.98	112.60
1	B	153	ILE	N-CA-CB	-5.59	102.26	111.44
1	A	60	GLY	CA-C-N	-5.58	113.69	122.79
1	A	60	GLY	C-N-CA	-5.58	113.69	122.79
1	A	133	SER	CA-CB-OG	-5.54	100.01	111.10
1	B	153	ILE	CA-CB-CG2	5.51	119.86	110.50
1	A	19	THR	O-C-N	-5.46	114.60	122.36
2	C	227	GLY	CA-C-O	-5.44	116.20	121.75
1	B	162	GLY	CA-C-N	-5.40	115.99	122.90
1	B	162	GLY	C-N-CA	-5.40	115.99	122.90
1	B	154	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	19	THR	CA-C-O	5.35	125.86	119.60
1	B	10	THR	CA-C-O	-5.35	113.02	118.90
1	B	95	THR	CB-CA-C	5.34	117.70	109.15
1	B	62	LYS	N-CA-C	5.31	117.54	110.53
1	B	27	ASN	CA-C-N	-5.30	113.84	121.42
1	B	27	ASN	C-N-CA	-5.30	113.84	121.42
1	B	52	CYS	CA-C-O	5.30	126.36	120.43
1	A	105	TYR	CA-CB-CG	-5.29	104.37	113.90
1	B	13	LEU	CA-C-O	-5.29	115.27	120.82
1	A	88	PRO	O-C-N	5.28	123.74	121.31
1	A	87	ALA	O-C-N	5.26	127.33	121.43
1	B	61	SER	CA-CB-OG	-5.26	100.59	111.10
1	B	43	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	34	GLN	CG-CD-NE2	5.24	124.25	116.40
1	A	41	GLN	N-CA-C	5.23	116.24	108.86
1	A	150	VAL	CA-CB-CG2	-5.22	101.53	110.40
1	B	130	ARG	CD-NE-CZ	-5.21	117.10	124.40
1	A	20	SER	CA-C-O	5.18	125.92	119.97
1	B	169	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	34	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	B	115	PRO	CA-C-O	5.08	126.67	121.23
1	A	27	ASN	OD1-CG-ND2	5.05	127.65	122.60
1	B	29	VAL	CA-C-O	-5.05	114.98	120.84
1	A	82	LEU	N-CA-C	5.04	117.18	109.07
1	A	130	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	99	CYS	CA-C-O	-5.03	114.19	119.97
1	A	7	SER	N-CA-CB	5.02	118.39	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	GLY	Mainchain

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	1283	0	1294	74	0
1	B	1283	0	1294	63	0
2	C	84	0	99	8	0
2	D	84	0	99	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	6	0	5	3	0
5	A	90	0	0	11	0
5	B	106	0	0	3	0
5	C	11	0	0	4	0
5	D	2	0	0	0	0
All	All	2951	0	2791	138	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 25.

All (138) 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)
4:B:202:GOL:C1	4:B:202:GOL:O1	1.63	1.44
1:A:160:THR:HG22	1:A:161:ARG:HG3	1.41	1.01
1:B:42:SER:HB3	1:B:109:ARG:NH2	1.74	1.01
2:C:232:SER:HB2	5:C:2009:HOH:O	1.69	0.92
1:A:75:TYR:OH	1:A:80:GLN:NE2	2.04	0.89
1:A:119:ARG:HH22	1:B:102:SER:HB3	1.42	0.84
1:B:46:THR:HB	1:B:153:ILE:HD11	1.63	0.80
1:B:18:ILE:O	1:B:22:THR:HG23	1.81	0.80
1:A:9:GLN:HG3	5:C:2007:HOH:O	1.82	0.78
1:B:11:ARG:HH21	1:B:25:ASP:CG	1.90	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:NH2	1:B:102:SER:HB3	1.98	0.77
1:A:23:GLY:HA3	1:A:70:PRO:HG3	1.66	0.75
1:B:77:ASN:CG	1:B:80:GLN:HG2	2.11	0.75
1:A:100:GLY:HA2	5:A:2068:HOH:O	1.86	0.75
1:A:10:THR:HG23	2:C:227:GLY:HA2	1.68	0.75
1:A:79:ASP:HB2	5:A:2054:HOH:O	1.87	0.74
1:A:42:SER:OG	1:A:109:ARG:NH2	2.21	0.74
1:A:22:THR:HB	5:A:2017:HOH:O	1.89	0.72
1:A:3:ILE:HD13	1:A:144:LEU:HD23	1.71	0.71
1:A:1:ALA:HB3	5:A:2002:HOH:O	1.90	0.71
1:A:28:GLN:C	1:A:28:GLN:HE21	1.98	0.71
1:A:77:ASN:OD1	1:A:80:GLN:NE2	2.26	0.69
1:A:77:ASN:HB3	1:A:80:GLN:HG2	1.74	0.68
1:A:24:ARG:HB3	5:A:2017:HOH:O	1.93	0.68
1:B:48:VAL:HG21	1:B:175:MET:HE1	1.75	0.68
1:A:28:GLN:NE2	2:C:228:ARG:HH12	1.92	0.68
1:A:62:LYS:HE3	5:A:2043:HOH:O	1.94	0.68
1:B:42:SER:HB3	1:B:109:ARG:CZ	2.23	0.68
1:B:112:ASP:HB2	1:B:134:TYR:OH	1.95	0.67
1:A:172:VAL:HA	1:A:175:MET:HG3	1.78	0.65
1:B:11:ARG:NH2	1:B:25:ASP:OD1	2.30	0.65
1:A:123:ARG:HH21	1:A:158:VAL:HG21	1.62	0.64
1:B:80:GLN:HG3	1:B:82:LEU:HB3	1.80	0.64
1:A:4:THR:OG1	2:C:232:SER:HB3	1.97	0.63
1:B:14:LEU:HD12	5:B:2019:HOH:O	1.97	0.63
1:A:3:ILE:HD11	1:A:148:GLY:HA2	1.79	0.63
1:A:77:ASN:CG	1:A:80:GLN:HG2	2.24	0.63
1:B:75:TYR:OH	1:B:80:GLN:NE2	2.33	0.62
1:A:118:ARG:HD2	1:A:120:GLY:O	2.00	0.61
1:B:142:PRO:HB2	1:B:144:LEU:HD13	1.81	0.61
1:A:74:MET:HE2	1:A:75:TYR:HB2	1.81	0.61
1:A:77:ASN:CB	1:A:80:GLN:HE21	2.13	0.61
1:A:77:ASN:CB	1:A:80:GLN:HG2	2.33	0.59
4:B:202:GOL:C1	4:B:202:GOL:HO1	2.07	0.58
1:A:22:THR:CB	5:A:2017:HOH:O	2.49	0.58
1:A:48:VAL:HG21	1:A:175:MET:HE1	1.84	0.58
1:A:72:THR:HG22	1:A:73:GLN:O	2.04	0.58
1:B:74:MET:HE3	1:B:75:TYR:HB3	1.85	0.57
1:B:137:GLY:H	4:B:202:GOL:C3	2.16	0.57
1:A:77:ASN:HA	5:A:2056:HOH:O	2.04	0.56
1:B:77:ASN:HB3	1:B:80:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:O	1:A:138:SER:HB2	2.06	0.56
1:B:115:PRO:HB2	1:B:127:LEU:HD12	1.89	0.55
1:A:28:GLN:HE22	2:C:228:ARG:HH12	1.54	0.54
1:B:77:ASN:CB	1:B:80:GLN:HG2	2.37	0.54
1:A:13:LEU:O	1:A:16:CYS:N	2.41	0.54
1:B:127:LEU:HD23	5:B:2090:HOH:O	2.08	0.54
1:B:42:SER:HB3	1:B:109:ARG:HH22	1.66	0.53
1:A:14:LEU:HD12	1:A:18:ILE:HD11	1.91	0.53
1:A:77:ASN:HB3	1:A:80:GLN:CG	2.39	0.53
1:B:8:GLN:HE21	2:D:228:ARG:HE	1.55	0.53
1:A:44:LEU:HD21	1:A:109:ARG:HA	1.90	0.52
1:B:52:CYS:O	1:B:84:GLY:HA2	2.09	0.52
1:A:123:ARG:NH2	1:A:158:VAL:HG11	2.24	0.52
1:A:119:ARG:HD3	1:B:117:ARG:NH2	2.25	0.52
1:A:1:ALA:HB1	1:A:2:PRO:HD2	1.91	0.51
1:B:112:ASP:CB	1:B:134:TYR:OH	2.58	0.51
1:B:14:LEU:HD13	1:B:18:ILE:CD1	2.40	0.51
1:B:74:MET:HE3	1:B:75:TYR:CB	2.40	0.51
1:A:77:ASN:CG	1:A:80:GLN:HE21	2.18	0.51
1:A:26:LYS:HB2	1:A:26:LYS:NZ	2.25	0.51
1:A:77:ASN:HD22	1:A:77:ASN:C	2.18	0.51
1:B:51:VAL:HG11	1:B:74:MET:HE2	1.93	0.51
1:A:119:ARG:HH22	1:B:102:SER:CB	2.18	0.50
1:A:46:THR:HG23	1:A:94:MET:HE2	1.93	0.50
1:A:80:GLN:HG3	1:A:82:LEU:HB3	1.93	0.50
1:B:23:GLY:HA3	1:B:70:PRO:HG3	1.94	0.50
1:B:104:LEU:HD13	1:B:151:VAL:HG21	1.95	0.49
1:A:44:LEU:O	1:A:140:GLY:HA3	2.13	0.48
1:A:104:LEU:HD22	1:A:151:VAL:HG11	1.96	0.48
1:B:32:GLU:HB3	1:B:94:MET:HE2	1.96	0.48
1:B:131:PRO:O	1:B:134:TYR:HB3	2.14	0.47
1:A:13:LEU:O	1:A:14:LEU:C	2.55	0.47
2:C:232:SER:HA	5:C:2011:HOH:O	2.13	0.47
1:B:132:VAL:HG13	1:B:133:SER:N	2.29	0.47
1:A:100:GLY:CA	5:A:2068:HOH:O	2.56	0.47
1:A:145:CYS:HB2	1:A:146:PRO:CD	2.45	0.46
1:B:5:ALA:HA	2:D:230:ILE:O	2.14	0.46
1:A:55:VAL:HG21	1:A:139:SER:HB3	1.97	0.46
1:A:14:LEU:HD12	1:A:18:ILE:CD1	2.45	0.46
1:A:123:ARG:NH2	1:A:158:VAL:HG21	2.27	0.46
1:B:25:ASP:O	1:B:67:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:N	1:B:109:ARG:HH12	2.14	0.46
1:B:14:LEU:HD13	1:B:14:LEU:O	2.16	0.46
1:A:145:CYS:CB	1:A:146:PRO:CD	2.94	0.46
1:B:44:LEU:O	1:B:140:GLY:HA3	2.16	0.46
1:A:3:ILE:HD11	1:A:148:GLY:CA	2.46	0.45
1:A:3:ILE:CD1	1:A:148:GLY:HA2	2.46	0.45
1:A:11:ARG:HH21	1:A:25:ASP:CG	2.24	0.45
1:A:65:ALA:HB3	5:A:2045:HOH:O	2.16	0.45
1:B:14:LEU:HD22	1:B:14:LEU:HA	1.74	0.45
1:B:14:LEU:CD1	1:B:18:ILE:HD11	2.47	0.45
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.39	0.44
1:B:135:LEU:O	1:B:138:SER:HB2	2.18	0.44
1:A:128:SER:HA	1:A:129:PRO:HD3	1.81	0.44
1:B:36:LEU:HA	2:D:224:VAL:O	2.18	0.43
1:B:19:THR:HG21	2:D:224:VAL:HG13	2.00	0.43
1:A:95:THR:HG22	5:A:2065:HOH:O	2.19	0.43
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.77	0.43
1:B:1:ALA:HB3	1:B:3:ILE:O	2.19	0.43
1:B:33:VAL:HB	2:D:229:ILE:HB	2.00	0.43
1:B:51:VAL:CG1	1:B:74:MET:HE2	2.49	0.43
1:A:28:GLN:C	1:A:28:GLN:NE2	2.74	0.43
1:B:10:THR:HG23	2:D:227:GLY:HA2	2.00	0.43
1:B:51:VAL:HG11	1:B:53:TRP:CE2	2.54	0.43
1:B:136:LYS:HD3	1:B:136:LYS:HA	1.89	0.43
1:A:80:GLN:HG3	1:A:82:LEU:CB	2.49	0.42
1:A:36:LEU:HD11	1:A:45:ALA:HB2	2.00	0.42
1:A:28:GLN:NE2	1:A:28:GLN:O	2.43	0.42
1:B:122:SER:HB2	1:B:169:PHE:O	2.20	0.42
1:B:54:THR:OG1	1:B:55:VAL:N	2.51	0.42
1:B:109:ARG:HH11	1:B:109:ARG:HD2	1.40	0.42
2:C:221:GLY:N	5:C:2006:HOH:O	2.53	0.42
1:A:160:THR:O	1:A:161:ARG:HB2	2.20	0.42
1:B:2:PRO:HD3	1:B:105:TYR:OH	2.20	0.41
1:B:160:THR:O	1:B:163:VAL:HG12	2.19	0.41
1:A:19:THR:HA	1:A:22:THR:OG1	2.20	0.41
1:A:145:CYS:HB2	1:A:146:PRO:HD3	2.02	0.41
1:B:13:LEU:O	1:B:16:CYS:N	2.52	0.41
1:A:126:LEU:HD22	1:A:164:ALA:O	2.21	0.41
1:B:27:ASN:HD22	1:B:27:ASN:HA	1.46	0.41
1:B:133:SER:OG	1:B:134:TYR:N	2.54	0.41
1:B:74:MET:CE	1:B:75:TYR:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:OG1	2:C:232:SER:CB	2.68	0.41
1:B:11:ARG:NH2	1:B:25:ASP:CG	2.68	0.41
1:A:102:SER:HB2	5:B:2092:HOH:O	2.21	0.41
1:B:36:LEU:HD11	1:B:45:ALA:HB2	2.03	0.40
1:B:134:TYR:O	1:B:134:TYR:CG	2.74	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	173/187 (92%)	165 (95%)	8 (5%)	0	100	100
1	B	173/187 (92%)	160 (92%)	13 (8%)	0	100	100
2	C	10/16 (62%)	9 (90%)	1 (10%)	0	100	100
2	D	10/16 (62%)	10 (100%)	0	0	100	100
All	All	366/406 (90%)	344 (94%)	22 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	142/154 (92%)	122 (86%)	20 (14%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	142/154 (92%)	124 (87%)	18 (13%)	4	6
2	C	10/13 (77%)	7 (70%)	3 (30%)	0	0
2	D	10/13 (77%)	6 (60%)	4 (40%)	0	0
All	All	304/334 (91%)	259 (85%)	45 (15%)	3	4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	14	LEU
1	A	28	GLN
1	A	37	SER
1	A	41	GLN
1	A	42	SER
1	A	97	CYS
1	A	98	THR
1	A	102	SER
1	A	118	ARG
1	A	123	ARG
1	A	128	SER
1	A	135	LEU
1	A	139	SER
1	A	144	LEU
1	A	147	SER
1	A	151	VAL
1	A	158	VAL
1	A	163	VAL
1	A	175	MET
1	B	14	LEU
1	B	17	ILE
1	B	22	THR
1	B	24	ARG
1	B	28	GLN
1	B	37	SER
1	B	68	LYS
1	B	88	PRO
1	B	102	SER
1	B	114	ILE
1	B	123	ARG
1	B	130	ARG
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	151	VAL
1	B	153	ILE
1	B	158	VAL
1	B	174	SER
2	C	222	SER
2	C	228	ARG
2	C	231	LEU
2	D	228	ARG
2	D	230	ILE
2	D	231	LEU
2	D	232	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	28	GLN
1	A	77	ASN
1	A	80	GLN
1	A	110	HIS
1	A	149	HIS
1	B	8	GLN
1	B	27	ASN

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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	202	-	5,5,5	4.61	4 (80%)	5,5,5	3.56	2 (40%)

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	GOL	B	202	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	GOL	C3-C2	-7.17	1.24	1.51
4	B	202	GOL	O1-C1	5.04	1.63	1.42
4	B	202	GOL	O3-C3	4.27	1.60	1.42
4	B	202	GOL	C1-C2	-3.03	1.40	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	GOL	O3-C3-C2	5.94	137.13	110.38
4	B	202	GOL	O1-C1-C2	5.07	133.18	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	202	GOL	C1-C2-C3-O3
4	B	202	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	GOL	3	0

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	175/187 (93%)	-0.24	2 (1%) 78 74	24, 43, 75, 92	0
1	B	175/187 (93%)	-0.26	2 (1%) 78 74	25, 41, 73, 91	0
2	C	12/16 (75%)	-0.18	1 (8%) 17 14	28, 35, 49, 74	0
2	D	12/16 (75%)	-0.13	1 (8%) 17 14	30, 36, 45, 75	0
All	All	374/406 (92%)	-0.24	6 (1%) 70 66	24, 42, 74, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	LEU	3.1
1	A	1	ALA	2.9
2	D	232	SER	2.7
2	C	232	SER	2.4
1	B	1	ALA	2.3
1	A	17	ILE	2.1

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
4	GOL	B	202	6/6	0.80	0.13	47,59,64,69	0
3	ZN	A	201	1/1	0.98	0.07	62,62,62,62	0
3	ZN	B	201	1/1	0.99	0.09	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.