Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 05:54 AM EST

PDB ID	:	1Q5M
Title	:	Binary complex of rabbit 20alpha-hydroxysteroid dehydrogenase with NADPH
Authors	:	Couture, J.F.; Legrand, P.; Cantin, L.; Labrie, F.; Luu-The, V.; Breton, R.
Deposited on	:	2003-08-08
Resolution	:	1.32 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:

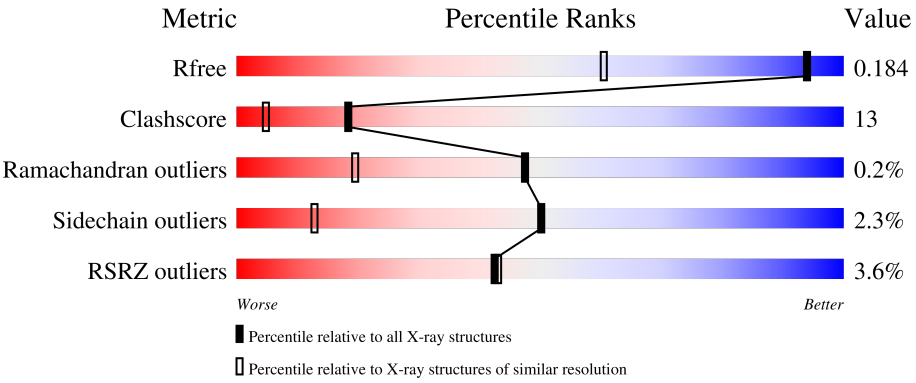
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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}	130704	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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 <=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	322	3% 77% 19% .
1	B	322	4% 79% 16% 5%

2 Entry composition

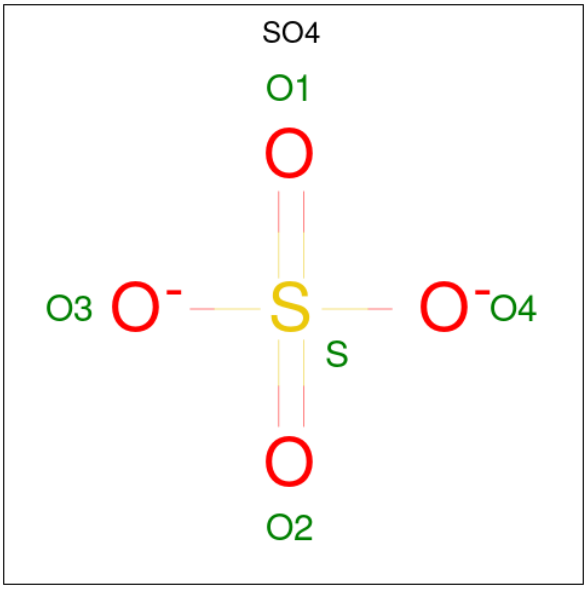
There are 4 unique types of molecules in this entry. The entry contains 6032 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Prostaglandin-E2 9-reductase.

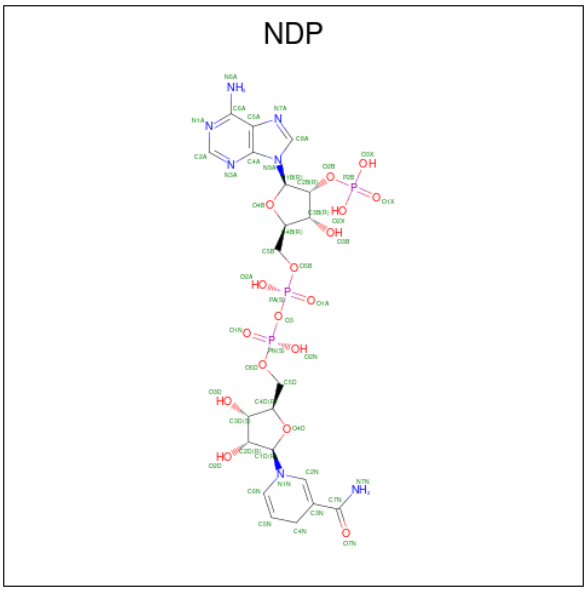
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	7	0
			2598	1671	438	479	10			
1	B	322	Total	C	N	O	S	0	5	0
			2595	1672	436	477	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 4 is water.

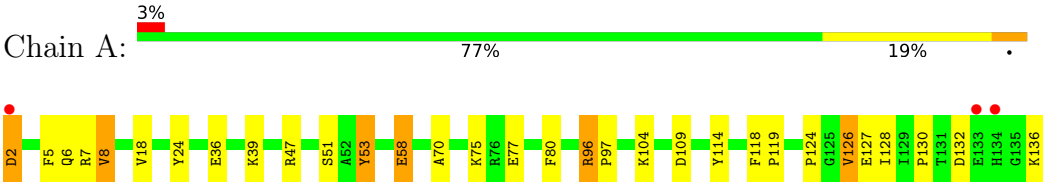
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	4	0
			333	333		
4	B	400	Total	O	22	0
			400	400		

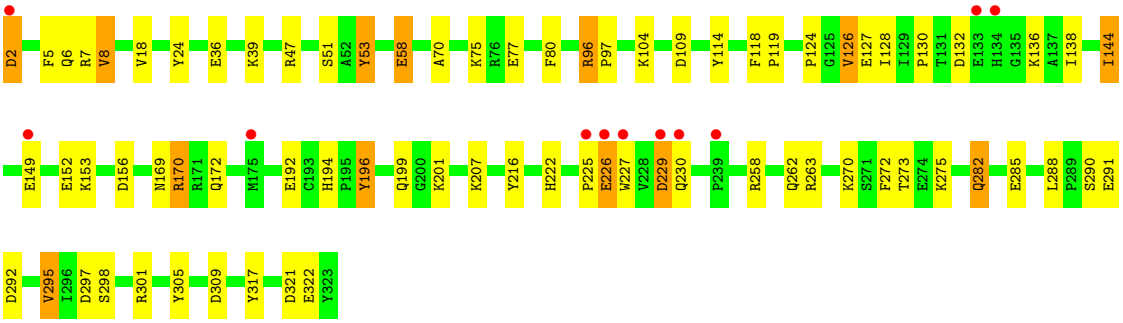
3 Residue-property plots (i)

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: Prostaglandin-E2 9-reductase

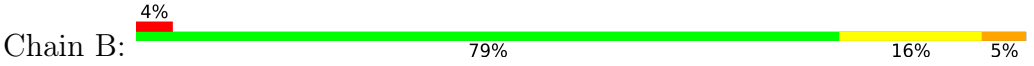
Chain A:

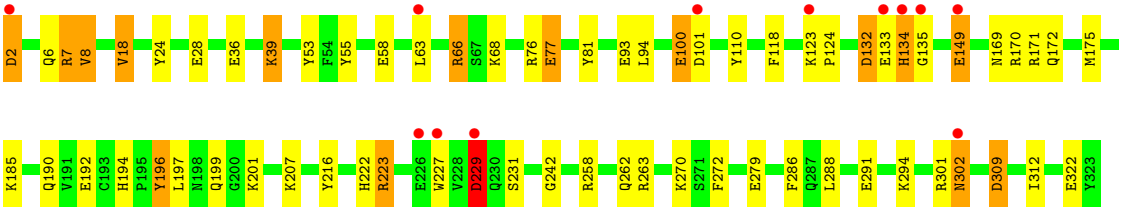




• Molecule 1: Prostaglandin-E2 9-reductase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.54Å 85.27Å 66.15Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	57.74 – 1.32 39.08 – 1.32	Depositor EDS
% Data completeness (in resolution range)	96.4 (57.74-1.32) 96.4 (39.08-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.148 , 0.177 0.157 , 0.184	Depositor DCC
R_{free} test set	5499 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, SO4

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	1.54	21/2700 (0.8%)	1.47	37/3653 (1.0%)
1	B	1.58	29/2683 (1.1%)	1.42	39/3632 (1.1%)
All	All	1.56	50/5383 (0.9%)	1.45	76/7285 (1.0%)

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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	GLU	CD-OE2	15.37	1.42	1.25
1	A	291	GLU	CD-OE2	10.31	1.36	1.25
1	B	291	GLU	CD-OE2	10.26	1.36	1.25
1	B	100	GLU	CD-OE1	10.18	1.36	1.25
1	A	8	VAL	CA-CB	10.16	1.76	1.54
1	A	53	TYR	CD1-CE1	10.02	1.54	1.39
1	B	100	GLU	CG-CD	10.00	1.67	1.51
1	B	93	GLU	CD-OE2	9.82	1.36	1.25
1	B	39	LYS	CE-NZ	8.56	1.70	1.49
1	B	6	GLN	CB-CG	-8.17	1.30	1.52
1	A	6	GLN	CB-CG	-7.82	1.31	1.52
1	A	53	TYR	CE2-CZ	-7.73	1.28	1.38
1	B	77	GLU	CD-OE1	7.43	1.33	1.25
1	A	118	PHE	CB-CG	-7.30	1.39	1.51
1	B	53	TYR	CD1-CE1	7.25	1.50	1.39
1	B	55	TYR	CG-CD2	7.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	SER	CA-CB	-6.75	1.42	1.52
1	B	301	ARG	CB-CG	-6.64	1.34	1.52
1	A	53	TYR	CD2-CE2	6.57	1.49	1.39
1	A	114	TYR	CE1-CZ	-6.57	1.30	1.38
1	B	242	GLY	N-CA	-6.51	1.36	1.46
1	B	302	ASN	CB-CG	6.50	1.66	1.51
1	A	24	TYR	CE2-CZ	-6.45	1.30	1.38
1	B	28	GLU	CD-OE1	6.42	1.32	1.25
1	A	124	PRO	CB-CG	-6.37	1.18	1.50
1	A	196	TYR	CD1-CE1	6.34	1.48	1.39
1	B	24	TYR	CE2-CZ	-5.98	1.30	1.38
1	B	196	TYR	CE2-CZ	-5.97	1.30	1.38
1	A	5	PHE	CG-CD1	-5.91	1.29	1.38
1	B	77	GLU	CG-CD	5.86	1.60	1.51
1	B	322	GLU	CG-CD	5.83	1.60	1.51
1	A	138	ILE	CA-CB	5.73	1.68	1.54
1	B	110	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	53	TYR	CZ-OH	5.67	1.47	1.37
1	B	227	TRP	CB-CG	5.63	1.60	1.50
1	A	298	SER	CB-OG	-5.62	1.34	1.42
1	B	68	LYS	CD-CE	-5.62	1.37	1.51
1	A	305	TYR	CE2-CZ	-5.56	1.31	1.38
1	A	58	GLU	CD-OE1	-5.54	1.19	1.25
1	B	8	VAL	CA-CB	5.52	1.66	1.54
1	A	70	ALA	CA-CB	-5.50	1.40	1.52
1	B	279	GLU	CD-OE1	5.40	1.31	1.25
1	B	39	LYS	CD-CE	-5.37	1.37	1.51
1	B	94	LEU	N-CA	-5.33	1.35	1.46
1	B	53	TYR	CG-CD1	-5.30	1.32	1.39
1	A	317	TYR	CZ-OH	5.26	1.46	1.37
1	A	263	ARG	CZ-NH2	-5.18	1.26	1.33
1	B	291	GLU	CD-OE1	5.13	1.31	1.25
1	B	286	PHE	CE1-CZ	-5.08	1.27	1.37
1	B	207	LYS	CD-CE	5.03	1.63	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	A	118	PHE	CB-CG-CD2	12.11	129.27	120.80
1	A	170	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	A	53	TYR	CZ-CE2-CD2	-11.85	109.14	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	301	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	A	2	ASP	CB-CG-OD1	-11.29	108.14	118.30
1	A	309[A]	ASP	CB-CG-OD2	10.74	127.97	118.30
1	A	309[B]	ASP	CB-CG-OD2	10.74	127.97	118.30
1	B	301	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	118	PHE	CB-CG-CD1	-10.26	113.62	120.80
1	B	196	TYR	CB-CG-CD1	10.18	127.11	121.00
1	A	53	TYR	CE1-CZ-CE2	10.14	136.03	119.80
1	A	229	ASP	CB-CG-OD2	9.95	127.26	118.30
1	B	263	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	132	ASP	CB-CG-OD2	9.62	126.96	118.30
1	B	223	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	2	ASP	CB-CG-OD2	9.56	126.91	118.30
1	A	263	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	53	TYR	CD1-CE1-CZ	-9.32	111.41	119.80
1	B	229	ASP	CB-CG-OD2	9.18	126.57	118.30
1	A	132	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	B	76	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	170	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	263	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	309[A]	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	A	309[B]	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	B	301	ARG	NH1-CZ-NH2	7.61	127.78	119.40
1	B	53	TYR	CZ-CE2-CD2	-7.60	112.96	119.80
1	A	47	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	66	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	B	132	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	170	ARG	CD-NE-CZ	7.04	133.45	123.60
1	B	322	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	A	126	VAL	CG1-CB-CG2	6.84	121.85	110.90
1	B	53	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	B	53	TYR	CE1-CZ-CE2	6.76	130.62	119.80
1	B	272	PHE	CB-CG-CD1	6.68	125.48	120.80
1	B	118	PHE	CB-CG-CD2	6.59	125.42	120.80
1	A	80	PHE	CB-CG-CD2	-6.49	116.25	120.80
1	B	196	TYR	CB-CG-CD2	-6.41	117.15	121.00
1	B	301	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	297	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	93	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	A	272	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	B	170	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	100	GLU	CG-CD-OE1	6.09	130.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	185	LYS	CD-CE-NZ	-6.03	97.83	111.70
1	A	263	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	207	LYS	CD-CE-NZ	-5.82	98.32	111.70
1	B	301	ARG	CG-CD-NE	-5.76	99.71	111.80
1	A	109	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	156	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	7	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	18	VAL	CG1-CB-CG2	5.58	119.82	110.90
1	B	66	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	309[A]	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	309[B]	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	295	VAL	CA-CB-CG2	5.52	119.17	110.90
1	A	47	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	118	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	96	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	80	PHE	CB-CG-CD1	5.44	124.61	120.80
1	A	39	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	B	196	TYR	CD1-CE1-CZ	-5.39	114.94	119.80
1	B	39	LYS	CD-CE-NZ	-5.38	99.31	111.70
1	B	53	TYR	CD1-CE1-CZ	-5.35	114.99	119.80
1	B	2	ASP	OD1-CG-OD2	-5.32	113.20	123.30
1	A	321	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	81	TYR	CB-CG-CD1	5.30	124.18	121.00
1	B	77	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	B	2	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	53	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	A	130	PRO	N-CD-CG	5.11	110.86	103.20
1	B	77	GLU	CG-CD-OE1	-5.08	108.13	118.30
1	A	118	PHE	CB-CA-C	-5.06	100.29	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain

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	2598	0	2598	64	0
1	B	2595	0	2605	75	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	48	0	26	4	0
3	B	48	0	26	5	0
4	A	333	0	0	23	2
4	B	400	0	0	35	2
All	All	6032	0	5255	141	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:CA	1:A:8:VAL:CB	1.76	1.60
1:B:39:LYS:CE	1:B:39:LYS:NZ	1.70	1.52
1:B:302:ASN:HB2	4:B:1374:HOH:O	1.38	1.21
1:A:53:TYR:OH	4:A:1199:HOH:O	1.63	1.17
3:B:1004:NDP:O2N	4:B:1360:HOH:O	1.67	1.11
1:B:149[A]:GLU:HG3	4:B:1210:HOH:O	1.53	1.06
1:A:8:VAL:HG23	1:A:18:VAL:HG12	1.35	1.03
1:A:77:GLU:OE1	4:A:1112:HOH:O	1.77	1.01
3:A:1003:NDP:O2N	4:A:1300:HOH:O	1.80	0.99
1:A:8:VAL:HG23	1:A:18:VAL:CG1	1.95	0.96
1:B:8:VAL:HG23	1:B:18:VAL:HG12	1.45	0.96
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.03	0.94
1:B:309[B]:ASP:OD1	4:B:1173:HOH:O	1.85	0.94
1:B:123[A]:LYS:HD2	4:B:1351:HOH:O	1.67	0.93
1:B:223:ARG:HD3	4:B:1328:HOH:O	1.69	0.93
1:B:258:ARG:HE	1:B:262:GLN:HE21	1.03	0.92
1:B:197:LEU:HD12	1:B:302:ASN:ND2	1.85	0.92
1:B:294:LYS:HG3	4:B:1030:HOH:O	1.69	0.91
1:A:262:GLN:HE22	1:A:288:LEU:H	1.14	0.90
1:B:8:VAL:HG23	1:B:18:VAL:CG1	2.02	0.89
1:B:2:ASP:N	4:B:1348:HOH:O	2.06	0.88
1:B:39:LYS:NZ	1:B:39:LYS:CD	2.35	0.88
1:A:8:VAL:CG2	1:A:18:VAL:HG12	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:HIS:CG	1:B:135:GLY:N	2.42	0.86
1:B:18:VAL:HG11	4:B:1321:HOH:O	1.75	0.86
1:B:100:GLU:HG2	4:B:1263:HOH:O	1.74	0.86
1:B:262:GLN:HE22	1:B:288:LEU:H	1.21	0.85
1:A:2:ASP:N	4:A:1174:HOH:O	2.11	0.83
1:B:149[B]:GLU:HG3	4:B:1210:HOH:O	1.78	0.83
1:B:123[B]:LYS:HD2	1:B:124:PRO:HD2	1.61	0.81
1:A:149[B]:GLU:OE1	1:A:153:LYS:HE3	1.84	0.78
1:B:132:ASP:O	1:B:134:HIS:O	2.02	0.77
1:B:149[A]:GLU:OE2	4:B:1308:HOH:O	2.01	0.76
1:A:282[A]:GLN:NE2	1:A:285:GLU:OE2	2.19	0.75
1:A:8:VAL:CA	1:A:8:VAL:CG2	2.65	0.74
1:B:77:GLU:HG3	4:B:1205:HOH:O	1.89	0.73
1:B:134:HIS:CG	1:B:135:GLY:H	2.05	0.73
1:B:149[B]:GLU:OE1	4:B:1210:HOH:O	2.06	0.73
1:B:8:VAL:CG2	1:B:18:VAL:HG12	2.18	0.72
1:B:201:LYS:HE3	4:B:1380:HOH:O	1.90	0.72
1:B:197:LEU:CD1	1:B:302:ASN:ND2	2.55	0.70
1:B:312:ILE:HD11	4:B:1173:HOH:O	1.90	0.70
1:A:8:VAL:CA	1:A:8:VAL:CG1	2.68	0.69
1:A:8:VAL:CB	1:A:8:VAL:N	2.55	0.69
1:B:123[A]:LYS:CD	4:B:1351:HOH:O	2.34	0.67
1:B:194:HIS:HD2	1:B:196:TYR:H	1.44	0.65
1:A:194:HIS:HD2	1:A:196:TYR:H	1.44	0.65
1:A:136:LYS:HD2	4:A:1187:HOH:O	1.97	0.64
1:B:101[B]:ASP:OD1	4:B:1153:HOH:O	2.07	0.64
1:A:77:GLU:HG3	4:A:1066:HOH:O	1.97	0.63
1:A:136:LYS:CD	4:A:1325:HOH:O	2.47	0.63
1:A:292:ASP:HA	1:A:295:VAL:HG22	1.80	0.62
1:A:8:VAL:CB	1:A:8:VAL:C	2.68	0.62
1:A:136:LYS:HD2	4:A:1325:HOH:O	2.00	0.61
1:A:128:ILE:HD13	4:A:1286:HOH:O	2.00	0.61
1:B:229:ASP:OD1	1:B:231:SER:OG	2.19	0.61
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.83	0.60
1:A:77:GLU:CG	4:A:1066:HOH:O	2.49	0.59
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.85	0.59
1:B:302:ASN:ND2	4:B:1342:HOH:O	2.23	0.59
1:A:169:ASN:H	1:A:172:GLN:HE21	1.49	0.58
1:A:149[A]:GLU:OE2	1:A:152:GLU:OE1	2.22	0.57
1:A:262:GLN:NE2	1:A:288:LEU:H	1.94	0.57
1:B:169:ASN:H	1:B:172:GLN:HE21	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201[A]:LYS:HE3	1:A:322:GLU:OE1	2.05	0.56
1:B:63[A]:LEU:HD23	1:B:66:ARG:NH2	2.21	0.55
1:B:302:ASN:CB	4:B:1374:HOH:O	2.17	0.54
1:B:100:GLU:OE2	4:B:1263:HOH:O	2.18	0.54
1:A:227:TRP:HE3	4:A:1104:HOH:O	1.91	0.54
1:A:270:LYS:O	3:A:1003:NDP:H8A	2.09	0.53
1:B:262:GLN:NE2	1:B:288:LEU:H	1.99	0.52
1:A:75:LYS:HE3	4:A:1066:HOH:O	2.09	0.52
1:A:77:GLU:H	1:A:77:GLU:CD	2.11	0.52
1:A:282[A]:GLN:OE1	4:A:1055:HOH:O	2.18	0.52
1:B:216:TYR:CE1	3:B:1004:NDP:H41N	2.44	0.52
1:A:275:LYS:HE2	4:A:1328:HOH:O	2.10	0.51
1:A:225:PRO:O	1:A:226:GLU:CG	2.59	0.51
1:B:63[A]:LEU:HD23	1:B:66:ARG:HH22	1.76	0.51
1:A:58:GLU:HG3	4:A:1108:HOH:O	2.11	0.51
1:A:75:LYS:HB3	1:A:77:GLU:OE2	2.10	0.51
1:A:36:GLU:HG2	4:A:1210:HOH:O	2.11	0.50
1:A:225:PRO:O	1:A:226:GLU:OE2	2.28	0.50
1:B:270:LYS:O	3:B:1004:NDP:H8A	2.12	0.49
1:A:273:THR:HG21	1:A:275:LYS:HE3	1.93	0.49
1:B:302:ASN:CB	4:B:1342:HOH:O	2.61	0.49
1:A:128:ILE:CD1	4:A:1286:HOH:O	2.58	0.49
1:B:309[B]:ASP:CG	4:B:1173:HOH:O	2.42	0.49
1:B:197:LEU:HD12	1:B:302:ASN:HD22	1.75	0.48
1:A:169:ASN:H	1:A:172:GLN:NE2	2.12	0.48
1:B:309[A]:ASP:OD1	1:B:312:ILE:CD1	2.62	0.48
1:B:100:GLU:CG	4:B:1263:HOH:O	2.45	0.48
1:A:222:HIS:HE1	4:A:1300:HOH:O	1.97	0.48
1:B:134:HIS:ND1	1:B:135:GLY:N	2.58	0.47
1:B:222:HIS:HE1	4:B:1360:HOH:O	1.98	0.47
1:B:216:TYR:CZ	3:B:1004:NDP:H41N	2.49	0.47
1:B:149[B]:GLU:OE2	4:B:1308:HOH:O	2.21	0.46
1:B:194:HIS:HD2	1:B:196:TYR:N	2.12	0.46
1:B:309[A]:ASP:OD1	1:B:312:ILE:HD12	2.15	0.46
1:B:63[B]:LEU:HG	1:B:66:ARG:NH2	2.29	0.46
1:B:123[B]:LYS:HD3	4:B:1351:HOH:O	2.15	0.46
1:A:149[B]:GLU:OE2	1:A:152:GLU:HB2	2.15	0.46
1:A:136:LYS:CD	4:A:1187:HOH:O	2.62	0.46
1:B:63[A]:LEU:CD2	1:B:66:ARG:HH22	2.29	0.46
1:A:201[A]:LYS:NZ	4:A:1127:HOH:O	2.32	0.45
1:A:226:GLU:HG2	1:A:227:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:CD	4:A:1066:HOH:O	2.55	0.44
1:A:136:LYS:HD3	4:A:1325:HOH:O	2.14	0.44
1:B:169:ASN:H	1:B:172:GLN:NE2	2.16	0.44
1:B:7:ARG:CZ	4:B:1280:HOH:O	2.66	0.44
1:B:123[A]:LYS:CE	4:B:1351:HOH:O	2.63	0.44
1:B:294:LYS:HD3	4:B:1239:HOH:O	2.17	0.44
1:A:216:TYR:CE1	3:A:1003:NDP:H41N	2.52	0.44
1:A:77:GLU:OE2	4:A:1066:HOH:O	2.20	0.43
1:B:190:GLN:OE1	3:B:1004:NDP:H2N	2.19	0.43
1:A:96:ARG:HB3	1:A:97:PRO:HD3	2.00	0.42
1:B:77:GLU:CG	4:B:1205:HOH:O	2.56	0.42
1:A:149[B]:GLU:OE2	1:A:152:GLU:OE1	2.38	0.42
1:B:302:ASN:HB2	4:B:1342:HOH:O	2.17	0.42
1:B:132:ASP:O	1:B:134:HIS:C	2.57	0.42
1:B:294:LYS:CE	4:B:1030:HOH:O	2.68	0.42
1:A:216:TYR:CZ	3:A:1003:NDP:H41N	2.55	0.42
1:A:258:ARG:HE	1:A:262:GLN:NE2	1.89	0.42
1:A:225:PRO:O	1:A:226:GLU:CB	2.67	0.41
1:B:58:GLU:HG3	4:B:1242:HOH:O	2.19	0.41
1:A:119:PRO:O	1:A:144:ILE:HD11	2.21	0.41
1:B:258:ARG:HE	1:B:262:GLN:NE2	1.89	0.41
1:B:36:GLU:HG2	4:B:1337:HOH:O	2.20	0.41
1:A:225:PRO:O	1:A:226:GLU:HG2	2.21	0.40
1:B:171:ARG:O	1:B:175:MET:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1294:HOH:O	4:B:1353:HOH:O[1_455]	2.02	0.18
4:A:1091:HOH:O	4:B:1006:HOH:O[2_646]	2.06	0.14

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	327/322 (102%)	318 (97%)	9 (3%)	0	100 100
1	B	325/322 (101%)	317 (98%)	7 (2%)	1 (0%)	41 17
All	All	652/644 (101%)	635 (97%)	16 (2%)	1 (0%)	47 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	HIS

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	287/280 (102%)	276 (96%)	11 (4%)	33 3
1	B	285/280 (102%)	280 (98%)	5 (2%)	59 22
All	All	572/560 (102%)	556 (97%)	16 (3%)	50 8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	126	VAL
1	A	144	ILE
1	A	199	GLN
1	A	226	GLU
1	A	229	ASP
1	A	230	GLN
1	A	282[A]	GLN
1	A	282[B]	GLN
1	A	290[A]	SER
1	A	290[B]	SER
1	B	133	GLU

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Mol	Chain	Res	Type
1	B	149[A]	GLU
1	B	149[B]	GLU
1	B	199	GLN
1	B	229	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	167	ASN
1	A	172	GLN
1	A	194	HIS
1	A	199	GLN
1	A	250	GLN
1	A	262	GLN
1	B	105	ASN
1	B	167	ASN
1	B	172	GLN
1	B	178	ASN
1	B	194	HIS
1	B	199	GLN
1	B	262	GLN
1	B	287	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 monosaccharides 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	$\#\|Z\| > 2$
3	NDP	A	1003	-	45,52,52	1.78	10 (22%)	53,80,80	1.41	7 (13%)
3	NDP	B	1004	-	45,52,52	1.75	9 (20%)	53,80,80	1.44	9 (16%)
2	SO4	B	1002	-	4,4,4	0.72	0	6,6,6	0.73	0
2	SO4	A	1001	-	4,4,4	0.74	0	6,6,6	1.29	1 (16%)

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	NDP	A	1003	-	-	4/30/77/77	0/5/5/5
3	NDP	B	1004	-	-	5/30/77/77	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	NDP	C4N-C3N	-5.88	1.38	1.49
3	A	1003	NDP	C4N-C3N	-5.41	1.39	1.49
3	B	1004	NDP	O4B-C1B	3.86	1.46	1.41
3	A	1003	NDP	C2A-N3A	3.83	1.38	1.32
3	A	1003	NDP	PN-O1N	-3.80	1.37	1.50
3	A	1003	NDP	O4B-C1B	3.71	1.46	1.41
3	B	1004	NDP	C6N-C5N	3.49	1.39	1.33
3	A	1003	NDP	PA-O2A	-3.28	1.39	1.55
3	A	1003	NDP	C4N-C5N	-3.22	1.40	1.48
3	A	1003	NDP	C6N-N1N	3.11	1.45	1.37
3	B	1004	NDP	PN-O1N	-3.02	1.40	1.50
3	B	1004	NDP	C2A-N3A	2.71	1.36	1.32
3	B	1004	NDP	C2A-N1A	2.64	1.38	1.33
3	B	1004	NDP	C3D-C4D	-2.53	1.46	1.53
3	A	1003	NDP	C3D-C4D	-2.53	1.46	1.53
3	A	1003	NDP	C5A-C4A	-2.26	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	NDP	C1D-N1N	2.19	1.52	1.46
3	B	1004	NDP	PA-O2A	-2.18	1.45	1.55
3	A	1003	NDP	C2A-N1A	-2.02	1.30	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1004	NDP	O7N-C7N-C3N	-3.71	113.91	120.90
3	A	1003	NDP	O7N-C7N-C3N	-3.61	114.11	120.90
3	B	1004	NDP	C3N-C2N-N1N	-3.40	118.25	123.10
3	A	1003	NDP	O4B-C4B-C3B	3.34	111.72	105.11
3	A	1003	NDP	C5A-C6A-N1A	-3.30	112.88	120.35
3	B	1004	NDP	C3N-C7N-N7N	3.03	123.05	117.67
3	A	1003	NDP	C5A-C6A-N6A	2.99	124.89	120.35
3	A	1003	NDP	C1B-N9A-C4A	2.89	131.71	126.64
3	B	1004	NDP	C5A-C6A-N1A	-2.76	114.09	120.35
3	B	1004	NDP	C4A-C5A-N7A	-2.50	106.80	109.40
3	B	1004	NDP	N3A-C2A-N1A	-2.43	124.89	128.68
2	A	1001	SO4	O4-S-O3	2.31	118.92	109.06
3	B	1004	NDP	PN-O3-PA	2.23	140.48	132.83
3	A	1003	NDP	PN-O3-PA	2.19	140.33	132.83
3	A	1003	NDP	O2N-PN-O1N	2.11	122.66	112.24
3	B	1004	NDP	O2N-PN-O1N	2.07	122.48	112.24
3	B	1004	NDP	C5A-C6A-N6A	2.02	123.42	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

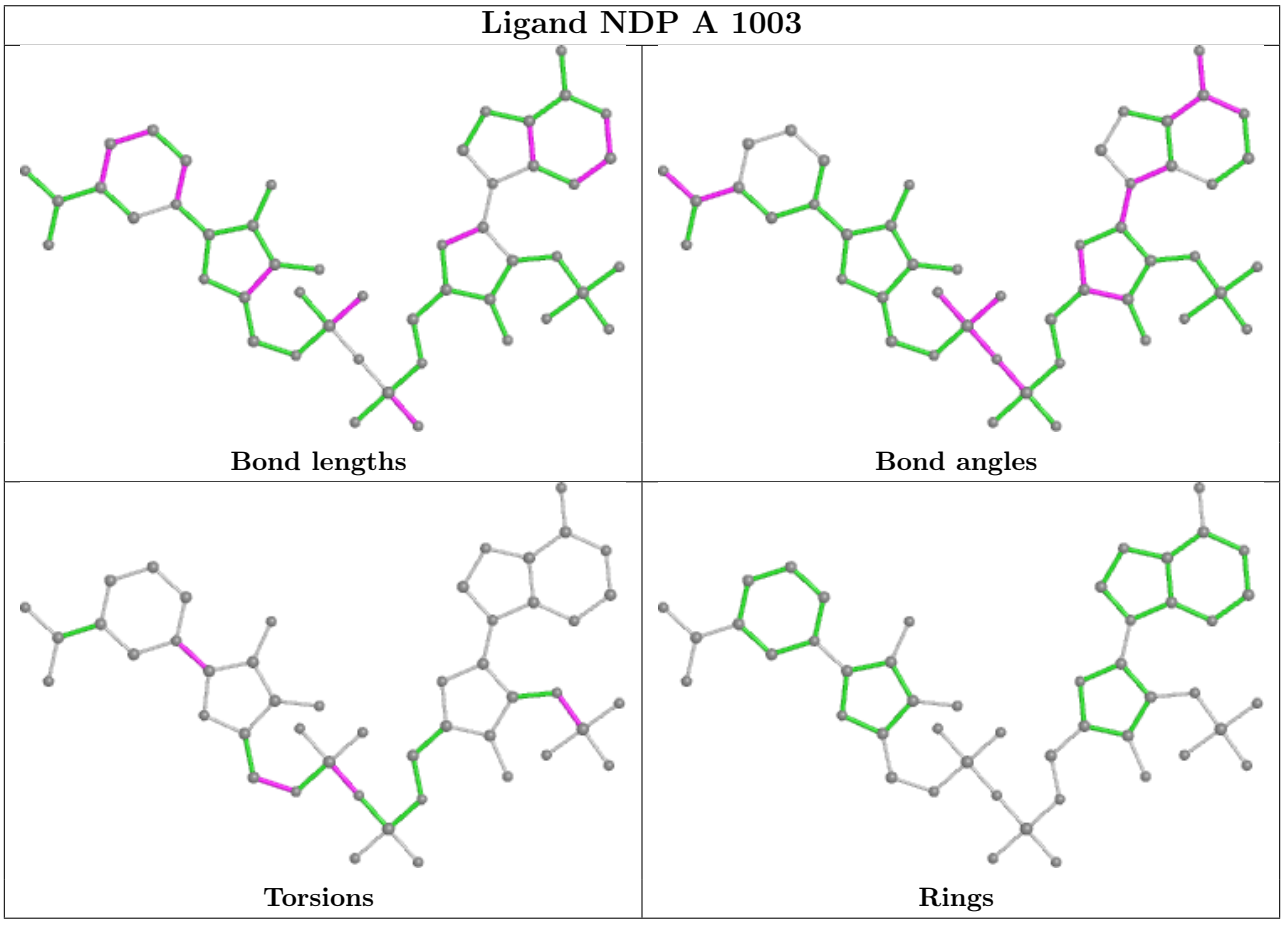
Mol	Chain	Res	Type	Atoms
3	A	1003	NDP	O4D-C1D-N1N-C2N
3	B	1004	NDP	O4D-C1D-N1N-C2N
3	A	1003	NDP	PA-O3-PN-O5D
3	B	1004	NDP	PA-O3-PN-O5D
3	B	1004	NDP	C4D-C5D-O5D-PN
3	A	1003	NDP	C4D-C5D-O5D-PN
3	A	1003	NDP	C2B-O2B-P2B-O2X
3	B	1004	NDP	C2B-O2B-P2B-O2X
3	B	1004	NDP	PA-O3-PN-O2N

There are no ring outliers.

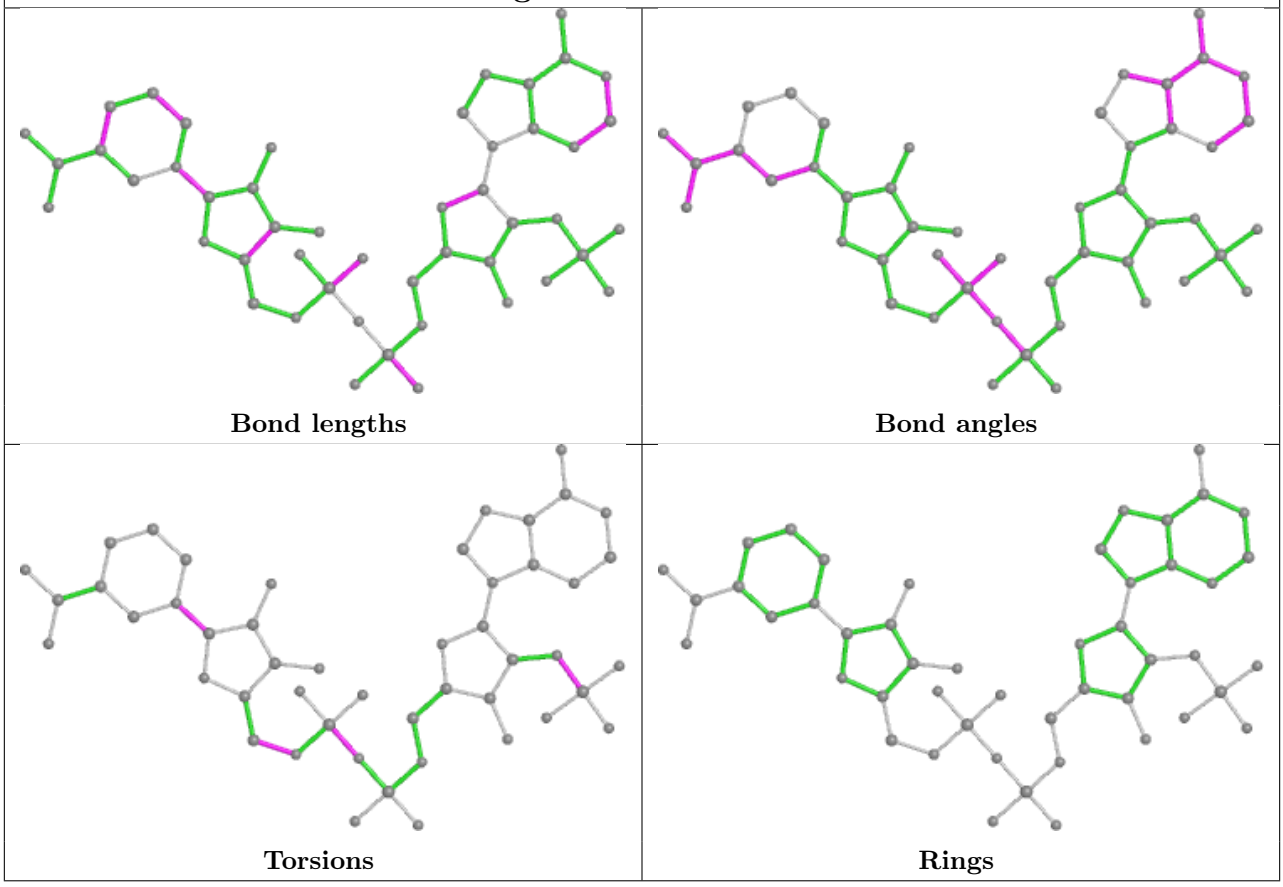
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	NDP	4	0
3	B	1004	NDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



Ligand NDP B 1004



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, 95^{th} 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	322/322 (100%)	0.23	11 (3%)	45	46	12, 15, 25, 50	0
1	B	322/322 (100%)	0.12	12 (3%)	41	42	12, 15, 26, 49	0
All	All	644/644 (100%)	0.17	23 (3%)	42	43	12, 15, 26, 50	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	TRP	18.1
1	B	227	TRP	5.5
1	B	134	HIS	4.4
1	B	135	GLY	3.7
1	A	229	ASP	3.7
1	A	226	GLU	3.6
1	A	230	GLN	3.3
1	A	133	GLU	3.2
1	B	63[A]	LEU	3.2
1	A	225	PRO	3.1
1	B	149[A]	GLU	2.7
1	A	134	HIS	2.7
1	B	229	ASP	2.6
1	A	149[A]	GLU	2.6
1	B	101[A]	ASP	2.5
1	B	133	GLU	2.5
1	B	302	ASN	2.5
1	A	175	MET	2.2
1	B	123[A]	LYS	2.2
1	A	2	ASP	2.1
1	B	226	GLU	2.0
1	B	2	ASP	2.0
1	A	239	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

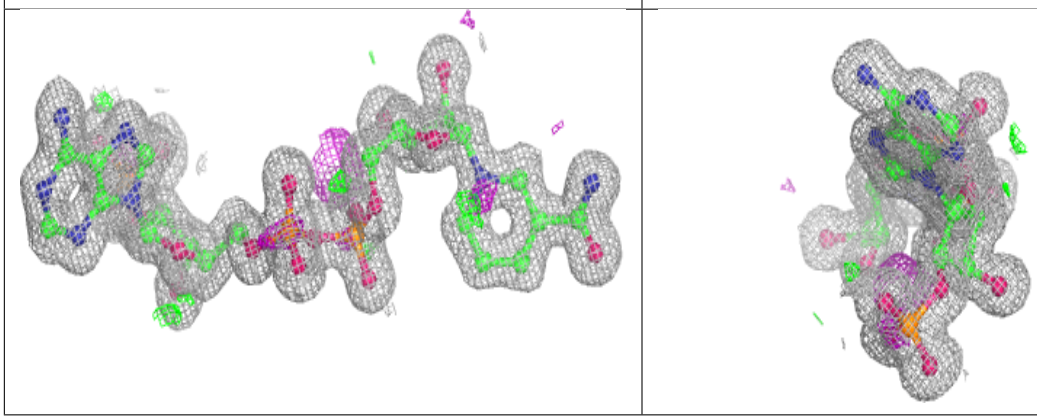
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1001	5/5	0.95	0.17	15,19,26,27	0
2	SO4	B	1002	5/5	0.97	0.12	19,20,22,29	0
3	NDP	A	1003	48/48	0.98	0.07	12,13,16,19	0
3	NDP	B	1004	48/48	0.98	0.07	11,13,15,18	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.

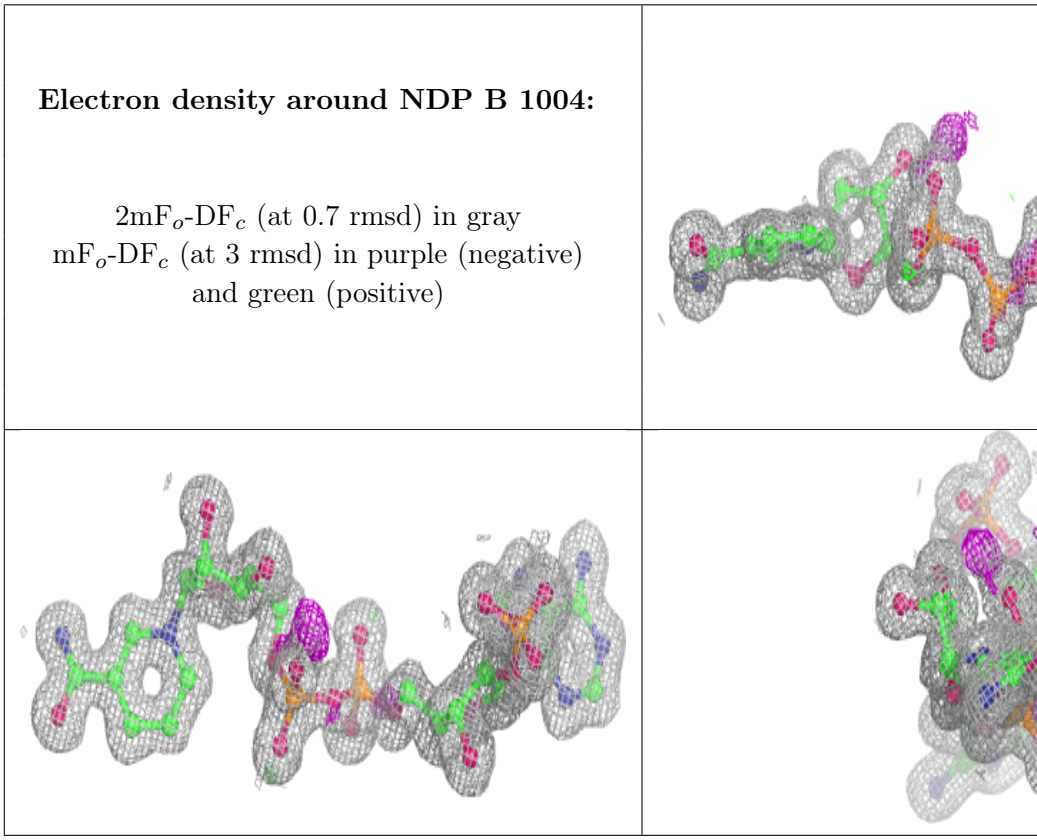
Electron density around NDP A 1003:

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



Electron density around NDP B 1004:

$2mF_o$-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.