Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 04:33 AM EDT

PDB ID	:	4GO0
Title	:	Crystal structure of the c707s mutant of c-terminal domain of 10'formyltetra hydrofolate dehydrogenase in complex with NADPH
Authors	:	Tsybovsky, Y.
Deposited on	:	2012-08-17
Resolution	:	3.38 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:

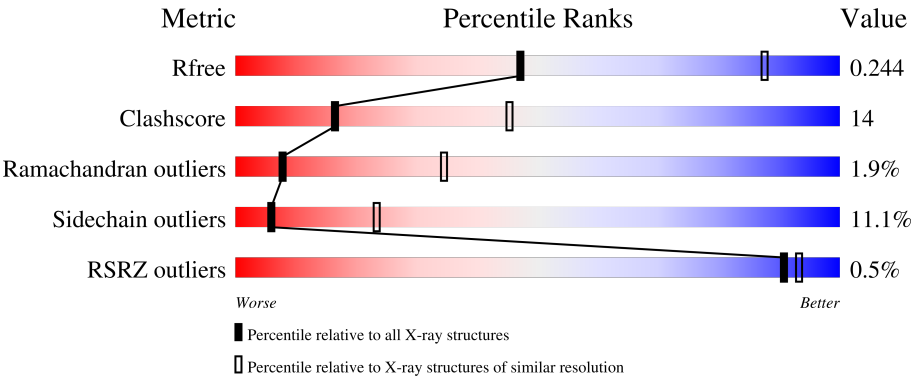
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	517	62% 30%
1	B	517	% 62% 31%
1	C	517	64% 28%
1	D	517	% 60% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15488 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 Cytosolic 10-formyltetrahydrofolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3824	2435	655	715	19			
1	B	498	Total	C	N	O	S	0	0	0
			3824	2435	655	715	19			
1	C	498	Total	C	N	O	S	0	0	0
			3824	2435	655	715	19			
1	D	498	Total	C	N	O	S	0	0	0
			3824	2435	655	715	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP P28037
A	387	ARG	-	expression tag	UNP P28037
A	388	GLY	-	expression tag	UNP P28037
A	389	SER	-	expression tag	UNP P28037
A	390	HIS	-	expression tag	UNP P28037
A	391	HIS	-	expression tag	UNP P28037
A	392	HIS	-	expression tag	UNP P28037
A	393	HIS	-	expression tag	UNP P28037
A	394	HIS	-	expression tag	UNP P28037
A	395	THR	-	expression tag	UNP P28037
A	396	THR	-	expression tag	UNP P28037
A	707	SER	CYS	engineered mutation	UNP P28037
B	386	MET	-	expression tag	UNP P28037
B	387	ARG	-	expression tag	UNP P28037
B	388	GLY	-	expression tag	UNP P28037
B	389	SER	-	expression tag	UNP P28037
B	390	HIS	-	expression tag	UNP P28037
B	391	HIS	-	expression tag	UNP P28037
B	392	HIS	-	expression tag	UNP P28037
B	393	HIS	-	expression tag	UNP P28037
B	394	HIS	-	expression tag	UNP P28037

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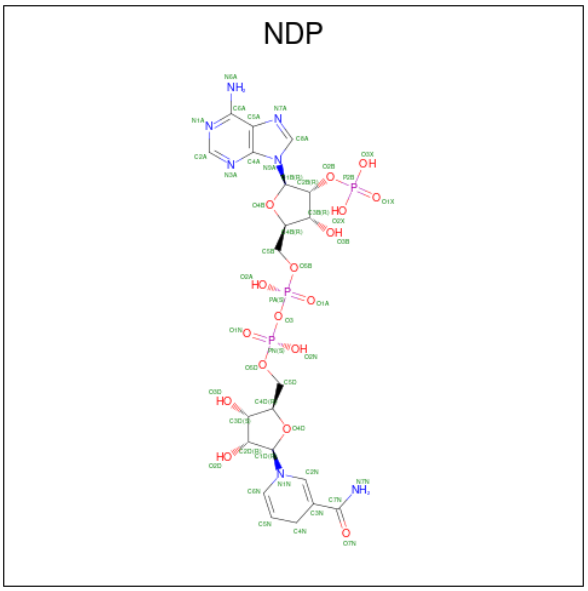
Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP P28037
B	396	THR	-	expression tag	UNP P28037
B	707	SER	CYS	engineered mutation	UNP P28037
C	386	MET	-	expression tag	UNP P28037
C	387	ARG	-	expression tag	UNP P28037
C	388	GLY	-	expression tag	UNP P28037
C	389	SER	-	expression tag	UNP P28037
C	390	HIS	-	expression tag	UNP P28037
C	391	HIS	-	expression tag	UNP P28037
C	392	HIS	-	expression tag	UNP P28037
C	393	HIS	-	expression tag	UNP P28037
C	394	HIS	-	expression tag	UNP P28037
C	395	THR	-	expression tag	UNP P28037
C	396	THR	-	expression tag	UNP P28037
C	707	SER	CYS	engineered mutation	UNP P28037
D	386	MET	-	expression tag	UNP P28037
D	387	ARG	-	expression tag	UNP P28037
D	388	GLY	-	expression tag	UNP P28037
D	389	SER	-	expression tag	UNP P28037
D	390	HIS	-	expression tag	UNP P28037
D	391	HIS	-	expression tag	UNP P28037
D	392	HIS	-	expression tag	UNP P28037
D	393	HIS	-	expression tag	UNP P28037
D	394	HIS	-	expression tag	UNP P28037
D	395	THR	-	expression tag	UNP P28037
D	396	THR	-	expression tag	UNP P28037
D	707	SER	CYS	engineered mutation	UNP P28037

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



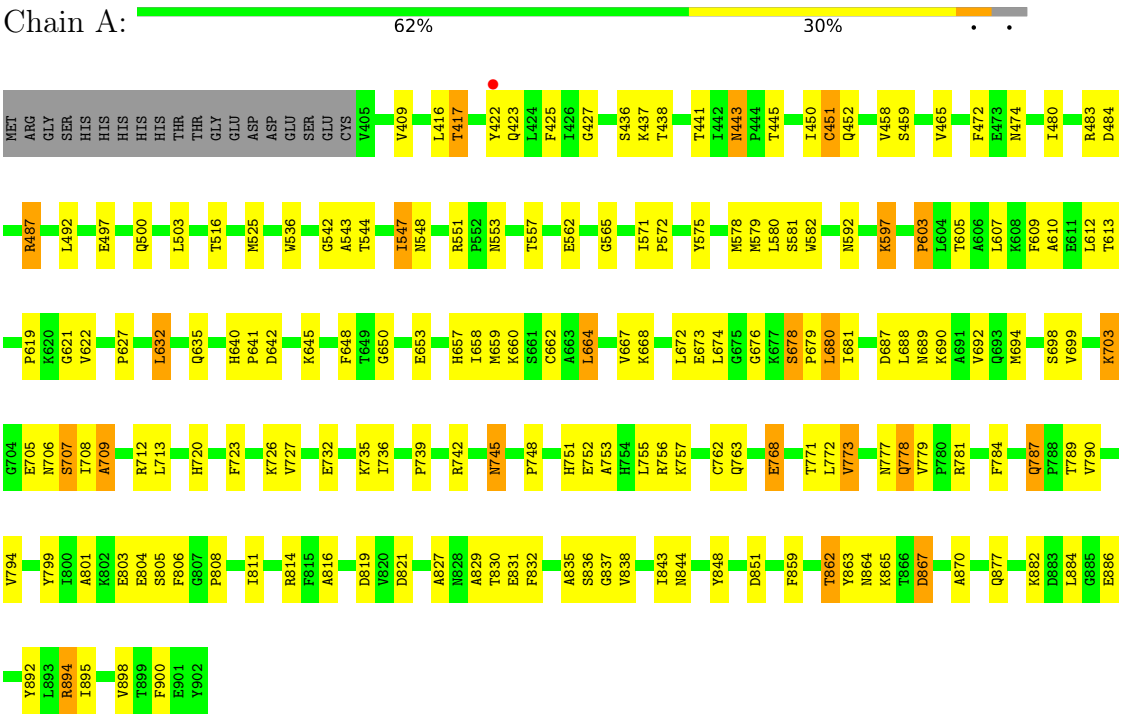
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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.

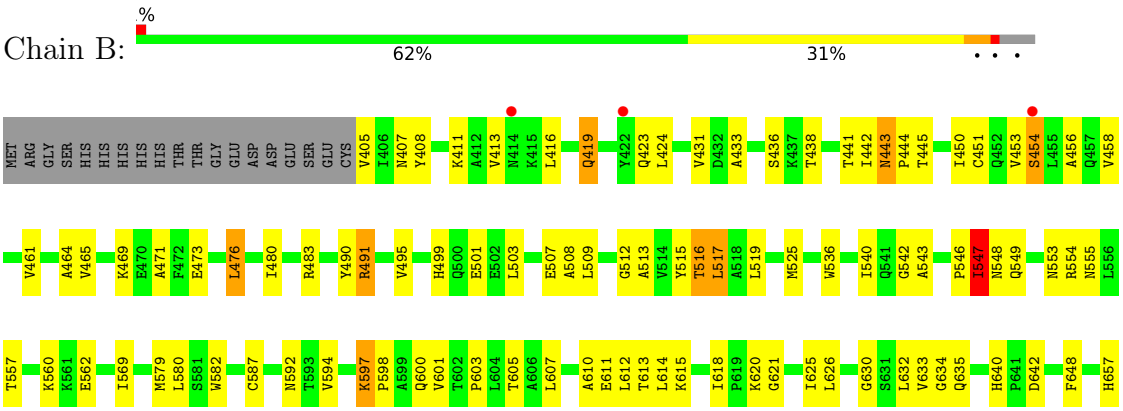
• Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase

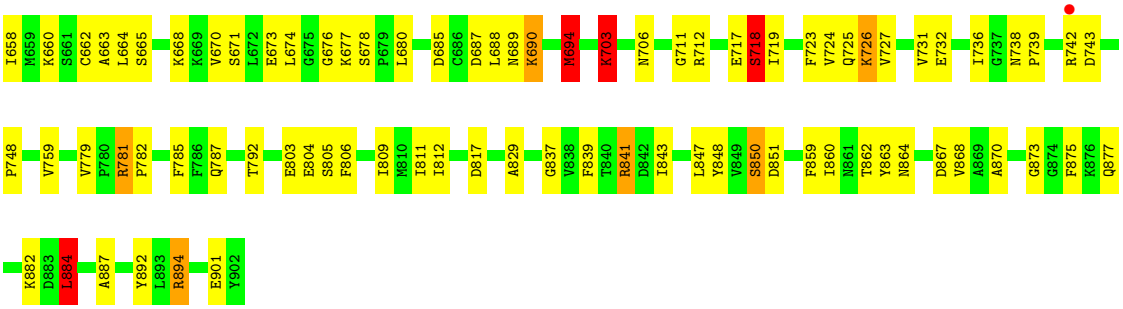
Chain A:



• Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase

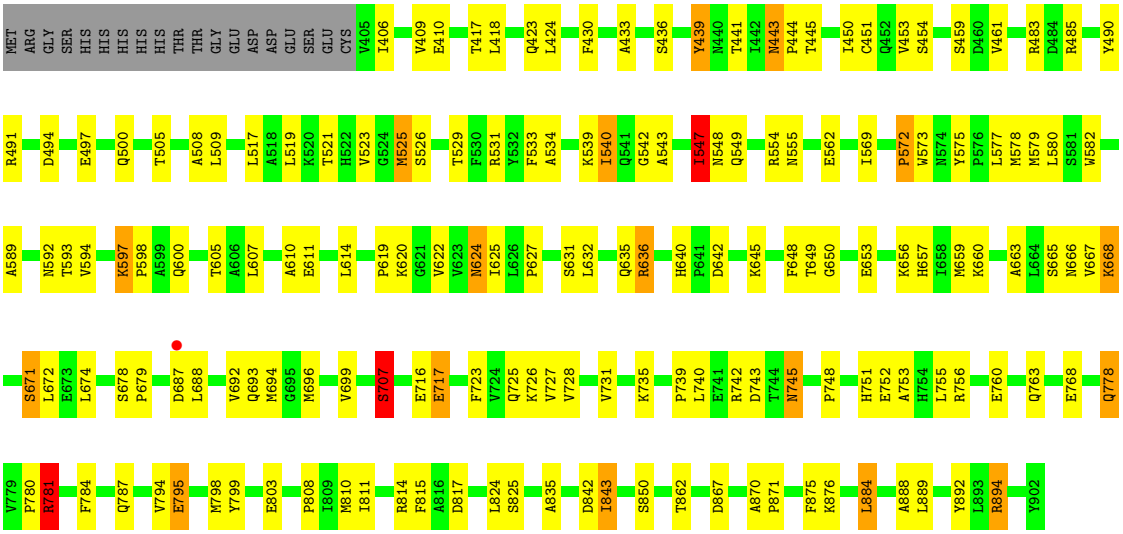
Chain B:





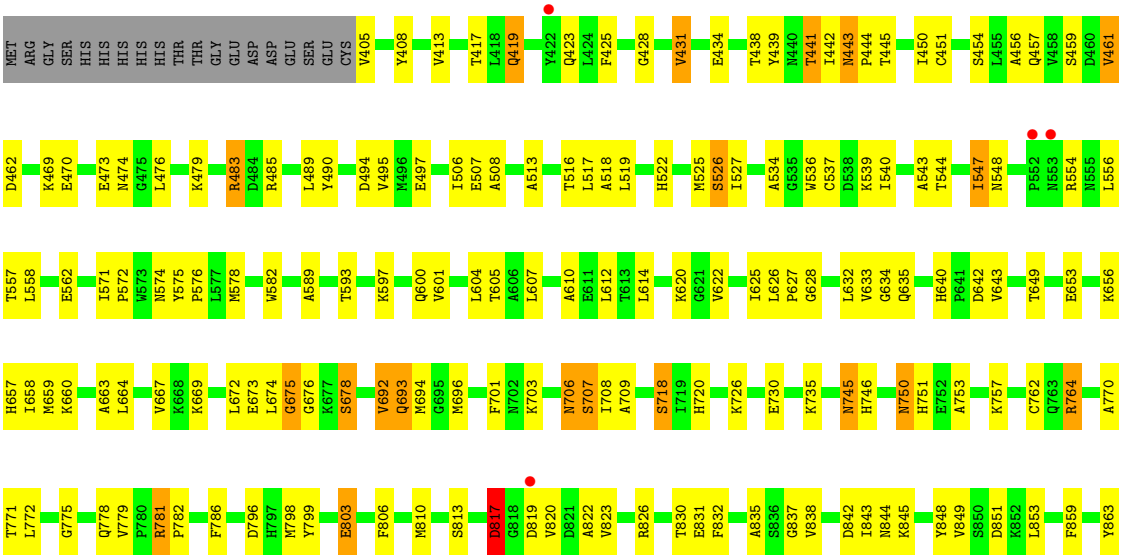
• Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase

Chain C:



• Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase

Chain D:




N864
K865
T866
D867
V868
A869
A870
P871
F872
G873
G874
F875
K876
Q877
D883
L884
R894
F900
E901
Y902

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	258.42Å 194.13Å 96.97Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	52.50 – 3.38 48.83 – 3.38	Depositor EDS
% Data completeness (in resolution range)	98.2 (52.50-3.38) 98.2 (48.83-3.38)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.252 0.194 , 0.244	Depositor DCC
R_{free} test set	3161 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15488	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

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	0.83	1/3898 (0.0%)	0.92	1/5274 (0.0%)
1	B	0.84	1/3898 (0.0%)	0.89	3/5274 (0.1%)
1	C	0.89	5/3898 (0.1%)	0.92	3/5274 (0.1%)
1	D	0.87	4/3898 (0.1%)	0.91	4/5274 (0.1%)
All	All	0.86	11/15592 (0.1%)	0.91	11/21096 (0.1%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	490	TYR	CE2-CZ	7.58	1.48	1.38
1	D	490	TYR	CE2-CZ	7.51	1.48	1.38
1	D	803	GLU	CG-CD	6.33	1.61	1.51
1	A	762	CYS	CB-SG	-6.16	1.71	1.82
1	B	490	TYR	CE2-CZ	6.04	1.46	1.38
1	D	762	CYS	CB-SG	-6.02	1.72	1.82
1	D	653	GLU	CG-CD	5.57	1.60	1.51
1	C	490	TYR	CG-CD1	5.41	1.46	1.39
1	C	490	TYR	CD2-CE2	5.38	1.47	1.39
1	C	653	GLU	CG-CD	5.32	1.59	1.51
1	C	717	GLU	CG-CD	5.32	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	687	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	C	687	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	781	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	554	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	694	MET	CG-SD-CE	6.07	109.91	100.20
1	B	503	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	B	517	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	669	LYS	CD-CE-NZ	-5.54	98.97	111.70
1	A	687	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	537	CYS	CA-CB-SG	-5.15	104.74	114.00
1	C	781	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	705	GLU	Peptide

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	3824	0	3851	121	0
1	B	3824	0	3851	133	0
1	C	3824	0	3851	117	0
1	D	3824	0	3851	123	0
2	A	48	0	26	3	0
2	B	48	0	26	4	0
2	C	48	0	26	2	0
2	D	48	0	26	7	0
All	All	15488	0	15508	443	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 14.

All (443) 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:497:GLU:O	1:A:500:GLN:HG2	1.58	1.03
1:A:676:GLY:O	1:A:804:GLU:HG3	1.66	0.95
1:B:443:ASN:C	1:B:443:ASN:HD22	1.75	0.90
1:B:443:ASN:ND2	1:B:445:THR:H	1.69	0.88
1:C:593:THR:HG22	1:C:622:VAL:HG13	1.54	0.87
1:C:485:ARG:NH1	1:C:589:ALA:O	2.09	0.86
1:D:593:THR:HG22	1:D:622:VAL:HA	1.58	0.85
1:C:751:HIS:HD2	1:C:753:ALA:HB3	1.42	0.85
1:A:894:ARG:HD3	1:B:875:PHE:CZ	2.16	0.80
1:B:483:ARG:NH1	1:D:868:VAL:HG22	1.96	0.80
1:C:756:ARG:HH22	1:C:778:GLN:HE22	1.29	0.80
1:C:607:LEU:O	1:C:610:ALA:HB3	1.83	0.78
1:C:692:VAL:O	1:C:696:MET:HG3	1.83	0.78
1:D:735:LYS:H	1:D:745:ASN:HD21	1.32	0.78
1:D:443:ASN:HD22	1:D:445:THR:H	1.32	0.77
1:C:751:HIS:CD2	1:C:753:ALA:HB3	2.21	0.76
1:B:610:ALA:HB2	1:B:625:ILE:HD12	1.67	0.76
1:A:777:ASN:O	1:A:787:GLN:HB2	1.84	0.76
1:B:508:ALA:HA	1:B:513:ALA:H	1.50	0.75
1:D:707:SER:OG	2:D:1001:NDP:H42N	1.87	0.75
1:A:735:LYS:N	1:A:745:ASN:HD21	1.85	0.74
1:B:806:PHE:CE1	2:B:1001:NDP:H2D	2.23	0.74
1:B:779:VAL:HG22	1:B:787:GLN:NE2	2.02	0.73
1:B:843:ILE:HD12	1:C:843:ILE:HG12	1.70	0.73
1:B:443:ASN:HD21	1:B:445:THR:H	1.38	0.72
1:B:670:VAL:HG22	1:B:671:SER:N	2.05	0.71
1:B:443:ASN:ND2	1:B:445:THR:N	2.39	0.70
1:B:843:ILE:HD12	1:C:843:ILE:CG1	2.21	0.70
1:C:640:HIS:CE1	1:C:642:ASP:HB2	2.27	0.69
1:A:723:PHE:O	1:A:727:VAL:HG23	1.92	0.69
1:B:443:ASN:HD22	1:B:444:PRO:N	1.91	0.69
1:A:752:GLU:HG2	1:A:756:ARG:NH2	2.07	0.69
1:C:875:PHE:CZ	1:D:894:ARG:HD3	2.27	0.69
1:D:735:LYS:N	1:D:745:ASN:HD21	1.91	0.68
1:D:556:LEU:HD23	1:D:900:PHE:CD1	2.29	0.68
1:A:640:HIS:ND1	1:A:641:PRO:HD2	2.09	0.68
1:B:677:LYS:HE3	1:B:711:GLY:O	1.93	0.68
1:C:423:GLN:HA	1:C:454:SER:OG	1.95	0.67
1:C:870:ALA:HB2	1:D:547:ILE:HD11	1.77	0.67
1:B:443:ASN:C	1:B:443:ASN:ND2	2.46	0.66
1:B:562:GLU:HB2	1:B:894:ARG:HD2	1.76	0.66
1:B:555:ASN:ND2	1:B:901:GLU:HB2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:LEU:HB3	1:A:674:LEU:HD21	1.77	0.66
1:A:465:VAL:HG11	1:A:640:HIS:CE1	2.31	0.65
1:D:772:LEU:HD21	1:D:775:GLY:O	1.96	0.65
1:B:536:TRP:CD1	1:D:539:LYS:HE3	2.31	0.65
1:C:894:ARG:HD3	1:D:875:PHE:CE1	2.32	0.65
1:C:424:LEU:HD23	1:C:627:PRO:HD2	1.78	0.65
1:B:711:GLY:O	1:B:712:ARG:HG3	1.96	0.64
1:B:718:SER:HB3	1:B:817:ASP:OD1	1.97	0.64
1:C:569:ILE:HD12	1:C:594:VAL:HG21	1.79	0.64
1:B:662:CYS:HB3	1:B:668:LYS:HG3	1.79	0.64
1:A:472:PHE:CE1	1:A:565:GLY:HA2	2.34	0.63
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.63	0.63
1:A:703:LYS:O	1:A:808:PRO:HD3	1.99	0.63
1:D:781:ARG:HB2	1:D:782:PRO:CD	2.29	0.62
1:D:408:TYR:CD1	1:D:419:GLN:HB3	2.35	0.62
1:A:427:GLY:HA2	1:A:621:GLY:HA2	1.81	0.62
1:A:806:PHE:CE1	2:A:1001:NDP:H2D	2.34	0.62
1:C:443:ASN:ND2	1:C:445:THR:H	1.97	0.62
1:B:408:TYR:CG	1:B:419:GLN:HB3	2.35	0.61
1:D:746:HIS:HE1	1:D:786:PHE:O	1.83	0.61
1:A:450:ILE:O	1:A:451:CYS:HB3	2.01	0.61
1:D:443:ASN:ND2	1:D:445:THR:H	1.99	0.61
1:C:688:LEU:O	1:C:688:LEU:HG	2.00	0.61
1:D:593:THR:CG2	1:D:622:VAL:HA	2.31	0.61
1:C:531:ARG:O	1:C:534:ALA:HB3	2.01	0.60
1:D:445:THR:O	1:D:445:THR:HG22	2.01	0.60
1:B:450:ILE:O	1:B:451:CYS:HB3	2.02	0.60
1:D:423:GLN:HA	1:D:454:SER:OG	2.02	0.60
1:A:735:LYS:H	1:A:745:ASN:HD21	1.48	0.60
1:C:674:LEU:O	2:C:1001:NDP:H2N	2.01	0.59
1:B:717:GLU:O	1:B:719:ILE:N	2.35	0.59
1:C:768:GLU:OE1	1:C:798:MET:HB3	2.02	0.59
1:A:894:ARG:HD3	1:B:875:PHE:CE2	2.37	0.59
1:B:809:ILE:O	1:B:811:ILE:HG13	2.03	0.59
1:D:562:GLU:HB2	1:D:894:ARG:HD2	1.84	0.59
1:D:547:ILE:HD13	1:D:557:THR:HB	1.85	0.59
1:A:425:PHE:CD2	1:A:610:ALA:HB1	2.38	0.59
1:B:724:VAL:HG21	1:B:792:THR:HG21	1.85	0.59
1:D:572:PRO:HD3	1:D:649:THR:O	2.02	0.59
1:A:886:GLU:O	1:A:886:GLU:HG2	2.03	0.58
1:B:555:ASN:HD21	1:B:901:GLU:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:GLU:HG2	1:A:756:ARG:HH21	1.68	0.58
1:C:443:ASN:C	1:C:443:ASN:HD22	2.07	0.58
1:A:863:TYR:O	1:A:864:ASN:HB2	2.03	0.58
1:B:543:ALA:HA	1:C:542:GLY:O	2.04	0.58
1:A:777:ASN:HB2	1:A:787:GLN:HE22	1.69	0.58
1:C:745:ASN:N	1:C:745:ASN:HD22	2.02	0.58
1:D:607:LEU:O	1:D:610:ALA:HB3	2.04	0.58
1:B:640:HIS:CE1	1:B:642:ASP:HB2	2.39	0.58
1:A:720:HIS:C	1:A:720:HIS:CD2	2.77	0.57
1:A:536:TRP:CE2	1:C:539:LYS:HD3	2.39	0.57
1:C:666:ASN:OD1	1:C:668:LYS:NZ	2.34	0.57
1:A:443:ASN:ND2	1:A:445:THR:H	2.03	0.57
1:A:673:GLU:HB3	2:A:1001:NDP:O7N	2.04	0.57
1:D:461:VAL:HA	1:D:626:LEU:HD11	1.86	0.57
1:D:675:GLY:HA3	1:D:832:PHE:HE1	1.69	0.57
1:D:751:HIS:CD2	1:D:753:ALA:HB3	2.41	0.56
1:C:439:TYR:CE2	1:C:453:VAL:HB	2.40	0.56
1:C:716:GLU:HG2	1:C:817:ASP:OD1	2.05	0.56
1:A:679:PRO:O	1:A:836:SER:HA	2.05	0.56
1:B:408:TYR:CD1	1:B:419:GLN:HB3	2.41	0.56
1:A:837:GLY:HA2	1:A:859:PHE:O	2.06	0.56
1:C:523:VAL:O	1:C:526:SER:HB2	2.06	0.56
1:C:799:TYR:CE2	1:C:803:GLU:HG2	2.42	0.56
1:A:543:ALA:HA	1:D:543:ALA:HA	1.87	0.55
1:A:794:VAL:HG11	1:A:811:ILE:CG2	2.36	0.55
1:C:696:MET:CE	1:C:731:VAL:HG23	2.36	0.55
1:A:409:VAL:HG21	1:A:451:CYS:HB2	1.87	0.55
1:D:640:HIS:CE1	1:D:642:ASP:HB2	2.42	0.55
1:C:529:THR:HG21	1:C:582:TRP:HA	1.89	0.55
1:D:849:VAL:HG12	1:D:853:LEU:CD1	2.36	0.55
1:A:712:ARG:NH1	1:A:801:ALA:HB1	2.22	0.55
1:D:635:GLN:OE1	1:D:657:HIS:HE1	1.89	0.55
1:A:664:LEU:HD21	1:B:660:LYS:HD2	1.89	0.55
1:C:461:VAL:HB	1:C:636:ARG:HG2	1.89	0.55
1:C:547:ILE:HG13	1:D:867:ASP:CB	2.36	0.55
1:C:799:TYR:CE2	1:C:803:GLU:CG	2.89	0.55
1:C:723:PHE:O	1:C:727:VAL:HG23	2.06	0.54
1:A:492:LEU:HD13	1:A:613:THR:HA	1.88	0.54
1:C:491:ARG:O	1:C:494:ASP:HB2	2.06	0.54
1:C:572:PRO:HG3	1:C:649:THR:HG22	1.88	0.54
1:C:656:LYS:HG2	1:D:663:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:THR:HG22	1:B:454:SER:HA	1.90	0.54
1:D:625:ILE:HG22	1:D:627:PRO:HD3	1.88	0.54
1:B:508:ALA:O	1:B:512:GLY:HA2	2.08	0.54
1:D:806:PHE:CE1	2:D:1001:NDP:H2D	2.43	0.54
1:B:670:VAL:HG22	1:B:671:SER:H	1.70	0.54
1:B:670:VAL:CG2	1:B:671:SER:N	2.71	0.54
1:C:611:GLU:O	1:C:614:LEU:HB2	2.09	0.54
1:D:456:ALA:HB3	1:D:633:VAL:HG21	1.90	0.54
1:A:548:ASN:HD21	1:D:483:ARG:HB3	1.73	0.53
1:B:469:LYS:HE2	1:B:473:GLU:OE1	2.07	0.53
1:B:843:ILE:HD12	1:C:843:ILE:HA	1.90	0.53
1:D:678:SER:HB3	1:D:835:ALA:O	2.08	0.53
1:D:750:ASN:HB3	1:D:751:HIS:ND1	2.23	0.53
1:A:851:ASP:OD1	1:B:560:LYS:HE2	2.08	0.53
1:B:689:ASN:OD1	1:B:726:LYS:NZ	2.40	0.53
1:C:678:SER:HB3	1:C:835:ALA:O	2.08	0.53
1:C:692:VAL:HG13	1:C:727:VAL:HG22	1.90	0.53
1:D:849:VAL:HG12	1:D:853:LEU:HD12	1.90	0.53
1:C:439:TYR:CE1	1:C:600:GLN:HG2	2.44	0.53
1:C:540:ILE:CD1	1:C:889:LEU:HD13	2.38	0.53
1:C:707:SER:HB3	2:C:1001:NDP:C3N	2.39	0.53
1:C:894:ARG:HD3	1:D:875:PHE:CZ	2.44	0.53
1:A:648:PHE:CZ	1:A:650:GLY:HA3	2.44	0.53
1:B:483:ARG:NH2	1:D:867:ASP:OD1	2.30	0.53
1:D:843:ILE:HG23	1:D:844:ASN:ND2	2.23	0.52
1:A:831:GLU:HB3	1:A:877:GLN:HG3	1.90	0.52
1:B:491:ARG:HG2	1:B:491:ARG:HH11	1.74	0.52
1:B:727:VAL:O	1:B:731:VAL:HG23	2.09	0.52
1:D:868:VAL:HA	1:D:884:LEU:HD22	1.91	0.52
1:A:443:ASN:C	1:A:443:ASN:HD22	2.12	0.52
1:C:672:LEU:HB3	1:C:674:LEU:HD21	1.91	0.52
1:A:417:THR:HG22	1:A:417:THR:O	2.08	0.52
1:A:640:HIS:CE1	1:A:642:ASP:HB2	2.43	0.52
1:B:483:ARG:HH22	1:D:867:ASP:CG	2.12	0.52
1:C:443:ASN:HD22	1:C:444:PRO:N	2.08	0.52
1:C:549:GLN:NE2	1:C:555:ASN:HB2	2.24	0.52
1:D:849:VAL:CG1	1:D:853:LEU:HD11	2.40	0.52
1:D:672:LEU:HB3	1:D:674:LEU:HD21	1.92	0.51
1:B:548:ASN:HD21	1:C:483:ARG:HB3	1.76	0.51
1:A:422:TYR:HB2	1:A:452:GLN:O	2.10	0.51
1:A:443:ASN:HD22	1:A:445:THR:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:755:LEU:HD22	1:C:784:PHE:HB3	1.92	0.51
1:D:485:ARG:NH1	1:D:589:ALA:O	2.44	0.51
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.45	0.51
1:A:707:SER:OG	2:A:1001:NDP:H42N	2.11	0.51
1:B:781:ARG:HG3	1:B:782:PRO:O	2.11	0.51
1:B:792:THR:HG22	1:B:812:ILE:HB	1.92	0.51
1:C:597:LYS:HD2	1:C:598:PRO:O	2.10	0.51
1:C:875:PHE:CE2	1:D:894:ARG:HD3	2.46	0.51
1:C:424:LEU:HG	1:C:454:SER:CB	2.41	0.51
1:A:862:THR:HB	1:B:901:GLU:HB3	1.93	0.51
1:D:536:TRP:O	1:D:540:ILE:HG13	2.11	0.51
1:A:619:PRO:HD2	1:A:622:VAL:HG21	1.92	0.50
1:B:542:GLY:O	1:C:543:ALA:HA	2.12	0.50
1:D:751:HIS:HD2	1:D:753:ALA:HB3	1.75	0.50
1:D:600:GLN:HB2	1:D:628:GLY:O	2.12	0.50
1:A:571:ILE:CD1	1:A:580:LEU:HB2	2.42	0.50
1:D:673:GLU:OE1	1:D:873:GLY:HA2	2.12	0.50
1:A:689:ASN:OD1	1:A:726:LYS:NZ	2.40	0.50
1:B:554:ARG:NH1	1:D:851:ASP:OD2	2.44	0.50
1:C:696:MET:HE1	1:C:731:VAL:CG2	2.42	0.50
1:D:764:ARG:CZ	1:D:799:TYR:CD2	2.95	0.50
1:B:687:ASP:OD1	1:B:690:LYS:HB2	2.11	0.50
1:A:544:THR:HG21	1:D:558:LEU:HD13	1.93	0.50
1:B:483:ARG:CB	1:C:548:ASN:HD21	2.25	0.50
1:B:499:HIS:CD2	1:B:612:LEU:HD21	2.46	0.50
1:A:660:LYS:HG3	1:B:660:LYS:HG3	1.94	0.49
1:D:707:SER:HB3	2:D:1001:NDP:C3N	2.42	0.49
1:C:533:PHE:HZ	1:C:884:LEU:HA	1.76	0.49
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.94	0.49
1:B:597:LYS:HD2	1:B:598:PRO:O	2.12	0.49
1:A:843:ILE:HG23	1:A:844:ASN:HD22	1.76	0.49
1:C:696:MET:HE1	1:C:731:VAL:HG23	1.93	0.49
1:C:418:LEU:HD21	1:C:505:THR:HG21	1.95	0.49
1:C:424:LEU:HG	1:C:454:SER:HB2	1.94	0.49
1:A:898:VAL:HG13	1:B:860:ILE:HD12	1.94	0.49
1:B:723:PHE:O	1:B:727:VAL:HG23	2.13	0.49
1:C:443:ASN:HD22	1:C:445:THR:H	1.58	0.49
1:D:796:ASP:OD1	1:D:826:ARG:HG2	2.13	0.49
1:B:549:GLN:NE2	1:B:555:ASN:H	2.10	0.49
1:A:640:HIS:CG	1:A:641:PRO:HD2	2.47	0.48
1:B:495:VAL:HG11	1:B:615:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:O	1:A:709:ALA:C	2.51	0.48
1:B:863:TYR:CD2	1:B:864:ASN:N	2.82	0.48
1:B:507:GLU:OE1	1:B:605:THR:HG21	2.14	0.48
1:B:676:GLY:O	1:B:804:GLU:HG3	2.14	0.48
1:A:680:LEU:HD12	1:A:680:LEU:C	2.33	0.48
1:B:670:VAL:CG2	1:B:671:SER:H	2.27	0.48
1:B:738:ASN:OD1	1:B:739:PRO:HD2	2.12	0.48
1:D:649:THR:HG23	2:D:1001:NDP:C3N	2.43	0.48
1:A:830:THR:HG23	1:A:832:PHE:O	2.13	0.48
1:C:505:THR:O	1:C:508:ALA:HB3	2.13	0.48
1:A:713:LEU:HD12	1:A:713:LEU:N	2.29	0.48
1:B:592:ASN:ND2	1:B:892:TYR:HB3	2.29	0.48
1:B:850:SER:HB3	1:B:860:ILE:HD11	1.95	0.48
1:C:575:TYR:HB3	1:C:578:MET:HB3	1.94	0.48
1:C:799:TYR:CE2	1:C:803:GLU:HG3	2.48	0.48
1:D:822:ALA:O	1:D:823:VAL:C	2.51	0.48
1:B:483:ARG:HB2	1:C:548:ASN:HD21	1.79	0.48
1:D:718:SER:HB3	1:D:817:ASP:OD2	2.13	0.48
1:A:592:ASN:ND2	1:A:892:TYR:HB3	2.29	0.48
1:A:692:VAL:HG13	1:A:727:VAL:HG22	1.95	0.48
1:A:816:ALA:HB3	1:A:819:ASP:OD1	2.14	0.48
1:B:868:VAL:O	1:B:884:LEU:HB3	2.14	0.48
1:A:547:ILE:HD12	1:A:547:ILE:HA	1.61	0.47
1:B:662:CYS:CB	1:B:668:LYS:HG3	2.44	0.47
1:C:540:ILE:HD13	1:C:889:LEU:HD13	1.96	0.47
1:C:862:THR:HB	1:D:901:GLU:HB3	1.96	0.47
1:D:445:THR:O	1:D:445:THR:CG2	2.62	0.47
1:B:680:LEU:C	1:B:680:LEU:HD12	2.34	0.47
1:C:577:LEU:HB2	1:C:605:THR:HB	1.97	0.47
1:A:635:GLN:OE1	1:A:657:HIS:CE1	2.67	0.47
1:A:898:VAL:CG1	1:B:860:ILE:HD12	2.44	0.47
1:B:443:ASN:HD22	1:B:445:THR:H	1.57	0.47
1:D:439:TYR:OH	1:D:600:GLN:O	2.27	0.47
1:D:842:ASP:HB3	1:D:845:LYS:HB2	1.95	0.47
1:B:613:THR:HB	1:B:618:ILE:HB	1.96	0.47
1:A:427:GLY:HA2	1:A:621:GLY:CA	2.45	0.47
1:A:678:SER:HB3	1:A:835:ALA:O	2.14	0.47
1:C:592:ASN:HD21	1:C:892:TYR:HB3	1.80	0.47
1:D:423:GLN:HB3	1:D:431:VAL:O	2.15	0.47
1:D:526:SER:OG	1:D:578:MET:HA	2.15	0.47
1:D:706:ASN:HD21	1:D:708:ILE:HG12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LYS:H	1:A:745:ASN:ND2	2.13	0.47
1:A:739:PRO:HD3	1:A:748:PRO:HD3	1.97	0.47
1:D:518:ALA:HA	1:D:522:HIS:HB2	1.97	0.47
1:A:895:ILE:HB	1:B:882:LYS:HE3	1.97	0.47
1:D:408:TYR:CG	1:D:419:GLN:HB3	2.49	0.47
1:D:434:GLU:HB3	1:D:457:GLN:HG3	1.97	0.47
1:B:738:ASN:OD1	1:B:739:PRO:CD	2.63	0.46
1:D:441:THR:C	1:D:442:ILE:HD13	2.36	0.46
1:C:521:THR:O	1:C:525:MET:HB2	2.15	0.46
1:C:547:ILE:HG13	1:D:867:ASP:HB3	1.98	0.46
1:C:745:ASN:N	1:C:745:ASN:ND2	2.63	0.46
1:D:489:LEU:HB2	1:D:534:ALA:HB2	1.98	0.46
1:A:547:ILE:HG13	1:B:867:ASP:CB	2.46	0.46
1:B:673:GLU:HB3	2:B:1001:NDP:O7N	2.15	0.46
1:A:667:VAL:CG2	1:B:877:GLN:HA	2.46	0.46
1:A:679:PRO:CB	1:A:827:ALA:HB1	2.46	0.46
1:C:799:TYR:CZ	1:C:803:GLU:HG3	2.50	0.46
1:D:848:TYR:O	1:D:851:ASP:HB2	2.15	0.46
1:A:579:MET:HE2	1:A:579:MET:HA	1.98	0.46
1:B:423:GLN:O	1:B:607:LEU:HD22	2.16	0.46
1:B:703:LYS:HD2	1:B:748:PRO:O	2.15	0.46
1:C:640:HIS:HE1	1:C:642:ASP:HB2	1.76	0.46
1:B:685:ASP:O	1:B:841:ARG:HB2	2.16	0.46
1:A:542:GLY:HA3	1:D:544:THR:OG1	2.16	0.46
1:A:688:LEU:HG	1:A:688:LEU:O	2.16	0.46
1:C:409:VAL:HG21	1:C:451:CYS:HB2	1.96	0.46
1:C:592:ASN:ND2	1:C:892:TYR:HB3	2.31	0.46
1:A:640:HIS:CE1	1:A:641:PRO:HD2	2.51	0.45
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.69	0.45
1:C:692:VAL:HG21	1:C:726:LYS:HB3	1.98	0.45
1:A:667:VAL:HG23	1:B:877:GLN:HA	1.99	0.45
1:B:862:THR:OG1	1:B:863:TYR:N	2.50	0.45
1:D:676:GLY:N	1:D:832:PHE:CD1	2.84	0.45
1:A:592:ASN:HD21	1:A:892:TYR:HB3	1.80	0.45
1:A:607:LEU:HD21	1:A:627:PRO:HD3	1.99	0.45
1:C:716:GLU:N	1:C:815:PHE:CE1	2.85	0.45
1:A:484:ASP:O	1:A:487:ARG:HB2	2.17	0.45
1:A:579:MET:HA	1:A:579:MET:CE	2.47	0.45
1:D:692:VAL:O	1:D:693:GLN:C	2.55	0.45
1:A:581:SER:O	1:A:582:TRP:C	2.54	0.45
1:D:425:PHE:CG	1:D:610:ALA:HB1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:VAL:HG12	1:D:612:LEU:HD13	1.99	0.45
1:D:707:SER:OG	2:D:1001:NDP:C4N	2.63	0.45
1:A:441:THR:HG23	1:A:450:ILE:HB	1.99	0.45
1:B:515:TYR:O	1:B:516:THR:C	2.55	0.45
1:D:497:GLU:HG3	1:D:527:ILE:HD13	1.98	0.45
1:B:443:ASN:HD22	1:B:445:THR:N	2.14	0.45
1:C:667:VAL:HG13	1:D:656:LYS:HG2	1.99	0.45
1:C:794:VAL:HG21	1:C:811:ILE:HG23	1.99	0.45
1:D:428:GLY:O	1:D:614:LEU:HD21	2.16	0.45
1:B:443:ASN:HD21	1:B:445:THR:CB	2.30	0.45
1:A:603:PRO:O	1:A:607:LEU:HG	2.17	0.45
1:C:870:ALA:HA	1:C:871:PRO:HD2	1.73	0.45
1:A:843:ILE:HG13	1:D:843:ILE:HD12	1.99	0.45
1:B:673:GLU:OE1	1:B:873:GLY:HA2	2.17	0.45
1:C:884:LEU:N	1:C:888:ALA:HB2	2.30	0.45
1:D:574:ASN:HD21	2:D:1001:NDP:H5N	1.83	0.45
1:A:777:ASN:HB2	1:A:787:GLN:NE2	2.31	0.44
1:B:648:PHE:CD1	1:B:658:ILE:HD12	2.51	0.44
1:B:863:TYR:HD2	1:B:864:ASN:N	2.15	0.44
1:D:865:LYS:HD2	1:D:865:LYS:HA	1.74	0.44
1:A:865:LYS:O	1:A:865:LYS:HG3	2.16	0.44
1:B:476:LEU:HD23	1:B:480:ILE:CG2	2.47	0.44
1:C:635:GLN:OE1	1:C:657:HIS:HE1	2.00	0.44
1:D:707:SER:HB3	2:D:1001:NDP:C2N	2.47	0.44
1:A:679:PRO:HD2	1:A:835:ALA:O	2.17	0.44
1:C:752:GLU:O	1:C:753:ALA:C	2.55	0.44
1:A:771:THR:O	1:A:773:VAL:HG12	2.18	0.44
1:C:795:GLU:O	1:C:798:MET:HG3	2.18	0.44
1:A:751:HIS:CD2	1:A:753:ALA:HB3	2.53	0.44
1:B:547:ILE:HD12	1:B:547:ILE:HA	1.44	0.44
1:B:549:GLN:HE22	1:B:555:ASN:H	1.64	0.44
1:D:582:TRP:CD1	1:D:884:LEU:HD21	2.53	0.44
1:D:837:GLY:HA2	1:D:859:PHE:O	2.18	0.44
1:D:838:VAL:HG13	1:D:838:VAL:O	2.18	0.44
1:C:444:PRO:HD2	1:C:509:LEU:O	2.18	0.44
1:A:778:GLN:HG3	1:A:779:VAL:N	2.33	0.44
1:B:413:VAL:O	1:B:416:LEU:HB2	2.17	0.44
1:B:443:ASN:HD21	1:B:445:THR:N	2.05	0.44
1:B:582:TRP:CD2	1:B:884:LEU:HD21	2.53	0.44
1:B:582:TRP:CG	1:B:884:LEU:HD21	2.53	0.44
1:D:640:HIS:HB3	1:D:643:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HD12	1:A:681:ILE:N	2.32	0.44
1:B:673:GLU:HB3	2:B:1001:NDP:C7N	2.47	0.44
1:A:562:GLU:OE1	1:A:894:ARG:NH1	2.48	0.43
1:A:612:LEU:HA	1:A:612:LEU:HD23	1.75	0.43
1:B:536:TRP:O	1:B:540:ILE:HG13	2.18	0.43
1:A:821:ASP:OD1	1:A:848:TYR:OH	2.33	0.43
1:B:736:ILE:CG2	1:B:785:PHE:HD1	2.31	0.43
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.78	0.43
1:C:671:SER:O	1:C:672:LEU:HD23	2.19	0.43
1:D:849:VAL:CG1	1:D:853:LEU:CD1	2.96	0.43
1:D:883:ASP:O	1:D:884:LEU:O	2.36	0.43
1:A:458:VAL:HG23	1:A:632:LEU:HD21	2.00	0.43
1:B:848:TYR:O	1:B:851:ASP:HB2	2.19	0.43
1:C:663:ALA:CB	1:D:659:MET:HB3	2.49	0.43
1:D:469:LYS:HE2	1:D:473:GLU:OE1	2.18	0.43
1:C:533:PHE:CZ	1:C:884:LEU:HA	2.52	0.43
1:C:562:GLU:OE1	1:C:894:ARG:NH1	2.48	0.43
1:C:659:MET:HG2	1:D:663:ALA:HB2	2.00	0.43
1:D:508:ALA:HA	1:D:513:ALA:O	2.17	0.43
1:C:573:TRP:CE2	1:C:751:HIS:HE1	2.36	0.43
1:A:900:PHE:CD2	1:C:843:ILE:HD11	2.54	0.43
1:B:837:GLY:HA2	1:B:859:PHE:O	2.19	0.43
1:D:778:GLN:O	1:D:779:VAL:C	2.56	0.43
1:B:635:GLN:OE1	1:B:657:HIS:HE1	2.02	0.43
1:B:694:MET:HB3	1:B:839:PHE:CZ	2.53	0.43
1:C:842:ASP:OD2	1:C:842:ASP:C	2.57	0.43
1:B:587:CYS:HB2	1:B:892:TYR:CE1	2.53	0.43
1:A:867:ASP:CG	1:B:547:ILE:HD12	2.39	0.43
1:B:443:ASN:H	1:B:450:ILE:HG13	1.84	0.43
1:A:609:PHE:O	1:A:613:THR:HG23	2.19	0.42
1:A:768:GLU:OE2	1:A:799:TYR:CB	2.67	0.42
1:B:658:ILE:HD13	1:B:658:ILE:HG21	1.75	0.42
1:C:780:PRO:O	1:C:781:ARG:HB3	2.19	0.42
1:D:575:TYR:O	1:D:576:PRO:C	2.57	0.42
1:C:696:MET:CE	1:C:731:VAL:CG2	2.97	0.42
1:C:497:GLU:O	1:C:500:GLN:HG2	2.19	0.42
1:C:678:SER:HA	1:C:679:PRO:HD3	1.94	0.42
1:D:556:LEU:HB3	1:D:900:PHE:HB2	2.00	0.42
1:A:698:SER:OG	1:A:699:VAL:N	2.51	0.42
1:B:579:MET:O	1:B:580:LEU:C	2.57	0.42
1:D:635:GLN:OE1	1:D:657:HIS:CE1	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:ASN:C	1:D:745:ASN:HD22	2.22	0.42
1:D:863:TYR:CD2	1:D:864:ASN:N	2.87	0.42
1:A:789:THR:HG22	1:A:790:VAL:N	2.35	0.42
1:D:831:GLU:HB3	1:D:877:GLN:HG3	2.00	0.42
1:B:443:ASN:HB2	1:B:450:ILE:HG12	2.01	0.42
1:B:610:ALA:HB2	1:B:625:ILE:CD1	2.44	0.42
1:C:678:SER:HB3	1:C:835:ALA:C	2.39	0.42
1:A:662:CYS:HB3	1:A:668:LYS:HG3	2.01	0.42
1:B:562:GLU:CB	1:B:894:ARG:HD2	2.45	0.42
1:D:720:HIS:CD2	1:D:720:HIS:C	2.93	0.42
1:A:575:TYR:HB3	1:A:578:MET:HB3	2.01	0.42
1:B:465:VAL:HG11	1:B:640:HIS:CE1	2.55	0.42
1:B:736:ILE:HG22	1:B:785:PHE:CD1	2.55	0.42
1:C:740:LEU:O	1:C:742:ARG:NH1	2.53	0.42
1:C:760:GLU:HA	1:C:763:GLN:OE1	2.20	0.42
1:C:424:LEU:CD2	1:C:627:PRO:HD2	2.46	0.42
1:C:441:THR:HG23	1:C:450:ILE:HB	2.01	0.41
1:C:648:PHE:CZ	1:C:650:GLY:HA3	2.55	0.41
1:C:739:PRO:HD3	1:C:748:PRO:HD3	2.02	0.41
1:A:557:THR:HG21	1:B:870:ALA:HB2	2.02	0.41
1:A:678:SER:HB3	1:A:835:ALA:C	2.39	0.41
1:A:752:GLU:HB2	1:A:784:PHE:CZ	2.54	0.41
1:A:755:LEU:O	1:A:756:ARG:C	2.58	0.41
1:B:569:ILE:CD1	1:B:594:VAL:HG21	2.50	0.41
1:B:592:ASN:HD21	1:B:892:TYR:HB3	1.85	0.41
1:B:630:GLY:O	1:B:634:GLY:HA3	2.21	0.41
1:B:677:LYS:CE	1:B:711:GLY:O	2.65	0.41
1:D:443:ASN:HD22	1:D:443:ASN:C	2.24	0.41
1:D:483:ARG:HE	1:D:483:ARG:HB2	1.30	0.41
1:A:503:LEU:HA	1:A:503:LEU:HD23	1.88	0.41
1:A:597:LYS:HB3	1:A:597:LYS:HE3	1.79	0.41
1:B:507:GLU:OE1	1:B:605:THR:CG2	2.69	0.41
1:B:748:PRO:HB3	1:B:785:PHE:CE2	2.55	0.41
1:D:470:GLU:CD	1:D:474:ASN:HD22	2.23	0.41
1:D:506:ILE:CG2	1:D:604:LEU:HB3	2.51	0.41
1:A:483:ARG:HD2	1:D:548:ASN:OD1	2.20	0.41
1:C:624:ASN:C	1:C:625:ILE:HG13	2.41	0.41
1:C:699:VAL:HG21	1:C:810:MET:HG3	2.03	0.41
1:D:708:ILE:HD11	1:D:864:ASN:HA	2.03	0.41
1:D:843:ILE:HG23	1:D:844:ASN:HD22	1.85	0.41
1:A:777:ASN:H	1:A:787:GLN:HE21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ALA:HB2	1:B:557:THR:HG21	2.03	0.41
1:B:464:ALA:CB	1:B:626:LEU:HD11	2.50	0.41
1:C:582:TRP:CD1	1:C:884:LEU:HD21	2.56	0.41
1:C:663:ALA:HB2	1:D:659:MET:HB3	2.03	0.41
1:D:693:GLN:O	1:D:696:MET:HB2	2.21	0.41
1:A:551:ARG:HA	1:A:553:ASN:N	2.36	0.41
1:A:735:LYS:N	1:A:745:ASN:ND2	2.62	0.41
1:A:838:VAL:O	1:A:838:VAL:HG13	2.21	0.41
1:B:461:VAL:HG22	1:B:633:VAL:HG13	2.03	0.41
1:B:674:LEU:O	2:B:1001:NDP:H2N	2.21	0.41
1:D:696:MET:HE3	1:D:696:MET:HB3	1.67	0.41
1:D:746:HIS:CE1	1:D:786:PHE:O	2.70	0.41
1:A:751:HIS:HD2	1:A:753:ALA:HB3	1.86	0.40
1:C:406:ILE:HG12	1:C:430:PHE:HD1	1.86	0.40
1:C:579:MET:O	1:C:580:LEU:C	2.59	0.40
1:A:497:GLU:O	1:A:500:GLN:CG	2.49	0.40
1:A:844:ASN:HD22	1:A:844:ASN:N	2.19	0.40
1:B:863:TYR:HD2	1:B:864:ASN:H	1.62	0.40
1:D:708:ILE:O	1:D:709:ALA:C	2.57	0.40
1:D:770:ALA:HB2	1:D:798:MET:SD	2.61	0.40
1:A:659:MET:HG2	1:B:663:ALA:HB2	2.01	0.40
1:A:773:VAL:HG13	1:A:790:VAL:O	2.21	0.40
1:B:611:GLU:O	1:B:614:LEU:HB2	2.22	0.40
1:C:418:LEU:HD11	1:C:505:THR:HG22	2.04	0.40
1:C:424:LEU:HD12	1:C:433:ALA:HA	2.02	0.40
1:C:540:ILE:HD11	1:C:889:LEU:HD13	2.03	0.40
1:B:424:LEU:HD22	1:B:456:ALA:HB2	2.04	0.40
1:B:471:ALA:HB2	1:B:621:GLY:HA3	2.02	0.40
1:D:547:ILE:N	1:D:547:ILE:HD12	2.36	0.40
1:D:870:ALA:HA	1:D:871:PRO:HD3	1.73	0.40
1:B:453:VAL:HG21	1:B:603:PRO:HG2	2.04	0.40
1:D:633:VAL:O	1:D:634:GLY:C	2.60	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	496/517 (96%)	452 (91%)	35 (7%)	9 (2%)	8 35
1	B	496/517 (96%)	449 (90%)	37 (8%)	10 (2%)	7 33
1	C	496/517 (96%)	436 (88%)	51 (10%)	9 (2%)	8 35
1	D	496/517 (96%)	428 (86%)	58 (12%)	10 (2%)	7 33
All	All	1984/2068 (96%)	1765 (89%)	181 (9%)	38 (2%)	8 34

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	772	LEU
1	B	436	SER
1	B	718	SER
1	C	707	SER
1	C	781	ARG
1	B	703	LYS
1	C	665	SER
1	D	462	ASP
1	D	817	ASP
1	D	884	LEU
1	A	436	SER
1	B	547	ILE
1	B	665	SER
1	B	829	ALA
1	B	884	LEU
1	B	887	ALA
1	C	825	SER
1	A	451	CYS
1	A	709	ALA
1	A	706	ASN
1	B	433	ALA
1	B	546	PRO
1	C	547	ILE
1	C	824	LEU
1	D	692	VAL
1	D	876	LYS
1	A	829	ALA
1	A	862	THR

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Mol	Chain	Res	Type
1	C	572	PRO
1	C	876	LYS
1	D	451	CYS
1	D	820	VAL
1	D	461	VAL
1	A	603	PRO
1	A	572	PRO
1	D	547	ILE
1	D	675	GLY
1	C	808	PRO

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	409/426 (96%)	365 (89%)	44 (11%)	6	25
1	B	409/426 (96%)	363 (89%)	46 (11%)	6	23
1	C	409/426 (96%)	368 (90%)	41 (10%)	7	28
1	D	409/426 (96%)	358 (88%)	51 (12%)	4	18
All	All	1636/1704 (96%)	1454 (89%)	182 (11%)	6	23

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LEU
1	A	417	THR
1	A	423	GLN
1	A	437	LYS
1	A	438	THR
1	A	443	ASN
1	A	459	SER
1	A	474	ASN
1	A	480	ILE
1	A	487	ARG
1	A	516	THR

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Mol	Chain	Res	Type
1	A	525	MET
1	A	547	ILE
1	A	597	LYS
1	A	605	THR
1	A	632	LEU
1	A	645	LYS
1	A	653	GLU
1	A	658	ILE
1	A	664	LEU
1	A	678	SER
1	A	680	LEU
1	A	690	LYS
1	A	694	MET
1	A	703	LYS
1	A	707	SER
1	A	732	GLU
1	A	736	ILE
1	A	742	ARG
1	A	745	ASN
1	A	757	LYS
1	A	763	GLN
1	A	768	GLU
1	A	773	VAL
1	A	778	GLN
1	A	781	ARG
1	A	787	GLN
1	A	803	GLU
1	A	805	SER
1	A	814	ARG
1	A	867	ASP
1	A	882	LYS
1	A	884	LEU
1	A	894	ARG
1	B	405	VAL
1	B	407	ASN
1	B	411	LYS
1	B	419	GLN
1	B	431	VAL
1	B	441	THR
1	B	442	ILE
1	B	443	ASN
1	B	454	SER

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Mol	Chain	Res	Type
1	B	458	VAL
1	B	476	LEU
1	B	491	ARG
1	B	501	GLU
1	B	509	LEU
1	B	516	THR
1	B	517	LEU
1	B	519	LEU
1	B	525	MET
1	B	547	ILE
1	B	553	ASN
1	B	597	LYS
1	B	600	GLN
1	B	601	VAL
1	B	620	LYS
1	B	632	LEU
1	B	664	LEU
1	B	678	SER
1	B	688	LEU
1	B	690	LYS
1	B	694	MET
1	B	703	LYS
1	B	706	ASN
1	B	718	SER
1	B	725	GLN
1	B	726	LYS
1	B	732	GLU
1	B	742	ARG
1	B	743	ASP
1	B	759	VAL
1	B	781	ARG
1	B	803	GLU
1	B	805	SER
1	B	841	ARG
1	B	850	SER
1	B	884	LEU
1	B	894	ARG
1	C	410	GLU
1	C	417	THR
1	C	436	SER
1	C	439	TYR
1	C	443	ASN

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Mol	Chain	Res	Type
1	C	459	SER
1	C	517	LEU
1	C	519	LEU
1	C	525	MET
1	C	540	ILE
1	C	547	ILE
1	C	554	ARG
1	C	597	LYS
1	C	619	PRO
1	C	620	LYS
1	C	624	ASN
1	C	631	SER
1	C	632	LEU
1	C	636	ARG
1	C	645	LYS
1	C	660	LYS
1	C	668	LYS
1	C	671	SER
1	C	693	GLN
1	C	694	MET
1	C	707	SER
1	C	717	GLU
1	C	725	GLN
1	C	728	VAL
1	C	735	LYS
1	C	743	ASP
1	C	745	ASN
1	C	778	GLN
1	C	787	GLN
1	C	795	GLU
1	C	814	ARG
1	C	843	ILE
1	C	850	SER
1	C	867	ASP
1	C	884	LEU
1	C	894	ARG
1	D	405	VAL
1	D	413	VAL
1	D	417	THR
1	D	419	GLN
1	D	431	VAL
1	D	438	THR

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Mol	Chain	Res	Type
1	D	441	THR
1	D	443	ASN
1	D	444	PRO
1	D	450	ILE
1	D	459	SER
1	D	476	LEU
1	D	479	LYS
1	D	483	ARG
1	D	494	ASP
1	D	507	GLU
1	D	516	THR
1	D	519	LEU
1	D	525	MET
1	D	526	SER
1	D	571	ILE
1	D	597	LYS
1	D	601	VAL
1	D	605	THR
1	D	620	LYS
1	D	632	LEU
1	D	658	ILE
1	D	660	LYS
1	D	664	LEU
1	D	667	VAL
1	D	678	SER
1	D	693	GLN
1	D	694	MET
1	D	703	LYS
1	D	706	ASN
1	D	707	SER
1	D	718	SER
1	D	726	LYS
1	D	730	GLU
1	D	745	ASN
1	D	750	ASN
1	D	757	LYS
1	D	764	ARG
1	D	771	THR
1	D	803	GLU
1	D	810	MET
1	D	813	SER
1	D	817	ASP

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Mol	Chain	Res	Type
1	D	819	ASP
1	D	830	THR
1	D	894	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	ASN
1	A	452	GLN
1	A	548	ASN
1	A	657	HIS
1	A	706	ASN
1	A	720	HIS
1	A	745	ASN
1	A	751	HIS
1	A	787	GLN
1	A	844	ASN
1	B	419	GLN
1	B	443	ASN
1	B	548	ASN
1	B	635	GLN
1	B	657	HIS
1	B	720	HIS
1	B	746	HIS
1	B	778	GLN
1	B	787	GLN
1	B	844	ASN
1	C	443	ASN
1	C	457	GLN
1	C	548	ASN
1	C	600	GLN
1	C	657	HIS
1	C	693	GLN
1	C	720	HIS
1	C	746	HIS
1	C	751	HIS
1	C	778	GLN
1	C	787	GLN
1	C	844	ASN
1	C	877	GLN
1	D	419	GLN
1	D	443	ASN

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Mol	Chain	Res	Type
1	D	452	GLN
1	D	474	ASN
1	D	481	ASN
1	D	548	ASN
1	D	657	HIS
1	D	706	ASN
1	D	745	ASN
1	D	746	HIS
1	D	778	GLN
1	D	844	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	C	1001	-	45,52,52	1.73	6 (13%)	53,80,80	1.50	7 (13%)
2	NDP	B	1001	-	45,52,52	1.67	5 (11%)	53,80,80	1.51	7 (13%)
2	NDP	D	1001	-	45,52,52	1.78	7 (15%)	53,80,80	1.58	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NDP	A	1001	-	45,52,52	1.78	5 (11%)	53,80,80	1.69	8 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	C	1001	-	-	7/30/77/77	0/5/5/5
2	NDP	B	1001	-	-	15/30/77/77	0/5/5/5
2	NDP	D	1001	-	-	12/30/77/77	0/5/5/5
2	NDP	A	1001	-	-	7/30/77/77	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NDP	O7N-C7N	6.89	1.40	1.24
2	C	1001	NDP	O7N-C7N	6.87	1.40	1.24
2	B	1001	NDP	O7N-C7N	6.78	1.40	1.24
2	D	1001	NDP	O7N-C7N	6.62	1.40	1.24
2	D	1001	NDP	C6N-C5N	5.25	1.42	1.33
2	B	1001	NDP	C6N-C5N	5.17	1.42	1.33
2	A	1001	NDP	C2A-N3A	5.15	1.40	1.32
2	A	1001	NDP	C6N-C5N	4.89	1.42	1.33
2	C	1001	NDP	C6N-C5N	4.65	1.41	1.33
2	D	1001	NDP	C2A-N3A	4.29	1.39	1.32
2	B	1001	NDP	C2A-N3A	3.86	1.38	1.32
2	C	1001	NDP	C2A-N3A	3.75	1.38	1.32
2	D	1001	NDP	C2N-C3N	3.42	1.44	1.34
2	C	1001	NDP	C2N-C3N	2.90	1.43	1.34
2	C	1001	NDP	C2A-N1A	2.76	1.39	1.33
2	A	1001	NDP	C2N-C3N	2.72	1.42	1.34
2	A	1001	NDP	C2A-N1A	2.59	1.38	1.33
2	B	1001	NDP	C2N-C3N	2.56	1.42	1.34
2	D	1001	NDP	C2A-N1A	2.53	1.38	1.33
2	B	1001	NDP	C2A-N1A	2.25	1.38	1.33
2	D	1001	NDP	C4N-C3N	2.11	1.54	1.49
2	C	1001	NDP	C1D-N1N	2.06	1.52	1.46
2	D	1001	NDP	C7N-C3N	2.05	1.53	1.48

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	NDP	O4D-C1D-N1N	6.01	119.80	108.06
2	B	1001	NDP	N3A-C2A-N1A	-5.28	120.42	128.68
2	C	1001	NDP	N3A-C2A-N1A	-5.14	120.65	128.68
2	A	1001	NDP	N3A-C2A-N1A	-5.11	120.68	128.68
2	D	1001	NDP	N3A-C2A-N1A	-4.92	120.99	128.68
2	D	1001	NDP	O4D-C1D-N1N	4.07	116.02	108.06
2	B	1001	NDP	O4D-C1D-N1N	3.72	115.32	108.06
2	A	1001	NDP	O4D-C4D-C5D	3.66	121.40	109.37
2	C	1001	NDP	O5D-C5D-C4D	3.48	120.97	108.99
2	B	1001	NDP	O4B-C1B-C2B	-3.42	100.66	106.59
2	C	1001	NDP	C3D-C2D-C1D	3.33	107.74	101.43
2	D	1001	NDP	O4B-C1B-C2B	-3.19	101.05	106.59
2	D	1001	NDP	C3D-C2D-C1D	3.11	107.33	101.43
2	A	1001	NDP	O4B-C1B-C2B	-2.99	101.39	106.59
2	B	1001	NDP	C1B-N9A-C4A	-2.87	121.60	126.64
2	A	1001	NDP	O2B-C2B-C1B	2.77	120.07	110.10
2	A	1001	NDP	O2X-P2B-O2B	2.77	118.39	105.99
2	D	1001	NDP	PN-O3-PA	-2.70	123.56	132.83
2	A	1001	NDP	O3D-C3D-C2D	2.57	120.12	111.82
2	C	1001	NDP	PN-O3-PA	-2.54	124.09	132.83
2	B	1001	NDP	O7N-C7N-C3N	-2.54	116.12	120.90
2	C	1001	NDP	C4D-O4D-C1D	2.45	114.88	109.47
2	D	1001	NDP	O7N-C7N-N7N	-2.41	117.24	122.88
2	B	1001	NDP	C3B-C2B-C1B	-2.40	98.37	102.89
2	D	1001	NDP	C3N-C7N-N7N	2.37	121.87	117.67
2	D	1001	NDP	C4A-C5A-N7A	-2.35	106.95	109.40
2	D	1001	NDP	O2B-C2B-C1B	2.34	118.54	110.10
2	D	1001	NDP	O2B-P2B-O1X	-2.32	100.45	109.39
2	B	1001	NDP	C4A-C5A-N7A	-2.28	107.02	109.40
2	D	1001	NDP	O4D-C1D-C2D	-2.26	101.72	106.64
2	A	1001	NDP	C5A-C6A-N6A	-2.21	116.99	120.35
2	C	1001	NDP	O2A-PA-O5B	2.20	117.95	107.75
2	C	1001	NDP	C3N-C7N-N7N	2.02	121.26	117.67

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NDP	O4D-C4D-C5D-O5D
2	A	1001	NDP	C3D-C4D-C5D-O5D
2	A	1001	NDP	O4D-C1D-N1N-C2N
2	A	1001	NDP	C2N-C3N-C7N-N7N
2	B	1001	NDP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	B	1001	NDP	C5B-O5B-PA-O3
2	B	1001	NDP	PN-O3-PA-O5B
2	B	1001	NDP	C5D-O5D-PN-O1N
2	B	1001	NDP	C5D-O5D-PN-O2N
2	B	1001	NDP	C2N-C3N-C7N-N7N
2	C	1001	NDP	C4D-C5D-O5D-PN
2	D	1001	NDP	C5B-O5B-PA-O1A
2	D	1001	NDP	C5B-O5B-PA-O3
2	D	1001	NDP	C5D-O5D-PN-O1N
2	D	1001	NDP	C4D-C5D-O5D-PN
2	D	1001	NDP	C3D-C4D-C5D-O5D
2	B	1001	NDP	C3D-C4D-C5D-O5D
2	C	1001	NDP	O4D-C4D-C5D-O5D
2	C	1001	NDP	C3D-C4D-C5D-O5D
2	B	1001	NDP	O4D-C1D-N1N-C2N
2	D	1001	NDP	O4D-C1D-N1N-C2N
2	D	1001	NDP	O4D-C4D-C5D-O5D
2	C	1001	NDP	O4D-C1D-N1N-C2N
2	B	1001	NDP	O4D-C4D-C5D-O5D
2	B	1001	NDP	C4B-C5B-O5B-PA
2	A	1001	NDP	C5D-O5D-PN-O3
2	D	1001	NDP	C5D-O5D-PN-O3
2	C	1001	NDP	PN-O3-PA-O2A
2	D	1001	NDP	PN-O3-PA-O2A
2	D	1001	NDP	C5D-O5D-PN-O2N
2	A	1001	NDP	PN-O3-PA-O1A
2	D	1001	NDP	O4B-C4B-C5B-O5B
2	B	1001	NDP	C2B-O2B-P2B-O1X
2	B	1001	NDP	C5D-O5D-PN-O3
2	C	1001	NDP	C2B-O2B-P2B-O2X
2	B	1001	NDP	C4D-C5D-O5D-PN
2	A	1001	NDP	PN-O3-PA-O2A
2	B	1001	NDP	PN-O3-PA-O1A
2	B	1001	NDP	PN-O3-PA-O2A
2	C	1001	NDP	PN-O3-PA-O1A
2	D	1001	NDP	PN-O3-PA-O1A

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	NDP	2	0

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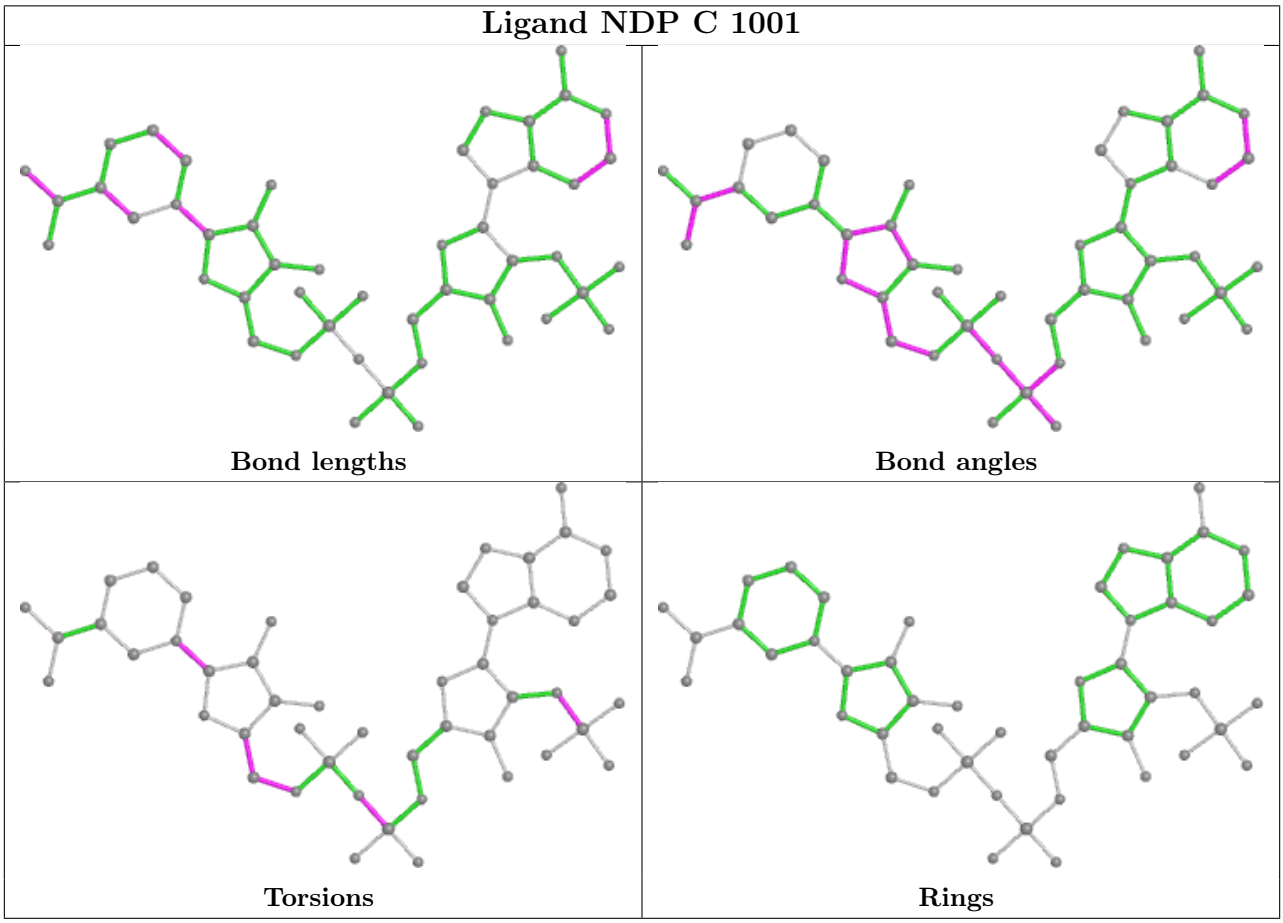
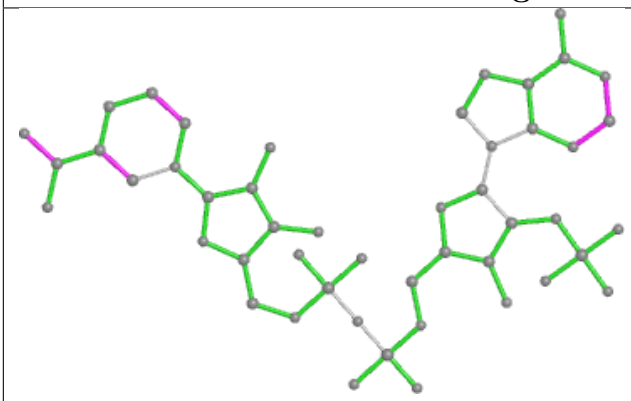
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	NDP	4	0
2	D	1001	NDP	7	0
2	A	1001	NDP	3	0

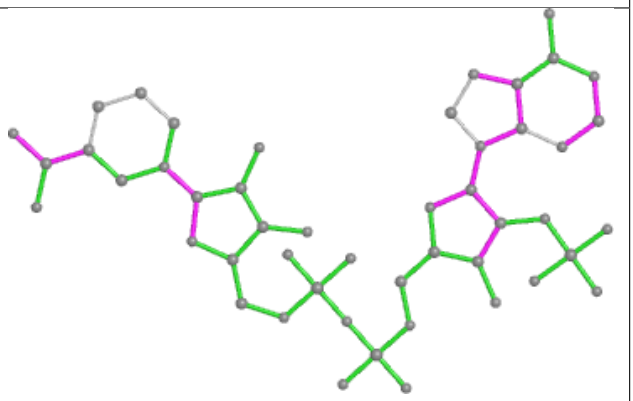
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



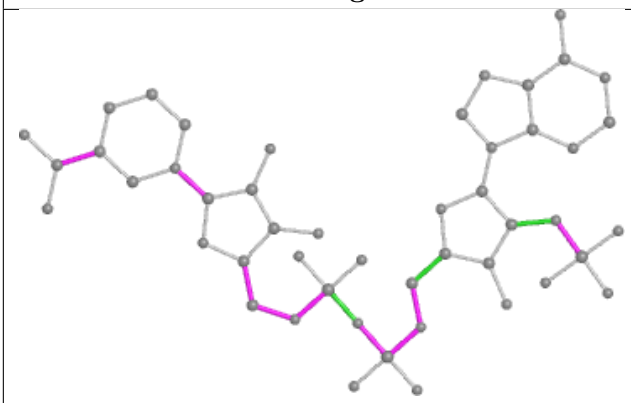
Ligand NDP B 1001



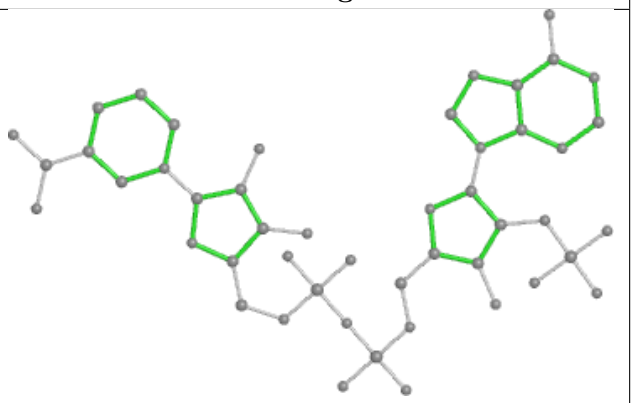
Bond lengths



Bond angles

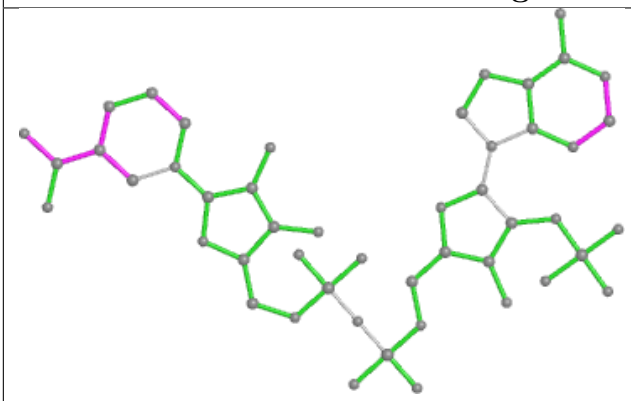


Torsions

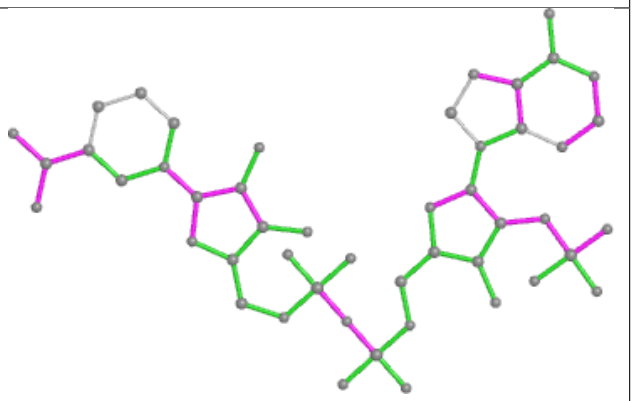


Rings

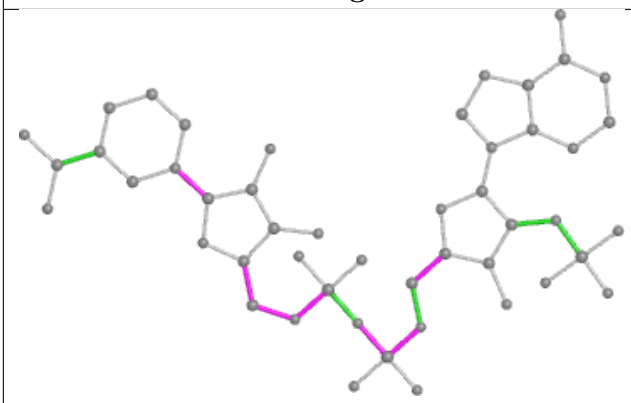
Ligand NDP D 1001



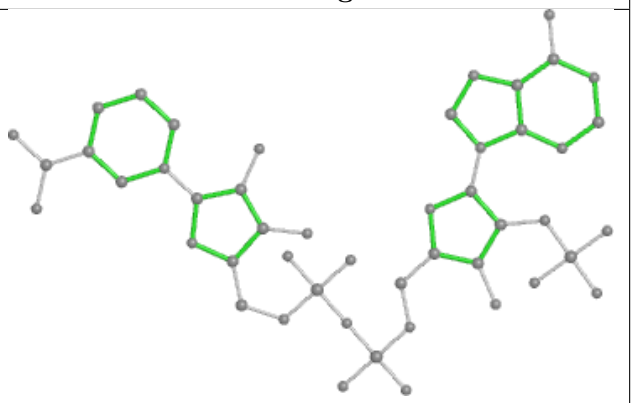
Bond lengths



Bond angles

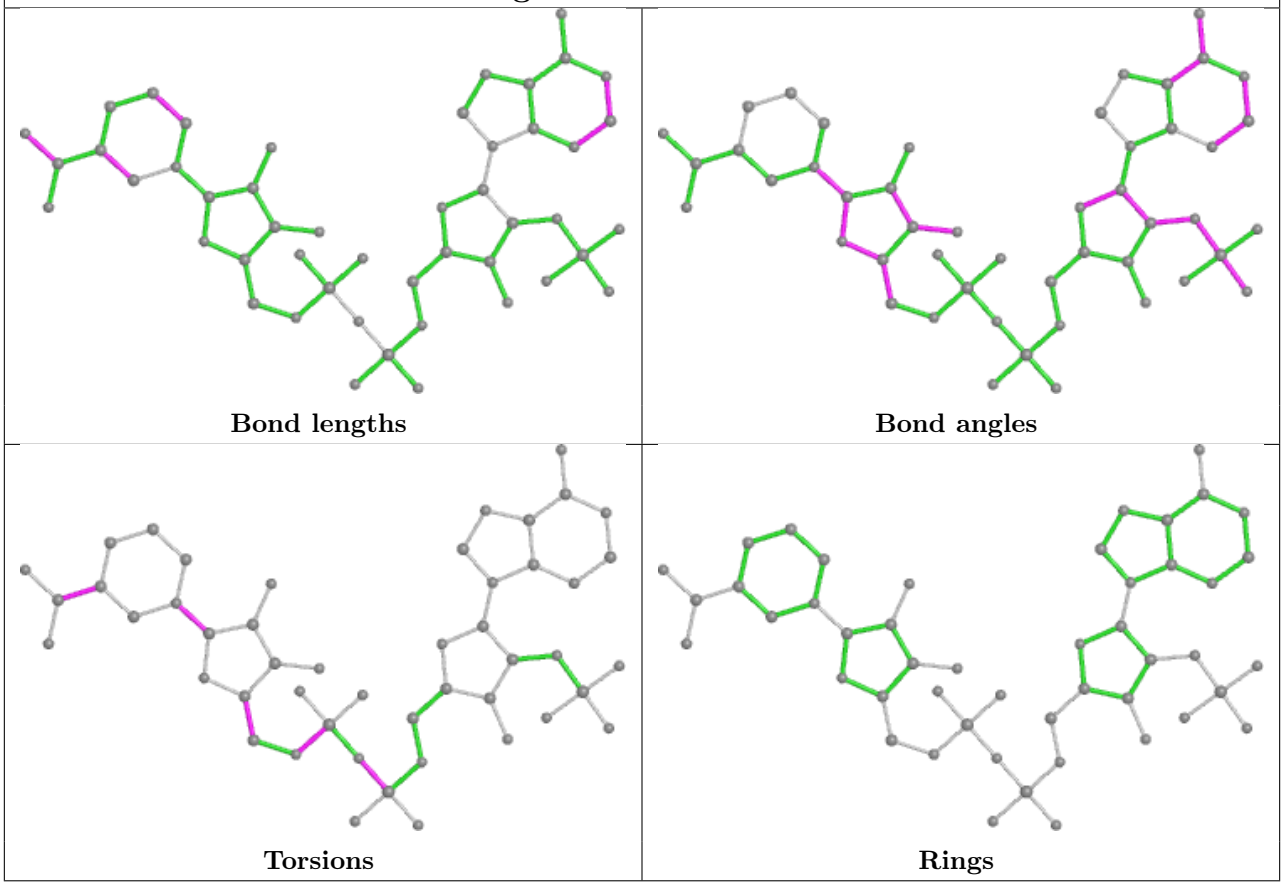


Torsions



Rings

Ligand NDP A 1001



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	498/517 (96%)	-0.21	1 (0%)	95	97	38, 52, 68, 78	0
1	B	498/517 (96%)	-0.20	4 (0%)	86	89	38, 53, 68, 87	0
1	C	498/517 (96%)	-0.34	1 (0%)	95	97	33, 49, 61, 74	0
1	D	498/517 (96%)	-0.28	4 (0%)	86	89	35, 51, 67, 80	0
All	All	1992/2068 (96%)	-0.26	10 (0%)	91	93	33, 51, 67, 87	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	TYR	2.9
1	B	422	TYR	2.6
1	D	552	PRO	2.6
1	C	687	ASP	2.3
1	D	553	ASN	2.3
1	B	454	SER	2.2
1	B	742	ARG	2.1
1	A	422	TYR	2.1
1	B	414	ASN	2.0
1	D	819	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

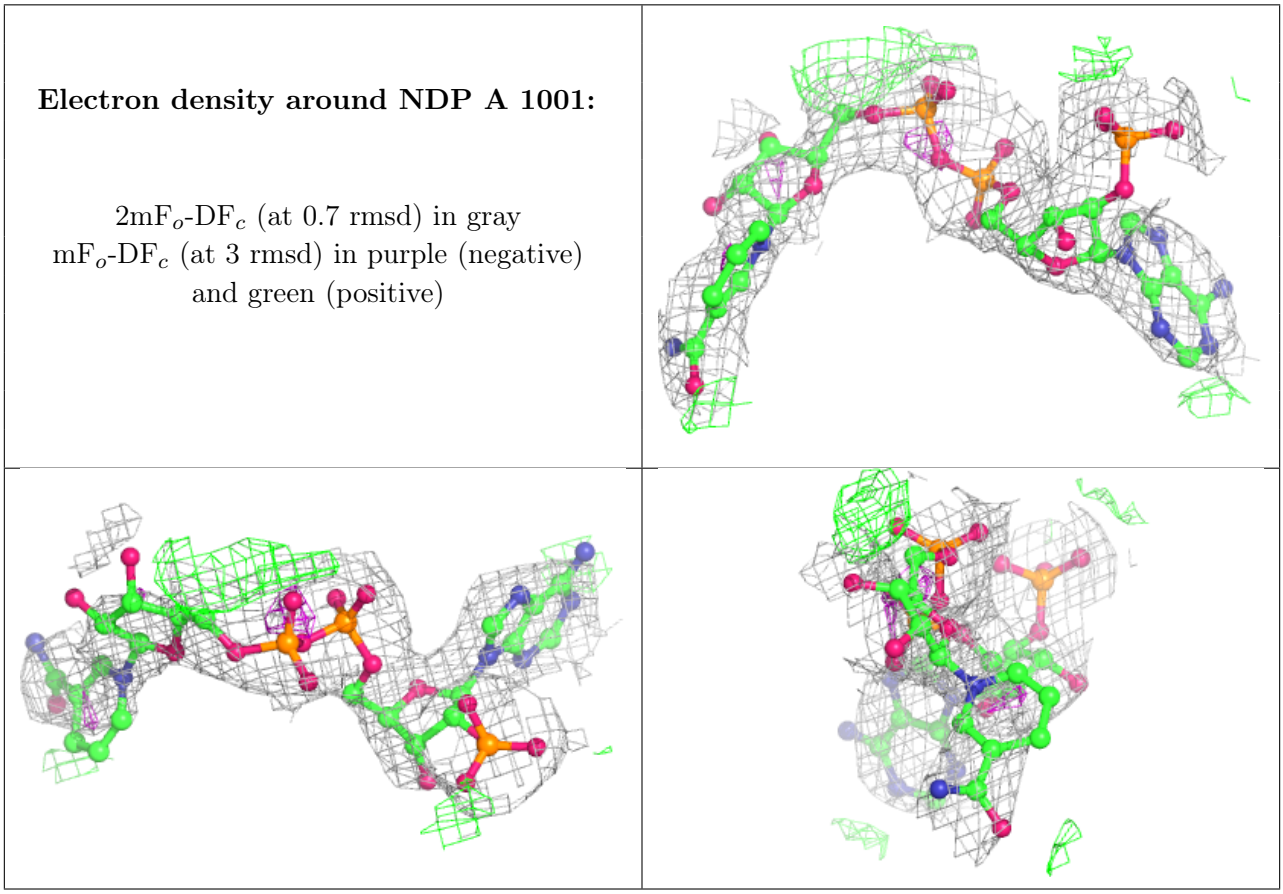
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NDP	A	1001	48/48	0.92	0.24	62,72,92,94	0
2	NDP	C	1001	48/48	0.92	0.27	51,65,81,82	0
2	NDP	B	1001	48/48	0.94	0.19	64,71,86,87	0
2	NDP	D	1001	48/48	0.95	0.20	51,62,80,83	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.

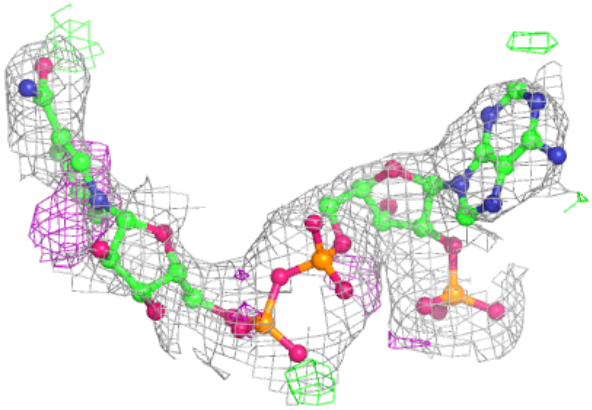
Electron density around NDP A 1001:

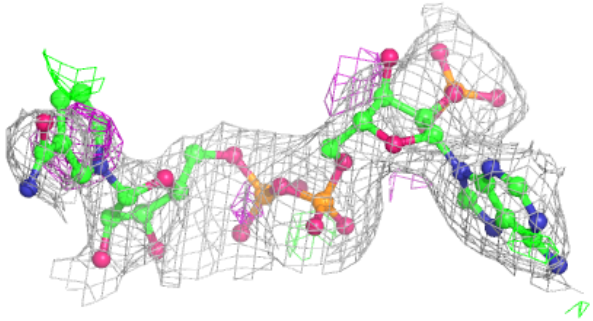
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

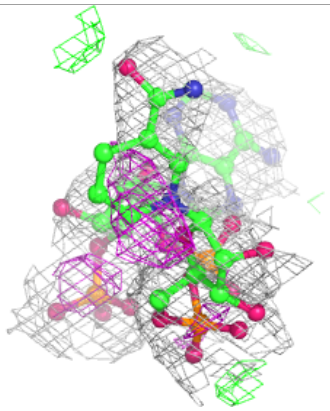


Electron density around NDP C 1001:

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

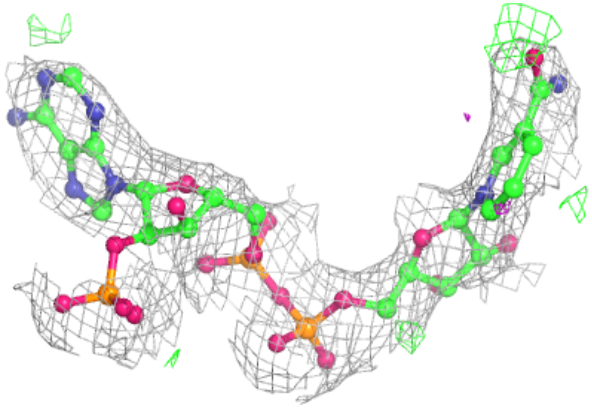


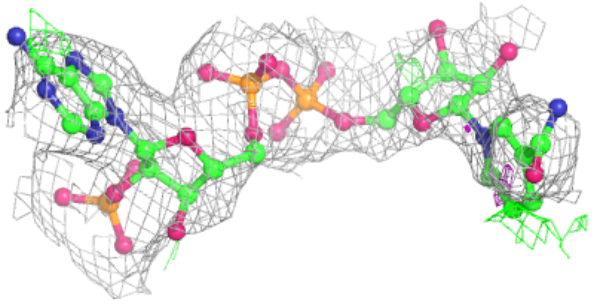


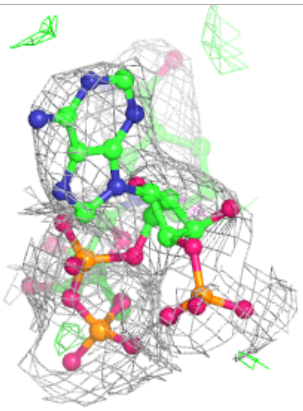


Electron density around NDP B 1001:

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

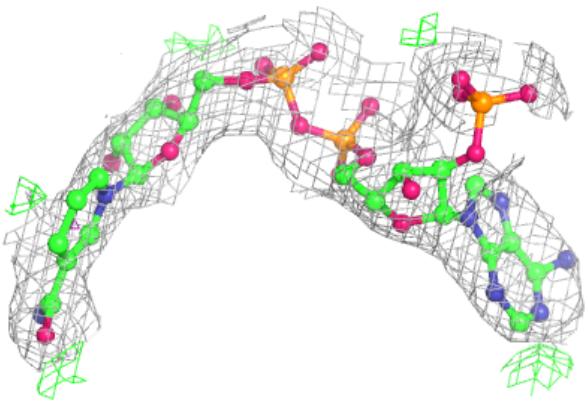


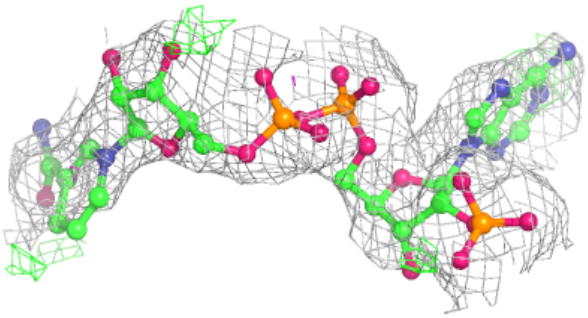


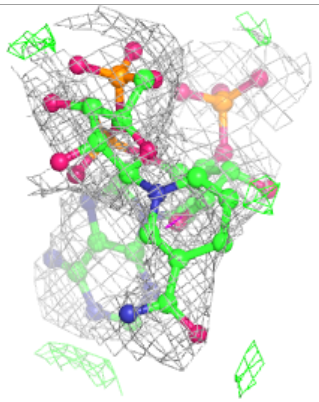


Electron density around NDP D 1001:

$2mF_o$-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.