Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:46 PM GMT

PDB ID	:	1QI1
Title	:	Ternary Complex of an NADP Dependent Aldehyde Dehydrogenase
Authors	:	Cobessi, D.; Tete-Favier, F.; Marchal, S.; Branlant, G.; Aubry, A.
Deposited on	:	1999-06-02
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

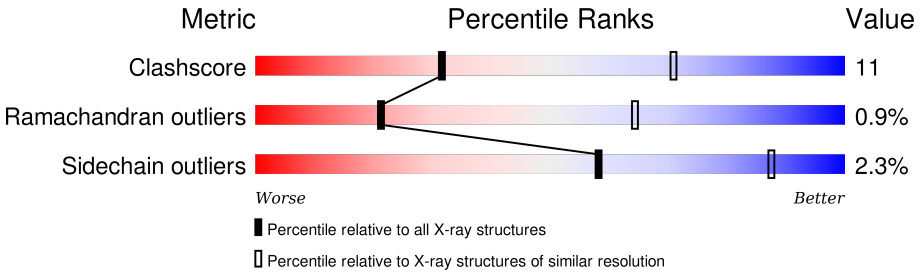
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	76% 23%
1	B	475	78% 21%
1	C	475	78% 21%
1	D	475	79% 20%

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
2	NAP	B	501	-	-	X	-
3	G3H	A	504	-	-	X	-
3	G3H	C	506	-	-	X	-
3	G3H	D	507	-	-	X	-
4	G3P	B	505	X	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14616 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.

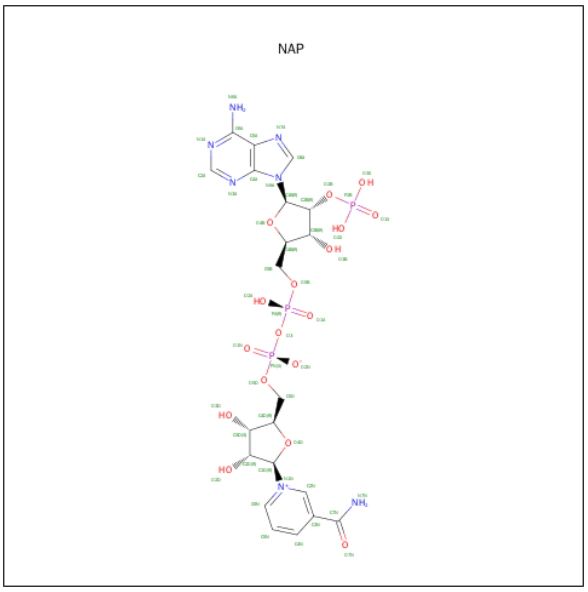
- Molecule 1 is a protein called PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	B	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	C	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	D	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			

There are 4 discrepancies between the modelled and reference sequences:

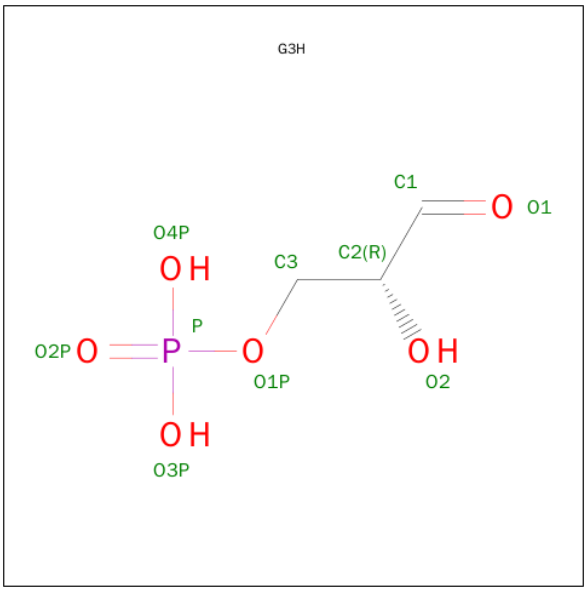
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	SER	CYS	ENGINEERED	UNP Q59931
B	284	SER	CYS	ENGINEERED	UNP Q59931
C	284	SER	CYS	ENGINEERED	UNP Q59931
D	284	SER	CYS	ENGINEERED	UNP Q59931

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



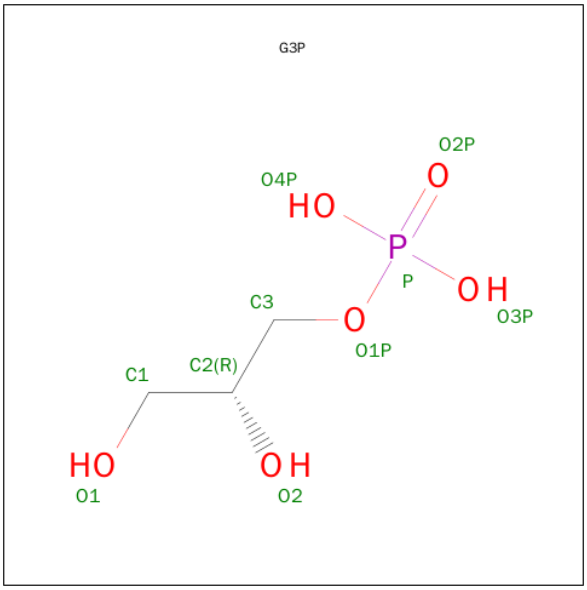
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 10 3 6 1	0	0
3	C	1	Total C O P 10 3 6 1	0	0
3	D	1	Total C O P 10 3 6 1	0	0

- Molecule 4 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O P 10 3 6 1	0	0

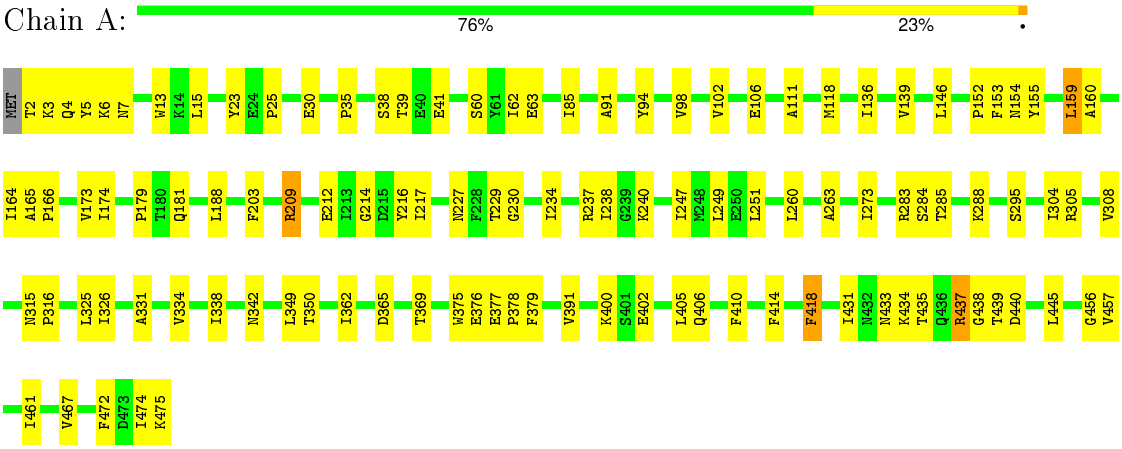
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

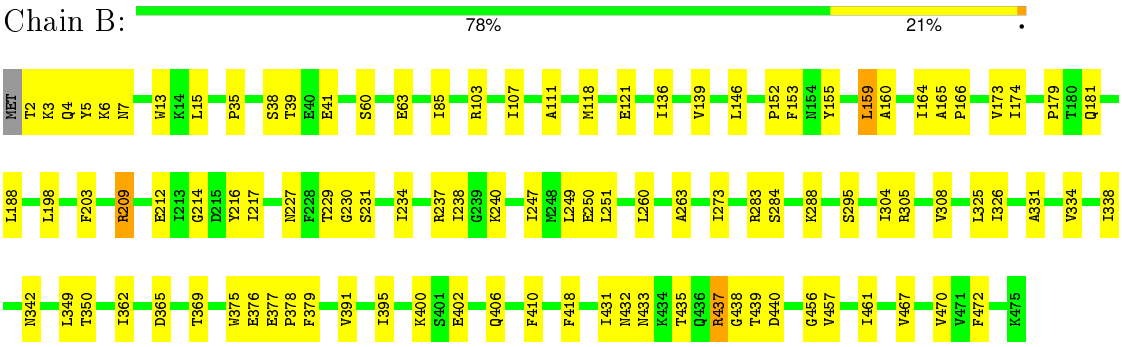
• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain A:



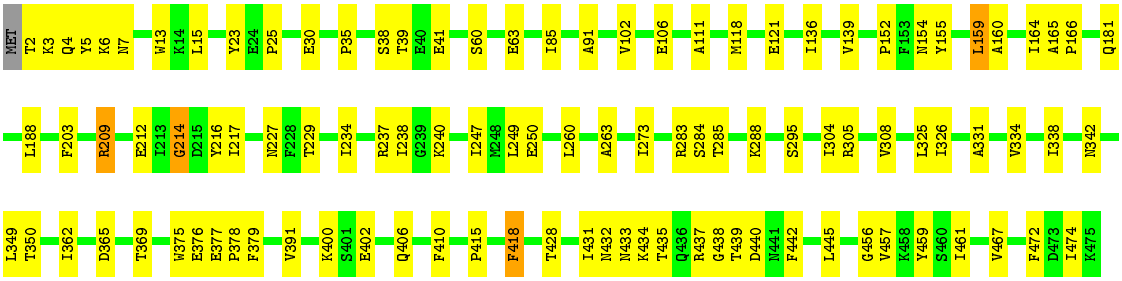
• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain B:



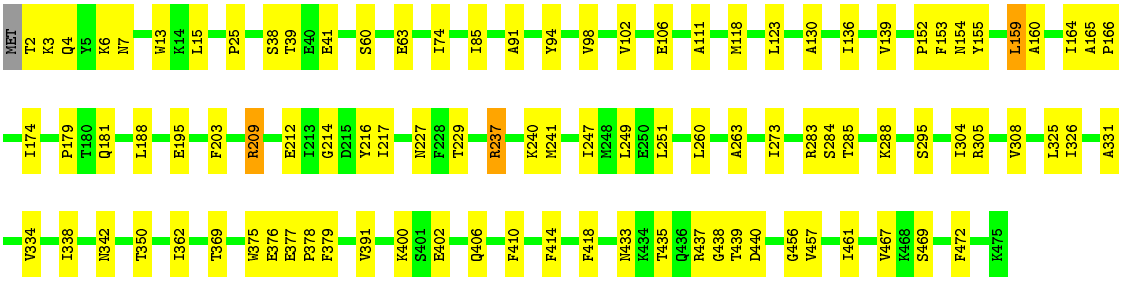
• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain C:



• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.50Å 158.50Å 282.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.0 (8.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.242 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14616	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G3P, NAP, G3H

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	0.50	0/3654	0.82	11/4942 (0.2%)
1	B	0.52	0/3654	0.72	11/4942 (0.2%)
1	C	0.50	0/3654	0.89	13/4942 (0.3%)
1	D	0.52	0/3654	0.90	13/4942 (0.3%)
All	All	0.51	0/14616	0.84	48/19768 (0.2%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	ARG	NE-CZ-NH2	-21.16	109.72	120.30
1	A	209	ARG	NE-CZ-NH1	20.22	130.41	120.30
1	C	283	ARG	NE-CZ-NH1	19.87	130.23	120.30
1	D	305	ARG	NE-CZ-NH2	-19.61	110.49	120.30
1	D	437	ARG	NE-CZ-NH1	19.03	129.81	120.30
1	D	437	ARG	NE-CZ-NH2	-18.94	110.83	120.30
1	D	305	ARG	NE-CZ-NH1	18.81	129.71	120.30
1	C	237	ARG	NE-CZ-NH1	18.57	129.58	120.30
1	C	237	ARG	NE-CZ-NH2	-18.24	111.18	120.30
1	C	283	ARG	NE-CZ-NH2	-18.19	111.20	120.30
1	A	209	ARG	CD-NE-CZ	9.79	137.30	123.60
1	C	283	ARG	CD-NE-CZ	9.69	137.17	123.60
1	D	437	ARG	CD-NE-CZ	9.05	136.27	123.60
1	D	305	ARG	CD-NE-CZ	8.66	135.72	123.60
1	C	237	ARG	CD-NE-CZ	7.77	134.48	123.60
1	B	305	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	305	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	C	437	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	237	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	209	ARG	NE-CZ-NH2	-6.73	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	C	437	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	237	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	437	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	283	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	283	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	283	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	283	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	209	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	209	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	437	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	C	305	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	437	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	237	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	283	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	437	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	305	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	209	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	305	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	209	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	237	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	C	305	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	237	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	456	GLY	N-CA-C	-5.28	99.89	113.10
1	D	209	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	456	GLY	N-CA-C	-5.10	100.35	113.10
1	B	456	GLY	N-CA-C	-5.03	100.52	113.10
1	D	456	GLY	N-CA-C	-5.01	100.57	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3596	0	3649	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3596	0	3649	70	0
1	C	3596	0	3649	81	0
1	D	3596	0	3649	71	0
2	A	48	0	25	16	0
2	B	48	0	25	21	0
2	C	48	0	25	19	0
2	D	48	0	25	13	0
3	A	10	0	5	9	0
3	C	10	0	5	7	0
3	D	10	0	5	8	0
4	B	10	0	6	11	0
All	All	14616	0	14717	312	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 11.

All (312) 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:D:284:SER:HB3	2:D:503:NAP:C4N	1.60	1.31
1:C:285:THR:OG1	3:C:506:G3H:H31	1.41	1.18
1:C:284:SER:HB3	2:C:502:NAP:C5N	1.78	1.14
1:D:284:SER:HB3	2:D:503:NAP:C5N	1.79	1.12
1:D:284:SER:CB	2:D:503:NAP:C4N	2.28	1.10
1:D:155:TYR:HD2	1:D:159:LEU:HD22	1.11	1.05
1:C:284:SER:CB	2:C:502:NAP:C5N	2.36	1.02
1:D:155:TYR:CD2	1:D:159:LEU:HD22	1.93	1.01
1:A:154:ASN:C	1:A:155:TYR:HD1	1.64	1.00
2:A:500:NAP:N7N	3:A:504:G3H:H11	1.75	1.00
2:B:501:NAP:H72N	4:B:505:G3P:C2	1.77	0.98
1:D:284:SER:CB	2:D:503:NAP:C5N	2.43	0.96
1:A:284:SER:HB3	2:A:500:NAP:C5N	1.95	0.95
2:B:501:NAP:N7N	4:B:505:G3P:H11	1.82	0.94
1:B:437:ARG:HH11	4:B:505:G3P:H32	1.31	0.93
1:A:154:ASN:O	1:A:155:TYR:CD1	2.23	0.92
2:D:503:NAP:H72N	3:D:507:G3H:C1	1.82	0.91
1:C:154:ASN:ND2	2:C:502:NAP:H71N	1.70	0.88
1:B:251:LEU:O	2:B:501:NAP:H5N	1.74	0.87
1:D:284:SER:OG	2:D:503:NAP:H4N	1.75	0.86
1:A:154:ASN:O	1:A:155:TYR:HD1	1.58	0.84
2:A:500:NAP:N7N	3:A:504:G3H:C1	2.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:TYR:HD2	1:D:159:LEU:CD2	1.91	0.83
1:A:240:LYS:HG3	1:B:240:LYS:HG3	1.60	0.82
1:B:153:PHE:HD2	2:B:501:NAP:H51N	1.44	0.81
1:C:155:TYR:HE2	3:C:506:G3H:O1	1.61	0.81
1:D:251:LEU:O	2:D:503:NAP:H5N	1.81	0.80
1:A:154:ASN:C	1:A:155:TYR:CD1	2.54	0.79
1:C:285:THR:OG1	3:C:506:G3H:H32	1.83	0.79
1:D:284:SER:CB	2:D:503:NAP:H4N	2.13	0.79
1:C:155:TYR:CE2	3:C:506:G3H:O1	2.36	0.79
1:D:285:THR:OG1	3:D:507:G3H:C3	2.31	0.78
1:A:153:PHE:HD2	2:A:500:NAP:H51N	1.48	0.78
1:C:155:TYR:HD2	2:C:502:NAP:H72N	1.31	0.78
2:B:501:NAP:N7N	4:B:505:G3P:C2	2.47	0.77
2:A:500:NAP:H71N	3:A:504:G3H:H11	1.48	0.77
1:A:284:SER:HB3	2:A:500:NAP:C4N	2.15	0.76
2:B:501:NAP:N7N	4:B:505:G3P:C1	2.50	0.74
1:D:285:THR:OG1	3:D:507:G3H:H32	1.88	0.73
1:A:152:PRO:HG3	2:A:500:NAP:O7N	1.90	0.72
1:D:402:GLU:H	1:D:402:GLU:CD	1.91	0.72
1:C:284:SER:CB	2:C:502:NAP:H5N	2.18	0.71
1:C:284:SER:OG	2:C:502:NAP:C4N	2.39	0.71
1:A:23:TYR:HD1	1:A:30:GLU:HA	1.54	0.71
2:B:501:NAP:N7N	4:B:505:G3P:O2	2.24	0.71
1:A:402:GLU:CD	1:A:402:GLU:H	1.93	0.70
1:D:288:LYS:HE2	1:D:377:GLU:HG3	1.71	0.70
1:A:288:LYS:HE2	1:A:377:GLU:HG3	1.71	0.70
1:B:288:LYS:HE2	1:B:377:GLU:HG3	1.74	0.70
1:C:402:GLU:H	1:C:402:GLU:CD	1.95	0.70
1:B:153:PHE:CD2	2:B:501:NAP:H51N	2.27	0.68
1:B:402:GLU:CD	1:B:402:GLU:H	1.94	0.68
2:D:503:NAP:N7N	3:D:507:G3H:C1	2.57	0.67
1:C:285:THR:HG1	3:C:506:G3H:H31	1.55	0.67
1:A:474:ILE:HG23	1:C:418:PHE:HB3	1.76	0.67
1:C:288:LYS:HE2	1:C:377:GLU:HG3	1.77	0.65
1:C:284:SER:CB	2:C:502:NAP:C4N	2.74	0.65
1:A:153:PHE:CD2	2:A:500:NAP:H51N	2.30	0.65
1:A:284:SER:CB	2:A:500:NAP:C5N	2.70	0.65
1:B:230:GLY:HA2	2:B:501:NAP:H1D	1.79	0.64
1:C:154:ASN:HD21	2:C:502:NAP:H71N	1.43	0.63
1:A:437:ARG:HD3	3:A:504:G3H:O2	1.98	0.63
1:C:284:SER:HB3	2:C:502:NAP:C4N	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:CE1	1:A:30:GLU:HG3	2.33	0.63
1:C:260:LEU:HD22	1:C:391:VAL:HG22	1.81	0.62
1:A:60:SER:OG	1:A:63:GLU:HG3	2.00	0.62
1:C:154:ASN:CG	2:C:502:NAP:H71N	2.03	0.62
1:A:209:ARG:HB2	1:A:212:GLU:HB3	1.81	0.62
1:C:273:ILE:HD11	1:C:304:ILE:HG23	1.81	0.61
1:D:152:PRO:HD3	1:D:229:THR:HB	1.83	0.61
1:A:284:SER:CB	2:A:500:NAP:C4N	2.79	0.61
1:D:155:TYR:CD2	1:D:159:LEU:CD2	2.76	0.60
1:D:85:ILE:HD12	1:D:188:LEU:HD11	1.84	0.60
1:D:273:ILE:HD11	1:D:304:ILE:HG23	1.83	0.60
1:A:273:ILE:HD11	1:A:304:ILE:HG23	1.82	0.60
1:B:260:LEU:HD22	1:B:391:VAL:HG22	1.83	0.60
1:C:284:SER:OG	2:C:502:NAP:H4N	2.01	0.60
1:C:209:ARG:HB2	1:C:212:GLU:HB3	1.84	0.60
1:C:60:SER:OG	1:C:63:GLU:HG3	2.02	0.59
1:B:273:ILE:HD11	1:B:304:ILE:HG23	1.84	0.59
1:D:60:SER:OG	1:D:63:GLU:HG3	2.02	0.59
1:D:155:TYR:CE2	3:D:507:G3H:C1	2.86	0.59
1:B:240:LYS:HB2	1:B:240:LYS:NZ	2.16	0.59
1:B:231:SER:N	2:B:501:NAP:O3D	2.35	0.59
1:A:260:LEU:HD22	1:A:391:VAL:HG22	1.85	0.58
1:A:152:PRO:HD3	1:A:229:THR:HB	1.85	0.58
1:D:164:ILE:HD13	1:D:203:PHE:HE1	1.69	0.58
1:C:2:THR:O	1:C:4:GLN:N	2.33	0.58
1:B:209:ARG:HB2	1:B:212:GLU:HB3	1.85	0.58
1:B:155:TYR:HE2	4:B:505:G3P:O1	1.86	0.57
1:A:23:TYR:CD1	1:A:30:GLU:HA	2.37	0.57
1:D:209:ARG:HB2	1:D:212:GLU:HB3	1.86	0.57
1:C:445:LEU:HD11	1:D:467:VAL:O	2.04	0.57
1:B:60:SER:OG	1:B:63:GLU:HG3	2.04	0.57
2:B:501:NAP:H72N	4:B:505:G3P:H2	1.68	0.57
1:A:240:LYS:HB2	1:A:240:LYS:NZ	2.19	0.57
1:D:284:SER:HB2	2:D:503:NAP:C5N	2.33	0.57
1:A:155:TYR:CE2	3:A:504:G3H:H2	2.40	0.56
1:C:240:LYS:HB2	1:C:240:LYS:NZ	2.21	0.56
1:D:240:LYS:HB2	1:D:240:LYS:NZ	2.20	0.56
1:A:159:LEU:HD21	2:A:500:NAP:H72N	1.70	0.56
1:C:406:GLN:OE1	1:C:435:THR:HB	2.06	0.56
1:D:251:LEU:O	2:D:503:NAP:C5N	2.52	0.56
1:A:285:THR:OG1	3:A:504:G3H:C3	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLU:OE2	2:B:501:NAP:H4N	2.05	0.56
1:A:164:ILE:HD13	1:A:203:PHE:HE1	1.69	0.56
1:C:38:SER:OG	1:C:41:GLU:HG3	2.05	0.56
1:D:260:LEU:HD22	1:D:391:VAL:HG22	1.86	0.56
1:B:406:GLN:OE1	1:B:435:THR:HB	2.06	0.55
1:B:153:PHE:HD2	2:B:501:NAP:C5D	2.17	0.55
1:D:406:GLN:OE1	1:D:435:THR:HB	2.07	0.55
1:B:38:SER:OG	1:B:41:GLU:HG3	2.06	0.55
1:A:263:ALA:HB2	1:A:410:PHE:O	2.06	0.55
1:A:375:TRP:CH2	1:A:400:LYS:HB3	2.42	0.54
1:A:285:THR:OG1	3:A:504:G3H:H32	2.05	0.54
1:C:376:GLU:O	1:C:378:PRO:HD3	2.07	0.54
1:B:284:SER:OG	2:B:501:NAP:C4N	2.55	0.54
1:D:263:ALA:HB2	1:D:410:PHE:O	2.08	0.54
1:C:152:PRO:HD3	1:C:229:THR:HB	1.88	0.54
1:A:38:SER:OG	1:A:41:GLU:HG3	2.07	0.54
1:B:2:THR:O	1:B:4:GLN:N	2.36	0.53
1:B:121:GLU:HA	1:C:121:GLU:HA	1.89	0.53
1:A:406:GLN:OE1	1:A:435:THR:HB	2.08	0.53
1:C:164:ILE:HD13	1:C:203:PHE:HE1	1.73	0.53
1:B:164:ILE:HD13	1:B:203:PHE:HE1	1.73	0.53
1:B:152:PRO:HD3	1:B:229:THR:HB	1.90	0.53
2:C:502:NAP:N7N	3:C:506:G3H:O1	2.41	0.53
1:A:376:GLU:O	1:A:378:PRO:HD3	2.08	0.53
1:C:260:LEU:CD2	1:C:391:VAL:HG22	2.39	0.52
1:C:263:ALA:HB2	1:C:410:PHE:O	2.09	0.52
1:A:375:TRP:CZ3	1:A:400:LYS:HB3	2.45	0.52
1:A:475:LYS:HG3	1:C:415:PRO:HB2	1.91	0.52
1:D:38:SER:OG	1:D:41:GLU:HG3	2.10	0.52
1:D:2:THR:O	1:D:4:GLN:N	2.37	0.51
1:C:284:SER:HB3	2:C:502:NAP:C6N	2.34	0.51
1:D:375:TRP:CH2	1:D:400:LYS:HB3	2.45	0.51
1:A:85:ILE:HD12	1:A:188:LEU:HD11	1.91	0.51
1:D:155:TYR:CE2	3:D:507:G3H:O1	2.64	0.51
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.93	0.51
1:B:284:SER:CB	2:B:501:NAP:C4N	2.89	0.51
1:C:85:ILE:HD12	1:C:188:LEU:HD11	1.93	0.51
1:A:251:LEU:O	2:A:500:NAP:H5N	2.10	0.51
1:B:181:GLN:HG2	1:B:326:ILE:HD11	1.93	0.51
1:C:375:TRP:CH2	1:C:400:LYS:HB3	2.46	0.51
1:B:7:ASN:O	1:B:13:TRP:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:503:NAP:H72N	3:D:507:G3H:H11	1.70	0.50
1:B:85:ILE:HD12	1:B:188:LEU:HD11	1.93	0.50
1:B:375:TRP:CH2	1:B:400:LYS:HB3	2.46	0.50
1:D:284:SER:HB2	2:D:503:NAP:H5N	1.93	0.50
1:C:250:GLU:OE2	2:C:502:NAP:H4N	2.12	0.50
1:B:284:SER:HB3	2:B:501:NAP:C5N	2.42	0.50
1:A:475:LYS:HG3	1:C:415:PRO:CB	2.42	0.50
1:B:139:VAL:HG13	1:B:467:VAL:HG13	1.94	0.50
1:D:7:ASN:O	1:D:13:TRP:HA	2.12	0.49
1:A:350:THR:OG1	1:A:362:ILE:HA	2.12	0.49
1:D:139:VAL:HG13	1:D:467:VAL:HG13	1.93	0.49
1:B:260:LEU:CD2	1:B:391:VAL:HG22	2.42	0.49
1:B:375:TRP:CZ3	1:B:400:LYS:HB3	2.47	0.49
1:A:325:LEU:HD12	1:A:331:ALA:HA	1.95	0.49
1:A:7:ASN:O	1:A:13:TRP:HA	2.13	0.49
1:C:442:PHE:HA	1:D:123:LEU:HD12	1.94	0.49
1:B:376:GLU:O	1:B:378:PRO:HD3	2.12	0.49
1:B:457:VAL:O	1:B:461:ILE:HG13	2.12	0.49
1:C:139:VAL:HG13	1:C:467:VAL:HG13	1.94	0.49
1:D:154:ASN:O	1:D:155:TYR:CD1	2.65	0.49
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.95	0.49
1:C:334:VAL:O	1:C:338:ILE:HG13	2.12	0.49
1:B:284:SER:HB3	2:B:501:NAP:C4N	2.43	0.49
1:C:7:ASN:O	1:C:13:TRP:HA	2.12	0.49
2:B:501:NAP:H3D	2:B:501:NAP:O1N	2.13	0.49
1:B:334:VAL:O	1:B:338:ILE:HG13	2.13	0.49
1:D:375:TRP:CZ3	1:D:400:LYS:HB3	2.47	0.48
1:D:350:THR:OG1	1:D:362:ILE:HA	2.13	0.48
1:A:2:THR:O	1:A:4:GLN:N	2.37	0.48
1:A:284:SER:OG	2:A:500:NAP:H4N	2.12	0.48
1:A:139:VAL:HG13	1:A:467:VAL:HG13	1.95	0.48
1:C:3:LYS:O	1:C:4:GLN:HB2	2.13	0.48
1:B:159:LEU:HD23	2:B:501:NAP:O7N	2.13	0.48
1:A:260:LEU:CD2	1:A:391:VAL:HG22	2.44	0.48
1:B:350:THR:OG1	1:B:362:ILE:HA	2.13	0.48
1:C:375:TRP:CZ3	1:C:400:LYS:HB3	2.49	0.48
1:D:39:THR:HB	1:D:216:TYR:CE2	2.49	0.48
1:C:350:THR:OG1	1:C:362:ILE:HA	2.13	0.47
1:B:437:ARG:NH1	4:B:505:G3P:H32	2.14	0.47
1:C:154:ASN:CG	2:C:502:NAP:N7N	2.67	0.47
1:B:111:ALA:HA	1:B:457:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG21	1:D:130:ALA:N	2.29	0.47
1:D:376:GLU:O	1:D:378:PRO:HD3	2.14	0.47
1:A:230:GLY:HA3	2:A:500:NAP:H51A	1.96	0.47
1:D:350:THR:HG1	1:D:362:ILE:HA	1.80	0.47
1:A:136:ILE:HD11	1:A:472:PHE:CZ	2.50	0.47
1:A:418:PHE:HB3	1:C:474:ILE:HG23	1.97	0.47
1:B:325:LEU:HD12	1:B:331:ALA:HA	1.97	0.47
1:A:111:ALA:HA	1:A:457:VAL:CG1	2.45	0.47
1:A:39:THR:HB	1:A:216:TYR:CZ	2.50	0.47
1:C:181:GLN:HG2	1:C:326:ILE:HD11	1.97	0.47
1:C:111:ALA:HA	1:C:457:VAL:CG1	2.45	0.47
1:A:334:VAL:O	1:A:338:ILE:HG13	2.15	0.47
1:C:247:ILE:HD12	1:C:249:LEU:HD11	1.97	0.47
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.96	0.46
1:C:39:THR:HB	1:C:216:TYR:CZ	2.50	0.46
1:B:247:ILE:HD12	1:B:249:LEU:HD11	1.96	0.46
1:C:284:SER:HB2	2:C:502:NAP:H5N	1.97	0.46
1:B:263:ALA:HB2	1:B:410:PHE:O	2.15	0.46
1:A:247:ILE:HD12	1:A:249:LEU:HD11	1.97	0.46
1:C:459:TYR:OH	1:D:123:LEU:HD11	2.16	0.46
1:B:5:TYR:O	1:B:35:PRO:HD3	2.16	0.46
1:C:136:ILE:HD11	1:C:472:PHE:CZ	2.51	0.46
1:B:284:SER:OG	2:B:501:NAP:H4N	2.14	0.46
1:A:350:THR:HG1	1:A:362:ILE:HA	1.81	0.46
1:D:3:LYS:O	1:D:4:GLN:HB2	2.16	0.46
1:D:325:LEU:HD12	1:D:331:ALA:HA	1.97	0.46
1:D:181:GLN:HG2	1:D:326:ILE:HD11	1.97	0.46
1:C:284:SER:OG	2:C:502:NAP:C5N	2.60	0.46
1:A:284:SER:CB	2:A:500:NAP:H5N	2.46	0.46
1:D:304:ILE:O	1:D:308:VAL:HG23	2.16	0.45
1:D:39:THR:HB	1:D:216:TYR:CZ	2.50	0.45
1:D:247:ILE:HD12	1:D:249:LEU:HD11	1.97	0.45
1:C:159:LEU:CD2	2:C:502:NAP:O7N	2.64	0.45
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.99	0.45
1:A:214:GLY:O	1:A:217:ILE:HG12	2.16	0.45
1:D:111:ALA:HA	1:D:457:VAL:CG1	2.47	0.45
1:C:325:LEU:HD12	1:C:331:ALA:HA	1.98	0.45
1:C:25:PRO:HB2	1:C:91:ALA:HB2	1.99	0.45
1:A:181:GLN:HG2	1:A:326:ILE:HD11	1.98	0.45
1:A:39:THR:HB	1:A:216:TYR:CE2	2.51	0.45
1:D:334:VAL:O	1:D:338:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:HB	1:B:216:TYR:CZ	2.52	0.44
1:D:136:ILE:HD11	1:D:472:PHE:CZ	2.52	0.44
1:C:234:ILE:O	1:C:238:ILE:HG13	2.17	0.44
1:D:260:LEU:CD2	1:D:391:VAL:HG22	2.46	0.44
1:A:3:LYS:O	1:A:4:GLN:HB2	2.17	0.44
1:D:457:VAL:O	1:D:461:ILE:HG13	2.17	0.44
1:C:457:VAL:O	1:C:461:ILE:HG13	2.17	0.44
1:D:94:TYR:O	1:D:98:VAL:HG23	2.18	0.44
1:A:304:ILE:O	1:A:308:VAL:HG23	2.18	0.44
1:C:285:THR:HG1	3:C:506:G3H:C3	2.18	0.44
1:B:349:LEU:HD11	1:B:365:ASP:HB2	2.00	0.44
1:D:153:PHE:HA	1:D:179:PRO:HG3	1.99	0.44
1:A:414:PHE:HB2	1:D:414:PHE:HB2	1.99	0.44
1:B:136:ILE:HD11	1:B:472:PHE:CZ	2.52	0.44
1:A:437:ARG:NH1	3:A:504:G3H:O2	2.41	0.44
1:C:6:LYS:HG2	1:C:15:LEU:HG	2.00	0.44
1:A:5:TYR:O	1:A:35:PRO:HD3	2.18	0.44
1:D:6:LYS:HG2	1:D:15:LEU:HG	1.99	0.43
1:D:285:THR:OG1	3:D:507:G3H:O1P	2.36	0.43
1:A:160:ALA:O	1:A:164:ILE:HG13	2.18	0.43
1:B:155:TYR:CZ	4:B:505:G3P:H31	2.53	0.43
1:A:25:PRO:HB2	1:A:91:ALA:HB2	2.00	0.43
1:D:214:GLY:O	1:D:217:ILE:HG12	2.18	0.43
1:C:214:GLY:O	1:C:217:ILE:HG12	2.19	0.43
1:A:240:LYS:HG3	1:B:240:LYS:CG	2.41	0.43
1:A:6:LYS:HG2	1:A:15:LEU:HG	2.01	0.43
1:B:431:ILE:HG22	1:B:432:ASN:HD22	1.83	0.43
1:B:160:ALA:O	1:B:164:ILE:HG13	2.18	0.43
1:B:234:ILE:O	1:B:238:ILE:HG13	2.19	0.43
1:B:39:THR:HB	1:B:216:TYR:CE2	2.53	0.43
1:C:431:ILE:HG22	1:C:432:ASN:HD22	1.84	0.43
1:A:230:GLY:HA2	2:A:500:NAP:H1D	2.01	0.43
1:C:160:ALA:O	1:C:164:ILE:HG13	2.18	0.43
1:C:39:THR:HB	1:C:216:TYR:CE2	2.54	0.43
1:C:304:ILE:O	1:C:308:VAL:HG23	2.19	0.42
1:B:391:VAL:O	1:B:395:ILE:HG13	2.19	0.42
1:B:3:LYS:O	1:B:4:GLN:HB2	2.19	0.42
1:D:160:ALA:O	1:D:164:ILE:HG13	2.19	0.42
1:D:154:ASN:O	1:D:155:TYR:HD1	2.02	0.42
1:B:304:ILE:O	1:B:308:VAL:HG23	2.20	0.42
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD12	1:D:159:LEU:HA	1.90	0.42
1:C:154:ASN:OD1	2:C:502:NAP:N7N	2.52	0.42
1:B:198:LEU:HD12	1:B:198:LEU:H	1.85	0.42
1:B:153:PHE:HA	1:B:179:PRO:HG3	2.01	0.42
1:D:74:ILE:HD13	1:D:195:GLU:HB3	2.02	0.42
1:A:159:LEU:HD12	1:A:159:LEU:HA	1.91	0.42
1:C:23:TYR:CD1	1:C:30:GLU:HA	2.54	0.42
1:A:153:PHE:HA	1:A:179:PRO:HG3	2.02	0.42
1:D:25:PRO:HB2	1:D:91:ALA:HB2	2.02	0.42
1:A:434:LYS:O	1:A:434:LYS:HG2	2.19	0.42
1:A:445:LEU:N	1:A:445:LEU:HD23	2.35	0.42
1:C:273:ILE:CD1	1:C:304:ILE:HG23	2.47	0.42
1:B:350:THR:HG1	1:B:362:ILE:HA	1.83	0.42
1:C:349:LEU:HD11	1:C:365:ASP:HB2	2.02	0.42
1:B:6:LYS:HG2	1:B:15:LEU:HG	2.00	0.42
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.89	0.41
1:A:102:VAL:O	1:A:106:GLU:HG3	2.20	0.41
1:B:273:ILE:CD1	1:B:304:ILE:HG23	2.48	0.41
1:C:434:LYS:HG2	1:C:434:LYS:O	2.19	0.41
1:A:155:TYR:N	1:A:155:TYR:HD1	2.14	0.41
1:C:102:VAL:O	1:C:106:GLU:HG3	2.21	0.41
1:B:214:GLY:O	1:B:217:ILE:HG12	2.19	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.88	0.41
1:D:237:ARG:O	1:D:241:MET:HG3	2.20	0.41
1:C:5:TYR:O	1:C:35:PRO:HD3	2.21	0.41
1:A:94:TYR:O	1:A:98:VAL:HG23	2.20	0.41
1:A:155:TYR:N	1:A:155:TYR:CD1	2.84	0.41
1:B:155:TYR:CE2	4:B:505:G3P:O1	2.71	0.41
1:A:23:TYR:HD1	1:A:30:GLU:CA	2.27	0.41
1:A:146:LEU:HA	1:A:173:VAL:HG23	2.01	0.41
1:A:155:TYR:CZ	3:A:504:G3H:H2	2.56	0.41
2:B:501:NAP:O2D	2:B:501:NAP:H6N	2.21	0.41
1:A:273:ILE:CD1	1:A:304:ILE:HG23	2.48	0.41
1:A:457:VAL:O	1:A:461:ILE:HG13	2.21	0.41
1:A:234:ILE:O	1:A:238:ILE:HG13	2.21	0.41
1:C:428:THR:HG23	1:D:469:SER:O	2.20	0.41
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.95	0.40
1:A:315:ASN:HA	1:A:316:PRO:HD3	1.94	0.40
1:D:102:VAL:O	1:D:106:GLU:HG3	2.22	0.40
1:C:350:THR:HG1	1:C:362:ILE:HA	1.85	0.40
1:B:103:ARG:O	1:B:107:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HA	1:B:173:VAL:HG23	2.04	0.40
1:A:431:ILE:HD11	1:B:470:VAL:CG1	2.52	0.40
1:A:349:LEU:HD11	1:A:365:ASP:HB2	2.04	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	472/475 (99%)	444 (94%)	24 (5%)	4 (1%)	24	66
1	B	472/475 (99%)	443 (94%)	25 (5%)	4 (1%)	24	66
1	C	472/475 (99%)	443 (94%)	24 (5%)	5 (1%)	17	58
1	D	472/475 (99%)	445 (94%)	23 (5%)	4 (1%)	24	66
All	All	1888/1900 (99%)	1775 (94%)	96 (5%)	17 (1%)	21	64

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	THR
1	B	439	THR
1	C	439	THR
1	D	439	THR
1	A	438	GLY
1	A	440	ASP
1	B	438	GLY
1	C	438	GLY
1	D	438	GLY
1	D	440	ASP
1	A	433	ASN
1	B	433	ASN

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Mol	Chain	Res	Type
1	B	440	ASP
1	C	433	ASN
1	C	440	ASP
1	D	433	ASN
1	C	214	GLY

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	378/379 (100%)	369 (98%)	9 (2%)	57	87
1	B	378/379 (100%)	369 (98%)	9 (2%)	57	87
1	C	378/379 (100%)	370 (98%)	8 (2%)	61	89
1	D	378/379 (100%)	369 (98%)	9 (2%)	57	87
All	All	1512/1516 (100%)	1477 (98%)	35 (2%)	58	87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	MET
1	A	159	LEU
1	A	174	ILE
1	A	227	ASN
1	A	295	SER
1	A	342	ASN
1	A	369	THR
1	A	379	PHE
1	A	418	PHE
1	B	118	MET
1	B	159	LEU
1	B	174	ILE
1	B	227	ASN
1	B	295	SER
1	B	342	ASN
1	B	369	THR

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Mol	Chain	Res	Type
1	B	379	PHE
1	B	418	PHE
1	C	118	MET
1	C	159	LEU
1	C	227	ASN
1	C	295	SER
1	C	342	ASN
1	C	369	THR
1	C	379	PHE
1	C	418	PHE
1	D	118	MET
1	D	159	LEU
1	D	174	ILE
1	D	227	ASN
1	D	295	SER
1	D	342	ASN
1	D	369	THR
1	D	379	PHE
1	D	418	PHE

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

Mol	Chain	Res	Type
1	A	227	ASN
1	A	342	ASN
1	A	412	ASN
1	B	227	ASN
1	B	342	ASN
1	B	412	ASN
1	B	432	ASN
1	C	227	ASN
1	C	342	ASN
1	C	412	ASN
1	C	432	ASN
1	C	433	ASN
1	D	227	ASN
1	D	342	ASN
1	D	412	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 carbohydrates in this entry.

5.6 Ligand geometry

8 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	NAP	A	500	-	42,52,52	1.87	4 (9%)	54,80,80	3.15	12 (22%)
3	G3H	A	504	-	9,9,9	1.26	1 (11%)	10,12,12	1.11	1 (10%)
2	NAP	B	501	-	42,52,52	1.91	3 (7%)	54,80,80	3.55	18 (33%)
4	G3P	B	505	-	9,9,9	1.43	1 (11%)	10,12,12	0.89	0
2	NAP	C	502	-	42,52,52	2.47	4 (9%)	54,80,80	2.71	12 (22%)
3	G3H	C	506	1	9,9,9	1.53	2 (22%)	10,12,12	1.05	0
2	NAP	D	503	-	42,52,52	1.96	6 (14%)	54,80,80	2.19	16 (29%)
3	G3H	D	507	-	9,9,9	1.24	0	10,12,12	1.15	1 (10%)

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	NAP	A	500	-	-	0/27/67/67	0/5/5/5
3	G3H	A	504	-	-	0/6/8/8	0/0/0/0
2	NAP	B	501	-	-	0/27/67/67	0/5/5/5
4	G3P	B	505	-	1/1/2/2	0/8/8/8	0/0/0/0
2	NAP	C	502	-	-	0/27/67/67	0/5/5/5
3	G3H	C	506	1	-	0/6/8/8	0/0/0/0
2	NAP	D	503	-	-	0/27/67/67	0/5/5/5
3	G3H	D	507	-	-	0/6/8/8	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAP	C3N-C7N	-14.68	1.27	1.50
2	B	501	NAP	C3N-C7N	-10.28	1.34	1.50
2	A	500	NAP	C3N-C7N	-10.19	1.34	1.50
2	D	503	NAP	C3N-C7N	-10.09	1.34	1.50
4	B	505	G3P	O1-C1	-3.22	1.28	1.42
3	C	506	G3H	P-O4P	-2.30	1.46	1.54
2	B	501	NAP	P2B-O2X	-2.26	1.46	1.54
2	C	502	NAP	P2B-O2X	-2.25	1.46	1.54
2	D	503	NAP	C5A-N7A	-2.01	1.32	1.39
2	A	500	NAP	P2B-O2X	-2.01	1.47	1.54
2	D	503	NAP	C6N-N1N	2.03	1.40	1.35
3	A	504	G3H	O1-C1	2.06	1.29	1.19
3	C	506	G3H	O1-C1	2.10	1.29	1.19
2	C	502	NAP	O4D-C1D	2.10	1.43	1.41
2	A	500	NAP	O4D-C1D	2.18	1.44	1.41
2	D	503	NAP	P2B-O3X	2.32	1.63	1.54
2	D	503	NAP	PN-O5D	2.54	1.70	1.59
2	C	502	NAP	O4B-C1B	2.55	1.44	1.41
2	A	500	NAP	O4B-C1B	2.70	1.44	1.41
2	B	501	NAP	O4B-C1B	3.33	1.45	1.41
2	D	503	NAP	O4B-C1B	3.34	1.45	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAP	C4D-O4D-C1D	-15.62	92.55	109.72
2	A	500	NAP	C4D-O4D-C1D	-14.04	94.29	109.72
2	C	502	NAP	C4D-O4D-C1D	-12.23	96.28	109.72
2	A	500	NAP	N3A-C2A-N1A	-9.68	121.48	128.89
2	B	501	NAP	N3A-C2A-N1A	-8.63	122.29	128.89
2	C	502	NAP	N3A-C2A-N1A	-8.44	122.43	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	503	NAP	N3A-C2A-N1A	-8.02	122.75	128.89
2	D	503	NAP	C4D-O4D-C1D	-7.37	101.62	109.72
2	C	502	NAP	P2B-O2B-C2B	-6.90	105.01	121.56
2	B	501	NAP	P2B-O2B-C2B	-6.50	105.99	121.56
2	A	500	NAP	P2B-O2B-C2B	-6.03	107.11	121.56
2	D	503	NAP	P2B-O2B-C2B	-5.29	108.87	121.56
2	B	501	NAP	O3-PN-O5D	-5.06	89.50	102.94
2	B	501	NAP	O4B-C1B-C2B	-4.42	98.60	106.60
2	A	500	NAP	C4B-O4B-C1B	-4.29	105.00	109.72
2	B	501	NAP	O7N-C7N-C3N	-4.14	115.07	119.59
2	A	500	NAP	C3B-C2B-C1B	-4.02	94.96	102.73
2	C	502	NAP	C1B-N9A-C4A	-3.45	121.73	126.94
2	C	502	NAP	C5B-C4B-C3B	-2.90	103.68	115.21
2	D	503	NAP	O4B-C1B-C2B	-2.85	101.45	106.60
2	A	500	NAP	C1B-N9A-C4A	-2.74	122.81	126.94
2	B	501	NAP	C3B-C2B-C1B	-2.66	97.58	102.73
2	D	503	NAP	C3N-C7N-N7N	-2.61	114.96	117.82
2	C	502	NAP	C4N-C3N-C7N	-2.60	114.21	121.09
2	B	501	NAP	C4N-C3N-C7N	-2.56	114.32	121.09
2	D	503	NAP	C5B-C4B-C3B	-2.48	105.36	115.21
3	D	507	G3H	O1-C1-C2	-2.47	119.11	125.35
2	B	501	NAP	O3D-C3D-C4D	-2.43	103.77	111.05
2	A	500	NAP	O4B-C1B-C2B	-2.27	102.50	106.60
2	A	500	NAP	O7N-C7N-C3N	-2.24	117.14	119.59
2	D	503	NAP	O4D-C4D-C5D	-2.14	101.65	109.32
2	D	503	NAP	C3B-C2B-C1B	-2.13	98.62	102.73
3	A	504	G3H	O1-C1-C2	-2.06	120.15	125.35
2	C	502	NAP	O4B-C1B-C2B	-2.04	102.91	106.60
2	B	501	NAP	C2N-C3N-C7N	2.01	125.14	119.31
2	B	501	NAP	C4A-C5A-N7A	2.03	111.35	109.48
2	D	503	NAP	O3-PA-O5B	2.04	108.34	102.94
2	B	501	NAP	O5D-PN-O1N	2.12	117.86	109.62
2	D	503	NAP	O4B-C1B-N9A	2.16	112.62	108.10
2	D	503	NAP	O2B-P2B-O1X	2.16	112.50	107.11
2	D	503	NAP	O4D-C1D-N1N	2.19	110.54	108.13
2	A	500	NAP	C4A-C5A-N7A	2.23	111.53	109.48
2	C	502	NAP	O3D-C3D-C4D	2.34	118.06	111.05
2	B	501	NAP	O7N-C7N-N7N	2.35	125.91	122.59
2	D	503	NAP	O3D-C3D-C4D	2.38	118.20	111.05
2	D	503	NAP	O2X-P2B-O1X	2.43	118.41	110.58
2	B	501	NAP	O2X-P2B-O1X	2.50	118.64	110.58
2	B	501	NAP	O3-PA-O5B	2.55	109.71	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	NAP	O2X-P2B-O1X	2.61	118.97	110.58
2	C	502	NAP	C2N-C3N-C7N	2.62	126.93	119.31
2	C	502	NAP	C4A-C5A-N7A	2.73	111.99	109.48
2	A	500	NAP	O3D-C3D-C4D	2.76	119.33	111.05
2	C	502	NAP	O2X-P2B-O1X	2.82	119.67	110.58
2	B	501	NAP	C2D-C3D-C4D	2.93	108.63	102.61
2	D	503	NAP	C4A-C5A-N7A	2.98	112.22	109.48
2	D	503	NAP	O3B-C3B-C2B	3.20	120.40	111.16
2	B	501	NAP	O4D-C4D-C5D	3.71	122.58	109.32
2	C	502	NAP	O4D-C1D-N1N	5.57	114.25	108.13
2	A	500	NAP	O4D-C1D-N1N	9.96	119.08	108.13
2	B	501	NAP	O4D-C1D-N1N	12.30	121.65	108.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	505	G3P	C2

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAP	16	0
3	A	504	G3H	9	0
2	B	501	NAP	21	0
4	B	505	G3P	11	0
2	C	502	NAP	19	0
3	C	506	G3H	7	0
2	D	503	NAP	13	0
3	D	507	G3H	8	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.