Full wwPDB X-ray Structure Validation Report

Sep 17, 2024 – 02:09 PM JST

PDB ID	:	8WHG
Title	:	imine reductase mutant - M3
Authors	:	Zhu, X.X.; Chen, X.R.; Zheng, G.W.
Deposited on	:	2023-09-23
Resolution	:	2.71 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 (i) 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 (i)) were used in the production of this report:

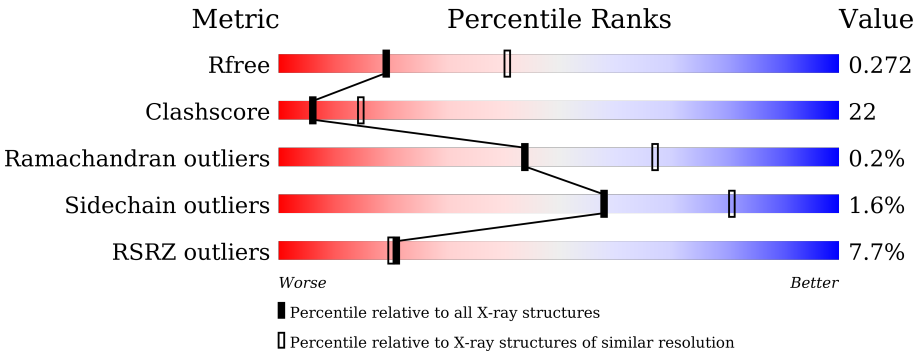
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.71 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}	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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	297	2% 68% 29% ·
1	B	297	70% 28% ·
1	C	297	% 60% 36% · ·
1	D	297	2% 66% 31% · ·
1	E	297	5% 63% 34% ·
1	F	297	29% 48% 44% · 7%

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Mol	Chain	Length	Quality of chain
1	G	297	
1	H	297	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16366 atoms, of which 50 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 6-phosphogluconate dehydrogenase NAD-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2125	1345	361	410	9			
1	B	291	Total	C	N	O	S	0	0	0
			2138	1352	364	413	9			
1	C	289	Total	C	N	O	S	0	0	0
			2125	1345	361	410	9			
1	D	290	Total	C	N	O	S	0	0	0
			2130	1348	362	411	9			
1	E	289	Total	C	N	O	S	0	0	0
			2125	1345	361	410	9			
1	F	276	Total	C	N	O	S	0	0	0
			2029	1286	343	391	9			
1	G	288	Total	C	N	O	S	0	0	0
			2114	1339	357	409	9			
1	H	160	Total	C	N	O	S	0	0	0
			1198	761	199	232	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ARG	THR	engineered mutation	UNP D9X416
A	73	SER	THR	engineered mutation	UNP D9X416
A	97	TYR	LEU	engineered mutation	UNP D9X416
A	126	GLY	ALA	engineered mutation	UNP D9X416
A	127	PRO	ILE	engineered mutation	UNP D9X416
A	130	TRP	ASP	engineered mutation	UNP D9X416
A	131	LEU	ILE	engineered mutation	UNP D9X416
A	135	ARG	ALA	engineered mutation	UNP D9X416
A	137	ILE	VAL	engineered mutation	UNP D9X416
A	214	LEU	MET	engineered mutation	UNP D9X416
A	217	LEU	VAL	engineered mutation	UNP D9X416
A	221	ARG	TYR	engineered mutation	UNP D9X416
B	40	ARG	THR	engineered mutation	UNP D9X416

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Chain	Residue	Modelled	Actual	Comment	Reference
B	73	SER	THR	engineered mutation	UNP D9X416
B	97	TYR	LEU	engineered mutation	UNP D9X416
B	126	GLY	ALA	engineered mutation	UNP D9X416
B	127	PRO	ILE	engineered mutation	UNP D9X416
B	130	TRP	ASP	engineered mutation	UNP D9X416
B	131	LEU	ILE	engineered mutation	UNP D9X416
B	135	ARG	ALA	engineered mutation	UNP D9X416
B	137	ILE	VAL	engineered mutation	UNP D9X416
B	214	LEU	MET	engineered mutation	UNP D9X416
B	217	LEU	VAL	engineered mutation	UNP D9X416
B	221	ARG	TYR	engineered mutation	UNP D9X416
C	40	ARG	THR	engineered mutation	UNP D9X416
C	73	SER	THR	engineered mutation	UNP D9X416
C	97	TYR	LEU	engineered mutation	UNP D9X416
C	126	GLY	ALA	engineered mutation	UNP D9X416
C	127	PRO	ILE	engineered mutation	UNP D9X416
C	130	TRP	ASP	engineered mutation	UNP D9X416
C	131	LEU	ILE	engineered mutation	UNP D9X416
C	135	ARG	ALA	engineered mutation	UNP D9X416
C	137	ILE	VAL	engineered mutation	UNP D9X416
C	214	LEU	MET	engineered mutation	UNP D9X416
C	217	LEU	VAL	engineered mutation	UNP D9X416
C	221	ARG	TYR	engineered mutation	UNP D9X416
D	40	ARG	THR	engineered mutation	UNP D9X416
D	73	SER	THR	engineered mutation	UNP D9X416
D	97	TYR	LEU	engineered mutation	UNP D9X416
D	126	GLY	ALA	engineered mutation	UNP D9X416
D	127	PRO	ILE	engineered mutation	UNP D9X416
D	130	TRP	ASP	engineered mutation	UNP D9X416
D	131	LEU	ILE	engineered mutation	UNP D9X416
D	135	ARG	ALA	engineered mutation	UNP D9X416
D	137	ILE	VAL	engineered mutation	UNP D9X416
D	214	LEU	MET	engineered mutation	UNP D9X416
D	217	LEU	VAL	engineered mutation	UNP D9X416
D	221	ARG	TYR	engineered mutation	UNP D9X416
E	40	ARG	THR	engineered mutation	UNP D9X416
E	73	SER	THR	engineered mutation	UNP D9X416
E	97	TYR	LEU	engineered mutation	UNP D9X416
E	126	GLY	ALA	engineered mutation	UNP D9X416
E	127	PRO	ILE	engineered mutation	UNP D9X416
E	130	TRP	ASP	engineered mutation	UNP D9X416
E	131	LEU	ILE	engineered mutation	UNP D9X416

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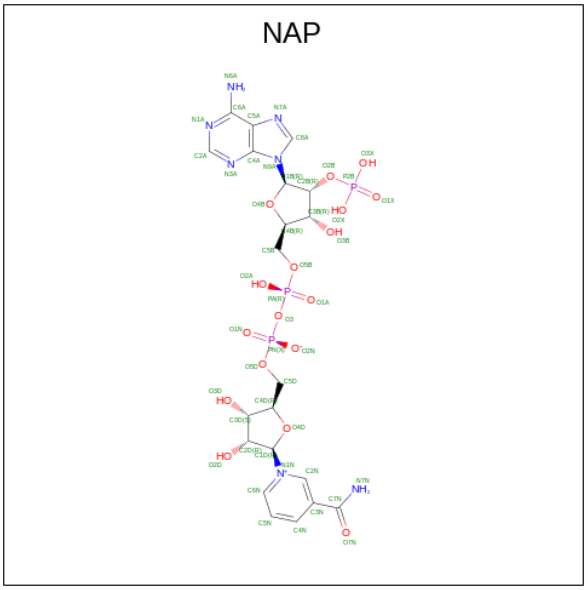
Chain	Residue	Modelled	Actual	Comment	Reference
E	135	ARG	ALA	engineered mutation	UNP D9X416
E	137	ILE	VAL	engineered mutation	UNP D9X416
E	214	LEU	MET	engineered mutation	UNP D9X416
E	217	LEU	VAL	engineered mutation	UNP D9X416
E	221	ARG	TYR	engineered mutation	UNP D9X416
F	40	ARG	THR	engineered mutation	UNP D9X416
F	73	SER	THR	engineered mutation	UNP D9X416
F	97	TYR	LEU	engineered mutation	UNP D9X416
F	126	GLY	ALA	engineered mutation	UNP D9X416
F	127	PRO	ILE	engineered mutation	UNP D9X416
F	130	TRP	ASP	engineered mutation	UNP D9X416
F	131	LEU	ILE	engineered mutation	UNP D9X416
F	135	ARG	ALA	engineered mutation	UNP D9X416
F	137	ILE	VAL	engineered mutation	UNP D9X416
F	214	LEU	MET	engineered mutation	UNP D9X416
F	217	LEU	VAL	engineered mutation	UNP D9X416
F	221	ARG	TYR	engineered mutation	UNP D9X416
G	40	ARG	THR	engineered mutation	UNP D9X416
G	73	SER	THR	engineered mutation	UNP D9X416
G	97	TYR	LEU	engineered mutation	UNP D9X416
G	126	GLY	ALA	engineered mutation	UNP D9X416
G	127	PRO	ILE	engineered mutation	UNP D9X416
G	130	TRP	ASP	engineered mutation	UNP D9X416
G	131	LEU	ILE	engineered mutation	UNP D9X416
G	135	ARG	ALA	engineered mutation	UNP D9X416
G	137	ILE	VAL	engineered mutation	UNP D9X416
G	214	LEU	MET	engineered mutation	UNP D9X416
G	217	LEU	VAL	engineered mutation	UNP D9X416
G	221	ARG	TYR	engineered mutation	UNP D9X416
H	40	ARG	THR	engineered mutation	UNP D9X416
H	73	SER	THR	engineered mutation	UNP D9X416
H	97	TYR	LEU	engineered mutation	UNP D9X416
H	126	GLY	ALA	engineered mutation	UNP D9X416
H	127	PRO	ILE	engineered mutation	UNP D9X416
H	130	TRP	ASP	engineered mutation	UNP D9X416
H	131	LEU	ILE	engineered mutation	UNP D9X416
H	135	ARG	ALA	engineered mutation	UNP D9X416
H	137	ILE	VAL	engineered mutation	UNP D9X416
H	214	LEU	MET	engineered mutation	UNP D9X416
H	217	LEU	VAL	engineered mutation	UNP D9X416
H	221	ARG	TYR	engineered mutation	UNP D9X416

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-

letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	E	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

- Molecule 3 is water.

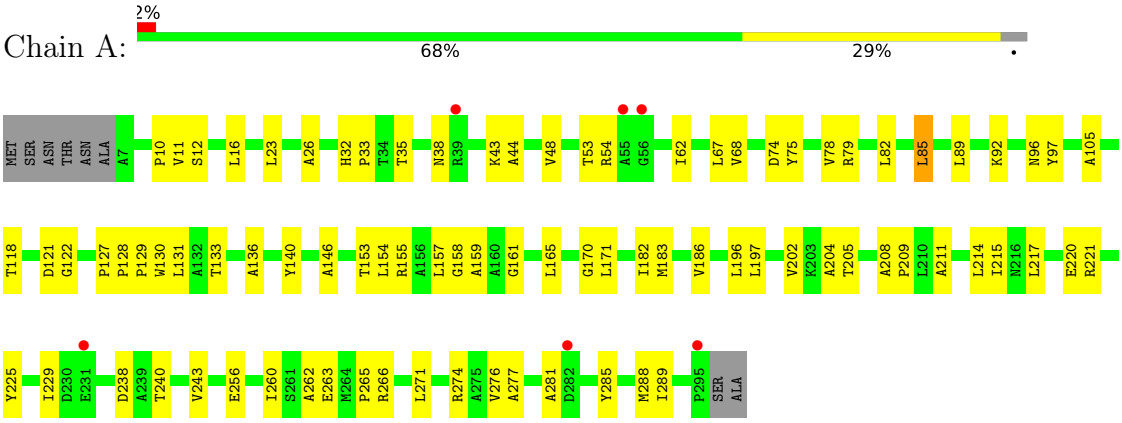
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	26	Total	O	0	0
			26	26		
3	C	16	Total	O	0	0
			16	16		
3	D	29	Total	O	0	0
			29	29		
3	E	35	Total	O	0	0
			35	35		
3	F	12	Total	O	0	0
			12	12		
3	G	40	Total	O	0	0
			40	40		
3	H	41	Total	O	0	0
			41	41		

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.

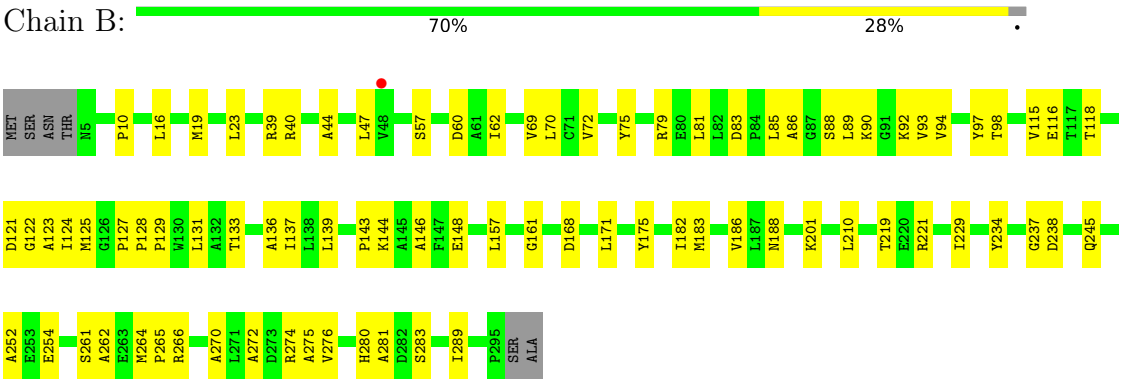
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

Chain A:



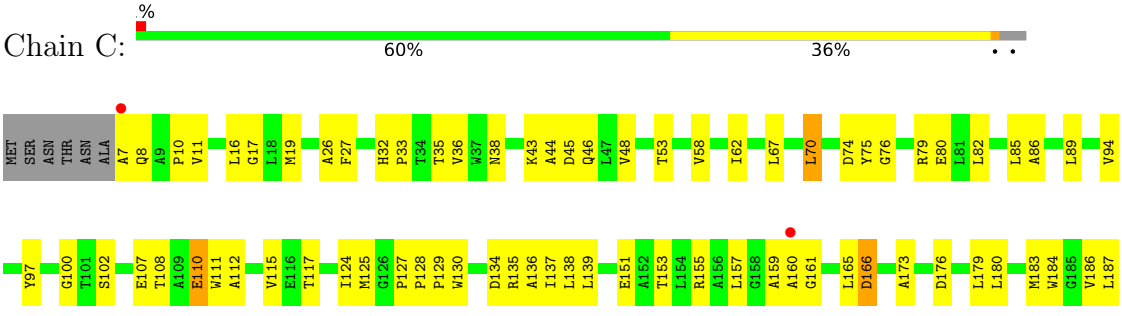
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

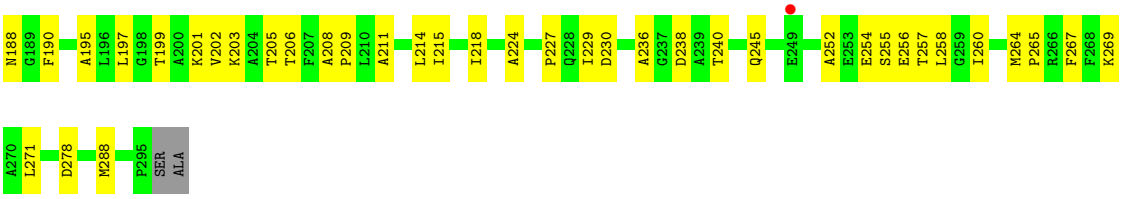
Chain B:



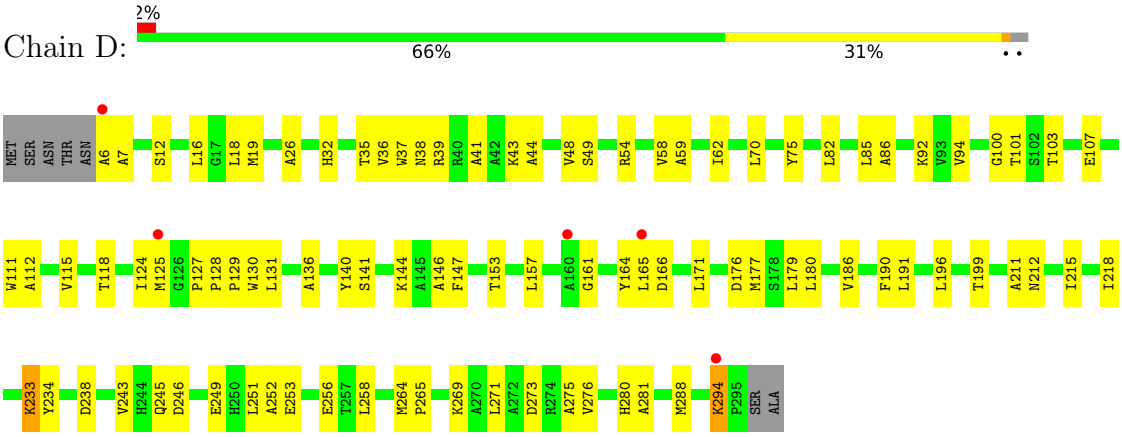
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

Chain C:

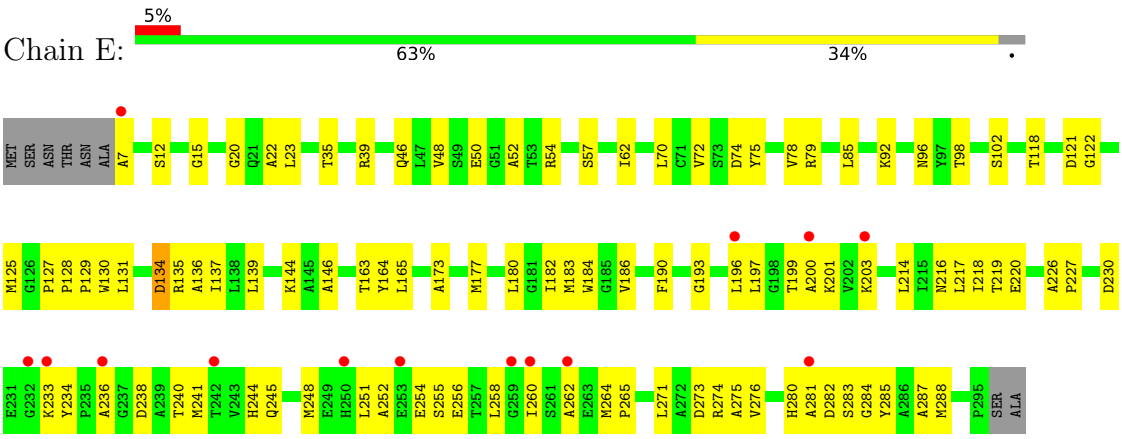




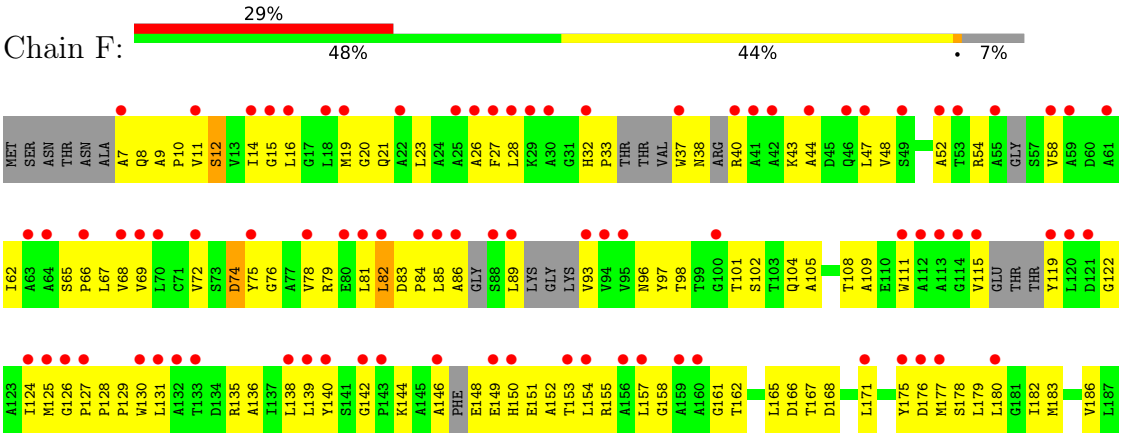
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

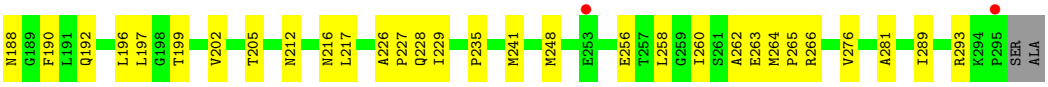


• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein



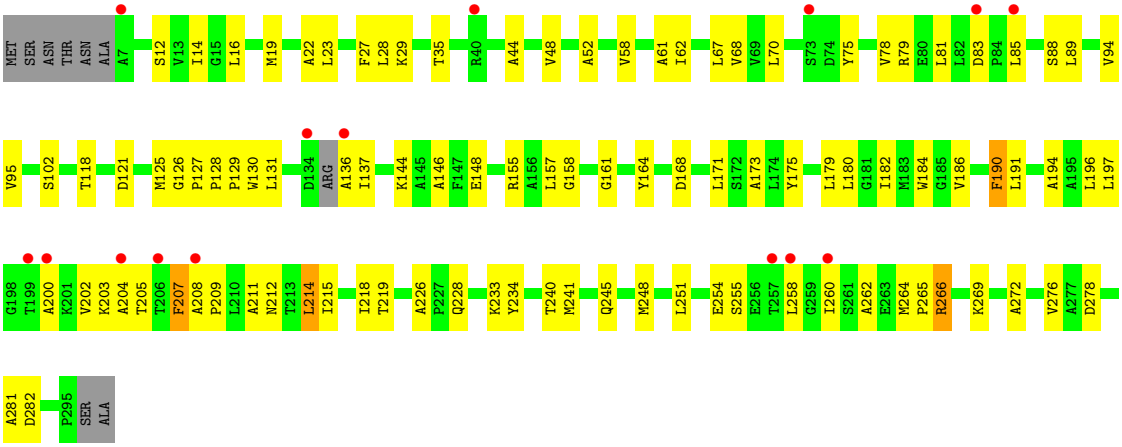
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein





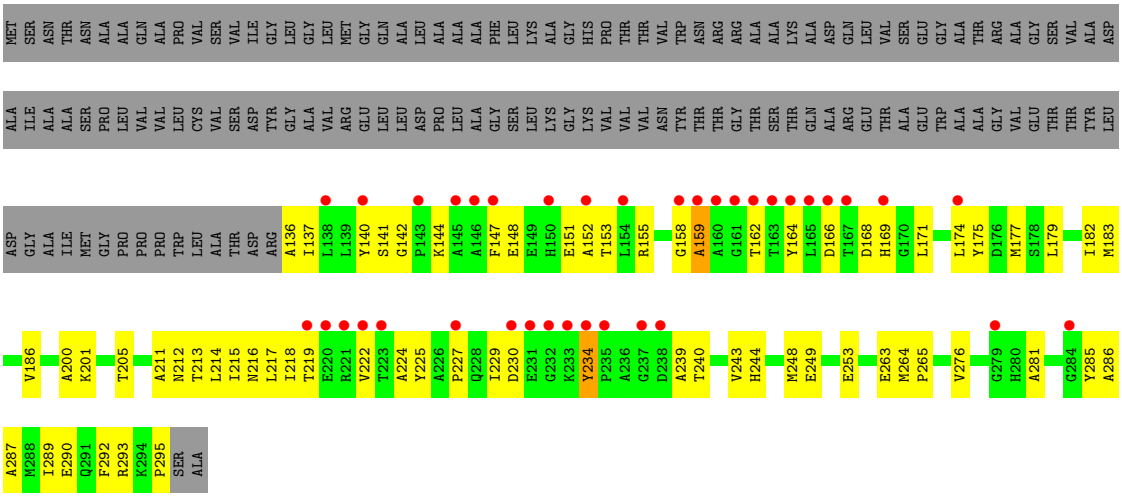
• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

Chain G:



• Molecule 1: 6-phosphogluconate dehydrogenase NAD-binding protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	335.10Å 96.07Å 103.79Å 90.00° 100.48° 90.00°	Depositor
Resolution (Å)	102.06 – 2.71 102.06 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.0 (102.06-2.71) 95.0 (102.06-2.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.230 , 0.271 0.232 , 0.272	Depositor DCC
R_{free} test set	86326 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16366	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: NAP

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	0.24	0/2167	0.43	0/2954
1	B	0.24	0/2180	0.44	0/2972
1	C	0.24	0/2167	0.44	0/2954
1	D	0.24	0/2172	0.44	0/2961
1	E	0.25	0/2167	0.45	0/2954
1	F	0.26	0/2063	0.44	0/2804
1	G	0.24	0/2155	0.44	0/2937
1	H	0.25	0/1222	0.42	0/1659
All	All	0.24	0/16293	0.44	0/22195

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2125	0	2114	80	0
1	B	2138	0	2125	58	0
1	C	2125	0	2114	103	0
1	D	2130	0	2119	83	0
1	E	2125	0	2114	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2029	0	2007	170	0
1	G	2114	0	2100	111	0
1	H	1198	0	1177	76	0
2	B	48	25	25	3	0
2	E	48	25	25	1	0
3	A	37	0	0	0	0
3	B	26	0	0	3	0
3	C	16	0	0	5	0
3	D	29	0	0	2	0
3	E	35	0	0	1	0
3	F	12	0	0	0	0
3	G	40	0	0	2	0
3	H	41	0	0	2	0
All	All	16316	50	15920	710	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 22.

All (710) 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:F:7:ALA:HA	1:F:33:PRO:HD3	1.37	1.05
1:A:276:VAL:HG13	1:A:281:ALA:HB2	1.40	1.03
1:B:186:VAL:HG22	1:D:186:VAL:HG22	1.40	0.99
1:D:70:LEU:HD11	1:D:82:LEU:HD11	1.47	0.97
1:D:19:MET:HE2	1:D:124:ILE:HD13	1.50	0.91
1:A:186:VAL:HG22	1:C:186:VAL:HG22	1.53	0.91
1:E:196:LEU:HD12	1:E:260:ILE:HD11	1.53	0.89
1:E:75:TYR:HA	1:E:78:VAL:HG23	1.54	0.88
1:A:74:ASP:OD1	1:A:75:TYR:N	2.09	0.86
1:E:48:VAL:HG21	1:E:54:ARG:HB2	1.58	0.85
1:E:75:TYR:HA	1:E:78:VAL:CG2	2.06	0.84
1:G:251:LEU:HD13	1:H:177:MET:HB3	1.59	0.84
1:F:11:VAL:HG12	1:F:67:LEU:HD22	1.59	0.84
1:F:96:ASN:OD1	1:F:98:THR:HG22	1.78	0.84
1:H:276:VAL:HG13	1:H:281:ALA:HB2	1.59	0.84
1:C:203:LYS:HG2	1:C:206:THR:HG23	1.60	0.83
1:G:168:ASP:HB3	1:G:171:LEU:HD23	1.59	0.82
1:G:62:ILE:HD13	1:G:68:VAL:HG21	1.61	0.82
1:F:28:LEU:HD11	1:F:52:ALA:HB2	1.62	0.80
1:E:244:HIS:O	1:E:248:MET:HG3	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:MET:HE2	1:D:124:ILE:HG21	1.63	0.80
1:G:264:MET:HB3	1:G:265:PRO:HD3	1.65	0.79
1:E:186:VAL:HG22	1:F:186:VAL:HG22	1.64	0.79
1:G:214:LEU:HD13	1:H:179:LEU:HB3	1.62	0.79
1:C:127:PRO:HB2	1:C:129:PRO:HD2	1.64	0.79
1:F:48:VAL:HG11	1:F:54:ARG:HB2	1.64	0.79
1:C:32:HIS:CE1	1:C:153:THR:HG23	2.18	0.79
1:F:176:ASP:O	1:F:180:LEU:HD23	1.83	0.78
1:E:251:LEU:HD13	1:F:177:MET:O	1.83	0.78
1:G:186:VAL:HG22	1:H:186:VAL:HG22	1.65	0.78
1:F:26:ALA:HB3	1:F:157:LEU:HD23	1.65	0.77
1:C:203:LYS:HE3	1:C:205:THR:OG1	1.85	0.77
1:C:62:ILE:HG13	1:C:85:LEU:HD13	1.66	0.76
1:F:166:ASP:HB3	1:F:171:LEU:CD1	2.15	0.76
1:G:211:ALA:O	1:G:215:ILE:HD12	1.84	0.76
1:A:48:VAL:HG21	1:A:54:ARG:HB2	1.67	0.75
1:D:127:PRO:HB2	1:D:129:PRO:HD2	1.68	0.75
1:E:70:LEU:CD2	1:E:78:VAL:HG13	2.17	0.75
1:F:58:VAL:HG21	1:F:81:LEU:HD12	1.67	0.75
1:A:127:PRO:HB2	1:A:129:PRO:HD2	1.68	0.75
1:F:62:ILE:HG13	1:F:85:LEU:HD11	1.68	0.75
1:B:210:LEU:HD21	1:D:179:LEU:HD11	1.69	0.75
1:C:211:ALA:O	1:C:215:ILE:HG13	1.87	0.75
1:F:44:ALA:HA	1:F:47:LEU:HD13	1.68	0.75
1:F:82:LEU:HD23	1:F:89:LEU:HD11	1.67	0.74
1:E:196:LEU:CD1	1:E:260:ILE:HD11	2.18	0.73
1:D:271:LEU:HB3	1:D:288:MET:HE3	1.71	0.72
1:F:177:MET:HE2	1:F:177:MET:HA	1.72	0.72
1:H:286:ALA:O	1:H:289:ILE:HG22	1.89	0.72
1:C:165:LEU:O	1:C:166:ASP:HB2	1.88	0.72
1:D:19:MET:CE	1:D:124:ILE:HD13	2.20	0.72
1:F:85:LEU:HD23	1:F:89:LEU:HD11	1.72	0.71
1:D:32:HIS:CE1	1:D:153:THR:HG23	2.25	0.71
1:G:203:LYS:HE2	1:G:204:ALA:HB3	1.70	0.71
1:F:12:SER:OG	1:F:68:VAL:HG13	1.90	0.71
1:A:118:THR:HG21	1:A:146:ALA:HB2	1.72	0.71
1:F:155:ARG:HH11	1:F:155:ARG:HB2	1.55	0.71
1:E:127:PRO:HB2	1:E:129:PRO:HD2	1.71	0.71
1:F:127:PRO:HD2	1:F:130:TRP:CD2	2.26	0.71
1:E:260:ILE:HA	1:F:293:ARG:O	1.91	0.71
1:H:249:GLU:O	1:H:253:GLU:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:CD1	1:D:82:LEU:HD11	2.20	0.70
1:F:168:ASP:HB3	1:F:171:LEU:HG	1.73	0.70
1:H:218:ILE:O	1:H:222:VAL:HG23	1.90	0.70
1:D:125:MET:HE3	1:D:125:MET:HA	1.74	0.70
1:F:78:VAL:HG21	1:F:98:THR:HG21	1.73	0.70
1:A:225:TYR:O	1:A:229:ILE:HG13	1.91	0.70
1:E:218:ILE:HD11	1:F:186:VAL:HG21	1.72	0.70
1:C:255:SER:HB3	1:C:260:ILE:HD11	1.73	0.70
1:D:44:ALA:O	1:D:48:VAL:HG23	1.91	0.70
1:G:125:MET:HE3	1:G:125:MET:HA	1.74	0.70
1:F:148:GLU:HA	1:F:151:GLU:HB2	1.72	0.69
1:E:70:LEU:HD21	1:E:78:VAL:HG13	1.73	0.69
1:G:212:ASN:OD1	1:H:219:THR:HB	1.92	0.69
1:G:245:GLN:HA	1:G:248:MET:HE2	1.74	0.69
1:F:62:ILE:HG13	1:F:85:LEU:HD21	1.74	0.69
1:A:214:LEU:HD11	1:C:183:MET:HG2	1.73	0.68
1:A:217:LEU:HD22	1:C:135:ARG:HG3	1.75	0.68
1:F:44:ALA:O	1:F:48:VAL:HG22	1.93	0.68
1:B:127:PRO:HB2	1:B:129:PRO:HD2	1.75	0.68
1:E:62:ILE:HG13	1:E:85:LEU:HD13	1.75	0.68
1:D:38:ASN:HD21	1:D:43:LYS:HE2	1.58	0.68
1:F:197:LEU:HB3	1:F:202:VAL:HB	1.77	0.67
1:F:166:ASP:HB3	1:F:171:LEU:HD13	1.75	0.67
1:E:7:ALA:N	3:E:404:HOH:O	2.28	0.67
1:E:177:MET:CE	1:E:180:LEU:HD12	2.23	0.67
1:F:16:LEU:HB2	1:F:38:ASN:HB2	1.74	0.67
1:G:197:LEU:HB3	1:G:202:VAL:HB	1.77	0.67
1:F:32:HIS:NE2	1:F:153:THR:HA	2.09	0.67
1:F:76:GLY:HA2	1:F:79:ARG:HH21	1.57	0.67
1:B:86:ALA:HB1	1:B:115:VAL:HG11	1.75	0.67
1:E:48:VAL:CG2	1:E:54:ARG:HB2	2.24	0.67
1:B:183:MET:HG2	1:D:218:ILE:HD13	1.76	0.67
1:F:125:MET:HG3	1:F:179:LEU:CD1	2.24	0.67
1:F:177:MET:HA	1:F:177:MET:CE	2.24	0.67
1:G:203:LYS:CE	1:H:230:ASP:HB2	2.25	0.66
1:H:239:ALA:HB1	1:H:243:VAL:CG1	2.25	0.66
1:C:255:SER:HB3	1:C:260:ILE:CD1	2.26	0.66
1:B:90:LYS:HE3	1:B:116:GLU:OE1	1.95	0.66
1:D:70:LEU:HD12	1:D:94:VAL:HG13	1.77	0.66
1:D:249:GLU:O	1:D:253:GLU:HG3	1.96	0.66
1:E:255:SER:HB2	1:E:262:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ILE:O	1:F:186:VAL:HG23	1.94	0.66
1:C:203:LYS:HE2	1:C:206:THR:HG23	1.76	0.66
1:G:179:LEU:HD22	1:H:214:LEU:HG	1.77	0.65
1:D:19:MET:CE	1:D:124:ILE:HG21	2.26	0.65
1:F:78:VAL:CG2	1:F:98:THR:HG21	2.27	0.65
1:G:62:ILE:HD12	1:G:89:LEU:CD2	2.25	0.65
1:C:125:MET:HB2	1:C:137:ILE:HB	1.77	0.65
1:E:57:SER:HB3	1:G:278:ASP:HA	1.78	0.65
1:H:168:ASP:CB	1:H:171:LEU:HG	2.26	0.65
1:B:72:VAL:O	1:B:98:THR:HG23	1.97	0.65
1:H:200:ALA:C	1:H:201:LYS:HD2	2.18	0.65
1:E:230:ASP:OD2	1:F:205:THR:HG23	1.97	0.64
1:H:212:ASN:ND2	3:H:302:HOH:O	2.24	0.64
1:D:103:THR:O	1:D:107:GLU:HG2	1.97	0.64
1:D:38:ASN:ND2	1:D:43:LYS:HE2	2.12	0.64
1:H:162:THR:HA	1:H:164:TYR:OH	1.98	0.64
1:D:19:MET:HE3	1:D:131:LEU:HD11	1.80	0.64
1:F:188:ASN:HB3	1:F:264:MET:CE	2.28	0.64
1:F:152:ALA:HA	1:F:155:ARG:NH2	2.13	0.63
1:G:127:PRO:HD2	1:G:130:TRP:CD2	2.33	0.63
1:G:207:PHE:CE1	1:G:211:ALA:HB2	2.33	0.63
1:E:74:ASP:O	1:E:78:VAL:HG23	1.99	0.63
1:F:82:LEU:HD23	1:F:85:LEU:HD23	1.80	0.63
1:F:86:ALA:HA	1:F:115:VAL:HG11	1.80	0.63
1:C:16:LEU:HD11	1:C:36:VAL:HB	1.80	0.63
1:C:70:LEU:HD12	1:C:94:VAL:HG13	1.81	0.63
1:A:127:PRO:HD2	1:A:130:TRP:CD2	2.34	0.63
1:B:182:ILE:O	1:B:186:VAL:HG23	1.99	0.63
1:F:89:LEU:HD23	1:F:115:VAL:HG12	1.81	0.63
1:D:211:ALA:O	1:D:215:ILE:HG13	1.99	0.62
1:C:107:GLU:O	1:C:110:GLU:HG3	1.99	0.62
1:F:158:GLY:O	1:F:162:THR:HG23	1.98	0.62
1:C:208:ALA:HB3	1:C:209:PRO:HD3	1.80	0.62
1:E:201:LYS:HE2	1:E:201:LYS:HA	1.82	0.62
1:F:11:VAL:HG12	1:F:67:LEU:CD2	2.28	0.62
1:F:74:ASP:O	1:F:78:VAL:HG23	1.99	0.62
1:F:125:MET:CE	1:F:176:ASP:HA	2.29	0.62
1:G:16:LEU:HD12	1:G:44:ALA:HB2	1.81	0.62
1:A:10:PRO:HA	1:A:33:PRO:HG2	1.81	0.61
1:H:162:THR:HG23	1:H:164:TYR:CE2	2.36	0.61
1:A:23:LEU:HD23	1:A:157:LEU:HD22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLY:O	1:C:80:GLU:HG3	1.99	0.61
1:F:14:ILE:HD12	1:F:58:VAL:HG23	1.83	0.61
1:A:16:LEU:HD12	1:A:44:ALA:HB2	1.81	0.61
1:H:213:THR:O	1:H:217:LEU:HG	2.01	0.61
1:F:76:GLY:HA2	1:F:79:ARG:NH2	2.15	0.61
1:A:131:LEU:O	1:A:133:THR:HG23	2.01	0.60
1:H:244:HIS:CE1	1:H:285:TYR:HB2	2.35	0.60
1:E:177:MET:HE2	1:E:180:LEU:HD12	1.82	0.60
1:D:136:ALA:O	1:D:161:GLY:HA3	2.01	0.60
1:E:234:TYR:CD2	1:E:287:ALA:HA	2.37	0.60
1:D:233:LYS:HD3	1:D:234:TYR:H	1.67	0.60
1:F:192:GLN:OE1	1:F:265:PRO:HD3	2.01	0.60
1:G:14:ILE:HD13	1:G:58:VAL:HG13	1.84	0.60
1:F:26:ALA:CB	1:F:157:LEU:HD23	2.31	0.60
1:B:168:ASP:HB3	1:B:171:LEU:HD23	1.83	0.60
1:E:236:ALA:HB2	1:E:283:SER:C	2.21	0.60
1:H:166:ASP:CB	1:H:171:LEU:HD12	2.32	0.60
1:C:97:TYR:HB3	1:C:124:ILE:HD12	1.83	0.60
1:F:58:VAL:HG21	1:F:81:LEU:CD1	2.31	0.59
1:F:125:MET:HG3	1:F:179:LEU:HD13	1.83	0.59
1:G:62:ILE:HD12	1:G:89:LEU:HD21	1.84	0.59
1:A:10:PRO:CA	1:A:33:PRO:HG2	2.33	0.59
1:A:136:ALA:O	1:A:161:GLY:HA3	2.03	0.59
1:C:115:VAL:HG23	1:C:117:THR:HG22	1.85	0.59
1:F:108:THR:HG23	1:F:119:TYR:CE2	2.37	0.59
1:A:16:LEU:HB2	1:A:38:ASN:HB2	1.83	0.59
1:F:9:ALA:O	1:F:33:PRO:HD2	2.03	0.59
1:F:152:ALA:HA	1:F:155:ARG:CZ	2.33	0.59
1:H:162:THR:HG23	1:H:164:TYR:HE2	1.68	0.59
1:H:239:ALA:HB1	1:H:243:VAL:HG11	1.85	0.59
1:B:57:SER:N	1:B:60:ASP:OD2	2.35	0.58
1:B:131:LEU:O	1:B:133:THR:HG23	2.03	0.58
1:B:276:VAL:HG13	1:B:281:ALA:HB2	1.84	0.58
1:C:197:LEU:O	1:C:202:VAL:HB	2.04	0.58
1:E:62:ILE:O	1:E:92:LYS:HE3	2.03	0.58
1:B:254:GLU:HB2	1:D:101:THR:HG22	1.85	0.58
1:A:75:TYR:O	1:A:79:ARG:HG3	2.04	0.58
1:A:140:TYR:CE2	1:A:154:LEU:HD13	2.39	0.58
1:A:205:THR:HG23	1:C:230:ASP:OD2	2.04	0.58
1:F:48:VAL:HG12	1:F:52:ALA:O	2.03	0.58
1:F:89:LEU:HD23	1:F:115:VAL:CG1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:TRP:O	1:D:115:VAL:HG22	2.04	0.58
1:F:139:LEU:HD23	1:F:165:LEU:HD11	1.85	0.58
1:F:75:TYR:HE2	1:F:108:THR:HG21	1.68	0.57
1:B:270:ALA:O	1:B:274:ARG:HG3	2.04	0.57
1:D:125:MET:HA	1:D:125:MET:CE	2.34	0.57
1:A:229:ILE:HG23	1:A:289:ILE:HG12	1.85	0.57
1:F:40:ARG:HB2	1:F:43:LYS:HG2	1.86	0.57
1:B:275:ALA:O	1:B:280:HIS:HB2	2.05	0.57
1:A:62:ILE:HG13	1:A:85:LEU:HD22	1.87	0.57
1:C:11:VAL:HG23	1:C:67:LEU:HD23	1.87	0.57
1:E:254:GLU:OE1	1:F:101:THR:HB	2.04	0.57
1:C:75:TYR:HD2	1:C:108:THR:HG1	1.52	0.57
1:E:197:LEU:HD13	1:F:178:SER:OG	2.04	0.57
1:C:26:ALA:HB3	1:C:157:LEU:HD23	1.87	0.57
1:C:58:VAL:O	1:C:62:ILE:HG12	2.04	0.57
1:D:127:PRO:HD2	1:D:130:TRP:CE3	2.40	0.57
1:D:127:PRO:HD2	1:D:130:TRP:CD2	2.40	0.56
1:G:190:PHE:HE1	1:G:194:ALA:HB2	1.69	0.56
1:G:203:LYS:NZ	1:H:230:ASP:HB2	2.19	0.56
1:G:264:MET:HB3	1:G:265:PRO:CD	2.33	0.56
1:C:17:GLY:CA	3:C:304:HOH:O	2.52	0.56
1:C:203:LYS:HE2	1:C:206:THR:CG2	2.34	0.56
1:A:82:LEU:HA	1:A:85:LEU:HD11	1.86	0.56
1:A:217:LEU:HD22	1:C:135:ARG:CG	2.34	0.56
1:D:196:LEU:HD11	1:D:251:LEU:CD1	2.35	0.56
1:E:23:LEU:HD23	1:E:131:LEU:HD13	1.87	0.56
1:F:138:LEU:HD11	1:F:157:LEU:HB2	1.85	0.56
1:G:35:THR:HG21	1:G:61:ALA:HA	1.86	0.56
1:G:44:ALA:O	1:G:48:VAL:HG23	2.04	0.56
1:G:179:LEU:HD22	1:H:214:LEU:CG	2.35	0.56
1:E:139:LEU:HD22	1:E:165:LEU:HD21	1.88	0.56
1:G:196:LEU:CD2	1:G:258:LEU:HD12	2.36	0.56
1:C:186:VAL:HG13	1:C:215:ILE:HD13	1.86	0.56
1:F:196:LEU:CD2	1:F:260:ILE:HD11	2.36	0.56
1:A:221:ARG:HD2	1:C:127:PRO:HG3	1.87	0.56
1:G:255:SER:OG	1:G:260:ILE:HD11	2.06	0.56
1:A:214:LEU:HD11	1:C:183:MET:CG	2.34	0.56
1:F:15:GLY:O	1:F:20:GLY:HA3	2.05	0.56
1:G:144:LYS:HG3	1:G:164:TYR:CE2	2.41	0.56
1:B:229:ILE:HG23	1:B:289:ILE:HG12	1.87	0.56
1:C:236:ALA:CB	1:C:240:THR:HG22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:VAL:HG22	1:E:281:ALA:HA	1.88	0.56
1:G:19:MET:HE2	1:G:19:MET:HA	1.88	0.56
1:B:234:TYR:HB2	1:B:283:SER:HB3	1.88	0.56
1:D:276:VAL:HG13	1:D:281:ALA:HB2	1.87	0.56
1:C:16:LEU:HD12	1:C:44:ALA:HB2	1.88	0.55
1:D:37:TRP:CH2	1:D:39:ARG:HG3	2.42	0.55
1:F:11:VAL:CG1	1:F:67:LEU:HD22	2.32	0.55
1:H:227:PRO:O	1:H:230:ASP:N	2.39	0.55
1:C:252:ALA:O	1:C:256:GLU:HG3	2.06	0.55
1:C:254:GLU:OE2	1:C:258:LEU:HD11	2.06	0.55
1:G:125:MET:HA	1:G:125:MET:CE	2.35	0.55
1:B:70:LEU:CD1	1:B:94:VAL:HG13	2.37	0.55
1:E:130:TRP:O	1:E:136:ALA:HB2	2.05	0.55
1:G:58:VAL:HG21	1:G:81:LEU:HD22	1.89	0.55
1:F:155:ARG:HB2	1:F:155:ARG:NH1	2.20	0.55
1:C:183:MET:O	1:C:187:LEU:HG	2.06	0.55
1:D:19:MET:CE	1:D:131:LEU:HD11	2.37	0.55
1:F:111:TRP:CZ2	1:F:115:VAL:HG21	2.42	0.55
1:G:130:TRP:O	1:G:136:ALA:HB2	2.07	0.55
1:A:240:THR:OG1	1:A:243:VAL:HG23	2.06	0.55
1:C:75:TYR:O	1:C:79:ARG:HG3	2.07	0.54
1:E:72:VAL:O	1:E:98:THR:HG23	2.08	0.54
1:E:262:ALA:C	1:E:265:PRO:HD2	2.27	0.54
1:G:212:ASN:HD21	1:H:222:VAL:HB	1.71	0.54
1:B:62:ILE:O	1:B:92:LYS:HE3	2.07	0.54
1:C:124:ILE:HG12	1:C:138:LEU:HD23	1.89	0.54
1:D:59:ALA:HA	1:D:85:LEU:HD13	1.89	0.54
1:D:252:ALA:O	1:D:256:GLU:HG3	2.07	0.54
1:G:197:LEU:CD2	1:H:174:LEU:HB3	2.37	0.54
1:F:7:ALA:O	1:F:8:GLN:HB3	2.07	0.54
1:G:276:VAL:HG13	1:G:281:ALA:HB2	1.90	0.54
1:H:155:ARG:HG2	1:H:162:THR:HG21	1.90	0.54
1:C:125:MET:HE1	1:C:176:ASP:HA	1.88	0.54
1:F:168:ASP:HB3	1:F:171:LEU:CG	2.36	0.54
1:H:244:HIS:HE1	1:H:285:TYR:HB2	1.72	0.54
1:H:287:ALA:O	1:H:290:GLU:HG3	2.07	0.54
1:E:241:MET:HE1	1:E:284:GLY:O	2.08	0.54
1:A:130:TRP:O	1:A:136:ALA:HB2	2.06	0.54
1:E:275:ALA:O	1:E:280:HIS:HB2	2.07	0.54
1:H:166:ASP:HB2	1:H:171:LEU:HD12	1.89	0.54
1:B:171:LEU:HD12	1:B:175:TYR:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:O	1:A:186:VAL:HG23	2.08	0.54
1:B:23:LEU:HD23	1:B:157:LEU:HD22	1.89	0.54
1:F:10:PRO:C	1:F:65:SER:HB2	2.29	0.54
1:A:26:ALA:HB3	1:A:157:LEU:HD23	1.89	0.53
1:B:118:THR:HG21	1:B:146:ALA:CB	2.38	0.53
1:F:97:TYR:CD1	1:F:122:GLY:HA3	2.42	0.53
1:C:264:MET:HB3	1:C:265:PRO:HD3	1.90	0.53
1:D:245:GLN:NE2	1:D:273:ASP:OD1	2.33	0.53
1:F:228:GLN:OE1	1:F:235:PRO:HD2	2.08	0.53
1:G:218:ILE:CD1	1:H:183:MET:HG3	2.37	0.53
1:H:168:ASP:HB3	1:H:171:LEU:HG	1.89	0.53
1:F:155:ARG:HH11	1:F:155:ARG:CB	2.22	0.53
1:A:262:ALA:C	1:A:265:PRO:HD2	2.28	0.53
1:B:237:GLY:O	1:D:18:LEU:HD22	2.08	0.53
1:C:45:ASP:OD1	1:C:46:GLN:N	2.42	0.53
1:C:127:PRO:HD2	1:C:130:TRP:CD2	2.44	0.53
1:D:118:THR:HG21	1:D:146:ALA:HB2	1.90	0.53
1:E:264:MET:HB3	1:E:265:PRO:HD3	1.91	0.53
1:F:7:ALA:CA	1:F:33:PRO:HD3	2.26	0.53
1:C:70:LEU:CD1	1:C:94:VAL:HG13	2.37	0.53
1:H:240:THR:O	1:H:243:VAL:HG12	2.09	0.53
1:A:155:ARG:HG2	1:A:159:ALA:HA	1.91	0.53
1:G:136:ALA:O	1:G:161:GLY:HA3	2.08	0.53
1:H:168:ASP:HB2	1:H:171:LEU:HG	1.90	0.53
1:A:35:THR:HA	1:A:53:THR:O	2.08	0.52
1:F:32:HIS:CE1	1:F:153:THR:HA	2.43	0.52
1:F:127:PRO:HB2	1:F:129:PRO:HD2	1.90	0.52
1:B:122:GLY:HA2	1:B:139:LEU:O	2.09	0.52
1:E:196:LEU:O	1:E:199:THR:OG1	2.27	0.52
1:F:125:MET:HG3	1:F:179:LEU:HD12	1.90	0.52
1:G:190:PHE:CE1	1:G:194:ALA:HB2	2.44	0.52
1:D:16:LEU:HB2	1:D:38:ASN:HB2	1.90	0.52
1:A:205:THR:O	1:A:209:PRO:HD3	2.09	0.52
1:H:211:ALA:O	1:H:215:ILE:HG13	2.09	0.52
1:D:58:VAL:HG12	1:D:85:LEU:CD1	2.40	0.52
1:E:218:ILE:CD1	1:F:186:VAL:HG21	2.38	0.52
1:F:188:ASN:HB3	1:F:264:MET:HE3	1.91	0.52
1:G:12:SER:HA	1:G:35:THR:O	2.10	0.52
1:A:32:HIS:CE1	1:A:153:THR:HG23	2.45	0.52
1:G:144:LYS:HE2	1:G:148:GLU:OE2	2.10	0.52
1:A:220:GLU:HG3	1:C:135:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ASP:O	1:C:48:VAL:HG22	2.10	0.52
1:E:125:MET:HG2	1:E:137:ILE:HG22	1.91	0.52
1:G:75:TYR:OH	1:G:121:ASP:OD1	2.27	0.52
1:F:8:GLN:O	1:F:8:GLN:HG2	2.10	0.51
1:F:226:ALA:HB3	1:F:227:PRO:CD	2.40	0.51
1:A:229:ILE:CG2	1:A:289:ILE:HG12	2.40	0.51
1:F:130:TRP:O	1:F:136:ALA:HB2	2.10	0.51
1:F:140:TYR:CZ	1:F:154:LEU:HD13	2.45	0.51
1:C:136:ALA:O	1:C:161:GLY:HA3	2.11	0.51
1:F:62:ILE:HG13	1:F:85:LEU:CD1	2.38	0.51
1:C:7:ALA:O	1:C:8:GLN:HB2	2.10	0.51
1:G:203:LYS:HE2	1:G:204:ALA:CB	2.38	0.51
1:F:66:PRO:O	1:F:93:VAL:N	2.44	0.51
1:F:226:ALA:HB3	1:F:227:PRO:HD3	1.93	0.51
1:G:218:ILE:HG21	1:H:186:VAL:CG1	2.41	0.51
1:H:248:MET:HE1	1:H:285:TYR:HE1	1.75	0.51
1:F:82:LEU:HA	1:F:85:LEU:CB	2.41	0.51
1:B:81:LEU:HD21	2:B:301:NAP:N1A	2.26	0.51
1:B:219:THR:HB	1:D:212:ASN:CG	2.30	0.51
1:B:245:GLN:NE2	3:B:404:HOH:O	2.35	0.51
1:C:17:GLY:HA3	3:C:304:HOH:O	2.11	0.51
1:F:21:GLN:HG2	1:F:47:LEU:HD11	1.93	0.51
1:G:85:LEU:HB3	1:G:88:SER:OG	2.11	0.51
1:F:138:LEU:CD1	1:F:157:LEU:HB2	2.41	0.51
1:G:128:PRO:HB2	1:G:129:PRO:HD3	1.92	0.51
1:B:81:LEU:HD21	2:B:301:NAP:C2A	2.41	0.51
1:E:216:ASN:O	1:E:219:THR:HG23	2.11	0.51
1:D:275:ALA:O	1:D:280:HIS:HB2	2.11	0.50
1:G:218:ILE:HG21	1:H:186:VAL:HG11	1.91	0.50
1:A:11:VAL:HG12	1:A:67:LEU:HD23	1.93	0.50
1:E:196:LEU:HD12	1:E:260:ILE:CD1	2.32	0.50
1:D:112:ALA:HA	1:D:115:VAL:CG2	2.41	0.50
1:E:240:THR:HB	1:E:281:ALA:O	2.11	0.50
1:H:151:GLU:O	1:H:153:THR:N	2.39	0.50
1:C:74:ASP:OD1	1:C:76:GLY:N	2.41	0.50
1:E:241:MET:O	1:E:245:GLN:HB2	2.12	0.50
1:F:82:LEU:HA	1:F:85:LEU:HB3	1.93	0.50
1:G:262:ALA:O	1:G:266:ARG:HG3	2.10	0.50
1:B:85:LEU:O	1:B:89:LEU:HD23	2.12	0.50
1:E:177:MET:CE	1:E:177:MET:HA	2.41	0.50
1:E:217:LEU:HB3	1:F:130:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ALA:O	1:F:161:GLY:HA3	2.11	0.50
1:D:186:VAL:HG13	1:D:215:ILE:HD13	1.94	0.50
1:D:269:LYS:NZ	1:D:273:ASP:OD1	2.45	0.50
1:F:144:LYS:O	1:F:144:LYS:HG3	2.10	0.50
1:G:155:ARG:HD2	3:G:305:HOH:O	2.11	0.50
1:E:48:VAL:HA	1:E:52:ALA:O	2.12	0.49
1:F:12:SER:HB3	1:F:65:SER:OG	2.12	0.49
1:G:23:LEU:HD22	1:G:157:LEU:HD13	1.94	0.49
1:H:162:THR:HA	1:H:164:TYR:CZ	2.47	0.49
1:E:245:GLN:NE2	1:E:273:ASP:OD1	2.36	0.49
1:G:28:LEU:HD11	1:G:52:ALA:HB2	1.92	0.49
1:B:125:MET:HB2	1:B:137:ILE:HB	1.93	0.49
1:C:128:PRO:N	1:C:129:PRO:CD	2.76	0.49
1:C:245:GLN:HG2	1:C:269:LYS:NZ	2.28	0.49
1:E:122:GLY:HA2	1:E:139:LEU:O	2.12	0.49
1:G:190:PHE:HD2	1:H:222:VAL:CG1	2.25	0.49
1:B:16:LEU:CD1	1:B:44:ALA:HB2	2.41	0.49
1:E:203:LYS:H	1:E:203:LYS:HD2	1.77	0.49
1:A:211:ALA:O	1:A:215:ILE:HG13	2.12	0.49
1:E:46:GLN:NE2	1:E:50:GLU:OE2	2.46	0.49
1:E:75:TYR:CA	1:E:78:VAL:HG23	2.35	0.49
1:F:75:TYR:HA	1:F:78:VAL:CG2	2.43	0.49
1:A:48:VAL:CG2	1:A:54:ARG:HB2	2.40	0.49
1:C:11:VAL:HG11	1:C:27:PHE:CG	2.47	0.49
1:C:19:MET:SD	1:C:124:ILE:HG21	2.53	0.49
1:F:83:ASP:HB2	1:F:84:PRO:HD3	1.95	0.49
1:A:62:ILE:HD13	1:A:68:VAL:HG11	1.94	0.49
1:C:195:ALA:O	1:C:199:THR:HG23	2.13	0.49
1:H:168:ASP:O	1:H:169:HIS:HB2	2.13	0.49
1:B:85:LEU:HB3	1:B:88:SER:OG	2.13	0.49
1:D:144:LYS:HE2	1:D:164:TYR:CE2	2.48	0.49
1:E:276:VAL:HG22	1:E:281:ALA:CA	2.42	0.49
1:F:85:LEU:HD23	1:F:89:LEU:CD1	2.43	0.49
1:G:240:THR:HG22	1:G:282:ASP:O	2.13	0.49
1:G:248:MET:CE	1:G:272:ALA:HB2	2.43	0.49
1:E:57:SER:CB	1:G:278:ASP:HA	2.43	0.48
1:E:193:GLY:O	1:E:197:LEU:HB2	2.13	0.48
1:D:199:THR:HG21	1:D:258:LEU:HB3	1.95	0.48
1:F:96:ASN:OD1	1:F:97:TYR:N	2.46	0.48
1:F:140:TYR:CE1	1:F:154:LEU:HD13	2.48	0.48
1:G:191:LEU:HB3	1:H:292:PHE:CD2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ALA:HB1	1:B:266:ARG:CZ	2.43	0.48
1:F:86:ALA:HA	1:F:115:VAL:CG1	2.42	0.48
1:A:186:VAL:HG22	1:C:186:VAL:CG2	2.35	0.48
1:H:142:GLY:HA2	1:H:169:HIS:HD2	1.78	0.48
1:A:62:ILE:HD12	1:A:89:LEU:HD21	1.94	0.48
1:H:166:ASP:HB3	1:H:171:LEU:HD12	1.96	0.48
1:H:225:TYR:O	1:H:229:ILE:HG13	2.13	0.48
1:E:193:GLY:CA	1:F:178:SER:HB3	2.44	0.48
1:F:146:ALA:HA	1:F:149:GLU:OE2	2.13	0.48
1:G:248:MET:HE3	1:G:272:ALA:CB	2.44	0.48
1:F:188:ASN:HB3	1:F:264:MET:HE1	1.95	0.48
1:B:16:LEU:HD12	1:B:44:ALA:HB2	1.96	0.48
1:C:16:LEU:HB2	1:C:38:ASN:HB2	1.95	0.48
1:F:75:TYR:CE2	1:F:108:THR:HG21	2.47	0.48
1:F:166:ASP:CG	1:F:167:THR:H	2.17	0.48
1:C:17:GLY:N	3:C:304:HOH:O	2.45	0.48
1:G:67:LEU:HD11	1:G:95:VAL:HG23	1.96	0.48
1:H:148:GLU:HA	1:H:151:GLU:HB2	1.95	0.48
1:H:234:TYR:CD2	1:H:287:ALA:HB2	2.49	0.48
1:E:199:THR:HB	1:E:258:LEU:HD23	1.96	0.48
1:F:62:ILE:HG13	1:F:85:LEU:CD2	2.42	0.48
1:F:125:MET:HE3	1:F:176:ASP:HA	1.96	0.48
1:G:118:THR:HG21	1:G:146:ALA:HB2	1.96	0.48
1:F:10:PRO:HB2	1:F:65:SER:HB2	1.95	0.47
1:F:23:LEU:HD12	1:F:131:LEU:CD1	2.44	0.47
1:G:245:GLN:HA	1:G:248:MET:CE	2.44	0.47
1:H:224:ALA:O	1:H:227:PRO:HD2	2.14	0.47
1:A:75:TYR:OH	1:A:121:ASP:OD1	2.32	0.47
1:G:208:ALA:HB3	1:G:209:PRO:HD3	1.96	0.47
1:A:97:TYR:HA	1:A:122:GLY:O	2.14	0.47
1:C:151:GLU:HG2	1:C:155:ARG:NH1	2.30	0.47
1:D:75:TYR:CE2	1:D:100:GLY:HA3	2.49	0.47
1:E:241:MET:HE1	1:E:285:TYR:HA	1.96	0.47
1:B:261:SER:HB2	1:D:294:LYS:O	2.14	0.47
1:D:12:SER:HA	1:D:35:THR:O	2.14	0.47
1:E:271:LEU:HB3	1:E:288:MET:CE	2.44	0.47
1:C:125:MET:HG3	1:C:179:LEU:HD13	1.95	0.47
1:H:182:ILE:O	1:H:186:VAL:HG23	2.15	0.47
1:B:79:ARG:NH1	1:B:83:ASP:OD1	2.47	0.47
1:C:16:LEU:CD1	1:C:44:ALA:HB2	2.45	0.47
1:F:124:ILE:HG21	1:F:131:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:HIS:HB3	1:F:153:THR:OG1	2.15	0.47
1:G:27:PHE:CE2	1:G:157:LEU:HD21	2.49	0.47
1:H:214:LEU:O	1:H:218:ILE:HG12	2.15	0.47
1:A:217:LEU:HD13	1:C:135:ARG:HG2	1.97	0.47
1:C:278:ASP:OD2	3:C:301:HOH:O	2.21	0.47
1:D:125:MET:HG3	1:D:179:LEU:HD12	1.96	0.47
1:E:75:TYR:HA	1:E:78:VAL:HG21	1.93	0.47
1:F:165:LEU:O	1:F:166:ASP:HB2	2.14	0.47
1:G:248:MET:HE1	1:G:272:ALA:HB2	1.97	0.47
1:A:183:MET:HE2	1:C:214:LEU:HD12	1.97	0.47
1:D:215:ILE:O	1:D:218:ILE:HG22	2.14	0.47
1:D:243:VAL:HG13	3:D:305:HOH:O	2.15	0.47
1:H:293:ARG:O	1:H:295:PRO:HD3	2.14	0.47
1:A:285:TYR:CZ	1:A:288:MET:HG3	2.51	0.46
1:D:125:MET:SD	1:D:176:ASP:HA	2.55	0.46
1:D:196:LEU:HD11	1:D:251:LEU:HD12	1.98	0.46
1:F:27:PHE:CE2	1:F:157:LEU:HD21	2.50	0.46
1:G:219:THR:HA	1:H:212:ASN:OD1	2.14	0.46
1:E:254:GLU:OE2	1:E:258:LEU:CD1	2.63	0.46
1:F:85:LEU:O	1:F:89:LEU:HD22	2.15	0.46
1:G:16:LEU:CD1	1:G:44:ALA:HB2	2.45	0.46
1:B:186:VAL:HG22	1:D:186:VAL:CG2	2.29	0.46
1:E:75:TYR:O	1:E:79:ARG:HG2	2.15	0.46
1:E:262:ALA:O	1:E:265:PRO:HD2	2.15	0.46
1:H:136:ALA:O	1:H:137:ILE:HG13	2.15	0.46
1:F:19:MET:O	1:F:23:LEU:HD13	2.16	0.46
1:G:127:PRO:HD2	1:G:130:TRP:CE3	2.50	0.46
3:B:413:HOH:O	1:D:243:VAL:HG21	2.16	0.46
1:C:45:ASP:HA	1:C:48:VAL:HG22	1.97	0.46
1:E:130:TRP:CH2	1:F:217:LEU:HB3	2.51	0.46
1:E:201:LYS:O	1:E:201:LYS:HD3	2.15	0.46
1:G:200:ALA:O	1:G:202:VAL:HG23	2.15	0.46
1:G:207:PHE:CD1	1:G:211:ALA:HB2	2.50	0.46
1:G:102:SER:HA	1:G:173:ALA:HB3	1.98	0.46
1:A:16:LEU:CD1	1:A:44:ALA:HB2	2.45	0.46
1:A:38:ASN:ND2	1:A:43:LYS:HB2	2.31	0.46
1:D:238:ASP:OD1	1:D:238:ASP:N	2.42	0.46
1:E:197:LEU:HD21	1:F:175:TYR:CD1	2.50	0.46
1:F:168:ASP:HB3	1:F:171:LEU:CD1	2.46	0.46
1:A:128:PRO:N	1:A:129:PRO:CD	2.78	0.46
1:D:62:ILE:O	1:D:92:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:MET:HE2	1:D:180:LEU:HD12	1.98	0.46
1:F:72:VAL:CG2	1:F:78:VAL:HG22	2.45	0.46
1:H:140:TYR:O	1:H:164:TYR:HB3	2.16	0.46
1:C:238:ASP:OD1	1:C:238:ASP:N	2.39	0.46
1:D:37:TRP:HH2	1:D:39:ARG:HG3	1.80	0.46
1:D:75:TYR:CD2	1:D:100:GLY:HA3	2.50	0.46
1:E:184:TRP:CZ2	1:F:248:MET:HG3	2.51	0.46
1:E:197:LEU:HD21	1:F:175:TYR:CE1	2.51	0.46
1:G:126:GLY:HA3	1:G:130:TRP:CE3	2.51	0.46
1:G:203:LYS:HE3	1:H:230:ASP:HB2	1.98	0.46
1:G:203:LYS:HD3	1:G:205:THR:H	1.80	0.45
1:A:271:LEU:HB3	1:A:288:MET:HE3	1.99	0.45
1:D:16:LEU:HD11	1:D:36:VAL:HB	1.97	0.45
1:F:11:VAL:HG21	1:F:27:PHE:HB3	1.98	0.45
1:F:62:ILE:CG1	1:F:85:LEU:HD11	2.44	0.45
1:G:190:PHE:C	1:G:190:PHE:CD1	2.90	0.45
1:H:264:MET:HB3	1:H:265:PRO:HD3	1.99	0.45
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.97	0.45
1:B:188:ASN:HB3	1:B:264:MET:CE	2.47	0.45
1:C:186:VAL:CG1	1:C:215:ILE:HD13	2.46	0.45
1:D:125:MET:HG3	1:D:179:LEU:CD1	2.46	0.45
1:E:22:ALA:HB2	1:E:128:PRO:HB3	1.99	0.45
1:H:158:GLY:O	1:H:159:ALA:HB2	2.17	0.45
1:D:19:MET:HE1	1:D:131:LEU:HG	1.99	0.45
1:E:128:PRO:N	1:E:129:PRO:CD	2.79	0.45
1:H:263:GLU:O	3:H:301:HOH:O	2.20	0.45
1:B:210:LEU:CD2	1:D:179:LEU:HD11	2.45	0.45
1:F:67:LEU:HD21	1:F:69:VAL:HG23	1.97	0.45
1:F:142:GLY:HA2	1:F:167:THR:O	2.17	0.45
1:G:226:ALA:HB1	1:H:205:THR:HA	1.99	0.45
1:G:228:GLN:HB3	1:G:233:LYS:O	2.17	0.45
1:G:248:MET:HE3	1:G:269:LYS:HA	1.97	0.45
1:B:118:THR:HG23	1:B:143:PRO:HG2	1.98	0.45
1:B:182:ILE:HD11	1:D:190:PHE:HA	1.99	0.45
1:C:257:THR:HG22	1:C:258:LEU:HD23	1.99	0.45
1:F:125:MET:HE1	1:F:176:ASP:HA	1.98	0.45
1:H:171:LEU:O	1:H:175:TYR:HD1	1.99	0.45
1:C:86:ALA:HB1	1:C:115:VAL:HG12	1.98	0.45
1:D:26:ALA:HB3	1:D:157:LEU:HD23	1.99	0.45
1:B:272:ALA:O	1:B:276:VAL:HG23	2.17	0.45
1:D:128:PRO:N	1:D:129:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LYS:HD2	1:E:164:TYR:CE2	2.51	0.45
1:G:19:MET:CE	1:G:128:PRO:HG3	2.46	0.45
1:G:67:LEU:HD11	1:G:95:VAL:CG2	2.47	0.45
1:H:171:LEU:HD23	1:H:171:LEU:HA	1.82	0.45
1:H:216:ASN:O	1:H:219:THR:OG1	2.24	0.45
1:H:239:ALA:HB1	1:H:243:VAL:HG13	1.98	0.45
1:A:62:ILE:O	1:A:92:LYS:HE3	2.17	0.45
1:E:127:PRO:HD2	1:E:130:TRP:CD2	2.52	0.45
1:E:184:TRP:CH2	1:F:248:MET:HG3	2.51	0.45
1:F:97:TYR:CE1	1:F:122:GLY:HA3	2.52	0.45
1:G:190:PHE:C	1:G:190:PHE:HD1	2.20	0.45
1:G:218:ILE:HD12	1:H:183:MET:HG3	1.99	0.45
1:C:125:MET:HG3	1:C:179:LEU:CD1	2.47	0.44
1:E:241:MET:HE3	1:E:241:MET:HB2	1.80	0.44
1:F:27:PHE:O	1:F:32:HIS:HB2	2.17	0.44
1:D:128:PRO:N	1:D:129:PRO:HD2	2.31	0.44
1:E:15:GLY:O	1:E:20:GLY:HA3	2.16	0.44
1:F:256:GLU:OE2	1:F:266:ARG:NH2	2.51	0.44
1:G:254:GLU:OE2	1:H:174:LEU:CD1	2.65	0.44
1:A:183:MET:HE2	1:C:218:ILE:HD13	1.99	0.44
1:A:197:LEU:HB3	1:A:202:VAL:HB	1.99	0.44
1:C:112:ALA:HB1	1:C:117:THR:HG23	1.99	0.44
1:C:203:LYS:CG	1:C:206:THR:HG23	2.41	0.44
1:E:70:LEU:HD23	1:E:78:VAL:HG13	1.97	0.44
1:F:226:ALA:HA	1:F:229:ILE:HD12	1.99	0.44
1:F:229:ILE:HG23	1:F:289:ILE:HG12	1.99	0.44
1:G:14:ILE:CD1	1:G:58:VAL:HG13	2.47	0.44
1:G:248:MET:HE3	1:G:272:ALA:HB3	2.00	0.44
1:B:69:VAL:HG13	1:B:97:TYR:CE2	2.52	0.44
1:C:10:PRO:HA	1:C:33:PRO:HG2	1.99	0.44
1:C:139:LEU:CD2	1:C:165:LEU:HD21	2.47	0.44
1:F:10:PRO:HB2	1:F:65:SER:CB	2.47	0.44
1:B:19:MET:CE	1:B:124:ILE:HG21	2.47	0.44
1:C:127:PRO:HD2	1:C:130:TRP:CE2	2.53	0.44
1:E:252:ALA:HA	1:E:265:PRO:HB2	1.98	0.44
1:F:69:VAL:HG13	1:F:97:TYR:CD2	2.52	0.44
1:A:44:ALA:O	1:A:48:VAL:HG23	2.17	0.44
1:D:264:MET:HB3	1:D:265:PRO:HD3	1.99	0.44
1:F:144:LYS:NZ	1:F:148:GLU:OE2	2.45	0.44
1:G:175:TYR:OH	3:G:301:HOH:O	2.20	0.44
1:A:197:LEU:O	1:A:202:VAL:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:NH1	1:B:238:ASP:OD2	2.47	0.44
1:E:214:LEU:HD11	1:F:183:MET:HB2	2.00	0.44
1:E:274:ARG:NH1	1:F:263:GLU:OE2	2.50	0.44
1:F:37:TRP:CZ3	1:F:81:LEU:HD11	2.53	0.44
1:G:19:MET:HE2	1:G:128:PRO:HG3	1.99	0.44
1:G:70:LEU:HD13	1:G:94:VAL:HG13	1.99	0.44
1:G:182:ILE:O	1:G:186:VAL:HG23	2.17	0.44
1:C:160:ALA:N	3:C:302:HOH:O	2.27	0.44
1:C:176:ASP:O	1:C:180:LEU:CD2	2.66	0.44
1:F:165:LEU:HD13	1:F:175:TYR:CD2	2.53	0.44
1:G:197:LEU:HD12	1:G:207:PHE:CD2	2.53	0.44
1:C:190:PHE:HE1	1:C:208:ALA:HA	1.82	0.43
1:E:12:SER:HA	1:E:35:THR:O	2.18	0.43
1:E:102:SER:HA	1:E:173:ALA:HB3	2.00	0.43
1:E:134:ASP:OD1	1:E:134:ASP:N	2.49	0.43
1:E:226:ALA:HB3	1:E:227:PRO:CD	2.48	0.43
1:F:83:ASP:CB	1:F:84:PRO:HD3	2.48	0.43
1:H:219:THR:HA	1:H:222:VAL:HG23	1.99	0.43
1:A:75:TYR:O	1:A:78:VAL:HB	2.18	0.43
1:F:128:PRO:N	1:F:129:PRO:CD	2.81	0.43
1:F:262:ALA:C	1:F:265:PRO:HD2	2.38	0.43
1:H:219:THR:HA	1:H:222:VAL:CG2	2.48	0.43
1:B:128:PRO:N	1:B:129:PRO:CD	2.80	0.43
1:C:155:ARG:HG2	1:C:159:ALA:HA	1.99	0.43
1:E:78:VAL:HG11	1:E:96:ASN:ND2	2.33	0.43
1:F:7:ALA:HA	1:F:33:PRO:CD	2.27	0.43
1:F:16:LEU:HD12	1:F:47:LEU:CD2	2.48	0.43
1:A:105:ALA:HB3	1:A:170:GLY:HA2	2.00	0.43
1:A:276:VAL:HG22	1:A:281:ALA:HA	2.00	0.43
1:G:197:LEU:HB3	1:G:202:VAL:CB	2.46	0.43
1:B:136:ALA:O	1:B:161:GLY:HA3	2.17	0.43
1:E:190:PHE:HA	1:F:182:ILE:HD11	1.99	0.43
1:A:229:ILE:HD13	1:A:289:ILE:HD13	2.01	0.43
1:B:229:ILE:HD11	1:D:191:LEU:CD2	2.49	0.43
1:C:236:ALA:HB1	1:C:240:THR:HG22	1.99	0.43
1:E:251:LEU:HA	1:F:177:MET:SD	2.59	0.43
1:G:27:PHE:CZ	1:G:157:LEU:HD21	2.53	0.43
1:H:144:LYS:O	1:H:144:LYS:HG2	2.18	0.43
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.88	0.43
1:C:100:GLY:O	1:C:173:ALA:HB1	2.19	0.43
1:F:126:GLY:HA3	1:F:130:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:PRO:N	1:F:129:PRO:HD2	2.34	0.43
1:E:75:TYR:OH	1:E:121:ASP:OD1	2.31	0.43
1:G:79:ARG:O	1:G:83:ASP:HB2	2.18	0.43
1:H:147:PHE:CE1	1:H:164:TYR:HD2	2.37	0.43
1:A:38:ASN:HD22	1:A:43:LYS:HB2	1.83	0.43
1:A:183:MET:CE	1:C:218:ILE:HD13	2.49	0.43
1:D:141:SER:HA	1:D:166:ASP:O	2.18	0.43
1:D:147:PHE:CE2	1:D:164:TYR:HB2	2.54	0.43
1:F:101:THR:OG1	1:F:104:GLN:HG3	2.18	0.43
1:G:22:ALA:CB	1:G:131:LEU:HD12	2.49	0.43
1:G:203:LYS:HE2	1:G:204:ALA:N	2.34	0.43
1:G:241:MET:HE3	1:G:241:MET:HA	2.00	0.43
1:F:166:ASP:OD1	1:F:167:THR:N	2.46	0.42
1:H:201:LYS:HD2	1:H:201:LYS:N	2.34	0.42
1:C:127:PRO:CB	1:C:129:PRO:HD2	2.44	0.42
1:D:246:ASP:HB2	3:D:305:HOH:O	2.20	0.42
1:E:220:GLU:HB2	1:F:135:ARG:HH21	1.84	0.42
1:E:254:GLU:OE1	1:F:101:THR:HA	2.20	0.42
1:A:26:ALA:CB	1:A:157:LEU:HD23	2.49	0.42
1:A:285:TYR:CE1	1:A:288:MET:HG3	2.54	0.42
1:B:10:PRO:O	3:B:401:HOH:O	2.21	0.42
1:F:109:ALA:HA	1:F:119:TYR:CD2	2.55	0.42
1:F:264:MET:HB3	1:F:265:PRO:HD3	2.00	0.42
1:G:180:LEU:HB3	1:G:184:TRP:CZ3	2.55	0.42
1:A:140:TYR:O	1:A:165:LEU:HB2	2.20	0.42
1:B:93:VAL:HG22	1:B:118:THR:HB	2.00	0.42
1:D:171:LEU:HD23	1:D:171:LEU:HA	1.79	0.42
1:D:177:MET:CE	1:D:180:LEU:HD12	2.49	0.42
1:E:255:SER:HB2	1:E:262:ALA:CB	2.47	0.42
1:F:26:ALA:HB3	1:F:157:LEU:CD2	2.44	0.42
1:G:196:LEU:HD21	1:G:258:LEU:HD12	2.02	0.42
1:C:254:GLU:O	1:C:258:LEU:HG	2.20	0.42
1:G:168:ASP:O	1:G:171:LEU:HB2	2.20	0.42
1:D:86:ALA:HB1	1:D:115:VAL:HG12	2.00	0.42
1:G:23:LEU:CD2	1:G:157:LEU:HD13	2.49	0.42
1:G:248:MET:CE	1:G:272:ALA:CB	2.97	0.42
1:H:183:MET:HE2	1:H:183:MET:HB3	1.91	0.42
1:A:204:ALA:HB2	1:C:229:ILE:HG21	2.01	0.42
1:D:19:MET:HE2	1:D:124:ILE:CD1	2.37	0.42
1:E:199:THR:CB	1:E:258:LEU:HD23	2.49	0.42
1:A:183:MET:CE	1:C:214:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLU:HG2	1:C:267:PHE:HE1	1.85	0.42
1:C:16:LEU:HD11	1:C:36:VAL:CG2	2.50	0.42
1:E:238:ASP:HB2	1:F:127:PRO:HB3	2.00	0.42
1:G:197:LEU:CB	1:G:202:VAL:HB	2.46	0.42
1:A:118:THR:HG21	1:A:146:ALA:CB	2.45	0.41
1:F:276:VAL:HG13	1:F:281:ALA:HB2	2.00	0.41
1:G:203:LYS:HZ2	1:H:230:ASP:HB2	1.84	0.41
1:B:39:ARG:HB3	2:B:301:NAP:O1X	2.20	0.41
1:E:256:GLU:H	1:E:256:GLU:HG2	1.67	0.41
1:G:203:LYS:CE	1:G:204:ALA:HB3	2.43	0.41
1:G:241:MET:HE2	1:G:241:MET:HB3	1.87	0.41
1:A:78:VAL:HG21	1:A:96:ASN:HD21	1.85	0.41
1:C:35:THR:HA	1:C:53:THR:O	2.20	0.41
1:C:102:SER:HA	1:C:173:ALA:HB3	2.02	0.41
1:F:212:ASN:O	1:F:216:ASN:OD1	2.39	0.41
1:B:75:TYR:OH	1:B:121:ASP:OD1	2.38	0.41
1:E:39:ARG:HB3	2:E:301:NAP:O2X	2.21	0.41
1:A:196:LEU:HG	1:A:260:ILE:HD11	2.01	0.41
1:A:217:LEU:HD12	1:C:137:ILE:HD11	2.02	0.41
1:C:184:TRP:O	1:C:188:ASN:HB2	2.20	0.41
1:D:6:ALA:O	1:D:7:ALA:HB3	2.21	0.41
1:D:271:LEU:HB3	1:D:288:MET:CE	2.47	0.41
1:E:125:MET:CG	1:E:137:ILE:HG22	2.50	0.41
1:E:193:GLY:HA3	1:F:178:SER:HB3	2.02	0.41
1:E:200:ALA:O	1:E:201:LYS:HB3	2.19	0.41
1:B:123:ALA:HB3	1:B:139:LEU:HB2	2.01	0.41
1:E:271:LEU:HB3	1:E:288:MET:HE1	2.02	0.41
1:F:11:VAL:HG21	1:F:27:PHE:CB	2.51	0.41
1:F:38:ASN:O	1:F:40:ARG:N	2.53	0.41
1:F:241:MET:HE2	1:F:241:MET:HB3	1.91	0.41
1:A:256:GLU:OE1	1:A:266:ARG:NH2	2.52	0.41
1:H:151:GLU:O	1:H:152:ALA:HB3	2.21	0.41
1:B:188:ASN:HB3	1:B:264:MET:HE3	2.02	0.41
1:C:89:LEU:HD23	1:C:89:LEU:HA	1.93	0.41
1:E:135:ARG:HG2	1:F:217:LEU:HD22	2.01	0.41
1:E:139:LEU:HD23	1:E:163:THR:HB	2.01	0.41
1:E:182:ILE:HD11	1:F:190:PHE:HA	2.01	0.41
1:G:137:ILE:HD13	1:G:137:ILE:HA	1.95	0.41
1:A:196:LEU:HG	1:A:260:ILE:CD1	2.51	0.41
1:B:47:LEU:N	1:B:47:LEU:HD22	2.36	0.41
1:B:69:VAL:HG13	1:B:97:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD23	1:C:165:LEU:HD21	2.03	0.41
1:C:197:LEU:HB3	1:C:202:VAL:HB	2.02	0.41
1:E:118:THR:HG21	1:E:146:ALA:CB	2.51	0.41
1:E:203:LYS:HD2	1:E:203:LYS:N	2.36	0.41
1:G:127:PRO:HB2	1:G:129:PRO:HD2	2.03	0.41
1:A:12:SER:HA	1:A:35:THR:O	2.21	0.41
1:A:215:ILE:HG22	1:C:215:ILE:HG22	2.03	0.41
1:B:262:ALA:C	1:B:265:PRO:HD2	2.40	0.41
1:C:271:LEU:HB3	1:C:288:MET:HE3	2.03	0.41
1:E:183:MET:HE3	1:E:183:MET:HB3	1.99	0.41
1:G:75:TYR:O	1:G:78:VAL:HB	2.21	0.41
1:G:128:PRO:HD2	1:G:129:PRO:HD2	2.03	0.41
1:E:193:GLY:HA2	1:F:178:SER:HB3	2.03	0.40
1:H:248:MET:CE	1:H:285:TYR:HE1	2.34	0.40
1:C:218:ILE:HD12	1:C:218:ILE:HA	1.93	0.40
1:D:86:ALA:HB1	1:D:115:VAL:CG1	2.51	0.40
1:F:75:TYR:HA	1:F:78:VAL:HG23	2.04	0.40
1:F:102:SER:HA	1:F:105:ALA:HB3	2.02	0.40
1:F:104:GLN:O	1:F:108:THR:HG22	2.21	0.40
1:F:199:THR:HG21	1:F:258:LEU:HB3	2.03	0.40
1:A:274:ARG:HA	1:A:277:ALA:HB3	2.03	0.40
1:D:140:TYR:O	1:D:165:LEU:HB2	2.20	0.40
1:E:251:LEU:O	1:E:255:SER:OG	2.37	0.40
1:G:168:ASP:CB	1:G:171:LEU:HD23	2.41	0.40
1:B:144:LYS:O	1:B:148:GLU:HG3	2.20	0.40
1:C:82:LEU:HB3	1:C:111:TRP:CH2	2.56	0.40
1:C:180:LEU:HB3	1:C:184:TRP:CZ3	2.57	0.40
1:C:224:ALA:O	1:C:227:PRO:HD2	2.21	0.40
1:D:41:ALA:HB1	1:D:54:ARG:NH1	2.37	0.40
1:E:233:LYS:HA	1:E:233:LYS:HD3	1.92	0.40
1:F:115:VAL:HG12	1:F:115:VAL:O	2.21	0.40
1:G:171:LEU:HD12	1:G:175:TYR:HE1	1.86	0.40
1:G:240:THR:HB	1:G:281:ALA:O	2.22	0.40
1:H:219:THR:CA	1:H:222:VAL:HG23	2.51	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	287/297 (97%)	275 (96%)	11 (4%)	1 (0%)	37 60
1	B	289/297 (97%)	276 (96%)	13 (4%)	0	100 100
1	C	287/297 (97%)	272 (95%)	14 (5%)	1 (0%)	37 60
1	D	288/297 (97%)	274 (95%)	14 (5%)	0	100 100
1	E	287/297 (97%)	278 (97%)	9 (3%)	0	100 100
1	F	260/297 (88%)	245 (94%)	15 (6%)	0	100 100
1	G	284/297 (96%)	268 (94%)	15 (5%)	1 (0%)	30 53
1	H	158/297 (53%)	143 (90%)	14 (9%)	1 (1%)	22 43
All	All	2140/2376 (90%)	2031 (95%)	105 (5%)	4 (0%)	44 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	ASP
1	H	159	ALA
1	G	158	GLY
1	A	158	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	210/216 (97%)	208 (99%)	2 (1%)	73 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	211/216 (98%)	209 (99%)	2 (1%)	75 89
1	C	210/216 (97%)	205 (98%)	5 (2%)	44 71
1	D	210/216 (97%)	207 (99%)	3 (1%)	62 83
1	E	210/216 (97%)	208 (99%)	2 (1%)	73 88
1	F	200/216 (93%)	197 (98%)	3 (2%)	60 82
1	G	209/216 (97%)	203 (97%)	6 (3%)	37 65
1	H	118/216 (55%)	116 (98%)	2 (2%)	56 80
All	All	1578/1728 (91%)	1553 (98%)	25 (2%)	58 81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	238	ASP
1	B	40	ARG
1	B	201	LYS
1	C	43	LYS
1	C	70	LEU
1	C	110	GLU
1	C	134	ASP
1	C	201	LYS
1	D	49	SER
1	D	233	LYS
1	D	294	LYS
1	E	134	ASP
1	E	282	ASP
1	F	12	SER
1	F	74	ASP
1	F	82	LEU
1	G	29	LYS
1	G	190	PHE
1	G	207	PHE
1	G	214	LEU
1	G	234	TYR
1	G	266	ARG
1	H	141	SER
1	H	234	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	B	8	GLN
1	G	46	GLN
1	G	216	ASN
1	H	169	HIS
1	H	244	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	E	301	-	45,52,52	0.72	1 (2%)	56,80,80	0.74	1 (1%)
2	NAP	B	301	-	45,52,52	0.72	1 (2%)	56,80,80	0.74	2 (3%)

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	E	301	-	-	5/31/67/67	0/5/5/5
2	NAP	B	301	-	-	11/31/67/67	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C2N-N1N	2.53	1.38	1.35
2	E	301	NAP	C2N-N1N	2.46	1.37	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	NAP	C5A-C6A-N6A	2.17	123.65	120.35
2	E	301	NAP	C5A-C6A-N6A	2.16	123.63	120.35
2	B	301	NAP	C6N-N1N-C2N	-2.08	120.08	121.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

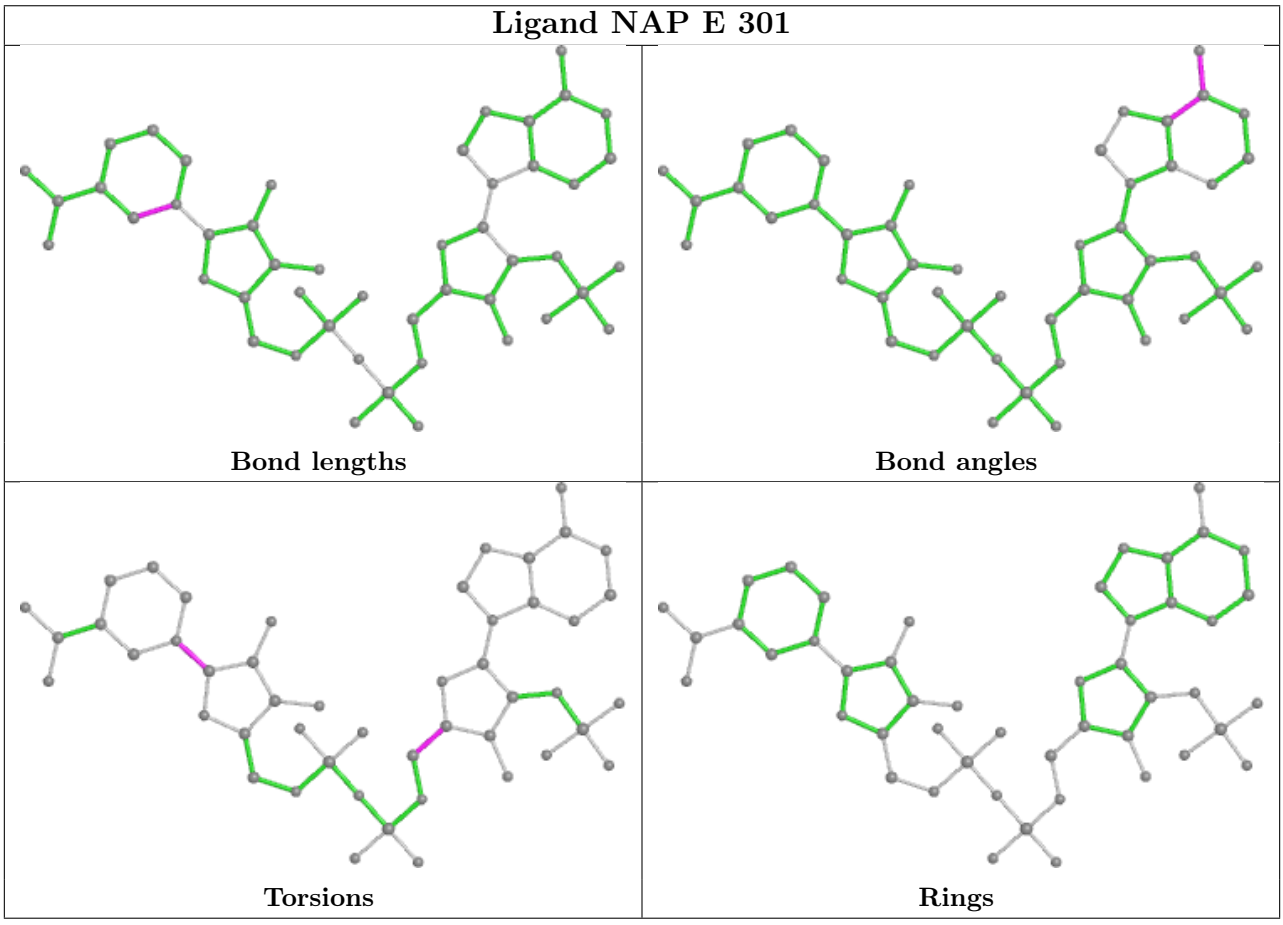
Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5B-O5B-PA-O1A
2	B	301	NAP	C5B-O5B-PA-O2A
2	B	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C2N
2	E	301	NAP	O4D-C1D-N1N-C6N
2	B	301	NAP	C4N-C3N-C7N-O7N
2	B	301	NAP	C4N-C3N-C7N-N7N
2	B	301	NAP	C2N-C3N-C7N-O7N
2	B	301	NAP	C2N-C3N-C7N-N7N
2	B	301	NAP	PN-O3-PA-O5B
2	B	301	NAP	C5B-O5B-PA-O3
2	B	301	NAP	PA-O3-PN-O2N
2	E	301	NAP	C2D-C1D-N1N-C2N
2	E	301	NAP	C2D-C1D-N1N-C6N
2	E	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

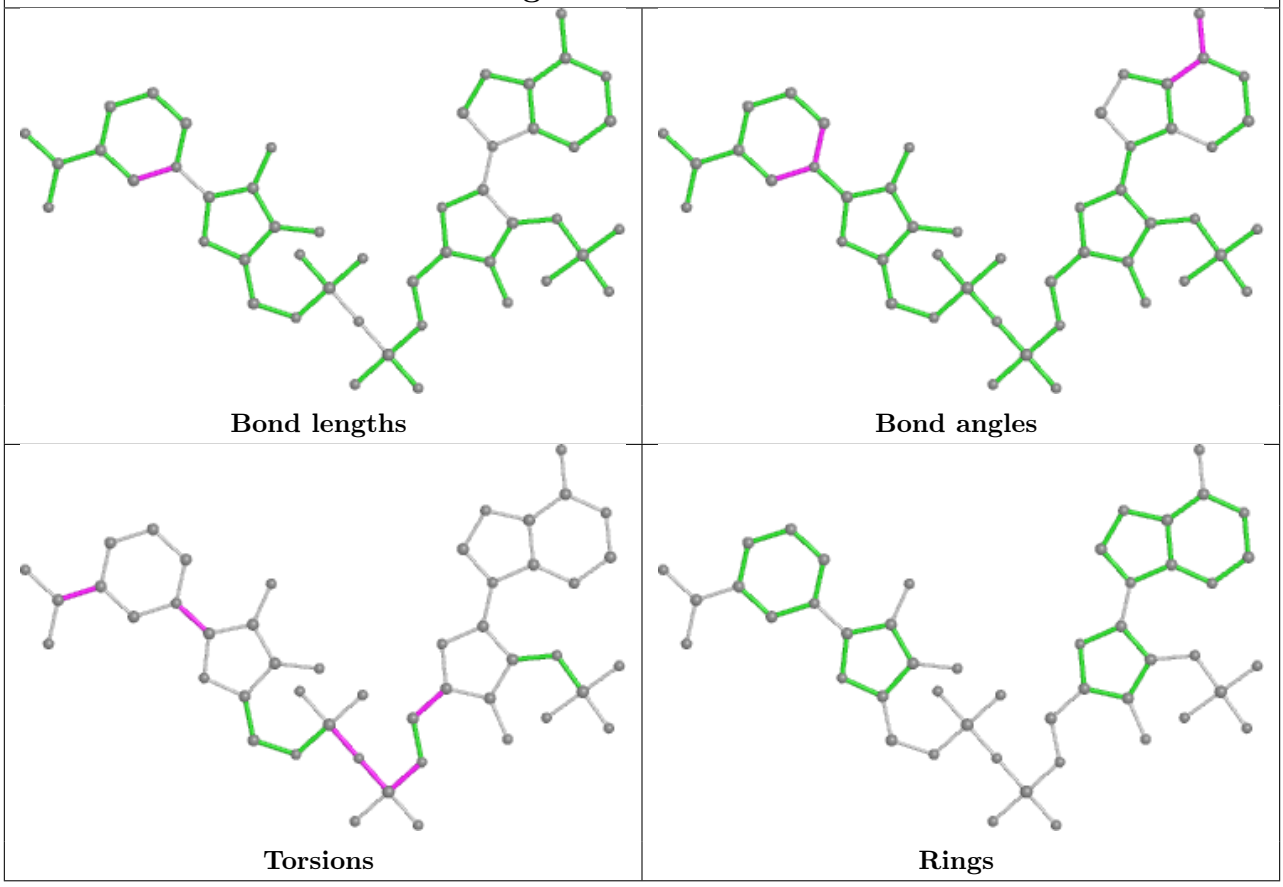
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	NAP	1	0
2	B	301	NAP	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 NAP B 301



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	289/297 (97%)	0.39	6 (2%) 63 63	37, 56, 71, 89	0
1	B	291/297 (97%)	0.15	1 (0%) 90 90	34, 49, 69, 80	0
1	C	289/297 (97%)	0.34	3 (1%) 79 79	38, 56, 71, 82	0
1	D	290/297 (97%)	0.24	5 (1%) 69 69	36, 50, 65, 78	0
1	E	289/297 (97%)	0.20	14 (4%) 36 35	28, 44, 72, 85	0
1	F	276/297 (92%)	1.39	87 (31%) 1 1	37, 88, 108, 114	0
1	G	288/297 (96%)	0.40	15 (5%) 34 32	38, 54, 73, 85	0
1	H	160/297 (53%)	1.09	37 (23%) 2 3	40, 62, 88, 96	0
All	All	2172/2376 (91%)	0.49	168 (7%) 21 20	28, 53, 93, 114	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	114	GLY	6.0
1	F	28	LEU	5.6
1	H	160	ALA	5.0
1	G	204	ALA	5.0
1	F	113	ALA	4.9
1	H	165	LEU	4.9
1	F	72	VAL	4.8
1	F	146	ALA	4.7
1	H	227	PRO	4.6
1	F	64	ALA	4.6
1	H	163	THR	4.6
1	F	55	ALA	4.5
1	F	26	ALA	4.5
1	G	136	ALA	4.4
1	F	86	ALA	4.4
1	H	162	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	47	LEU	4.2
1	H	159	ALA	4.2
1	H	161	GLY	4.1
1	F	53	THR	4.0
1	E	7	ALA	3.9
1	F	66	PRO	3.9
1	F	112	ALA	3.9
1	F	115	VAL	3.8
1	E	259	GLY	3.8
1	F	61	ALA	3.7
1	F	19	MET	3.7
1	F	88	SER	3.7
1	F	111	TRP	3.7
1	G	73	SER	3.6
1	F	18	LEU	3.6
1	F	94	VAL	3.5
1	F	85	LEU	3.5
1	F	154	LEU	3.5
1	F	82	LEU	3.5
1	D	6	ALA	3.4
1	F	150	HIS	3.4
1	F	84	PRO	3.3
1	F	171	LEU	3.3
1	C	7	ALA	3.3
1	F	22	ALA	3.3
1	H	279	GLY	3.2
1	H	232	GLY	3.2
1	F	14	ILE	3.2
1	F	124	ILE	3.2
1	F	159	ALA	3.1
1	F	58	VAL	3.1
1	F	11	VAL	3.1
1	H	138	LEU	3.0
1	G	208	ALA	3.0
1	D	125	MET	3.0
1	H	235	PRO	3.0
1	F	63	ALA	3.0
1	F	75	TYR	3.0
1	F	131	LEU	3.0
1	F	89	LEU	3.0
1	F	139	LEU	3.0
1	H	164	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	121	ASP	3.0
1	H	233	LYS	2.9
1	F	143	PRO	2.9
1	F	70	LEU	2.9
1	H	219	THR	2.9
1	F	120	LEU	2.9
1	E	200	ALA	2.9
1	F	93	VAL	2.9
1	F	132	ALA	2.9
1	F	157	LEU	2.9
1	F	126	GLY	2.9
1	F	138	LEU	2.9
1	G	134	ASP	2.8
1	F	30	ALA	2.8
1	A	39	ARG	2.8
1	E	203	LYS	2.8
1	H	230	ASP	2.8
1	H	221	ARG	2.8
1	F	153	THR	2.8
1	F	160	ALA	2.8
1	G	199	THR	2.8
1	F	127	PRO	2.8
1	F	100	GLY	2.8
1	F	29	LYS	2.7
1	H	158	GLY	2.7
1	H	238	ASP	2.7
1	H	140	TYR	2.7
1	H	166	ASP	2.7
1	E	236	ALA	2.7
1	F	44	ALA	2.7
1	E	242	THR	2.7
1	F	40	ARG	2.7
1	H	146	ALA	2.6
1	F	95	VAL	2.6
1	H	220	GLU	2.6
1	F	140	TYR	2.6
1	H	234	TYR	2.6
1	H	223	THR	2.6
1	F	37	TRP	2.6
1	F	42	ALA	2.6
1	H	237	GLY	2.6
1	F	16	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	150	HIS	2.5
1	G	40	ARG	2.5
1	F	15	GLY	2.5
1	D	160	ALA	2.5
1	F	52	ALA	2.5
1	F	78	VAL	2.5
1	F	25	ALA	2.5
1	H	152	ALA	2.5
1	F	81	LEU	2.4
1	A	295	PRO	2.4
1	F	295	PRO	2.4
1	H	167	THR	2.4
1	H	231	GLU	2.4
1	G	258	LEU	2.4
1	A	55	ALA	2.4
1	G	200	ALA	2.4
1	G	260	ILE	2.4
1	A	282	ASP	2.4
1	F	180	LEU	2.4
1	F	176	ASP	2.4
1	G	83	ASP	2.4
1	A	56	GLY	2.3
1	F	133	THR	2.3
1	F	80	GLU	2.3
1	F	7	ALA	2.3
1	F	59	ALA	2.3
1	H	143	PRO	2.3
1	H	169	HIS	2.3
1	G	85	LEU	2.3
1	F	46	GLN	2.2
1	E	281	ALA	2.2
1	F	142	GLY	2.2
1	F	119	TYR	2.2
1	F	68	VAL	2.2
1	H	222	VAL	2.2
1	E	260	ILE	2.2
1	F	130	TRP	2.2
1	F	41	ALA	2.2
1	F	125	MET	2.2
1	F	156	ALA	2.2
1	B	48	VAL	2.2
1	H	284	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLU	2.1
1	G	206	THR	2.1
1	G	257	THR	2.1
1	F	27	PHE	2.1
1	F	69	VAL	2.1
1	E	196	LEU	2.1
1	C	160	ALA	2.1
1	H	145	ALA	2.1
1	C	249	GLU	2.1
1	E	250	HIS	2.1
1	F	177	MET	2.1
1	H	147	PHE	2.1
1	D	165	LEU	2.1
1	F	149	GLU	2.1
1	F	32	HIS	2.1
1	E	233	LYS	2.1
1	F	49	SER	2.1
1	H	174	LEU	2.1
1	E	262	ALA	2.1
1	E	253	GLU	2.1
1	H	154	LEU	2.1
1	G	7	ALA	2.1
1	E	232	GLY	2.1
1	F	175	TYR	2.0
1	D	294	LYS	2.0
1	F	253	GLU	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)

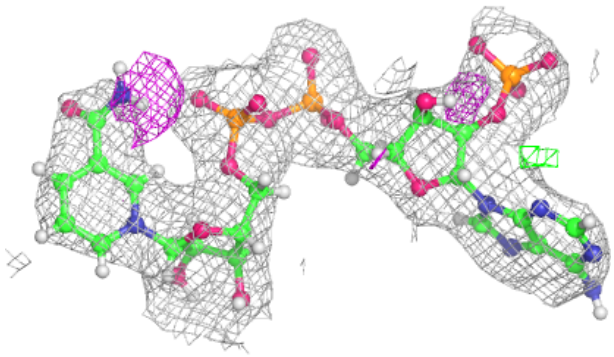
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

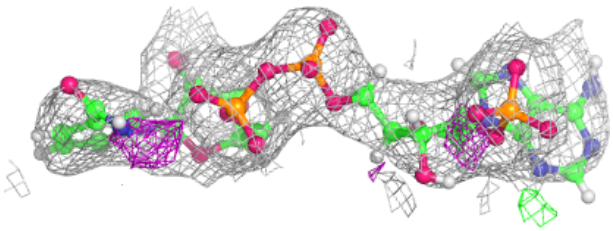
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	B	301	48/48	0.90	0.10	53,71,92,101	0
2	NAP	E	301	48/48	0.95	0.08	36,46,58,61	0

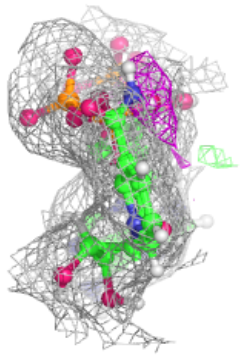
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP B 301:

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

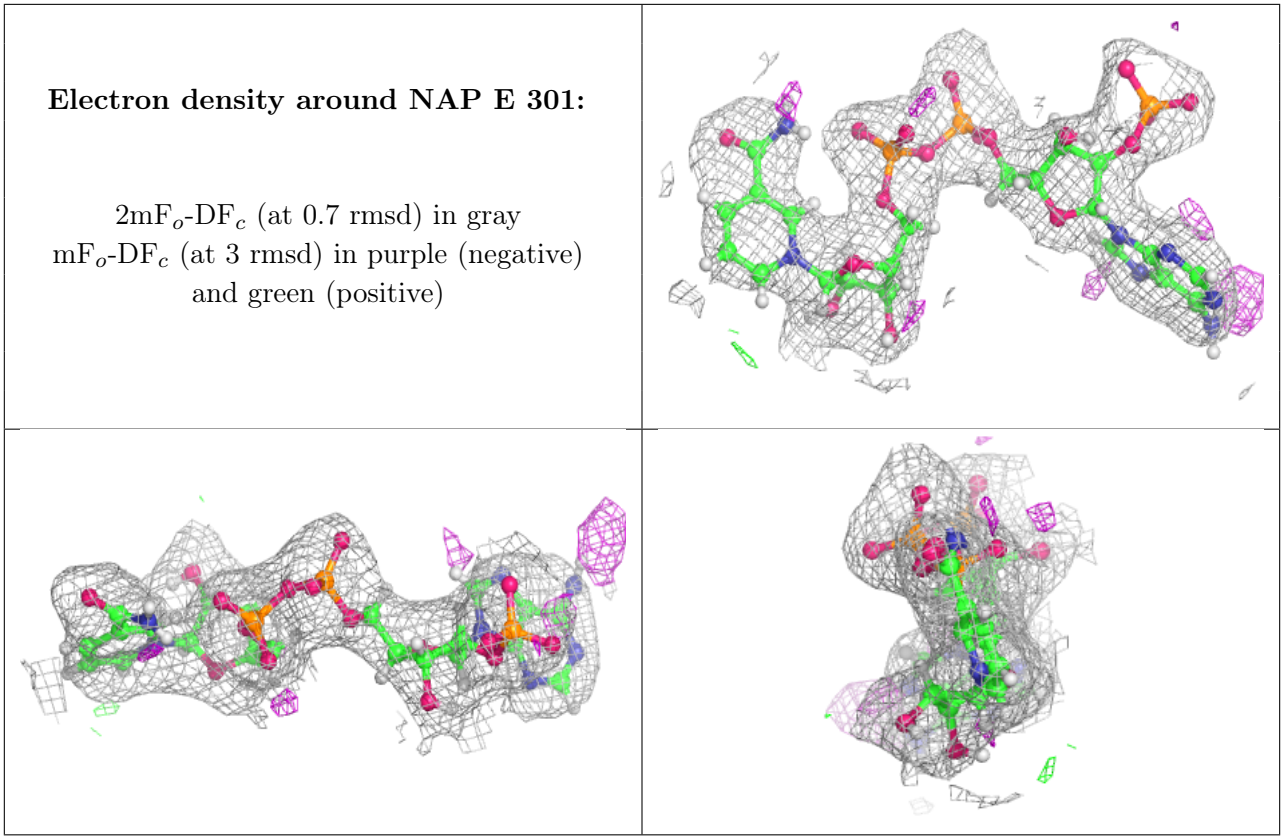






Electron density around NAP E 301:

$2mF_o$-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.