



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID : 2AZN
Title : X-RAY Structure of 2,5-diamino-6-ribosylamino-4(3h)-pyrimidinone 5-phosphate reductase
Authors : Chatwell, L.; Bacher, A.; Huber, R.; Fischer, M.; Krojer, T.
Deposited on : 2005-09-12
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

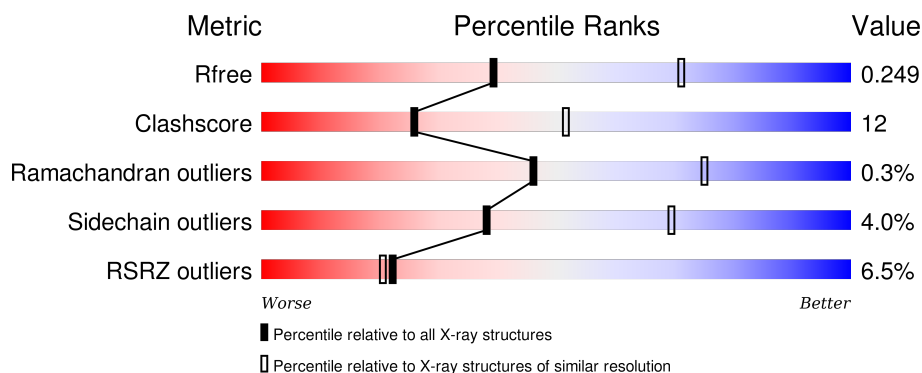
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>6%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>
1	B	219	<div> <div>7%</div> <div>77%</div> <div>22%</div> <div>•</div> </div>
1	C	219	<div> <div>6%</div> <div>76%</div> <div>22%</div> <div>•</div> </div>
1	D	219	<div> <div>7%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
1	E	219	<div> <div>5%</div> <div>78%</div> <div>21%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	219	

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	MA5	B	1002	-	-	-	X
2	MA5	B	1007	-	-	-	X
2	MA5	C	1003	-	-	-	X
2	MA5	D	1001	-	-	-	X
2	MA5	F	1005	-	-	-	X
2	MA5	F	1008	-	-	-	X
4	EPE	B	3001	-	-	-	X
4	EPE	F	3002	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11090 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 Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	Se	26	0	0
			1710	1087	292	323	3	5			
1	B	219	Total	C	N	O	S	Se	35	0	0
			1710	1087	292	323	3	5			
1	C	219	Total	C	N	O	S	Se	25	0	0
			1710	1087	292	323	3	5			
1	D	219	Total	C	N	O	S	Se	25	0	0
			1710	1087	292	323	3	5			
1	E	219	Total	C	N	O	S	Se	29	0	0
			1710	1087	292	323	3	5			
1	F	219	Total	C	N	O	S	Se	29	0	0
			1710	1087	292	323	3	5			

There are 30 discrepancies between the modelled and reference sequences:

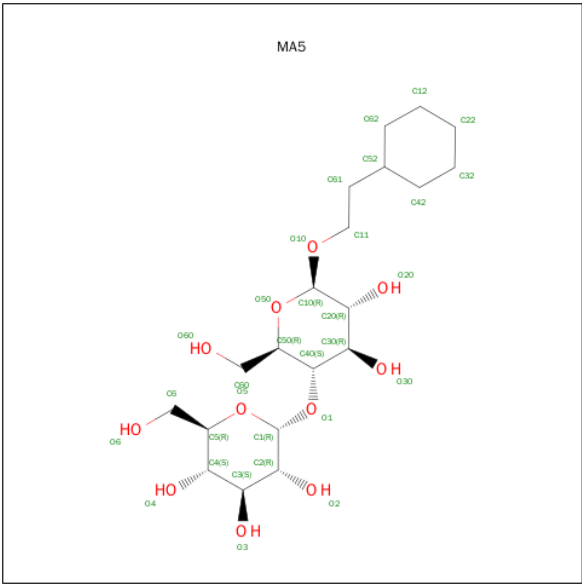
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
A	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085
A	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
A	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
B	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085
B	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
B	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085
C	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
C	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085
C	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
C	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085
D	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
D	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085

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Chain	Residue	Modelled	Actual	Comment	Reference
D	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
D	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085
E	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
E	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085
E	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
E	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
E	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085
F	17	MSE	MET	MODIFIED RESIDUE	UNP Q58085
F	52	MSE	MET	MODIFIED RESIDUE	UNP Q58085
F	122	MSE	MET	MODIFIED RESIDUE	UNP Q58085
F	140	MSE	MET	MODIFIED RESIDUE	UNP Q58085
F	163	MSE	MET	MODIFIED RESIDUE	UNP Q58085

- Molecule 2 is 2-(6-(2-CYCLOHEXYLETHOXY)-TETRAHYDRO-4,5-DIHYDROXY-2(HYDROXYMETHYL)-2H-PYRAN-3-YLOXY)-TETRAHYDRO-6(HYDROXYMETHYL)-2H-PYRAN-3,4,5-TRIOL (three-letter code: MA5) (formula: C₂₀H₃₆O₁₁).



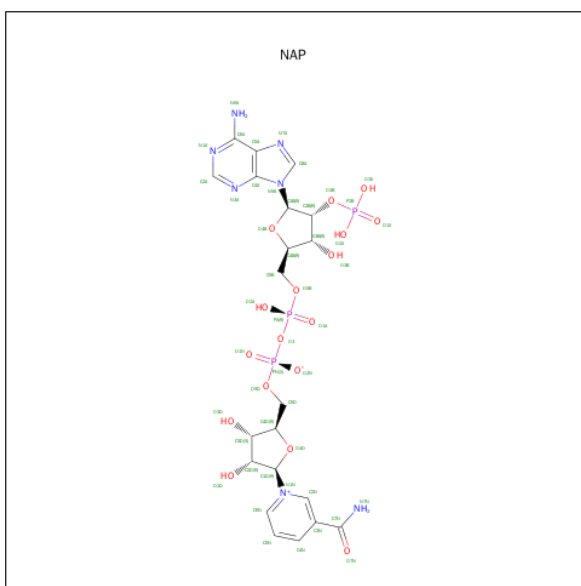
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	15	0
			31	20	11		
2	B	1	Total	C	O	13	0
			31	20	11		
2	C	1	Total	C	O	0	0
			31	20	11		
2	A	1	Total	C	O	15	0
			31	20	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	15	0
			31	20	11		
2	C	1	Total	C	O	0	0
			31	20	11		
2	B	1	Total	C	O	12	0
			31	20	11		
2	F	1	Total	C	O	7	0
			31	20	11		

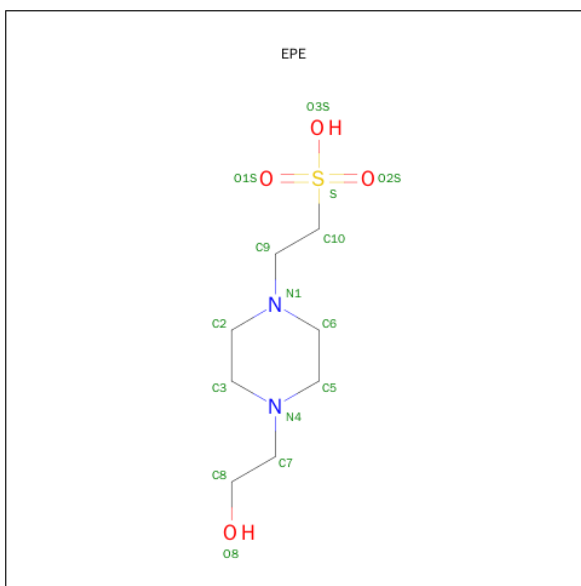
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
4	F	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

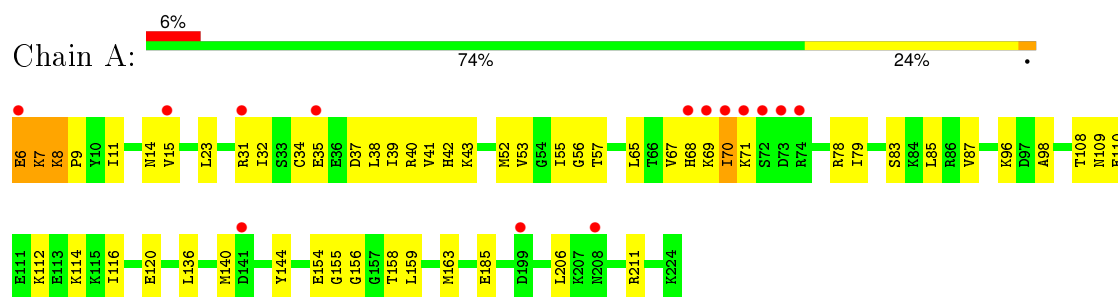
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	35	Total	O	0	0
			35	35		
5	C	50	Total	O	0	0
			50	50		
5	D	49	Total	O	0	0
			49	49		
5	E	56	Total	O	0	0
			56	56		
5	F	43	Total	O	0	0
			43	43		

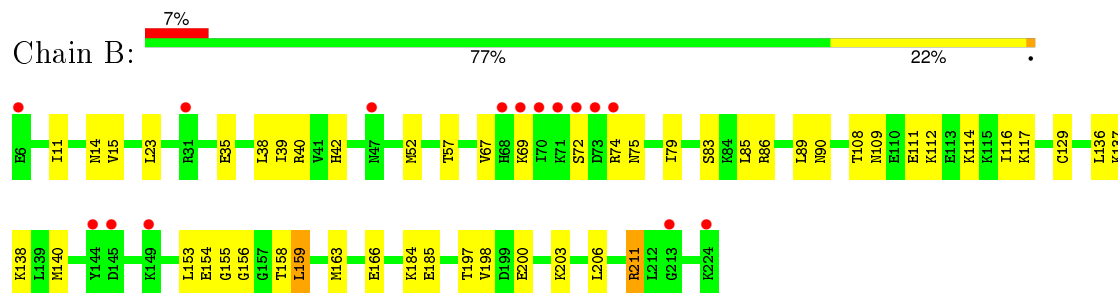
3 Residue-property plots [i](#)

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.

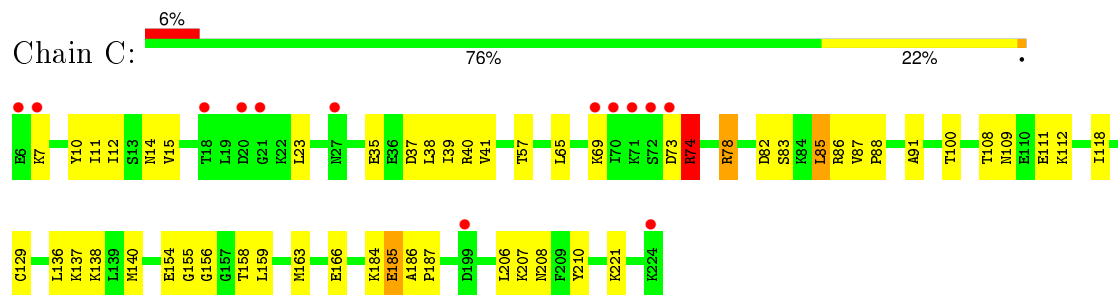
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



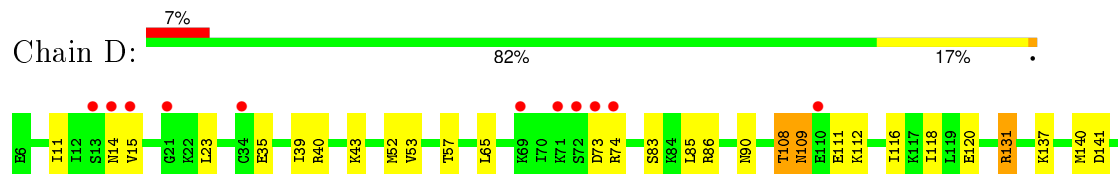
- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase

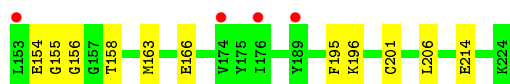


- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase

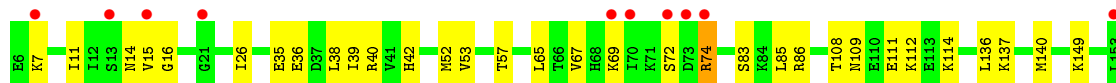
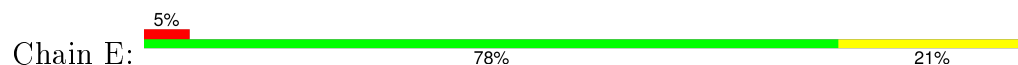


- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase

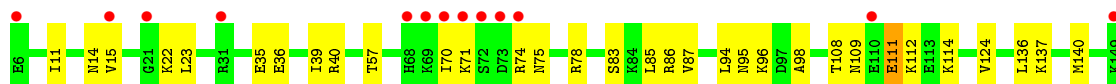
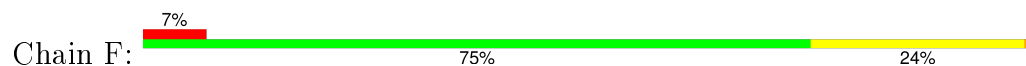




- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



- Molecule 1: Putative 5-amino-6-(5-phosphoribosylamino)uracil reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.17Å 137.17Å 213.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 99.4 (29.82-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.253 0.229 , 0.249	Depositor DCC
R_{free} test set	2784 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 133909 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11090	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.9778e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, EPE, MA5

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	0.38	0/1724	0.67	0/2304
1	B	0.41	0/1724	0.67	0/2304
1	C	0.39	0/1724	0.67	0/2304
1	D	0.38	0/1724	0.67	0/2304
1	E	0.38	0/1724	0.66	0/2304
1	F	0.38	0/1724	0.68	0/2304
All	All	0.39	0/10344	0.67	0/13824

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	1710	0	1801	52	0
1	B	1710	0	1801	44	0
1	C	1710	0	1801	45	0
1	D	1710	0	1801	36	0
1	E	1710	0	1801	43	0
1	F	1710	0	1801	43	0
2	A	31	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	62	0	72	6	0
2	C	62	0	72	12	0
2	D	31	0	36	4	0
2	F	62	0	72	3	0
3	A	48	0	25	13	0
3	B	48	0	25	7	0
3	C	48	0	25	8	0
3	D	48	0	25	8	0
3	E	48	0	25	6	0
3	F	48	0	25	6	0
4	B	12	0	13	4	0
4	F	12	0	13	5	0
5	A	37	0	0	2	0
5	B	35	0	0	2	0
5	C	50	0	0	7	0
5	D	49	0	0	3	0
5	E	56	0	0	6	0
5	F	43	0	0	6	0
All	All	11090	0	11270	268	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 12.

All (268) 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:C:78:ARG:HG2	5:C:2042:HOH:O	1.59	1.00
1:B:14:ASN:HD21	1:B:40:ARG:HH22	1.10	0.98
1:C:65:LEU:HB2	5:C:2042:HOH:O	1.63	0.96
1:F:111:GLU:HG2	4:F:3002:EPE:H61	1.46	0.96
1:C:14:ASN:HD21	1:C:40:ARG:HH22	1.13	0.96
1:F:14:ASN:HD21	1:F:40:ARG:HH22	1.15	0.94
1:A:14:ASN:HD21	1:A:40:ARG:HH22	1.16	0.89
1:B:111:GLU:HG2	4:B:3001:EPE:H61	1.55	0.89
1:B:89:LEU:HB3	2:B:1002:MA5:H61	1.55	0.88
1:A:110:GLU:HB3	2:A:1004:MA5:O6	1.74	0.88
1:B:114:LYS:HD2	4:B:3001:EPE:H62	1.59	0.85
1:D:14:ASN:HD21	1:D:40:ARG:HH22	1.24	0.82
1:E:14:ASN:HD21	1:E:40:ARG:HH22	1.27	0.81
1:B:158:THR:HB	3:B:2002:NAP:H52A	1.64	0.80
1:A:56:GLY:H	3:A:2001:NAP:C5B	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:PHE:HB3	5:E:2009:HOH:O	1.86	0.74
1:A:114:LYS:HG2	4:B:3001:EPE:H31	1.70	0.74
2:C:1006:MA5:O20	2:C:1006:MA5:H112	1.89	0.73
1:E:74:ARG:HH11	1:E:74:ARG:HG3	1.55	0.72
1:E:57:THR:OG1	3:E:2005:NAP:H6N	1.90	0.72
1:B:38:LEU:HD13	1:B:69:LYS:NZ	2.04	0.71
1:D:109:ASN:ND2	1:D:112:LYS:H	1.88	0.71
1:C:11:ILE:HD11	1:C:140:MSE:SE	2.39	0.71
1:F:11:ILE:HD11	1:F:140:MSE:SE	2.41	0.71
1:E:194:GLY:HA3	5:E:2060:HOH:O	1.88	0.71
1:A:55:ILE:HG22	3:A:2001:NAP:H4B	1.72	0.70
1:C:186:ALA:N	5:C:2033:HOH:O	2.23	0.70
1:F:111:GLU:HG3	4:F:3002:EPE:H91	1.73	0.69
1:E:158:THR:HB	3:E:2005:NAP:H52A	1.75	0.69
1:B:11:ILE:HD11	1:B:140:MSE:SE	2.42	0.69
1:E:11:ILE:HD11	1:E:140:MSE:SE	2.43	0.69
1:A:14:ASN:HD21	1:A:40:ARG:NH2	1.91	0.68
1:A:56:GLY:H	3:A:2001:NAP:H51A	1.55	0.68
1:A:55:ILE:CG2	3:A:2001:NAP:H4B	2.23	0.68
1:B:35:GLU:O	1:B:39:ILE:HD13	1.94	0.68
1:A:42:HIS:HB3	1:A:70:ILE:HG21	1.78	0.66
1:D:214:GLU:HG2	5:D:2051:HOH:O	1.96	0.66
1:B:14:ASN:HD21	1:B:40:ARG:NH2	1.91	0.65
1:A:109:ASN:ND2	1:A:112:LYS:H	1.95	0.65
1:F:158:THR:HB	3:F:2006:NAP:H52A	1.79	0.65
1:F:14:ASN:HD21	1:F:40:ARG:NH2	1.92	0.64
1:A:57:THR:OG1	3:A:2001:NAP:H6N	1.98	0.64
1:C:109:ASN:ND2	1:C:112:LYS:H	1.96	0.64
1:E:109:ASN:ND2	1:E:112:LYS:H	1.97	0.63
1:D:158:THR:HB	3:D:2004:NAP:H52A	1.79	0.63
1:C:14:ASN:HD21	1:C:40:ARG:NH2	1.93	0.63
1:C:108:THR:CG2	1:C:109:ASN:N	2.62	0.62
1:F:137:LYS:HE2	1:F:166:GLU:OE1	2.00	0.62
1:E:35:GLU:O	1:E:39:ILE:HD13	2.00	0.62
1:F:35:GLU:O	1:F:39:ILE:HD13	1.98	0.62
1:A:42:HIS:HB3	1:A:70:ILE:CG2	2.30	0.62
1:F:108:THR:CG2	1:F:109:ASN:N	2.63	0.62
1:E:16:GLY:H	3:E:2005:NAP:H72N	1.48	0.61
1:A:52:MSE:HE1	1:A:140:MSE:HE1	1.80	0.61
1:D:11:ILE:HD13	1:D:163:MSE:CE	2.30	0.61
1:C:12:ILE:HD11	2:C:1006:MA5:H612	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ILE:HD13	1:F:163:MSE:CE	2.31	0.61
1:C:137:LYS:HE2	1:C:166:GLU:OE1	2.00	0.60
1:E:11:ILE:HD13	1:E:163:MSE:HE1	1.82	0.60
1:E:74:ARG:HH11	1:E:74:ARG:CG	2.14	0.60
1:D:11:ILE:HD13	1:D:163:MSE:HE1	1.83	0.60
1:C:158:THR:HB	3:C:2003:NAP:H52A	1.83	0.60
1:A:38:LEU:HB3	1:A:69:LYS:HD2	1.84	0.60
1:B:57:THR:OG1	3:B:2002:NAP:H6N	2.02	0.59
1:C:12:ILE:CD1	2:C:1006:MA5:H612	2.32	0.59
1:D:14:ASN:HD21	1:D:40:ARG:NH2	1.99	0.59
1:E:108:THR:CG2	1:E:109:ASN:N	2.66	0.59
1:C:78:ARG:HD3	1:C:100:THR:OG1	2.02	0.59
1:D:57:THR:OG1	3:D:2004:NAP:H6N	2.03	0.59
1:F:86:ARG:HD3	5:F:3016:HOH:O	2.03	0.59
1:E:137:LYS:HE2	1:E:166:GLU:OE1	2.01	0.59
1:A:108:THR:CG2	1:A:109:ASN:N	2.66	0.58
1:F:109:ASN:ND2	1:F:112:LYS:H	2.01	0.58
1:F:57:THR:OG1	3:F:2006:NAP:H6N	2.03	0.58
1:E:42:HIS:CG	1:E:69:LYS:HB2	2.39	0.58
1:A:32:ILE:HD12	5:A:2027:HOH:O	2.03	0.58
1:B:197:THR:OG1	1:B:200:GLU:HG2	2.04	0.58
1:B:137:LYS:HE2	1:B:166:GLU:OE1	2.03	0.57
1:F:114:LYS:NZ	4:F:3002:EPE:O3S	2.31	0.57
1:D:108:THR:HG23	1:D:109:ASN:N	2.18	0.57
1:D:158:THR:HB	3:D:2004:NAP:C5B	2.34	0.57
1:A:11:ILE:HD11	1:A:140:MSE:SE	2.55	0.57
1:B:108:THR:CG2	1:B:109:ASN:N	2.67	0.57
1:C:154:GLU:O	3:C:2003:NAP:H5N	2.05	0.57
1:B:158:THR:HB	3:B:2002:NAP:C5B	2.32	0.57
1:A:6:GLU:HA	1:A:144:TYR:CD1	2.39	0.56
1:F:154:GLU:O	3:F:2006:NAP:C5N	2.54	0.56
1:C:38:LEU:HD13	1:C:69:LYS:HE2	1.87	0.56
1:A:31:ARG:NH2	5:A:2018:HOH:O	2.37	0.56
1:A:11:ILE:HD13	1:A:163:MSE:CE	2.35	0.56
1:F:111:GLU:CG	4:F:3002:EPE:H61	2.29	0.56
1:D:11:ILE:HD11	1:D:140:MSE:SE	2.56	0.56
3:A:2001:NAP:H1B	3:A:2001:NAP:O2X	2.05	0.55
1:C:184:LYS:C	5:C:2033:HOH:O	2.44	0.55
1:A:110:GLU:CB	2:A:1004:MA5:O6	2.53	0.55
1:E:214:GLU:HG2	5:E:2026:HOH:O	2.06	0.55
1:B:117:LYS:HB3	2:B:1007:MA5:H621	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLY:H	3:A:2001:NAP:H52A	1.71	0.55
1:B:109:ASN:ND2	1:B:112:LYS:H	2.05	0.54
1:C:12:ILE:HD13	2:C:1006:MA5:H422	1.90	0.54
1:C:35:GLU:O	1:C:39:ILE:HD13	2.06	0.54
1:B:111:GLU:HG2	4:B:3001:EPE:C6	2.33	0.54
1:E:11:ILE:HD13	1:E:163:MSE:CE	2.37	0.54
1:E:158:THR:HB	3:E:2005:NAP:C5B	2.38	0.54
1:B:52:MSE:HE1	1:B:140:MSE:HE1	1.90	0.54
1:D:52:MSE:HE1	1:D:140:MSE:HE1	1.90	0.53
1:F:111:GLU:CG	4:F:3002:EPE:H91	2.39	0.53
1:F:83:SER:HB2	3:F:2006:NAP:O3X	2.09	0.53
1:C:158:THR:HB	3:C:2003:NAP:C5B	2.39	0.53
2:B:1007:MA5:H321	1:C:118:ILE:HD12	1.89	0.53
1:B:38:LEU:HD13	1:B:69:LYS:HZ3	1.71	0.53
1:A:43:LYS:HG2	1:A:70:ILE:HD12	1.89	0.53
1:E:26:ILE:HG12	5:E:2049:HOH:O	2.07	0.53
1:C:108:THR:HG22	1:C:109:ASN:N	2.24	0.53
1:F:158:THR:HB	3:F:2006:NAP:C5B	2.39	0.53
1:C:136:LEU:O	1:C:140:MSE:HG2	2.08	0.53
1:B:112:LYS:O	1:B:116:ILE:HG13	2.09	0.53
1:A:53:VAL:HG11	1:A:65:LEU:HD11	1.92	0.52
1:E:108:THR:HG22	1:E:109:ASN:N	2.25	0.52
1:D:109:ASN:HD21	1:D:112:LYS:H	1.53	0.52
1:C:73:ASP:O	1:C:74:ARG:HB2	2.09	0.52
1:F:14:ASN:ND2	1:F:40:ARG:HH22	1.96	0.51
1:A:14:ASN:ND2	1:A:40:ARG:HH22	1.98	0.51
1:E:26:ILE:HG23	5:E:2049:HOH:O	2.10	0.51
1:C:11:ILE:HD13	1:C:163:MSE:CE	2.41	0.51
1:B:75:ASN:HB3	5:B:3003:HOH:O	2.10	0.51
1:D:118:ILE:HG12	2:D:1001:MA5:H122	1.92	0.51
1:B:86:ARG:HD3	5:B:3031:HOH:O	2.10	0.51
1:B:158:THR:HG21	3:B:2002:NAP:H3B	1.92	0.51
1:E:83:SER:HB2	3:E:2005:NAP:O3X	2.11	0.51
1:E:7:LYS:HG3	1:E:7:LYS:O	2.10	0.51
1:E:67:VAL:HG11	1:E:72:SER:HB2	1.93	0.51
1:F:11:ILE:HD13	1:F:163:MSE:HE1	1.92	0.51
1:D:83:SER:HB2	3:D:2004:NAP:O1X	2.11	0.51
1:F:75:ASN:HB3	5:F:3033:HOH:O	2.11	0.51
1:B:83:SER:HB2	3:B:2002:NAP:O1X	2.11	0.51
1:C:86:ARG:HD3	5:C:2021:HOH:O	2.11	0.50
1:A:11:ILE:HD13	1:A:163:MSE:HE1	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HB3	3:D:2004:NAP:H2N	1.93	0.50
1:C:82:ASP:OD2	1:C:85:LEU:HA	2.12	0.49
1:C:10:TYR:CD1	2:C:1006:MA5:H50	2.47	0.49
1:D:154:GLU:O	3:D:2004:NAP:H5N	2.13	0.49
1:D:158:THR:HG21	3:D:2004:NAP:H3B	1.94	0.49
1:C:83:SER:HB2	3:C:2003:NAP:O3X	2.12	0.49
1:C:208:ASN:HD21	2:C:1003:MA5:C60	2.25	0.49
1:F:198:VAL:O	1:F:203:LYS:NZ	2.40	0.49
1:E:38:LEU:HD13	1:E:69:LYS:HE2	1.94	0.49
1:E:14:ASN:HD21	1:E:40:ARG:NH2	2.04	0.49
1:A:67:VAL:CG1	1:A:70:ILE:HG23	2.42	0.49
1:C:88:PRO:HG2	1:C:91:ALA:HB2	1.93	0.49
1:B:38:LEU:HD13	1:B:69:LYS:HZ1	1.77	0.49
1:E:36:GLU:HB3	1:E:212:LEU:HD11	1.95	0.49
2:C:1006:MA5:O10	2:C:1006:MA5:H622	2.12	0.49
1:E:74:ARG:CG	1:E:74:ARG:NH1	2.76	0.48
1:B:11:ILE:HD13	1:B:163:MSE:HE1	1.95	0.48
1:F:205:GLU:OE2	1:F:207:LYS:NZ	2.42	0.48
1:B:154:GLU:O	3:B:2002:NAP:C5N	2.62	0.48
1:F:136:LEU:O	1:F:140:MSE:HG2	2.13	0.48
1:D:90:ASN:OD1	1:F:96:LYS:HE2	2.13	0.48
1:D:154:GLU:O	3:D:2004:NAP:C5N	2.61	0.48
1:B:11:ILE:HD13	1:B:163:MSE:CE	2.43	0.48
1:F:15:VAL:HG12	1:F:174:VAL:HG22	1.96	0.48
1:C:57:THR:OG1	3:C:2003:NAP:H6N	2.13	0.48
1:A:116:ILE:O	1:A:120:GLU:HG3	2.14	0.48
1:F:214:GLU:HG2	5:F:3017:HOH:O	2.14	0.48
1:A:70:ILE:HG12	1:A:71:LYS:N	2.28	0.47
2:F:1005:MA5:C11	2:F:1005:MA5:O20	2.62	0.47
1:F:108:THR:HG22	1:F:109:ASN:N	2.29	0.47
1:B:136:LEU:HD13	1:B:163:MSE:SE	2.64	0.47
2:D:1001:MA5:H111	1:E:114:LYS:HD2	1.96	0.47
1:E:155:GLY:HA3	1:E:156:GLY:HA2	1.65	0.47
1:D:137:LYS:HE2	1:D:166:GLU:OE1	2.14	0.47
1:B:23:LEU:HB3	3:B:2002:NAP:H2N	1.97	0.47
1:F:155:GLY:HA3	1:F:156:GLY:HA2	1.61	0.47
1:E:53:VAL:HG11	1:E:65:LEU:HD11	1.96	0.47
1:C:14:ASN:ND2	1:C:40:ARG:HH22	1.97	0.47
1:F:195:PHE:CD1	1:F:201:CYS:HA	2.50	0.47
1:A:114:LYS:NZ	2:A:1004:MA5:H62	2.30	0.47
1:A:83:SER:OG	3:A:2001:NAP:H8A	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLU:HB2	5:C:2053:HOH:O	2.14	0.47
1:B:155:GLY:HA3	1:B:156:GLY:HA2	1.62	0.47
1:E:86:ARG:HD3	5:E:2020:HOH:O	2.14	0.47
1:B:67:VAL:CG1	1:B:72:SER:HB3	2.45	0.46
1:F:36:GLU:HB3	1:F:212:LEU:HD11	1.97	0.46
1:F:211:ARG:HG2	5:F:3019:HOH:O	2.15	0.46
1:A:158:THR:N	3:A:2001:NAP:O2A	2.49	0.46
1:C:208:ASN:HD21	2:C:1003:MA5:H601	1.81	0.46
1:D:86:ARG:HD3	5:D:2044:HOH:O	2.15	0.46
1:A:52:MSE:HE3	1:A:79:ILE:HG21	1.97	0.46
1:F:95:ASN:HA	5:F:3034:HOH:O	2.16	0.46
1:A:78:ARG:HD2	1:A:98:ALA:HB3	1.96	0.45
1:E:52:MSE:HE1	1:E:140:MSE:HE1	1.98	0.45
1:A:34:CYS:O	1:A:38:LEU:HG	2.16	0.45
1:D:116:ILE:O	1:D:120:GLU:HG3	2.17	0.45
1:B:52:MSE:HE3	1:B:79:ILE:HG21	1.97	0.45
1:A:108:THR:HG23	1:A:109:ASN:N	2.32	0.45
1:A:136:LEU:HD13	1:A:163:MSE:SE	2.66	0.45
1:E:42:HIS:CD2	1:E:69:LYS:HB2	2.52	0.45
1:C:187:PRO:HA	5:C:2008:HOH:O	2.17	0.45
1:C:23:LEU:HB3	3:C:2003:NAP:H2N	1.99	0.44
2:C:1006:MA5:O30	2:C:1006:MA5:O2	2.30	0.44
1:C:37:ASP:O	1:C:41:VAL:HG23	2.18	0.44
1:A:42:HIS:CE1	1:A:68:HIS:H	2.36	0.44
1:B:117:LYS:HG3	2:B:1007:MA5:H111	2.00	0.44
1:C:11:ILE:HD13	1:C:163:MSE:HE1	2.00	0.44
2:D:1001:MA5:O60	1:E:114:LYS:HE3	2.17	0.44
1:C:155:GLY:HA3	1:C:156:GLY:HA2	1.64	0.44
1:A:8:LYS:HG3	1:A:9:PRO:N	2.31	0.44
1:D:108:THR:CG2	1:D:109:ASN:N	2.79	0.43
1:F:15:VAL:HG21	1:F:23:LEU:HD21	2.00	0.43
1:E:195:PHE:CD1	1:E:201:CYS:HA	2.53	0.43
1:A:155:GLY:HA3	1:A:156:GLY:HA2	1.63	0.43
1:C:129:CYS:SG	1:C:138:LYS:HB2	2.58	0.43
1:E:53:VAL:CG1	1:E:65:LEU:HD11	2.49	0.43
1:F:195:PHE:CE1	1:F:202:VAL:HG23	2.53	0.43
1:B:42:HIS:CD2	1:B:69:LYS:HB2	2.53	0.43
1:B:153:LEU:HD11	1:B:159:LEU:HD13	2.00	0.43
1:B:136:LEU:O	1:B:140:MSE:HG2	2.18	0.43
1:A:55:ILE:HG22	3:A:2001:NAP:C4B	2.45	0.43
1:A:23:LEU:HB3	3:A:2001:NAP:H2N	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG13	1:A:87:VAL:O	2.19	0.43
1:B:129:CYS:SG	1:B:138:LYS:HB2	2.58	0.43
1:F:22:LYS:HE3	5:F:3042:HOH:O	2.19	0.43
1:D:73:ASP:OD2	1:D:74:ARG:N	2.52	0.43
1:C:87:VAL:HG13	1:C:87:VAL:O	2.19	0.43
1:F:94:LEU:HD22	1:F:124:VAL:HG21	2.01	0.43
1:F:154:GLU:O	3:F:2006:NAP:H5N	2.19	0.42
1:C:23:LEU:HB3	3:C:2003:NAP:C2N	2.49	0.42
1:B:108:THR:HG23	1:B:109:ASN:N	2.34	0.42
1:A:154:GLU:O	3:A:2001:NAP:H5N	2.20	0.42
1:E:154:GLU:O	3:E:2005:NAP:C4N	2.68	0.42
1:D:112:LYS:O	1:D:116:ILE:HG13	2.20	0.42
1:D:53:VAL:HG11	1:D:65:LEU:HD11	2.02	0.42
1:D:155:GLY:HA3	1:D:156:GLY:HA2	1.64	0.42
1:C:83:SER:OG	3:C:2003:NAP:H8A	2.19	0.42
1:A:35:GLU:O	1:A:39:ILE:HD13	2.19	0.42
1:E:136:LEU:O	1:E:140:MSE:HG2	2.20	0.42
1:C:210:TYR:CD2	2:C:1003:MA5:H601	2.55	0.42
1:D:131:ARG:HG3	1:D:131:ARG:HH11	1.84	0.42
1:A:114:LYS:CE	2:A:1004:MA5:H62	2.49	0.41
1:D:109:ASN:HD22	1:D:111:GLU:H	1.68	0.41
1:A:114:LYS:HZ2	2:A:1004:MA5:H62	1.85	0.41
1:A:96:LYS:HE2	1:B:90:ASN:CG	2.40	0.41
1:C:210:TYR:CB	2:C:1003:MA5:H40	2.50	0.41
1:B:211:ARG:HG2	1:B:211:ARG:H	1.61	0.41
1:F:87:VAL:O	1:F:87:VAL:HG13	2.20	0.41
1:A:154:GLU:O	3:A:2001:NAP:C5N	2.69	0.41
2:C:1006:MA5:H2	2:C:1006:MA5:HO2	1.63	0.41
1:E:15:VAL:HG12	1:E:174:VAL:HG22	2.02	0.41
1:B:117:LYS:HG3	2:B:1007:MA5:C11	2.51	0.41
2:F:1005:MA5:O20	2:F:1005:MA5:H111	2.20	0.41
1:A:37:ASP:O	1:A:41:VAL:HG23	2.21	0.41
1:A:53:VAL:CG1	1:A:65:LEU:HD11	2.50	0.41
2:D:1001:MA5:H612	1:E:111:GLU:HA	2.03	0.41
1:D:109:ASN:HD22	1:D:111:GLU:N	2.18	0.41
1:E:38:LEU:CD1	1:E:69:LYS:HE2	2.51	0.41
1:B:90:ASN:HA	2:B:1002:MA5:O30	2.21	0.41
1:A:109:ASN:HD21	1:A:112:LYS:H	1.68	0.41
1:D:195:PHE:CD1	1:D:201:CYS:HA	2.55	0.41
1:B:198:VAL:O	1:B:203:LYS:NZ	2.44	0.41
1:E:195:PHE:CE1	1:E:202:VAL:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:O	1:D:43:LYS:HG3	2.21	0.40
1:D:35:GLU:O	1:D:39:ILE:HD13	2.21	0.40
1:F:153:LEU:HD11	1:F:159:LEU:HD13	2.03	0.40
1:D:15:VAL:HG21	1:D:23:LEU:HD21	2.03	0.40
1:F:78:ARG:HD2	1:F:98:ALA:HB3	2.03	0.40
1:F:210:TYR:CD2	2:F:1005:MA5:H20	2.57	0.40
1:D:196:LYS:HD2	5:D:2021:HOH:O	2.21	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	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	34	63
1	B	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	C	217/219 (99%)	207 (95%)	8 (4%)	2 (1%)	21	49
1	D	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	E	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	F	217/219 (99%)	208 (96%)	8 (4%)	1 (0%)	34	63
All	All	1302/1314 (99%)	1249 (96%)	49 (4%)	4 (0%)	46	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	LYS
1	A	7	LYS
1	C	74	ARG
1	F	70	ILE

5.3.2 Protein sidechains ⓘ

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	191/187 (102%)	181 (95%)	10 (5%)	29	58
1	B	191/187 (102%)	183 (96%)	8 (4%)	36	68
1	C	191/187 (102%)	181 (95%)	10 (5%)	29	58
1	D	191/187 (102%)	185 (97%)	6 (3%)	47	78
1	E	191/187 (102%)	186 (97%)	5 (3%)	54	83
1	F	191/187 (102%)	184 (96%)	7 (4%)	41	72
All	All	1146/1122 (102%)	1100 (96%)	46 (4%)	38	69

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	LYS
1	A	8	LYS
1	A	15	VAL
1	A	70	ILE
1	A	85	LEU
1	A	159	LEU
1	A	185	GLU
1	A	206	LEU
1	A	211	ARG
1	B	15	VAL
1	B	74	ARG
1	B	85	LEU
1	B	159	LEU
1	B	184	LYS
1	B	185	GLU
1	B	206	LEU
1	B	211	ARG
1	C	15	VAL
1	C	74	ARG
1	C	78	ARG
1	C	85	LEU

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Mol	Chain	Res	Type
1	C	111	GLU
1	C	159	LEU
1	C	185	GLU
1	C	206	LEU
1	C	207	LYS
1	C	221	LYS
1	D	85	LEU
1	D	108	THR
1	D	109	ASN
1	D	131	ARG
1	D	141	ASP
1	D	206	LEU
1	E	74	ARG
1	E	85	LEU
1	E	149	LYS
1	E	185	GLU
1	E	206	LEU
1	F	71	LYS
1	F	74	ARG
1	F	85	LEU
1	F	111	GLU
1	F	159	LEU
1	F	185	GLU
1	F	206	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	27	ASN
1	A	109	ASN
1	B	14	ASN
1	B	27	ASN
1	B	109	ASN
1	C	14	ASN
1	C	109	ASN
1	D	14	ASN
1	D	27	ASN
1	D	109	ASN
1	E	14	ASN
1	E	27	ASN
1	E	109	ASN

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Mol	Chain	Res	Type
1	F	14	ASN
1	F	27	ASN
1	F	109	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 ⓘ

16 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	MA5	A	1004	-	33,33,33	0.58	1 (3%)	44,46,46	0.93	2 (4%)
3	NAP	A	2001	-	42,52,52	1.09	3 (7%)	54,80,80	2.19	8 (14%)
2	MA5	B	1002	-	33,33,33	0.58	1 (3%)	44,46,46	0.88	2 (4%)
2	MA5	B	1007	-	33,33,33	0.58	1 (3%)	44,46,46	0.82	1 (2%)
3	NAP	B	2002	-	42,52,52	1.10	4 (9%)	54,80,80	2.12	8 (14%)
4	EPE	B	3001	-	11,12,15	0.92	0	12,16,20	1.59	2 (16%)
2	MA5	C	1003	-	33,33,33	0.59	1 (3%)	44,46,46	1.14	4 (9%)
2	MA5	C	1006	-	33,33,33	0.59	1 (3%)	44,46,46	0.84	2 (4%)
3	NAP	C	2003	-	42,52,52	1.09	3 (7%)	54,80,80	2.06	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MA5	D	1001	-	33,33,33	0.58	1 (3%)	44,46,46	0.87	2 (4%)
3	NAP	D	2004	-	42,52,52	1.10	4 (9%)	54,80,80	2.13	9 (16%)
3	NAP	E	2005	-	42,52,52	1.10	3 (7%)	54,80,80	2.08	8 (14%)
2	MA5	F	1005	-	33,33,33	0.60	1 (3%)	44,46,46	1.00	2 (4%)
2	MA5	F	1008	-	33,33,33	0.58	1 (3%)	44,46,46	1.01	2 (4%)
3	NAP	F	2006	-	42,52,52	1.09	3 (7%)	54,80,80	2.14	8 (14%)
4	EPE	F	3002	-	11,12,15	0.92	0	12,16,20	1.53	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA5	A	1004	-	-	0/14/62/62	0/3/3/3
3	NAP	A	2001	-	-	0/27/67/67	0/5/5/5
2	MA5	B	1002	-	-	0/14/62/62	0/3/3/3
2	MA5	B	1007	-	-	0/14/62/62	0/3/3/3
3	NAP	B	2002	-	-	0/27/67/67	0/5/5/5
4	EPE	B	3001	-	-	0/6/14/19	1/1/1/1
2	MA5	C	1003	-	-	0/14/62/62	0/3/3/3
2	MA5	C	1006	-	-	0/14/62/62	0/3/3/3
3	NAP	C	2003	-	-	0/27/67/67	0/5/5/5
2	MA5	D	1001	-	-	0/14/62/62	0/3/3/3
3	NAP	D	2004	-	-	0/27/67/67	0/5/5/5
3	NAP	E	2005	-	-	0/27/67/67	0/5/5/5
2	MA5	F	1005	-	-	1/14/62/62	0/3/3/3
2	MA5	F	1008	-	-	0/14/62/62	0/3/3/3
3	NAP	F	2006	-	-	0/27/67/67	0/5/5/5
4	EPE	F	3002	-	-	0/6/14/19	1/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	NAP	C3N-C7N	2.02	1.53	1.50
3	D	2004	NAP	C3N-C7N	2.10	1.53	1.50
2	A	1004	MA5	O10-C10	2.17	1.44	1.40
3	B	2002	NAP	O4D-C1D	2.19	1.44	1.41
2	B	1002	MA5	O10-C10	2.20	1.44	1.40
2	B	1007	MA5	O10-C10	2.20	1.44	1.40
2	F	1008	MA5	O10-C10	2.20	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2006	NAP	O4D-C1D	2.21	1.44	1.41
2	D	1001	MA5	O10-C10	2.21	1.44	1.40
3	C	2003	NAP	O4D-C1D	2.23	1.44	1.41
3	D	2004	NAP	O4D-C1D	2.27	1.44	1.41
2	C	1006	MA5	O10-C10	2.29	1.44	1.40
2	C	1003	MA5	O10-C10	2.29	1.44	1.40
3	E	2005	NAP	O4D-C1D	2.30	1.44	1.41
3	A	2001	NAP	O4D-C1D	2.35	1.44	1.41
2	F	1005	MA5	O10-C10	2.37	1.44	1.40
3	A	2001	NAP	O4B-C1B	2.54	1.44	1.41
3	F	2006	NAP	O4B-C1B	2.64	1.44	1.41
3	B	2002	NAP	O4B-C1B	2.65	1.44	1.41
3	C	2003	NAP	O4B-C1B	2.65	1.44	1.41
3	D	2004	NAP	O4B-C1B	2.71	1.44	1.41
3	E	2005	NAP	O4B-C1B	2.74	1.44	1.41
3	B	2002	NAP	P2B-O1X	3.09	1.61	1.51
3	D	2004	NAP	P2B-O1X	3.09	1.61	1.51
3	A	2001	NAP	P2B-O1X	3.12	1.61	1.51
3	F	2006	NAP	P2B-O1X	3.12	1.61	1.51
3	C	2003	NAP	P2B-O1X	3.14	1.61	1.51
3	E	2005	NAP	P2B-O1X	3.15	1.61	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2004	NAP	N3A-C2A-N1A	-10.22	121.07	128.89
3	E	2005	NAP	N3A-C2A-N1A	-10.17	121.11	128.89
3	F	2006	NAP	N3A-C2A-N1A	-10.15	121.12	128.89
3	B	2002	NAP	N3A-C2A-N1A	-10.13	121.14	128.89
3	A	2001	NAP	N3A-C2A-N1A	-10.08	121.17	128.89
3	C	2003	NAP	N3A-C2A-N1A	-10.05	121.20	128.89
3	F	2006	NAP	C4D-O4D-C1D	-7.08	101.94	109.72
3	B	2002	NAP	C4D-O4D-C1D	-6.98	102.05	109.72
3	A	2001	NAP	C4B-O4B-C1B	-6.91	102.12	109.72
3	C	2003	NAP	C4D-O4D-C1D	-6.85	102.19	109.72
3	D	2004	NAP	C4D-O4D-C1D	-6.69	102.36	109.72
3	E	2005	NAP	C4D-O4D-C1D	-6.44	102.64	109.72
3	A	2001	NAP	C4D-O4D-C1D	-6.35	102.75	109.72
3	D	2004	NAP	C4B-O4B-C1B	-4.58	104.69	109.72
3	F	2006	NAP	C4B-O4B-C1B	-4.45	104.83	109.72
3	B	2002	NAP	C4B-O4B-C1B	-4.39	104.89	109.72
3	E	2005	NAP	C4B-O4B-C1B	-4.35	104.94	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	NAP	C4B-O4B-C1B	-3.78	105.57	109.72
3	F	2006	NAP	PN-O3-PA	-3.18	123.79	132.73
2	A	1004	MA5	C1-O1-C40	-3.12	109.86	118.01
3	B	2002	NAP	PN-O3-PA	-3.03	124.21	132.73
3	A	2001	NAP	PN-O3-PA	-2.99	124.34	132.73
2	F	1005	MA5	C1-O1-C40	-2.82	110.63	118.01
3	D	2004	NAP	PN-O3-PA	-2.82	124.81	132.73
2	C	1006	MA5	C1-O1-C40	-2.82	110.65	118.01
3	E	2005	NAP	PN-O3-PA	-2.76	124.99	132.73
3	C	2003	NAP	PN-O3-PA	-2.68	125.21	132.73
2	C	1003	MA5	C30-C40-C50	-2.45	105.29	110.84
3	B	2002	NAP	C3N-C7N-N7N	-2.34	115.26	117.82
2	D	1001	MA5	C11-O10-C10	-2.34	109.86	113.94
3	A	2001	NAP	O4B-C4B-C3B	-2.31	100.48	105.15
3	F	2006	NAP	C3N-C7N-N7N	-2.27	115.33	117.82
3	C	2003	NAP	C4A-C5A-N7A	-2.22	107.43	109.48
3	D	2004	NAP	O4B-C4B-C3B	-2.18	100.76	105.15
3	F	2006	NAP	O4B-C4B-C3B	-2.16	100.79	105.15
3	B	2002	NAP	O4B-C4B-C3B	-2.16	100.79	105.15
3	D	2004	NAP	C3N-C7N-N7N	-2.12	115.50	117.82
3	A	2001	NAP	C3N-C7N-N7N	-2.12	115.50	117.82
3	E	2005	NAP	O4B-C4B-C3B	-2.10	100.91	105.15
3	C	2003	NAP	C3N-C7N-N7N	-2.10	115.52	117.82
3	D	2004	NAP	C4A-C5A-N7A	-2.09	107.55	109.48
3	E	2005	NAP	C3N-C7N-N7N	-2.07	115.55	117.82
2	B	1002	MA5	C11-O10-C10	-2.05	110.36	113.94
3	B	2002	NAP	C4A-C5A-N7A	-2.03	107.61	109.48
3	E	2005	NAP	C4A-C5A-N7A	-2.01	107.63	109.48
3	F	2006	NAP	C4A-C5A-N7A	-2.00	107.64	109.48
2	A	1004	MA5	O10-C10-C20	2.10	110.69	108.04
3	D	2004	NAP	O4B-C1B-N9A	2.13	112.56	108.10
2	C	1003	MA5	O1-C40-C50	2.27	115.30	109.32
2	B	1002	MA5	O1-C40-C30	2.29	113.07	107.17
2	C	1006	MA5	O10-C10-C20	2.30	110.95	108.04
3	A	2001	NAP	O4B-C1B-N9A	2.30	112.92	108.10
2	B	1007	MA5	O1-C40-C30	2.36	113.25	107.17
2	D	1001	MA5	O1-C40-C30	2.54	113.72	107.17
2	C	1003	MA5	O10-C10-C20	2.87	111.67	108.04
4	B	3001	EPE	O2S-S-C10	3.26	109.68	106.91
4	F	3002	EPE	O2S-S-C10	3.29	109.71	106.91
2	F	1008	MA5	O10-C10-C20	3.31	112.22	108.04
4	F	3002	EPE	O1S-S-C10	3.42	109.83	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1008	MA5	O1-C40-C30	3.52	116.24	107.17
4	B	3001	EPE	O1S-S-C10	3.65	110.02	106.91
3	A	2001	NAP	O4D-C1D-N1N	3.72	112.22	108.13
2	F	1005	MA5	O10-C10-C20	3.81	112.86	108.04
3	C	2003	NAP	O4D-C1D-N1N	4.08	112.61	108.13
2	C	1003	MA5	O1-C40-C30	4.08	117.71	107.17
3	E	2005	NAP	O4D-C1D-N1N	4.27	112.82	108.13
3	D	2004	NAP	O4D-C1D-N1N	4.47	113.04	108.13
3	F	2006	NAP	O4D-C1D-N1N	4.47	113.05	108.13
3	B	2002	NAP	O4D-C1D-N1N	4.55	113.13	108.13

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1005	MA5	C11-O10-C10-O50

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3001	EPE	C2-C3-C5-C6-N1-N4
4	F	3002	EPE	C2-C3-C5-C6-N1-N4

15 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1004	MA5	5	0
3	A	2001	NAP	13	0
2	B	1002	MA5	2	0
2	B	1007	MA5	4	0
3	B	2002	NAP	7	0
4	B	3001	EPE	4	0
2	C	1003	MA5	4	0
2	C	1006	MA5	8	0
3	C	2003	NAP	8	0
2	D	1001	MA5	4	0
3	D	2004	NAP	8	0
3	E	2005	NAP	6	0
2	F	1005	MA5	3	0
3	F	2006	NAP	6	0
4	F	3002	EPE	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	214/219 (97%)	0.25	14 (6%)	22 20	39, 51, 76, 103	9 (4%)
1	B	214/219 (97%)	0.31	15 (7%)	19 17	39, 54, 77, 101	13 (6%)
1	C	214/219 (97%)	0.20	13 (6%)	25 23	37, 50, 73, 98	8 (3%)
1	D	214/219 (97%)	0.22	15 (7%)	19 17	36, 48, 72, 93	8 (3%)
1	E	214/219 (97%)	0.24	11 (5%)	32 30	36, 49, 74, 88	9 (4%)
1	F	214/219 (97%)	0.29	16 (7%)	17 15	38, 52, 76, 101	9 (4%)
All	All	1284/1314 (97%)	0.25	84 (6%)	22 20	36, 51, 75, 103	56 (4%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	70	ILE	7.1
1	A	6	GLU	6.8
1	E	73	ASP	6.4
1	F	69	LYS	6.1
1	B	6	GLU	5.7
1	A	71	LYS	5.6
1	D	73	ASP	5.5
1	C	6	GLU	5.3
1	B	72	SER	5.1
1	F	73	ASP	5.1
1	A	73	ASP	5.0
1	B	70	ILE	5.0
1	C	71	LYS	4.7
1	B	69	LYS	4.7
1	B	73	ASP	4.6
1	F	71	LYS	4.5
1	C	72	SER	4.4
1	F	72	SER	4.3
1	C	73	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	6	GLU	4.2
1	F	74	ARG	4.0
1	D	72	SER	4.0
1	B	71	LYS	3.7
1	F	31	ARG	3.5
1	A	70	ILE	3.3
1	B	144	TYR	3.3
1	D	21	GLY	3.2
1	A	68	HIS	3.1
1	B	68	HIS	3.1
1	E	72	SER	3.1
1	A	69	LYS	3.0
1	F	68	HIS	3.0
1	F	189	TYR	2.9
1	D	74	ARG	2.9
1	E	74	ARG	2.9
1	D	34	CYS	2.9
1	D	153	LEU	2.8
1	B	224	LYS	2.8
1	A	72	SER	2.8
1	A	15	VAL	2.8
1	D	69	LYS	2.8
1	C	70	ILE	2.7
1	B	149	LYS	2.7
1	D	15	VAL	2.7
1	D	189	TYR	2.6
1	C	224	LYS	2.6
1	A	199	ASP	2.6
1	C	199	ASP	2.6
1	E	70	ILE	2.6
1	D	71	LYS	2.6
1	C	27	ASN	2.6
1	E	69	LYS	2.5
1	F	110	GLU	2.5
1	B	47	ASN	2.4
1	C	18	THR	2.4
1	F	149	LYS	2.4
1	A	35	GLU	2.3
1	B	74	ARG	2.3
1	B	213	GLY	2.3
1	F	207	LYS	2.3
1	D	176	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	14	ASN	2.3
1	B	31	ARG	2.2
1	C	7	LYS	2.2
1	D	110	GLU	2.2
1	D	174	VAL	2.2
1	E	7	LYS	2.2
1	A	141	ASP	2.2
1	B	145	ASP	2.2
1	E	13	SER	2.2
1	A	208	ASN	2.2
1	C	21	GLY	2.2
1	A	31	ARG	2.2
1	E	153	LEU	2.2
1	C	69	LYS	2.2
1	F	21	GLY	2.1
1	E	15	VAL	2.1
1	C	20	ASP	2.1
1	F	15	VAL	2.1
1	E	21	GLY	2.1
1	D	13	SER	2.1
1	E	176	ILE	2.1
1	F	224	LYS	2.0
1	A	74	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MA5	B	1002	31/31	0.53	0.46	8.00	105,107,108,108	13
4	EPE	F	3002	12/15	0.35	0.44	6.45	104,107,117,118	0
2	MA5	D	1001	31/31	0.42	0.59	6.28	103,118,120,121	15
2	MA5	F	1008	31/31	0.55	0.43	6.06	71,91,95,95	7
2	MA5	F	1005	31/31	0.43	0.41	5.17	107,109,110,111	15
2	MA5	C	1003	31/31	0.73	0.36	4.73	68,77,81,83	0
2	MA5	B	1007	31/31	0.56	0.45	4.24	113,123,124,124	12
4	EPE	B	3001	12/15	0.78	0.38	3.23	104,104,105,105	0
2	MA5	C	1006	31/31	0.76	0.31	1.75	99,104,107,107	0
3	NAP	A	2001	48/48	0.81	0.29	1.45	79,88,103,103	0
3	NAP	F	2006	48/48	0.89	0.25	0.91	72,79,104,105	0
3	NAP	D	2004	48/48	0.85	0.27	0.84	67,80,96,97	0
3	NAP	C	2003	48/48	0.88	0.23	0.83	56,64,87,88	0
3	NAP	B	2002	48/48	0.86	0.24	0.68	72,77,104,104	0
3	NAP	E	2005	48/48	0.91	0.22	0.37	58,67,101,102	0
2	MA5	A	1004	31/31	0.63	0.46	-	115,118,122,122	15

6.5 Other polymers ⓘ

There are no such residues in this entry.