



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:06 PM GMT

PDB ID : 3SXN
Title : Mycobacterium tuberculosis Eis protein initiates modulation of host immune responses by acetylation of DUSP16/MKP-7
Authors : Kim, K.H.; An, D.R.; Yoon, J.Y.; Kim, H.S.; Yoon, H.J.; Song, J.S.; Im, H.N.; Kim, J.; Kim, D.J.; Lee, S.J.; Kim, H.J.; Lee, J.Y.; Suh, S.W.
Deposited on : 2011-07-15
Resolution : 2.03 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:

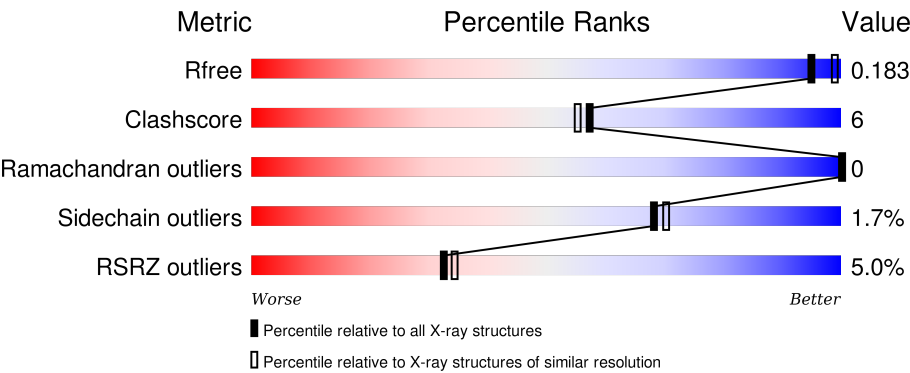
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div><div>4%</div><div>86%9%5%</div></div>
1	B	422	<div><div>4%</div><div>82%13%5%</div></div>
1	C	422	<div><div>5%</div><div>84%11%5%</div></div>
1	D	422	<div><div>4%</div><div>87%8%5%</div></div>
1	E	422	<div><div>6%</div><div>83%12%5%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	422	 6% 83% 11% • 5%

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	COA	F	500	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20893 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 Enhanced intracellular survival protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			
1	B	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			
1	C	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			
1	D	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			
1	E	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			
1	F	402	Total	C	N	O	S	0	0	0
			3100	1946	568	578	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP A0QY29
A	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
A	-17	SER	-	EXPRESSION TAG	UNP A0QY29
A	-16	SER	-	EXPRESSION TAG	UNP A0QY29
A	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
A	-9	SER	-	EXPRESSION TAG	UNP A0QY29
A	-8	SER	-	EXPRESSION TAG	UNP A0QY29
A	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
A	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
A	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
A	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
A	-3	ARG	-	EXPRESSION TAG	UNP A0QY29

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
A	-1	SER	-	EXPRESSION TAG	UNP A0QY29
A	0	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-19	MET	-	EXPRESSION TAG	UNP A0QY29
B	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
B	-17	SER	-	EXPRESSION TAG	UNP A0QY29
B	-16	SER	-	EXPRESSION TAG	UNP A0QY29
B	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
B	-9	SER	-	EXPRESSION TAG	UNP A0QY29
B	-8	SER	-	EXPRESSION TAG	UNP A0QY29
B	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
B	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
B	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
B	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
B	-3	ARG	-	EXPRESSION TAG	UNP A0QY29
B	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
B	-1	SER	-	EXPRESSION TAG	UNP A0QY29
B	0	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-19	MET	-	EXPRESSION TAG	UNP A0QY29
C	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
C	-17	SER	-	EXPRESSION TAG	UNP A0QY29
C	-16	SER	-	EXPRESSION TAG	UNP A0QY29
C	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
C	-9	SER	-	EXPRESSION TAG	UNP A0QY29
C	-8	SER	-	EXPRESSION TAG	UNP A0QY29
C	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
C	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
C	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
C	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
C	-3	ARG	-	EXPRESSION TAG	UNP A0QY29
C	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
C	-1	SER	-	EXPRESSION TAG	UNP A0QY29

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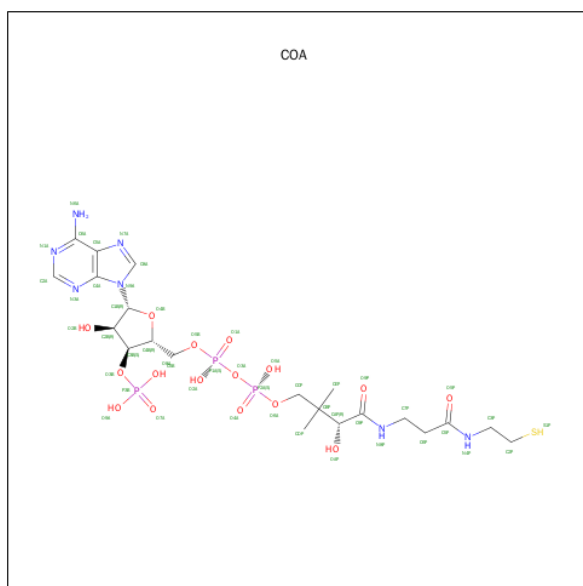
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-19	MET	-	EXPRESSION TAG	UNP A0QY29
D	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
D	-17	SER	-	EXPRESSION TAG	UNP A0QY29
D	-16	SER	-	EXPRESSION TAG	UNP A0QY29
D	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
D	-9	SER	-	EXPRESSION TAG	UNP A0QY29
D	-8	SER	-	EXPRESSION TAG	UNP A0QY29
D	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
D	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
D	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
D	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
D	-3	ARG	-	EXPRESSION TAG	UNP A0QY29
D	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
D	-1	SER	-	EXPRESSION TAG	UNP A0QY29
D	0	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-19	MET	-	EXPRESSION TAG	UNP A0QY29
E	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
E	-17	SER	-	EXPRESSION TAG	UNP A0QY29
E	-16	SER	-	EXPRESSION TAG	UNP A0QY29
E	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
E	-9	SER	-	EXPRESSION TAG	UNP A0QY29
E	-8	SER	-	EXPRESSION TAG	UNP A0QY29
E	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
E	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
E	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
E	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
E	-3	ARG	-	EXPRESSION TAG	UNP A0QY29
E	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
E	-1	SER	-	EXPRESSION TAG	UNP A0QY29
E	0	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-19	MET	-	EXPRESSION TAG	UNP A0QY29

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP A0QY29
F	-17	SER	-	EXPRESSION TAG	UNP A0QY29
F	-16	SER	-	EXPRESSION TAG	UNP A0QY29
F	-15	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-14	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-13	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-12	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-11	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-10	HIS	-	EXPRESSION TAG	UNP A0QY29
F	-9	SER	-	EXPRESSION TAG	UNP A0QY29
F	-8	SER	-	EXPRESSION TAG	UNP A0QY29
F	-7	GLY	-	EXPRESSION TAG	UNP A0QY29
F	-6	LEU	-	EXPRESSION TAG	UNP A0QY29
F	-5	VAL	-	EXPRESSION TAG	UNP A0QY29
F	-4	PRO	-	EXPRESSION TAG	UNP A0QY29
F	-3	ARG	-	EXPRESSION TAG	UNP A0QY29
F	-2	GLY	-	EXPRESSION TAG	UNP A0QY29
F	-1	SER	-	EXPRESSION TAG	UNP A0QY29
F	0	HIS	-	EXPRESSION TAG	UNP A0QY29

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	E	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

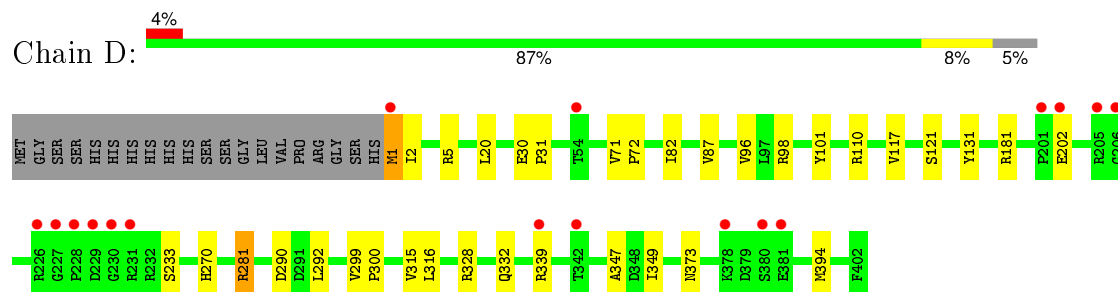
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	396	Total 396	O 396	0	0
3	B	394	Total 394	O 394	0	0
3	C	349	Total 349	O 349	0	0
3	D	361	Total 361	O 361	0	0
3	E	234	Total 234	O 234	0	0
3	F	271	Total 271	O 271	0	0

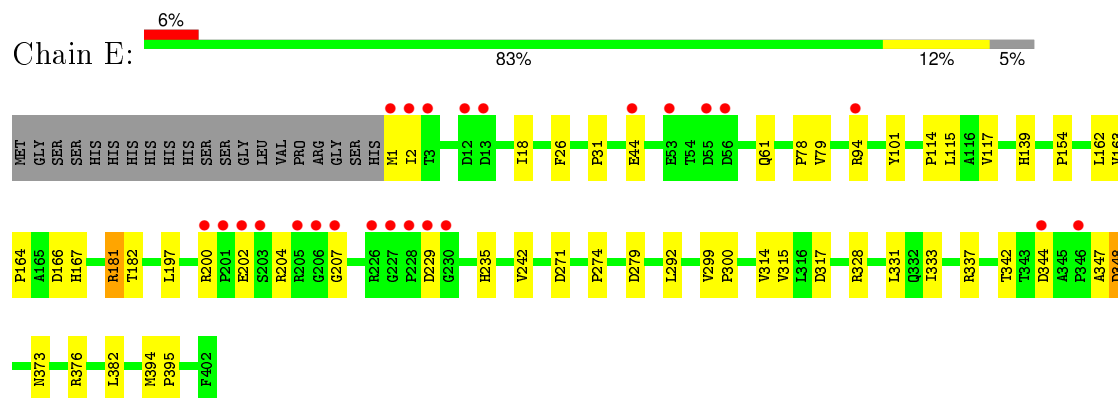
- Molecule 1: Enhanced intracellular survival protein



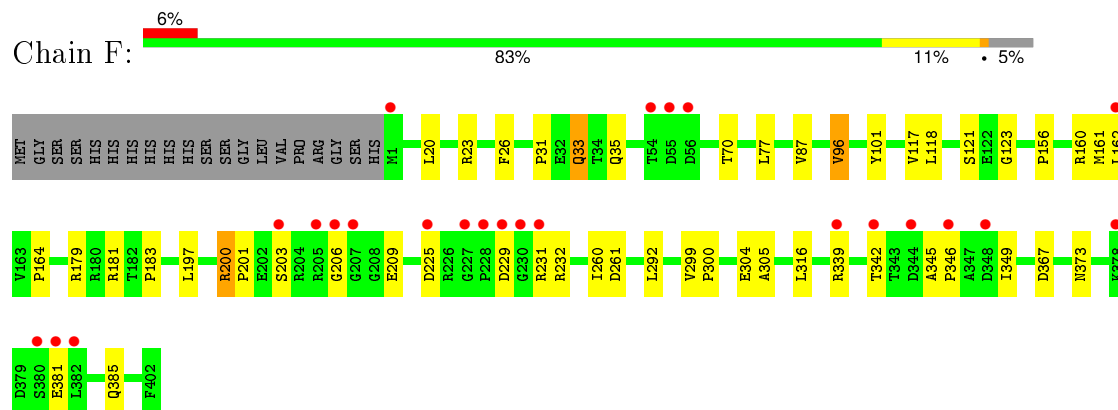
- Molecule 1: Enhanced intracellular survival protein



- Molecule 1: Enhanced intracellular survival protein



- Molecule 1: Enhanced intracellular survival protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.74Å 126.52Å 238.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.03 29.85 – 2.02	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.03) 92.0 (29.85-2.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.181 , 0.217 0.182 , 0.183	Depositor DCC
R_{free} test set	20113 reflections (11.52%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 203766 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20893	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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: COA

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	0.48	0/3172	0.63	3/4321 (0.1%)
1	B	0.46	0/3172	0.62	4/4321 (0.1%)
1	C	0.36	0/3172	0.55	0/4321
1	D	0.39	0/3172	0.56	1/4321 (0.0%)
1	E	0.34	0/3172	0.54	0/4321
1	F	0.34	0/3172	0.55	0/4321
All	All	0.40	0/19032	0.57	8/25926 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	374	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	374	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	B	323	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	323	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	323	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	281	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	291	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3100	0	3020	35	0
1	B	3100	0	3020	41	0
1	C	3100	0	3020	38	0
1	D	3100	0	3020	43	0
1	E	3100	0	3020	35	0
1	F	3100	0	3020	36	0
2	A	48	0	32	4	0
2	B	48	0	31	0	0
2	C	48	0	32	4	0
2	D	48	0	31	4	0
2	E	48	0	32	1	0
2	F	48	0	32	6	0
3	A	396	0	0	6	0
3	B	394	0	0	8	0
3	C	349	0	0	6	0
3	D	361	0	0	8	0
3	E	234	0	0	2	0
3	F	271	0	0	4	0
All	All	20893	0	18310	222	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 6.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH11	1:A:231:ARG:CG	1.68	1.06
1:A:231:ARG:NH1	1:A:231:ARG:HG3	1.56	1.03
1:E:1:MET:CB	1:E:2:ILE:HA	1.92	0.99
1:E:1:MET:HB3	1:E:2:ILE:CA	1.92	0.97
1:E:1:MET:HB3	1:E:2:ILE:HA	1.00	0.97
1:C:290:ASP:OD1	1:D:281:ARG:HD2	1.68	0.93
1:C:281:ARG:HD2	1:D:290:ASP:OD1	1.73	0.88
1:D:110:ARG:HD3	3:D:852:HOH:O	1.73	0.87
1:A:231:ARG:HH11	1:A:231:ARG:HG3	0.75	0.84
1:C:33:GLN:HE21	1:C:33:GLN:H	1.30	0.79
2:C:500:COA:H2A	2:C:500:COA:H122	1.64	0.78
1:D:1:MET:H3	1:D:2:ILE:HA	1.50	0.76
1:B:1:MET:HG3	3:B:984:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA2	1:A:225:ASP:HB3	1.72	0.72
1:A:33:GLN:OE1	1:A:200:ARG:NH2	2.23	0.72
1:D:87:VAL:HG21	1:D:96:VAL:HG23	1.70	0.72
1:F:206:GLY:O	1:F:225:ASP:HB2	1.90	0.71
2:C:500:COA:H2A	2:C:500:COA:CCP	2.22	0.70
1:C:344:ASP:HB2	3:C:625:HOH:O	1.92	0.69
1:D:96:VAL:HG22	3:D:809:HOH:O	1.93	0.68
1:B:350:GLU:HB2	1:B:376:ARG:HG2	1.75	0.67
1:C:28:ASP:CG	1:C:29:ILE:H	1.98	0.66
1:A:374:ARG:HD2	3:A:961:HOH:O	1.94	0.66
1:A:110:ARG:NH1	3:A:864:HOH:O	2.28	0.65
1:D:87:VAL:CG2	1:D:96:VAL:HG23	2.26	0.65
1:C:307:ARG:NH2	1:C:337:ARG:HH22	1.94	0.65
1:E:204:ARG:HG2	1:E:207:GLY:HA2	1.80	0.64
1:C:290:ASP:OD1	1:D:281:ARG:CD	2.44	0.64
1:B:309:GLN:NE2	3:B:880:HOH:O	2.31	0.64
1:A:121:SER:HB3	2:A:500:COA:H21	1.79	0.64
1:E:79:VAL:HG12	1:E:115:LEU:HB2	1.81	0.63
1:B:202:GLU:CD	1:B:202:GLU:H	2.02	0.63
1:A:117:VAL:HB	1:A:292:LEU:HD11	1.82	0.62
1:B:207:GLY:O	1:B:223:ARG:HB3	1.99	0.62
1:A:366:VAL:HG13	1:A:375:LEU:HD23	1.83	0.61
1:A:328:ARG:NH1	1:A:346:PRO:HA	2.16	0.61
1:C:307:ARG:NH2	1:C:337:ARG:NH2	2.50	0.60
1:E:44:GLU:CD	1:E:44:GLU:H	2.03	0.59
1:C:209:GLU:HB2	1:F:23:ARG:NH2	2.18	0.59
1:A:53:GLU:CD	1:A:53:GLU:H	2.06	0.59
1:B:311:ASP:OD1	1:B:334:SER:HA	2.03	0.59
1:A:200:ARG:HG2	1:A:202:GLU:OE2	2.03	0.58
1:F:209:GLU:HG2	3:F:850:HOH:O	2.02	0.58
1:E:181:ARG:CZ	1:E:242:VAL:O	2.52	0.58
1:A:32:GLU:HG2	3:A:743:HOH:O	2.03	0.58
1:B:156:PRO:HG2	1:B:249:ALA:HB2	1.84	0.58
1:D:87:VAL:CG1	1:D:96:VAL:HG21	2.35	0.57
1:C:228:PRO:HA	1:C:229:ASP:OD1	2.04	0.57
1:C:204:ARG:O	1:C:205:ARG:HB2	2.04	0.57
1:D:1:MET:N	1:D:2:ILE:HA	2.14	0.57
1:F:181:ARG:HB3	1:F:181:ARG:NH1	2.20	0.56
1:F:87:VAL:HG23	2:F:500:COA:H132	1.88	0.56
1:B:164:PRO:HG3	1:B:212:ALA:HB2	1.87	0.56
1:D:121:SER:HB3	2:D:500:COA:H21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:CB	1:D:2:ILE:HA	2.35	0.56
1:F:121:SER:CB	2:F:500:COA:H21	2.36	0.55
1:E:164:PRO:HB2	1:E:197:LEU:HD22	1.89	0.55
1:A:231:ARG:NH1	1:A:231:ARG:CG	2.40	0.55
1:E:163:VAL:HG13	1:E:166:ASP:HB2	1.89	0.55
2:D:500:COA:O5P	2:D:500:COA:H141	2.07	0.55
1:C:207:GLY:HA2	1:C:225:ASP:HB3	1.89	0.54
1:F:121:SER:HB3	2:F:500:COA:H21	1.88	0.54
1:F:121:SER:OG	2:F:500:COA:H21	2.07	0.54
1:E:299:VAL:HB	1:E:300:PRO:HD3	1.88	0.54
1:D:87:VAL:HG13	1:D:96:VAL:HG21	1.88	0.54
1:C:33:GLN:NE2	1:C:33:GLN:H	2.05	0.53
1:B:339:ARG:HG3	1:B:339:ARG:HH11	1.73	0.53
1:F:304:GLU:OE1	1:F:339:ARG:HD2	2.08	0.53
1:A:374:ARG:HD3	1:B:150:HIS:CE1	2.44	0.53
1:E:181:ARG:NH2	1:E:242:VAL:O	2.42	0.52
1:B:339:ARG:CG	1:B:339:ARG:HH11	2.21	0.52
1:E:139:HIS:HB2	3:E:820:HOH:O	2.08	0.52
1:C:228:PRO:HA	1:C:229:ASP:CG	2.29	0.52
1:B:333:ILE:HG12	1:B:338:ALA:HB2	1.92	0.52
1:F:96:VAL:HG13	3:F:772:HOH:O	2.09	0.52
1:F:26:PHE:CZ	2:F:500:COA:O5P	2.62	0.52
1:B:33:GLN:OE1	1:B:200:ARG:NH2	2.43	0.52
1:F:345:ALA:HB1	1:F:346:PRO:HD2	1.91	0.52
1:D:315:VAL:HB	1:D:347:ALA:HA	1.93	0.51
1:F:118:LEU:HD12	1:F:118:LEU:C	2.31	0.51
1:E:26:PHE:CZ	2:E:500:COA:O5P	2.64	0.51
2:C:500:COA:H61	3:C:689:HOH:O	2.08	0.51
1:A:33:GLN:CD	1:A:200:ARG:HH22	2.13	0.51
1:F:20:LEU:C	1:F:20:LEU:HD23	2.30	0.51
1:C:110:ARG:HD3	3:C:925:HOH:O	2.10	0.51
1:F:381:GLU:O	1:F:385:GLN:HG3	2.11	0.50
1:A:168:ARG:HH22	1:A:190:ASP:CG	2.13	0.50
1:D:1:MET:HB2	1:D:2:ILE:CA	2.41	0.50
1:B:33:GLN:OE1	1:B:200:ARG:NE	2.43	0.50
1:E:315:VAL:H	1:E:348:ASP:HB2	1.77	0.50
1:D:1:MET:HB2	1:D:2:ILE:HA	1.93	0.50
1:A:121:SER:CB	2:A:500:COA:H21	2.41	0.50
1:D:181:ARG:O	1:D:394:MET:SD	2.69	0.50
1:F:299:VAL:HB	1:F:300:PRO:HD3	1.94	0.50
1:D:31:PRO:HB3	1:D:202:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD22	1:E:167:HIS:CE1	2.46	0.49
1:F:33:GLN:H	1:F:33:GLN:NE2	2.11	0.49
1:F:161:MET:O	1:F:162:LEU:HD23	2.12	0.49
1:D:82:ILE:HD11	1:D:131:TYR:OH	2.12	0.49
1:F:231:ARG:HB3	1:F:261:ASP:OD2	2.13	0.49
1:D:316:LEU:O	1:D:328:ARG:HA	2.13	0.49
1:C:315:VAL:HB	1:C:347:ALA:HA	1.95	0.48
1:F:77:LEU:HD21	1:F:305:ALA:HB1	1.94	0.48
1:F:31:PRO:O	1:F:35:GLN:HG3	2.14	0.48
1:B:44:GLU:CD	1:B:44:GLU:H	2.17	0.48
1:C:316:LEU:O	1:C:328:ARG:HA	2.14	0.48
1:B:348:ASP:HB3	1:B:382:LEU:HD23	1.96	0.48
1:B:51:PRO:HD2	3:B:950:HOH:O	2.13	0.47
1:A:20:LEU:HD23	1:A:20:LEU:C	2.34	0.47
1:A:384:GLN:HA	3:A:735:HOH:O	2.13	0.47
1:D:82:ILE:HD12	1:D:117:VAL:O	2.15	0.47
1:B:206:GLY:O	1:B:225:ASP:HB2	2.14	0.47
1:B:373:ASN:HB2	3:B:815:HOH:O	2.14	0.47
1:C:154:PRO:C	1:C:156:PRO:HD3	2.34	0.47
1:E:279:ASP:OD1	1:F:123:GLY:HA3	2.14	0.47
1:D:299:VAL:HB	1:D:300:PRO:HD3	1.96	0.47
2:A:500:COA:H61	3:A:685:HOH:O	2.14	0.47
1:B:200:ARG:HH11	1:B:200:ARG:HG2	1.78	0.47
1:A:26:PHE:CZ	2:A:500:COA:O5P	2.68	0.47
1:E:317:ASP:HB2	1:E:347:ALA:CB	2.44	0.47
1:D:98:ARG:NH1	2:D:500:COA:O9A	2.40	0.46
1:B:181:ARG:CZ	1:B:242:VAL:O	2.63	0.46
1:C:18:ILE:HA	1:C:61:GLN:OE1	2.16	0.46
1:B:200:ARG:NH1	1:B:200:ARG:HG2	2.30	0.46
1:C:56:ASP:HA	3:C:943:HOH:O	2.15	0.46
1:D:121:SER:CB	2:D:500:COA:H21	2.46	0.46
1:D:30:GLU:HB3	1:D:31:PRO:HD2	1.98	0.46
1:B:232:ARG:HB3	1:B:260:ILE:HD13	1.97	0.46
1:A:350:GLU:HB2	1:A:376:ARG:HB2	1.98	0.46
1:E:200:ARG:HB3	1:E:202:GLU:OE1	2.15	0.46
1:E:18:ILE:HA	1:E:61:GLN:OE1	2.16	0.45
1:E:31:PRO:HG3	1:E:202:GLU:HB2	1.98	0.45
1:C:155:ASP:N	1:C:156:PRO:HD3	2.32	0.45
1:E:78:PRO:O	1:E:114:PRO:HD2	2.16	0.45
1:E:235:HIS:HE1	3:E:802:HOH:O	1.98	0.45
1:B:17:ARG:HD3	1:B:56:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:CD	3:A:961:HOH:O	2.60	0.45
1:C:128:ARG:CZ	2:C:500:COA:H1B	2.47	0.45
1:B:339:ARG:NH1	1:B:341:THR:HG21	2.32	0.45
1:F:232:ARG:HB3	1:F:260:ILE:HD13	1.99	0.45
1:E:182:THR:HG23	1:E:394:MET:SD	2.57	0.45
1:D:394:MET:CE	3:D:655:HOH:O	2.64	0.44
1:C:270:HIS:HD2	3:C:853:HOH:O	2.00	0.44
1:A:231:ARG:NH1	1:A:261:ASP:OD2	2.50	0.44
1:A:379:ASP:OD1	1:A:381:GLU:HB2	2.17	0.44
1:C:17:ARG:CZ	1:C:56:ASP:O	2.66	0.44
1:E:182:THR:HA	1:E:394:MET:SD	2.58	0.44
1:B:164:PRO:HD2	3:B:640:HOH:O	2.17	0.44
1:B:188:ARG:HD3	1:B:193:TRP:CE2	2.52	0.44
1:F:200:ARG:HA	1:F:201:PRO:HD3	1.90	0.44
1:C:142:VAL:HG21	1:C:273:LEU:HD21	2.00	0.44
1:D:20:LEU:HD23	1:D:20:LEU:C	2.38	0.44
1:C:117:VAL:HB	1:C:292:LEU:HD11	1.99	0.44
1:D:332:GLN:CD	1:D:339:ARG:NH1	2.70	0.44
1:C:28:ASP:CG	1:C:29:ILE:N	2.68	0.44
1:C:209:GLU:HB2	1:F:23:ARG:HH21	1.80	0.44
1:C:377:SER:HB3	1:C:383:LEU:HG	1.99	0.43
1:D:181:ARG:CZ	3:D:856:HOH:O	2.66	0.43
1:A:18:ILE:HA	1:A:61:GLN:OE1	2.17	0.43
1:F:87:VAL:HG13	1:F:96:VAL:HG21	2.01	0.43
1:D:5:ARG:HD3	3:D:953:HOH:O	2.18	0.43
1:F:20:LEU:O	1:F:20:LEU:HD23	2.19	0.43
1:D:117:VAL:HB	1:D:292:LEU:HD11	2.00	0.43
1:E:271:ASP:O	1:E:274:PRO:HD2	2.19	0.43
1:F:203:SER:HB3	3:F:695:HOH:O	2.18	0.43
1:A:231:ARG:HA	1:A:231:ARG:HD2	1.72	0.43
1:E:117:VAL:HB	1:E:292:LEU:HD11	1.99	0.43
1:F:70:THR:O	1:F:183:PRO:HA	2.18	0.43
1:B:20:LEU:HD23	1:B:20:LEU:C	2.38	0.43
1:E:328:ARG:HH21	1:E:344:ASP:HB2	1.83	0.43
2:F:500:COA:H61	3:F:654:HOH:O	2.19	0.43
1:E:314:VAL:HG12	1:E:382:LEU:HD21	2.00	0.43
1:A:150:HIS:NE2	1:B:374:ARG:HD3	2.33	0.42
1:C:309:GLN:HG2	3:C:850:HOH:O	2.19	0.42
1:F:164:PRO:HB2	1:F:197:LEU:CD2	2.49	0.42
1:A:44:GLU:H	1:A:44:GLU:CD	2.22	0.42
1:D:181:ARG:NH2	3:D:856:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HD3	1:B:260:ILE:O	2.19	0.42
1:D:87:VAL:HG11	1:D:96:VAL:CG2	2.50	0.42
1:F:316:LEU:HD12	1:F:349:ILE:HB	2.01	0.42
1:C:299:VAL:HB	1:C:300:PRO:HD3	2.00	0.42
1:D:316:LEU:HD23	1:D:349:ILE:HB	2.02	0.42
1:B:78:PRO:O	1:B:114:PRO:HD2	2.20	0.42
1:C:212:ALA:HA	1:C:220:ALA:O	2.20	0.42
1:B:18:ILE:HA	1:B:61:GLN:OE1	2.20	0.42
1:F:181:ARG:CZ	1:F:181:ARG:HB3	2.49	0.42
1:C:365:ARG:HD3	1:D:270:HIS:CG	2.55	0.42
1:D:71:VAL:HB	1:D:72:PRO:CD	2.50	0.42
1:A:172:ALA:HA	1:A:193:TRP:CZ2	2.55	0.42
1:B:44:GLU:HG3	3:B:949:HOH:O	2.20	0.41
1:A:20:LEU:HD23	1:A:20:LEU:O	2.19	0.41
1:B:181:ARG:NH2	3:B:779:HOH:O	2.53	0.41
1:E:394:MET:HG2	1:E:395:PRO:HD2	2.02	0.41
1:D:332:GLN:CD	1:D:339:ARG:HH11	2.23	0.41
1:E:44:GLU:CD	1:E:44:GLU:N	2.71	0.41
1:D:82:ILE:HD12	1:D:82:ILE:H	1.85	0.41
1:D:87:VAL:CG1	1:D:96:VAL:CG2	2.98	0.41
1:D:394:MET:HE3	3:D:655:HOH:O	2.20	0.41
1:B:178:TRP:CH2	1:B:399:GLY:HA2	2.55	0.41
1:D:181:ARG:O	1:D:394:MET:CE	2.68	0.41
1:C:54:THR:O	1:C:54:THR:HG22	2.21	0.41
1:F:229:ASP:OD1	1:F:229:ASP:N	2.53	0.41
1:A:33:GLN:CD	1:A:200:ARG:NH2	2.73	0.41
1:D:87:VAL:CG2	1:D:96:VAL:CG2	2.98	0.41
1:C:204:ARG:O	1:C:205:ARG:CB	2.67	0.41
1:E:317:ASP:HB2	1:E:347:ALA:HB2	2.03	0.41
1:E:154:PRO:HG3	1:F:373:ASN:ND2	2.36	0.41
1:D:373:ASN:ND2	3:D:799:HOH:O	2.54	0.41
1:F:117:VAL:HB	1:F:292:LEU:HD11	2.02	0.41
1:B:79:VAL:HG12	1:B:115:LEU:HB2	2.02	0.41
1:A:226:ARG:NH1	1:C:205:ARG:HH12	2.18	0.41
1:B:339:ARG:NH1	1:B:339:ARG:CG	2.81	0.41
1:A:205:ARG:HG3	1:A:205:ARG:O	2.20	0.41
1:B:1:MET:HG2	1:B:2:ILE:N	2.36	0.40
1:E:242:VAL:HG23	1:E:242:VAL:O	2.20	0.40
1:B:330:ALA:O	1:B:340:CYS:HA	2.21	0.40
1:C:189:PRO:HD2	1:C:192:LEU:HD12	2.02	0.40
1:C:211:PHE:CE1	1:F:23:ARG:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB3	1:B:383:LEU:HG	2.03	0.40
1:E:333:ILE:HA	1:E:337:ARG:O	2.21	0.40
1:B:362:GLY:HA2	3:B:861:HOH:O	2.21	0.40
1:E:373:ASN:ND2	1:E:376:ARG:HG2	2.35	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	400/422 (95%)	393 (98%)	7 (2%)	0	100	100
1	B	400/422 (95%)	396 (99%)	4 (1%)	0	100	100
1	C	400/422 (95%)	393 (98%)	7 (2%)	0	100	100
1	D	400/422 (95%)	396 (99%)	4 (1%)	0	100	100
1	E	400/422 (95%)	390 (98%)	10 (2%)	0	100	100
1	F	400/422 (95%)	395 (99%)	5 (1%)	0	100	100
All	All	2400/2532 (95%)	2363 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	311/328 (95%)	306 (98%)	5 (2%)	70	72
1	B	311/328 (95%)	307 (99%)	4 (1%)	76	78
1	C	311/328 (95%)	307 (99%)	4 (1%)	76	78
1	D	311/328 (95%)	308 (99%)	3 (1%)	82	85
1	E	311/328 (95%)	304 (98%)	7 (2%)	58	58
1	F	311/328 (95%)	302 (97%)	9 (3%)	50	48
All	All	1866/1968 (95%)	1834 (98%)	32 (2%)	68	70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	TYR
1	A	202	GLU
1	A	231	ARG
1	A	342	THR
1	A	367	ASP
1	B	101	TYR
1	B	339	ARG
1	B	342	THR
1	B	376	ARG
1	C	33	GLN
1	C	101	TYR
1	C	332	GLN
1	C	342	THR
1	D	1	MET
1	D	101	TYR
1	D	233	SER
1	E	94	ARG
1	E	101	TYR
1	E	181	ARG
1	E	229	ASP
1	E	331	LEU
1	E	342	THR
1	E	348	ASP
1	F	33	GLN
1	F	96	VAL
1	F	101	TYR
1	F	156	PRO
1	F	160	ARG
1	F	179	ARG
1	F	200	ARG

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Mol	Chain	Res	Type
1	F	342	THR
1	F	367	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	B	309	GLN
1	C	33	GLN
1	C	235	HIS
1	C	270	HIS
1	C	385	GLN
1	D	235	HIS
1	D	385	GLN
1	E	167	HIS
1	E	373	ASN
1	F	33	GLN
1	F	385	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	COA	A	500	-	40,50,50	1.85	13 (32%)	50,75,75	3.06	16 (32%)
2	COA	B	500	-	40,50,50	1.82	14 (35%)	50,75,75	3.12	16 (32%)
2	COA	C	500	-	40,50,50	2.18	14 (35%)	50,75,75	2.72	16 (32%)
2	COA	D	500	-	40,50,50	1.75	13 (32%)	50,75,75	3.13	15 (30%)
2	COA	E	500	-	40,50,50	1.48	8 (20%)	50,75,75	3.25	15 (30%)
2	COA	F	500	-	40,50,50	1.69	14 (35%)	50,75,75	3.10	15 (30%)

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	COA	A	500	-	-	1/44/64/64	0/3/3/3
2	COA	B	500	-	-	0/44/64/64	0/3/3/3
2	COA	C	500	-	-	0/44/64/64	0/3/3/3
2	COA	D	500	-	-	0/44/64/64	0/3/3/3
2	COA	E	500	-	-	1/44/64/64	0/3/3/3
2	COA	F	500	-	-	1/44/64/64	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	COA	C4A-N3A	-5.19	1.27	1.35
2	C	500	COA	O5P-C5P	-4.45	1.13	1.23
2	C	500	COA	C3P-N4P	-4.08	1.36	1.46
2	D	500	COA	C5P-N4P	-3.38	1.25	1.33
2	C	500	COA	P3B-O9A	-3.36	1.42	1.54
2	D	500	COA	P2A-O5A	-3.31	1.40	1.54
2	B	500	COA	P2A-O5A	-3.27	1.41	1.54
2	B	500	COA	P1A-O2A	-3.21	1.41	1.54
2	C	500	COA	P2A-O5A	-3.20	1.41	1.54
2	A	500	COA	P2A-O5A	-3.15	1.41	1.54
2	B	500	COA	O5P-C5P	-3.15	1.16	1.23
2	A	500	COA	P3B-O8A	-3.15	1.43	1.54
2	A	500	COA	C6P-C5P	-3.13	1.45	1.51
2	A	500	COA	O5P-C5P	-3.09	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	COA	P1A-O2A	-3.08	1.41	1.54
2	A	500	COA	P1A-O2A	-3.07	1.41	1.54
2	C	500	COA	C2A-N3A	-2.96	1.27	1.32
2	D	500	COA	C5A-N7A	-2.88	1.29	1.39
2	C	500	COA	C5P-N4P	-2.87	1.26	1.33
2	F	500	COA	P2A-O5A	-2.85	1.42	1.54
2	C	500	COA	P1A-O2A	-2.84	1.42	1.54
2	C	500	COA	P3B-O8A	-2.82	1.44	1.54
2	A	500	COA	C3P-N4P	-2.81	1.39	1.46
2	D	500	COA	P2A-O4A	-2.81	1.40	1.51
2	A	500	COA	O9P-C9P	-2.80	1.17	1.23
2	F	500	COA	P1A-O2A	-2.79	1.43	1.54
2	C	500	COA	O9P-C9P	-2.78	1.18	1.23
2	B	500	COA	P3B-O9A	-2.78	1.44	1.54
2	B	500	COA	P2A-O4A	-2.76	1.41	1.51
2	B	500	COA	C3P-N4P	-2.74	1.39	1.46
2	F	500	COA	C3P-N4P	-2.71	1.39	1.46
2	E	500	COA	P2A-O5A	-2.71	1.43	1.54
2	A	500	COA	P3B-O9A	-2.64	1.45	1.54
2	B	500	COA	P3B-O8A	-2.63	1.45	1.54
2	A	500	COA	C5A-N7A	-2.62	1.30	1.39
2	F	500	COA	C5A-N7A	-2.59	1.30	1.39
2	B	500	COA	C5A-N7A	-2.59	1.30	1.39
2	F	500	COA	P3B-O9A	-2.57	1.45	1.54
2	E	500	COA	P1A-O2A	-2.56	1.44	1.54
2	F	500	COA	P3B-O8A	-2.52	1.45	1.54
2	E	500	COA	P3B-O8A	-2.51	1.45	1.54
2	A	500	COA	P2A-O4A	-2.46	1.42	1.51
2	D	500	COA	CEP-CBP	-2.44	1.48	1.53
2	B	500	COA	C7P-N8P	-2.44	1.40	1.46
2	C	500	COA	P2A-O4A	-2.43	1.42	1.51
2	B	500	COA	P1A-O1A	-2.42	1.42	1.51
2	F	500	COA	C7P-N8P	-2.42	1.40	1.46
2	B	500	COA	O9P-C9P	-2.41	1.18	1.23
2	E	500	COA	P3B-O9A	-2.40	1.46	1.54
2	A	500	COA	C4A-N3A	-2.39	1.32	1.35
2	F	500	COA	C6P-C5P	-2.39	1.46	1.51
2	E	500	COA	C5A-N7A	-2.39	1.31	1.39
2	A	500	COA	P1A-O1A	-2.37	1.42	1.51
2	F	500	COA	C4A-N3A	-2.36	1.32	1.35
2	B	500	COA	C6P-C5P	-2.35	1.46	1.51
2	F	500	COA	O9P-C9P	-2.33	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	COA	O9P-C9P	-2.32	1.18	1.23
2	D	500	COA	O9P-C9P	-2.30	1.18	1.23
2	B	500	COA	CEP-CBP	-2.29	1.48	1.53
2	D	500	COA	P3B-O8A	-2.29	1.46	1.54
2	D	500	COA	C4A-N3A	-2.28	1.32	1.35
2	C	500	COA	P1A-O1A	-2.25	1.43	1.51
2	D	500	COA	O5P-C5P	-2.23	1.18	1.23
2	C	500	COA	C2P-S1P	-2.20	1.73	1.80
2	A	500	COA	P3B-O7A	-2.17	1.44	1.51
2	E	500	COA	C6P-C5P	-2.13	1.47	1.51
2	F	500	COA	O5P-C5P	-2.09	1.18	1.23
2	D	500	COA	C3P-N4P	-2.09	1.41	1.46
2	E	500	COA	P2A-O4A	-2.07	1.43	1.51
2	F	500	COA	O4B-C4B	-2.05	1.40	1.45
2	F	500	COA	P1A-O1A	-2.04	1.43	1.51
2	D	500	COA	P3B-O9A	-2.04	1.47	1.54
2	D	500	COA	C2P-S1P	-2.03	1.73	1.80
2	F	500	COA	CEP-CBP	-2.03	1.49	1.53
2	B	500	COA	C5A-C4A	2.04	1.45	1.40
2	C	500	COA	C5A-C4A	2.47	1.46	1.40

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	COA	N3A-C2A-N1A	-10.55	120.82	128.89
2	E	500	COA	CEP-CBP-CAP	-10.12	90.87	109.34
2	A	500	COA	CEP-CBP-CAP	-9.89	91.30	109.34
2	D	500	COA	CEP-CBP-CAP	-9.22	92.51	109.34
2	B	500	COA	CEP-CBP-CAP	-9.09	92.75	109.34
2	F	500	COA	CEP-CBP-CAP	-8.84	93.20	109.34
2	B	500	COA	CDP-CBP-CAP	-8.68	93.50	109.34
2	A	500	COA	CDP-CBP-CAP	-7.34	95.94	109.34
2	D	500	COA	CDP-CBP-CAP	-7.34	95.95	109.34
2	F	500	COA	CDP-CBP-CAP	-6.96	96.64	109.34
2	E	500	COA	CDP-CBP-CAP	-6.79	96.94	109.34
2	A	500	COA	N3A-C2A-N1A	-6.25	124.11	128.89
2	C	500	COA	C3P-N4P-C5P	-6.04	110.91	122.79
2	B	500	COA	N3A-C2A-N1A	-5.96	124.33	128.89
2	E	500	COA	N3A-C2A-N1A	-5.91	124.37	128.89
2	F	500	COA	N3A-C2A-N1A	-5.15	124.95	128.89
2	D	500	COA	C2P-C3P-N4P	-5.05	102.39	112.37
2	C	500	COA	O5P-C5P-N4P	-4.91	113.20	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	COA	O5P-C5P-C6P	-4.71	113.86	121.98
2	D	500	COA	N3A-C2A-N1A	-4.37	125.55	128.89
2	D	500	COA	C4A-C5A-N7A	-4.20	105.62	109.48
2	E	500	COA	O5P-C5P-C6P	-4.08	114.94	121.98
2	F	500	COA	OAP-CAP-C9P	-3.98	101.25	110.38
2	E	500	COA	C7P-C6P-C5P	-3.74	106.14	112.31
2	F	500	COA	C4A-C5A-N7A	-3.59	106.17	109.48
2	A	500	COA	O5P-C5P-C6P	-3.55	115.86	121.98
2	A	500	COA	C4A-C5A-N7A	-3.50	106.26	109.48
2	F	500	COA	P2A-O3A-P1A	-3.48	122.95	132.73
2	D	500	COA	O5P-C5P-N4P	-3.39	116.20	122.94
2	B	500	COA	C7P-C6P-C5P	-3.37	106.76	112.31
2	D	500	COA	P2A-O3A-P1A	-3.18	123.79	132.73
2	D	500	COA	OAP-CAP-C9P	-3.12	103.22	110.38
2	E	500	COA	C4A-C5A-N7A	-3.07	106.65	109.48
2	F	500	COA	C6P-C7P-N8P	-3.07	105.14	111.88
2	C	500	COA	C1B-N9A-C4A	-2.97	122.46	126.94
2	B	500	COA	OAP-CAP-C9P	-2.97	103.57	110.38
2	B	500	COA	O5P-C5P-C6P	-2.91	116.97	121.98
2	C	500	COA	C2P-C3P-N4P	-2.90	106.65	112.37
2	C	500	COA	P2A-O3A-P1A	-2.84	124.75	132.73
2	A	500	COA	C7P-C6P-C5P	-2.76	107.76	112.31
2	C	500	COA	C4B-O4B-C1B	-2.69	106.76	109.72
2	B	500	COA	C4A-C5A-N7A	-2.60	107.09	109.48
2	A	500	COA	C1B-N9A-C4A	-2.56	123.07	126.94
2	A	500	COA	OAP-CAP-C9P	-2.41	104.85	110.38
2	A	500	COA	P2A-O3A-P1A	-2.30	126.26	132.73
2	E	500	COA	C7P-N8P-C9P	-2.25	118.08	122.53
2	E	500	COA	P2A-O3A-P1A	-2.20	126.55	132.73
2	F	500	COA	C7P-C6P-C5P	-2.19	108.70	112.31
2	D	500	COA	O5A-P2A-O6A	-2.10	97.85	108.46
2	C	500	COA	O5A-P2A-O4A	2.02	123.46	112.53
2	B	500	COA	O6A-CCP-CBP	2.09	113.90	110.55
2	A	500	COA	O9A-P3B-O8A	2.14	115.54	107.38
2	B	500	COA	O5A-P2A-O4A	2.17	124.29	112.53
2	C	500	COA	O9A-P3B-O7A	2.17	117.58	110.58
2	D	500	COA	O3A-P2A-O6A	2.28	109.00	102.94
2	C	500	COA	OAP-CAP-C9P	2.29	115.63	110.38
2	C	500	COA	C7P-N8P-C9P	2.30	127.08	122.53
2	E	500	COA	O3A-P2A-O6A	2.36	109.20	102.94
2	A	500	COA	O3A-P2A-O6A	2.50	109.58	102.94
2	C	500	COA	C4A-C5A-N7A	2.52	111.79	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	COA	O6A-CCP-CBP	2.52	114.60	110.55
2	F	500	COA	O9A-P3B-O8A	2.58	117.19	107.38
2	B	500	COA	O4B-C1B-N9A	2.95	114.27	108.10
2	F	500	COA	O6A-CCP-CBP	3.04	115.44	110.55
2	E	500	COA	CDP-CBP-CCP	3.17	112.61	108.50
2	B	500	COA	C3P-N4P-C5P	3.21	129.11	122.79
2	D	500	COA	O9A-P3B-O8A	3.42	120.40	107.38
2	F	500	COA	C6P-C5P-N4P	3.54	122.61	116.46
2	A	500	COA	C6P-C5P-N4P	3.58	122.68	116.46
2	A	500	COA	O6A-CCP-CBP	3.80	116.66	110.55
2	E	500	COA	C6P-C5P-N4P	3.93	123.28	116.46
2	B	500	COA	C6P-C5P-N4P	4.31	123.95	116.46
2	F	500	COA	CEP-CBP-CDP	4.35	118.01	109.28
2	E	500	COA	C2P-C3P-N4P	4.48	121.21	112.37
2	C	500	COA	C6P-C5P-N4P	4.79	124.79	116.46
2	B	500	COA	C7P-N8P-C9P	5.01	132.46	122.53
2	A	500	COA	CDP-CBP-CCP	5.28	115.35	108.50
2	C	500	COA	O6A-CCP-CBP	5.29	119.05	110.55
2	C	500	COA	O4B-C1B-N9A	5.35	119.30	108.10
2	C	500	COA	C2A-N1A-C6A	5.65	128.87	118.77
2	D	500	COA	CEP-CBP-CDP	5.66	120.65	109.28
2	D	500	COA	O6A-CCP-CBP	5.69	119.69	110.55
2	E	500	COA	CEP-CBP-CDP	6.24	121.80	109.28
2	B	500	COA	CEP-CBP-CDP	6.45	122.23	109.28
2	A	500	COA	CEP-CBP-CDP	6.53	122.38	109.28
2	D	500	COA	CEP-CBP-CCP	6.98	117.56	108.50
2	B	500	COA	CDP-CBP-CCP	7.11	117.72	108.50
2	B	500	COA	CEP-CBP-CCP	7.79	118.59	108.50
2	F	500	COA	CDP-CBP-CCP	7.79	118.60	108.50
2	D	500	COA	CDP-CBP-CCP	9.19	120.41	108.50
2	A	500	COA	CEP-CBP-CCP	9.83	121.25	108.50
2	F	500	COA	CEP-CBP-CCP	10.61	122.26	108.50
2	E	500	COA	CEP-CBP-CCP	12.69	124.95	108.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	500	COA	C6P-C5P-N4P-C3P
2	F	500	COA	C6P-C5P-N4P-C3P
2	A	500	COA	C6P-C5P-N4P-C3P

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	COA	4	0
2	C	500	COA	4	0
2	D	500	COA	4	0
2	E	500	COA	1	0
2	F	500	COA	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	402/422 (95%)	-0.08	17 (4%) 40 42	17, 25, 46, 83	0
1	B	402/422 (95%)	0.02	18 (4%) 37 39	17, 25, 50, 82	0
1	C	402/422 (95%)	0.03	20 (4%) 32 34	19, 28, 55, 81	0
1	D	402/422 (95%)	-0.11	17 (4%) 40 42	15, 27, 49, 73	0
1	E	402/422 (95%)	0.12	24 (5%) 25 27	22, 34, 58, 77	0
1	F	402/422 (95%)	0.10	24 (5%) 25 27	22, 32, 57, 80	0
All	All	2412/2532 (95%)	0.01	120 (4%) 32 34	15, 29, 54, 83	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	10.6
1	F	206	GLY	9.2
1	E	206	GLY	8.6
1	F	205	ARG	7.3
1	B	227	GLY	7.1
1	F	228	PRO	6.9
1	A	203	SER	6.5
1	D	228	PRO	6.5
1	E	228	PRO	6.5
1	B	228	PRO	6.4
1	F	1	MET	6.4
1	C	227	GLY	6.3
1	C	228	PRO	6.2
1	E	227	GLY	5.9
1	E	203	SER	5.9
1	B	1	MET	5.9
1	B	205	ARG	5.8
1	C	1	MET	5.7
1	A	227	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	227	GLY	5.3
1	B	206	GLY	5.0
1	C	207	GLY	4.9
1	C	206	GLY	4.9
1	B	230	GLY	4.7
1	F	56	ASP	4.7
1	C	229	ASP	4.7
1	B	207	GLY	4.6
1	E	1	MET	4.6
1	F	227	GLY	4.6
1	B	231	ARG	4.5
1	A	205	ARG	4.4
1	A	206	GLY	4.4
1	F	381	GLU	4.3
1	C	205	ARG	4.1
1	D	205	ARG	4.1
1	B	229	ASP	4.1
1	B	203	SER	4.1
1	F	231	ARG	4.0
1	D	1	MET	4.0
1	F	229	ASP	3.9
1	E	205	ARG	3.9
1	A	229	ASP	3.9
1	B	226	ARG	3.9
1	E	229	ASP	3.9
1	F	54	THR	3.8
1	F	344	ASP	3.8
1	A	231	ARG	3.7
1	A	1	MET	3.7
1	C	231	ARG	3.4
1	F	346	PRO	3.4
1	E	3	THR	3.3
1	E	56	ASP	3.3
1	D	378	LYS	3.3
1	C	394	MET	3.3
1	C	381	GLU	3.3
1	A	56	ASP	3.3
1	E	202	GLU	3.2
1	B	394	MET	3.2
1	D	206	GLY	3.1
1	E	230	GLY	3.1
1	C	226	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	55	ASP	3.1
1	F	207	GLY	3.1
1	E	346	PRO	2.9
1	D	380	SER	2.9
1	F	203	SER	2.8
1	A	230	GLY	2.8
1	E	200	ARG	2.8
1	B	202	GLU	2.8
1	D	54	THR	2.7
1	C	56	ASP	2.7
1	D	202	GLU	2.7
1	C	294	ILE	2.7
1	D	230	GLY	2.7
1	C	55	ASP	2.7
1	E	207	GLY	2.6
1	F	382	LEU	2.6
1	D	381	GLU	2.6
1	E	53	GLU	2.6
1	D	229	ASP	2.5
1	E	44	GLU	2.5
1	A	201	PRO	2.5
1	F	162	LEU	2.5
1	F	348	ASP	2.5
1	A	200	ARG	2.4
1	E	226	ARG	2.4
1	F	380	SER	2.4
1	E	55	ASP	2.4
1	F	342	THR	2.4
1	E	2	ILE	2.4
1	D	339	ARG	2.4
1	F	378	LYS	2.4
1	A	207	GLY	2.4
1	B	200	ARG	2.3
1	C	230	GLY	2.3
1	E	12	ASP	2.3
1	E	344	ASP	2.3
1	C	342	THR	2.3
1	D	201	PRO	2.3
1	E	13	ASP	2.3
1	F	339	ARG	2.3
1	D	226	ARG	2.2
1	E	94	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	361	LEU	2.2
1	A	226	ARG	2.2
1	B	201	PRO	2.2
1	B	168	ARG	2.2
1	A	2	ILE	2.2
1	B	225	ASP	2.2
1	F	225	ASP	2.2
1	E	201	PRO	2.2
1	C	253	ALA	2.1
1	F	230	GLY	2.1
1	C	54	THR	2.1
1	D	342	THR	2.1
1	D	231	ARG	2.1
1	B	339	ARG	2.1
1	A	346	PRO	2.0
1	C	378	LYS	2.0
1	A	44	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 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(Å ²)	Q<0.9
2	COA	F	500	48/48	0.93	0.16	2.35	16,24,35,42	0
2	COA	C	500	48/48	0.92	0.13	1.61	16,24,35,42	0
2	COA	E	500	48/48	0.94	0.15	0.71	16,24,35,42	0
2	COA	D	500	48/48	0.94	0.12	0.62	16,24,35,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	COA	A	500	48/48	0.95	0.12	0.27	16,24,35,42	0
2	COA	B	500	48/48	0.94	0.10	0.02	16,24,35,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.