Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EAN
Title	:	Crystal structure of recombinant rat selenoprotein thioredoxin reductase 1 with reduced C-terminal tail
Authors	:	Sandalova, T.; Cheng, Q.; Lindqvist, Y.; Arner, E.
Deposited on	:	2008-08-26
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

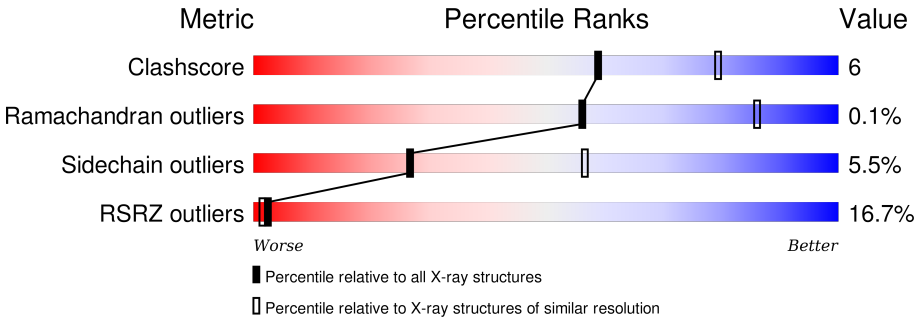
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	499	8% 83% 13%
1	B	499	7% 84% 12%
1	C	499	25% 84% 12%
1	D	499	12% 86% 10%
1	E	499	11% 83% 13%
1	F	499	34% 84% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23214 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.

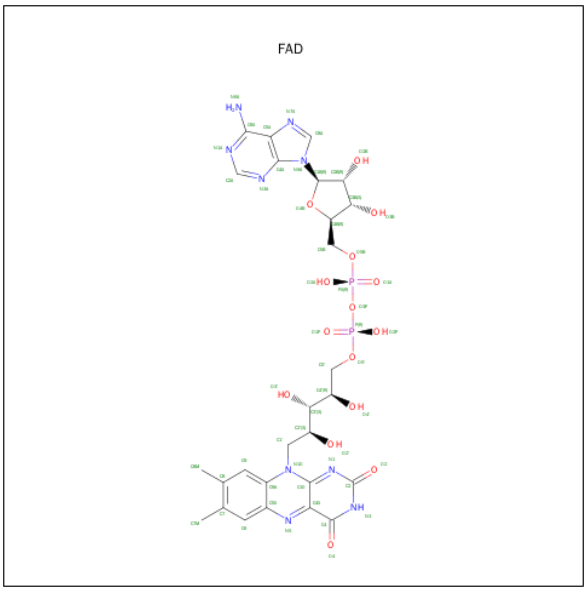
- Molecule 1 is a protein called Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	B	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	C	486	Total	C	N	O	S	Se	0	0	0
			3731	2368	633	708	21	1			
1	D	491	Total	C	N	O	S	Se	0	0	0
			3777	2399	639	717	21	1			
1	E	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	F	489	Total	C	N	O	S	Se	0	0	0
			3762	2390	636	714	21	1			

There are 12 discrepancies between the modelled and reference sequences:

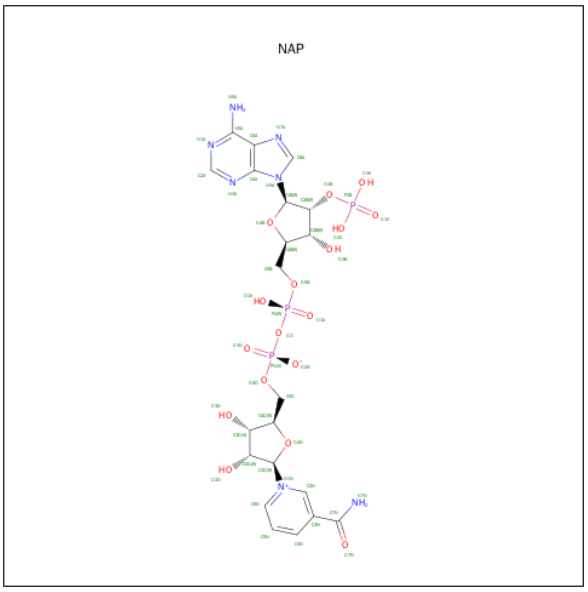
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ARG	ASN	CONFLICT	UNP O89049
A	53	TRP	GLY	CONFLICT	UNP O89049
B	52	ARG	ASN	CONFLICT	UNP O89049
B	53	TRP	GLY	CONFLICT	UNP O89049
C	52	ARG	ASN	CONFLICT	UNP O89049
C	53	TRP	GLY	CONFLICT	UNP O89049
D	52	ARG	ASN	CONFLICT	UNP O89049
D	53	TRP	GLY	CONFLICT	UNP O89049
E	52	ARG	ASN	CONFLICT	UNP O89049
E	53	TRP	GLY	CONFLICT	UNP O89049
F	52	ARG	ASN	CONFLICT	UNP O89049
F	53	TRP	GLY	CONFLICT	UNP O89049

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 4 is water.

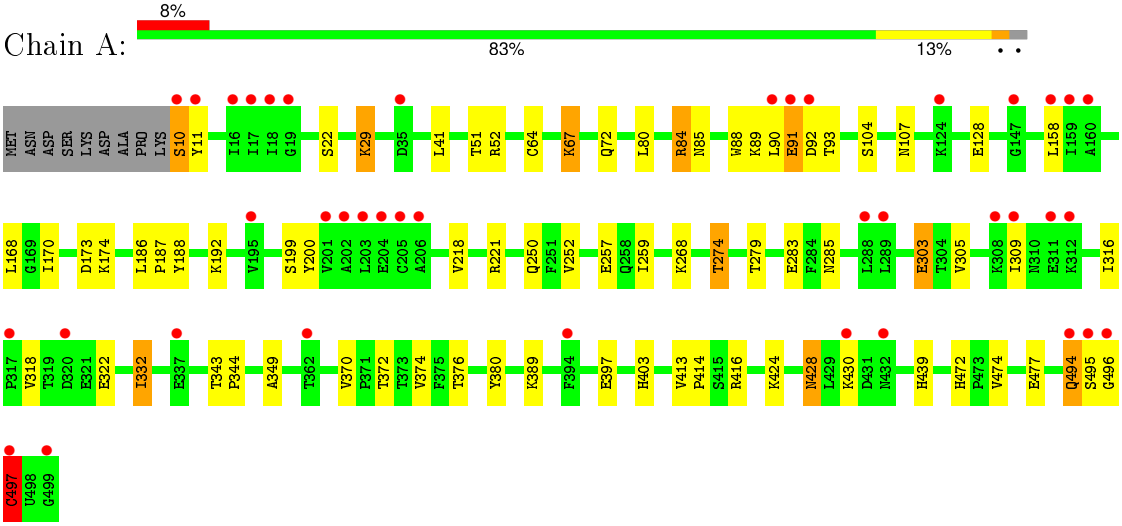
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	20	Total	O	0	0
			20	20		
4	C	14	Total	O	0	0
			14	14		
4	D	35	Total	O	0	0
			35	35		
4	E	26	Total	O	0	0
			26	26		
4	F	12	Total	O	0	0
			12	12		

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.

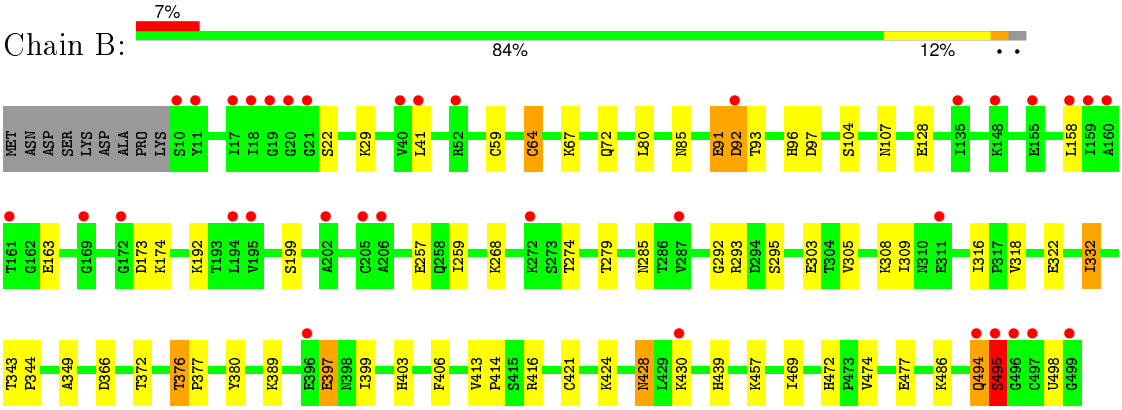
- Molecule 1: Thioredoxin reductase 1

Chain A:



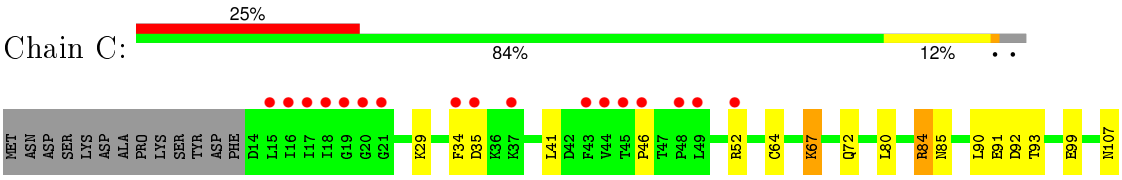
- Molecule 1: Thioredoxin reductase 1

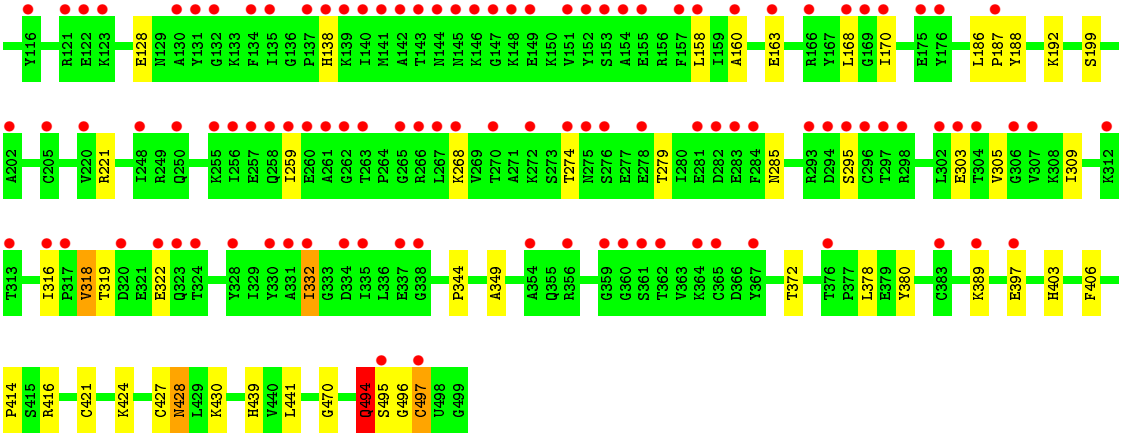
Chain B:



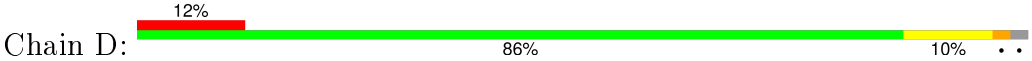
- Molecule 1: Thioredoxin reductase 1

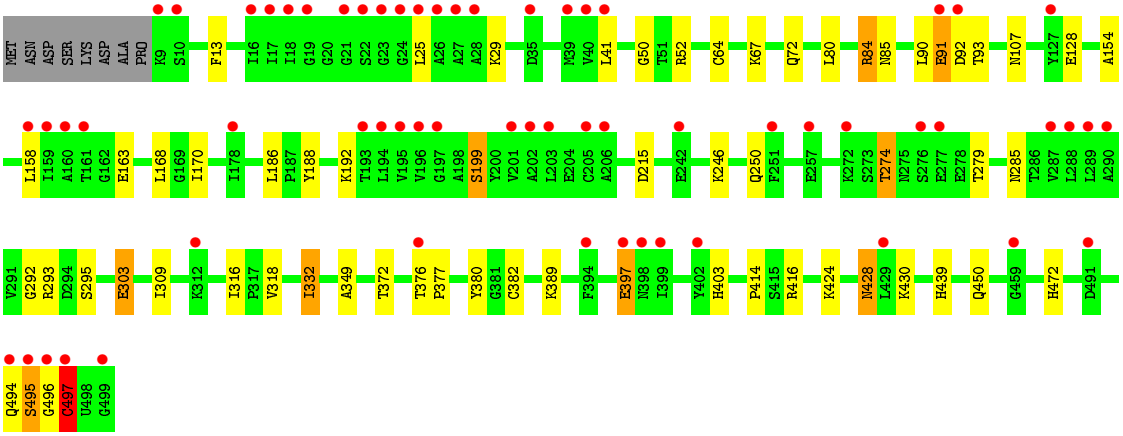
Chain C:



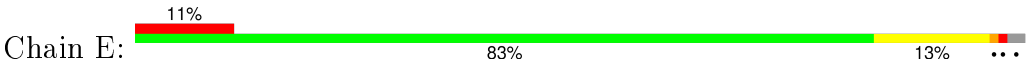


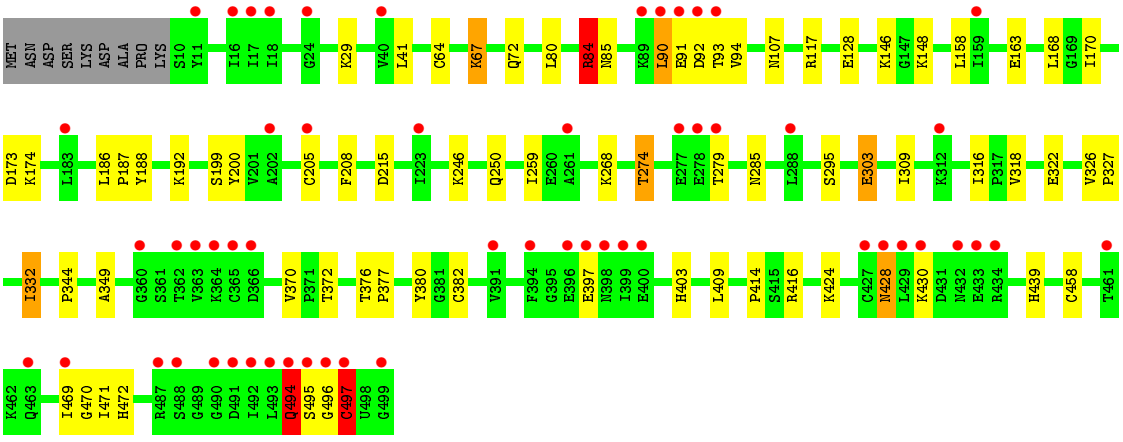
• Molecule 1: Thioredoxin reductase 1



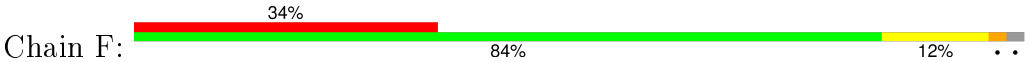


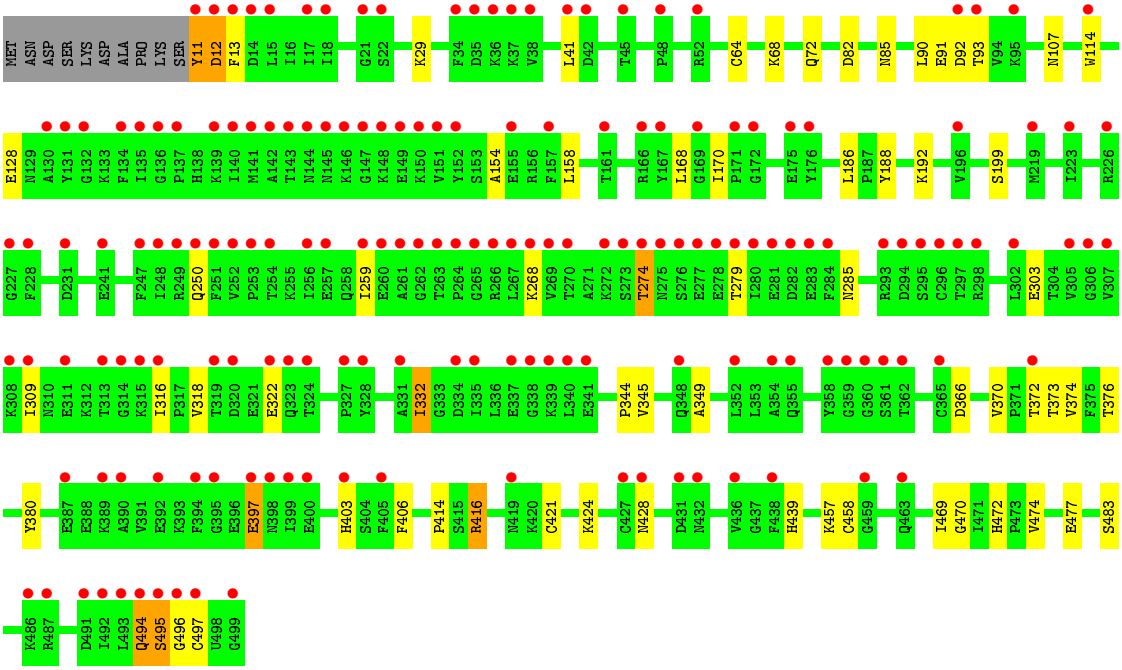
• Molecule 1: Thioredoxin reductase 1





• Molecule 1: Thioredoxin reductase 1




MET ASN ASP SER LYS ASP ALA PRO LYS SER Y11 D12 F13 D14 L15 I16 I17 I18 G21 S22 K29 F34 D35 K36 K37 V38 L41 D42 T45 P48 R52 G64 K68 Q72 D82 N85 L90 E91 D92 T93 V94 K95 N107 W114
E128 N129 A130 Y131 G132 K133 F134 I135 G136 P137 H138 K139 I140 M141 A142 T143 N144 N145 K146 G147 K148 E149 K150 V151 Y152 S153 A154 E155 R156 F157 L158 T161 R166 Y167 L168 G169 I170 P171 G172 E175 Y176 L186 P187 Y188 K192 V196 S199 M219 I223 R226
G227 F228 D231 E241 F247 I248 R249 Q250 F251 V252 P253 T254 K255 I256 E257 Q258 I259 E260 A261 G262 T263 P264 G265 R266 L267 K268 V269 T270 A271 K272 S273 T274 N275 S276 E277 E278 T279 I280 E281 D282 E283 F284 N285 R293 D294 S295 C296 T297 R298 L302 E303 T304 V305 G306 V307
K308 I309 M310 E311 K312 T313 G314 K315 I316 P317 V318 T319 D320 E321 E322 Q323 T324 P327 Y328 A331 I332 G333 D334 I335 L336 E337 G338 K339 L340 E341 P344 V345 Q348 A349 L352 L353 A354 Q355 Y358 G359 G360 S361 T362 C365 D366 V370 P371 T372 T373 V374 F375 T376
Y380 E387 E388 K389 A390 V391 E392 K393 F394 G395 E396 E397 M398 I399 E400 H403 S404 F405 F406 P414 S415 R416 N419 K420 C421 K424 C427 N428 D431 M432 V436 G437 F438 H439 K457 C458 G459 Q463 I469 G470 I471 H472 P473 V474 E477 S483
K486 R487 D491 I492 L493 Q494 S495 G496 C497 U498 G499

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.57Å 140.67Å 171.17Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	29.74 – 2.75 29.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.74-2.75) 99.5 (29.74-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.236 0.285 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 95820 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	23214	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 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, SEC, FAD

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	0.77	3/3835 (0.1%)	0.70	0/5185
1	B	0.78	1/3835 (0.0%)	0.71	0/5185
1	C	0.65	1/3796 (0.0%)	0.67	1/5132 (0.0%)
1	D	0.79	2/3844 (0.1%)	0.73	0/5196
1	E	0.75	3/3835 (0.1%)	0.71	2/5185 (0.0%)
1	F	0.63	1/3829 (0.0%)	0.66	1/5177 (0.0%)
All	All	0.73	11/22974 (0.0%)	0.70	4/31060 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	495	SER	CB-OG	5.96	1.50	1.42
1	F	11	TYR	N-CA	5.94	1.58	1.46
1	E	200	TYR	CD2-CE2	5.79	1.48	1.39
1	D	495	SER	CB-OG	5.78	1.49	1.42
1	E	382	CYS	CB-SG	-5.63	1.72	1.81
1	E	200	TYR	CD1-CE1	5.54	1.47	1.39
1	A	200	TYR	CE2-CZ	5.36	1.45	1.38
1	A	200	TYR	CD2-CE2	5.34	1.47	1.39
1	C	427	CYS	CB-SG	-5.28	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CB-CG2	-5.15	1.42	1.52
1	D	382	CYS	CB-SG	-5.01	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	114	TRP	CA-CB-CG	-7.31	99.81	113.70
1	E	84	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	E	117	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	221	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	494	GLN	Peptide
1	C	496	GLY	Peptide
1	E	494	GLN	Peptide
1	F	11	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3768	0	3767	56	0
1	B	3768	0	3769	50	0
1	C	3731	0	3740	53	0
1	D	3777	0	3780	34	0
1	E	3768	0	3767	55	0
1	F	3762	0	3762	46	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	32	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	11	2	0
3	C	32	0	11	1	0
3	D	32	0	11	1	0
3	E	32	0	11	1	0
3	F	32	0	11	1	0
4	A	23	0	0	2	0
4	B	20	0	0	5	0
4	C	14	0	0	7	0
4	D	35	0	0	0	0
4	E	26	0	0	0	0
4	F	12	0	0	1	0
All	All	23214	0	22837	266	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 (266) 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:192:LYS:H	1:C:285:ASN:HD22	1.24	0.85
1:E:496:GLY:N	1:E:497:CYS:HB2	1.92	0.84
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.62	0.83
1:A:10:SER:O	1:A:11:TYR:CG	2.35	0.80
1:B:192:LYS:H	1:B:285:ASN:HD22	1.28	0.78
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.64	0.78
1:A:192:LYS:H	1:A:285:ASN:HD22	1.28	0.77
1:A:10:SER:O	1:A:11:TYR:CD1	2.38	0.77
1:E:192:LYS:H	1:E:285:ASN:HD22	1.30	0.76
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.70	0.75
1:C:494:GLN:HA	1:C:494:GLN:HE21	1.52	0.74
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.71	0.74
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.70	0.73
1:E:469:ILE:HB	1:F:370:VAL:HG13	1.70	0.72
1:D:192:LYS:H	1:D:285:ASN:HD22	1.38	0.71
1:A:221:ARG:HG3	1:A:252:VAL:CG2	2.21	0.70
1:C:84:ARG:HH22	1:C:90:LEU:HB3	1.57	0.70
1:C:46:PRO:HB3	1:C:52:ARG:NH1	2.06	0.69
1:C:138:HIS:HB3	4:C:613:HOH:O	1.93	0.69
1:C:90:LEU:HD11	1:D:90:LEU:HD11	1.75	0.69
1:C:84:ARG:NH2	1:C:90:LEU:HB3	2.07	0.69
1:A:494:GLN:HB3	1:A:495:SER:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.77	0.68
1:F:192:LYS:H	1:F:285:ASN:HD22	1.42	0.67
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.10	0.67
1:D:84:ARG:NH2	1:D:90:LEU:HB3	2.11	0.66
1:E:496:GLY:H	1:E:497:CYS:CB	2.09	0.66
1:C:494:GLN:HA	1:C:494:GLN:NE2	2.10	0.66
1:C:494:GLN:HE21	1:C:494:GLN:CA	2.09	0.65
1:B:494:GLN:HA	1:B:494:GLN:HE21	1.61	0.65
1:E:72:GLN:HA	1:E:72:GLN:HE21	1.60	0.65
1:D:50:GLY:O	1:D:52:ARG:NH1	2.30	0.64
1:F:494:GLN:HB3	1:F:495:SER:HB2	1.79	0.64
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.80	0.64
1:E:496:GLY:H	1:E:497:CYS:HB2	1.62	0.63
1:E:84:ARG:NH2	1:E:90:LEU:HB3	2.15	0.62
1:F:494:GLN:HA	1:F:494:GLN:HE21	1.65	0.61
1:D:186:LEU:HD11	1:D:188:TYR:CZ	2.35	0.61
1:B:486:LYS:CE	4:B:603:HOH:O	2.47	0.61
1:C:46:PRO:CG	1:C:52:ARG:NH1	2.65	0.60
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.82	0.60
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.85	0.59
1:D:84:ARG:HH22	1:D:90:LEU:HB3	1.67	0.59
1:A:91:GLU:CD	1:A:92:ASP:H	2.07	0.58
1:E:84:ARG:HH22	1:E:90:LEU:HB3	1.68	0.58
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.86	0.58
1:E:332:ILE:HD12	1:E:349:ALA:HB1	1.86	0.58
1:F:85:ASN:HD22	1:F:414:PRO:HA	1.69	0.57
1:E:380:TYR:OH	1:E:439:HIS:CD2	2.54	0.57
1:C:192:LYS:N	1:C:285:ASN:HD22	2.00	0.57
1:A:85:ASN:HD22	1:A:414:PRO:HA	1.70	0.57
1:C:46:PRO:CB	1:C:52:ARG:NH1	2.68	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.86	0.56
1:B:332:ILE:HD12	1:B:349:ALA:CB	2.35	0.56
1:D:309:ILE:HG22	1:D:316:ILE:HG12	1.87	0.56
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.87	0.56
1:F:158:LEU:HD11	1:F:332:ILE:HG12	1.88	0.56
1:B:332:ILE:HD12	1:B:349:ALA:HB1	1.86	0.56
1:E:496:GLY:N	1:E:497:CYS:CB	2.64	0.55
1:E:309:ILE:HG22	1:E:316:ILE:HG12	1.88	0.55
3:B:601:NAP:H51A	4:B:612:HOH:O	2.05	0.55
1:F:332:ILE:HD12	1:F:349:ALA:HB1	1.89	0.55
1:B:380:TYR:OH	1:B:439:HIS:CD2	2.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ILE:HG22	1:F:316:ILE:HG12	1.89	0.55
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.42	0.55
3:B:601:NAP:C5B	4:B:612:HOH:O	2.55	0.54
1:D:158:LEU:HD11	1:D:332:ILE:HG12	1.89	0.54
1:A:72:GLN:NE2	1:A:72:GLN:HA	2.23	0.54
1:B:486:LYS:HE3	4:B:603:HOH:O	2.06	0.54
1:A:221:ARG:HG3	1:A:252:VAL:HG22	1.89	0.54
1:B:22:SER:OG	1:B:343:THR:HG23	2.07	0.54
1:D:84:ARG:CZ	1:D:84:ARG:HB2	2.38	0.54
1:A:84:ARG:NH2	1:A:90:LEU:HB3	2.23	0.54
1:E:192:LYS:N	1:E:285:ASN:HD22	2.04	0.54
1:B:332:ILE:CD1	1:B:349:ALA:HB1	2.37	0.54
1:A:259:ILE:HD11	1:A:268:LYS:HB2	1.89	0.54
1:C:72:GLN:NE2	1:C:72:GLN:HA	2.22	0.53
1:C:138:HIS:CB	4:C:613:HOH:O	2.55	0.53
1:F:332:ILE:HD12	1:F:349:ALA:CB	2.39	0.52
1:D:199:SER:HB3	3:D:601:NAP:O1N	2.09	0.52
1:E:332:ILE:HD12	1:E:349:ALA:CB	2.39	0.52
1:E:85:ASN:HD22	1:E:414:PRO:HA	1.74	0.52
1:A:29:LYS:NZ	1:B:498:SEC:SE	2.93	0.52
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.75	0.52
1:C:380:TYR:OH	1:C:439:HIS:CD2	2.57	0.52
1:C:428:ASN:ND2	1:C:430:LYS:H	2.07	0.52
1:B:308:LYS:HD2	4:B:614:HOH:O	2.09	0.51
1:B:259:ILE:HD11	1:B:268:LYS:HB2	1.92	0.51
1:F:72:GLN:HA	1:F:72:GLN:NE2	2.25	0.51
1:A:168:LEU:HB2	1:A:170:ILE:HG12	1.92	0.51
1:C:199:SER:HB3	3:C:601:NAP:O1N	2.10	0.51
1:A:380:TYR:OH	1:A:439:HIS:CD2	2.60	0.51
1:D:496:GLY:N	1:D:497:CYS:HB2	2.25	0.51
1:C:84:ARG:HB2	1:C:84:ARG:CZ	2.40	0.51
1:F:494:GLN:CA	1:F:494:GLN:HE21	2.23	0.51
1:E:332:ILE:CD1	1:E:349:ALA:HB1	2.40	0.51
1:A:374:VAL:HG12	1:A:376:THR:HG23	1.93	0.51
1:C:46:PRO:HG3	1:C:52:ARG:NH1	2.26	0.51
1:A:89:LYS:HE3	1:B:97:ASP:HB2	1.93	0.51
1:F:494:GLN:HB3	1:F:495:SER:CB	2.41	0.50
1:B:59:CYS:CB	1:B:64:CYS:HG	2.23	0.50
1:F:13:PHE:O	1:F:154:ALA:HA	2.11	0.50
1:C:309:ILE:HG22	1:C:316:ILE:HG12	1.94	0.50
1:F:406:PHE:CZ	1:F:421:CYS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ILE:HD11	1:C:268:LYS:HB2	1.93	0.50
1:B:72:GLN:NE2	1:B:72:GLN:HA	2.26	0.50
1:A:84:ARG:HB2	1:A:84:ARG:CZ	2.41	0.49
1:A:104:SER:HB3	1:B:413:VAL:HG13	1.94	0.49
1:E:163:GLU:HG2	1:E:295:SER:HA	1.94	0.49
1:B:494:GLN:CA	1:B:494:GLN:HE21	2.24	0.49
1:D:91:GLU:CD	1:D:92:ASP:H	2.15	0.49
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.26	0.49
1:F:374:VAL:HG12	1:F:376:THR:HG23	1.94	0.49
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.95	0.49
1:B:85:ASN:HD22	1:B:414:PRO:HA	1.77	0.49
1:D:303:GLU:CD	1:D:303:GLU:H	2.17	0.48
1:F:72:GLN:HA	1:F:72:GLN:HE21	1.78	0.48
1:B:366:ASP:OD2	1:B:457:LYS:HE3	2.13	0.48
1:D:13:PHE:O	1:D:154:ALA:HA	2.14	0.48
1:D:85:ASN:HD22	1:D:414:PRO:HA	1.78	0.48
1:C:186:LEU:HD11	1:C:188:TYR:CZ	2.48	0.47
1:B:474:VAL:O	1:B:477:GLU:HG2	2.14	0.47
1:F:168:LEU:HB2	1:F:170:ILE:HG12	1.95	0.47
1:F:41:LEU:HD23	1:F:128:GLU:HB3	1.95	0.47
1:A:67:LYS:HB3	1:A:67:LYS:HE2	1.75	0.47
1:A:428:ASN:ND2	1:A:430:LYS:H	2.13	0.47
1:C:168:LEU:HB2	1:C:170:ILE:HG12	1.97	0.47
1:E:471:ILE:HG21	1:F:373:THR:OG1	2.14	0.47
1:D:332:ILE:HD12	1:D:349:ALA:HB1	1.97	0.46
1:A:199:SER:HB3	3:A:601:NAP:O1N	2.15	0.46
1:C:46:PRO:CG	1:C:52:ARG:HH12	2.28	0.46
1:A:494:GLN:HE21	1:A:494:GLN:N	2.13	0.46
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.98	0.46
1:D:84:ARG:HB2	1:D:84:ARG:NH2	2.31	0.46
1:B:332:ILE:HA	1:B:332:ILE:HD13	1.70	0.46
1:F:474:VAL:O	1:F:477:GLU:HG2	2.16	0.46
1:F:332:ILE:CD1	1:F:349:ALA:HB1	2.45	0.46
1:A:332:ILE:HD12	1:A:349:ALA:HB1	1.97	0.46
1:B:158:LEU:HD11	1:B:332:ILE:HG12	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:NE2	2.31	0.46
1:A:22:SER:OG	1:A:343:THR:HG23	2.16	0.46
1:C:332:ILE:HD12	1:C:349:ALA:HB1	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:HE21	1.79	0.46
1:C:35:ASP:CB	4:C:614:HOH:O	2.63	0.46
1:E:496:GLY:H	1:E:497:CYS:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:GLU:HG2	1:E:332:ILE:CD1	2.46	0.45
1:D:250:GLN:HB3	1:D:274:THR:HB	1.97	0.45
1:D:397:GLU:HG2	1:D:397:GLU:O	2.16	0.45
1:A:413:VAL:HG13	1:B:104:SER:HB3	1.98	0.45
1:E:158:LEU:HD11	1:E:332:ILE:HG12	1.97	0.45
1:A:370:VAL:HG13	1:B:469:ILE:HB	1.99	0.45
1:B:67:LYS:HE2	1:B:67:LYS:HB3	1.82	0.45
1:E:303:GLU:CD	1:E:303:GLU:H	2.19	0.45
1:F:250:GLN:HB3	1:F:274:THR:HB	1.98	0.45
1:B:322:GLU:HG2	1:B:332:ILE:HD13	1.98	0.45
1:C:160:ALA:HB1	4:C:605:HOH:O	2.16	0.45
1:C:67:LYS:HE2	1:C:67:LYS:HB3	1.67	0.45
1:A:84:ARG:HH22	1:A:90:LEU:HB3	1.79	0.45
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.51	0.45
1:B:91:GLU:CD	1:B:92:ASP:H	2.20	0.45
1:E:322:GLU:HG2	1:E:332:ILE:HD13	1.98	0.45
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.99	0.45
1:B:309:ILE:HG22	1:B:316:ILE:HG12	1.98	0.45
1:B:494:GLN:HB3	1:B:495:SER:HA	1.99	0.45
1:A:332:ILE:HD12	1:A:349:ALA:CB	2.46	0.45
1:B:173:ASP:OD1	1:B:174:LYS:N	2.50	0.45
1:E:84:ARG:CZ	1:E:84:ARG:HB2	2.47	0.44
1:E:332:ILE:HD13	1:E:332:ILE:HA	1.70	0.44
1:B:163:GLU:HG2	1:B:295:SER:HA	2.00	0.44
1:E:205:CYS:HA	1:E:208:PHE:CE2	2.52	0.44
1:A:186:LEU:HD11	1:A:188:TYR:CZ	2.53	0.44
1:E:250:GLN:HB3	1:E:274:THR:HB	1.99	0.44
1:A:389:LYS:HA	1:A:389:LYS:HD2	1.82	0.44
1:E:173:ASP:OD1	1:E:174:LYS:N	2.51	0.44
1:E:494:GLN:HB3	1:E:495:SER:HA	2.00	0.44
1:C:99:GLU:OE1	1:E:148:LYS:HE3	2.18	0.44
1:B:322:GLU:HG2	1:B:332:ILE:CD1	2.47	0.44
1:C:322:GLU:HG2	1:C:332:ILE:CD1	2.48	0.43
1:E:469:ILE:HG21	1:F:345:VAL:HG23	1.99	0.43
1:D:168:LEU:HB2	1:D:170:ILE:HG12	2.00	0.43
1:E:67:LYS:HE2	1:E:67:LYS:HB3	1.67	0.43
1:A:84:ARG:HB2	1:A:84:ARG:NH2	2.33	0.43
1:B:41:LEU:HD23	1:B:128:GLU:HB3	2.00	0.43
1:E:458:CYS:HB2	1:F:458:CYS:HB2	2.01	0.43
1:E:469:ILE:CB	1:F:370:VAL:HG13	2.44	0.43
1:C:187:PRO:HB3	1:E:146:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LEU:HD11	1:F:188:TYR:CZ	2.52	0.43
1:E:370:VAL:HG13	1:F:469:ILE:HB	2.00	0.43
1:A:173:ASP:OD1	1:A:174:LYS:N	2.51	0.43
1:A:494:GLN:HB3	1:A:495:SER:CA	2.44	0.43
1:A:72:GLN:HE21	1:A:72:GLN:HA	1.81	0.43
1:B:72:GLN:HA	1:B:72:GLN:HE21	1.83	0.43
1:E:428:ASN:ND2	1:E:430:LYS:H	2.16	0.43
1:B:389:LYS:HD2	1:B:389:LYS:HA	1.78	0.43
1:F:397:GLU:O	1:F:397:GLU:HG2	2.17	0.43
1:C:318:VAL:HG13	1:C:319:THR:O	2.19	0.43
1:F:199:SER:HB3	3:F:601:NAP:O1N	2.19	0.43
1:C:85:ASN:HD22	1:C:414:PRO:HA	1.83	0.43
1:A:250:GLN:HB3	1:A:274:THR:HB	2.01	0.43
1:F:322:GLU:HG2	1:F:332:ILE:HD13	2.00	0.43
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.80	0.43
1:D:428:ASN:ND2	1:D:430:LYS:H	2.16	0.43
1:D:41:LEU:HD23	1:D:128:GLU:HB3	1.99	0.43
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.99	0.43
1:C:80:LEU:HD23	1:D:80:LEU:HD23	2.00	0.43
1:C:35:ASP:HB2	4:C:614:HOH:O	2.19	0.43
1:F:259:ILE:HD11	1:F:268:LYS:HB2	2.01	0.43
1:C:138:HIS:CG	4:C:613:HOH:O	2.71	0.43
1:A:283:GLU:HG3	4:A:620:HOH:O	2.18	0.43
1:B:292:GLY:C	1:B:293:ARG:HG2	2.39	0.43
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.88	0.43
1:A:309:ILE:HG22	1:A:316:ILE:HG12	2.01	0.43
1:E:90:LEU:HD11	1:F:90:LEU:HD11	2.01	0.42
1:D:163:GLU:HG2	1:D:295:SER:HA	2.01	0.42
1:C:163:GLU:HG2	1:C:295:SER:HA	2.01	0.42
1:F:483:SER:N	4:F:606:HOH:O	2.50	0.42
1:E:41:LEU:HD23	1:E:128:GLU:HB3	2.02	0.42
1:F:496:GLY:N	1:F:497:CYS:HB3	2.34	0.42
1:A:303:GLU:H	1:A:303:GLU:CD	2.21	0.42
1:A:322:GLU:HG2	1:A:332:ILE:CD1	2.50	0.42
1:C:389:LYS:HD2	1:C:389:LYS:HA	1.82	0.42
1:E:470:GLY:O	1:F:344:PRO:HG2	2.20	0.42
1:D:292:GLY:C	1:D:293:ARG:HG2	2.40	0.42
1:C:322:GLU:HG2	1:C:332:ILE:HD13	2.01	0.42
1:E:215:ASP:OD1	1:E:246:LYS:NZ	2.52	0.42
1:B:428:ASN:ND2	1:B:430:LYS:H	2.18	0.42
1:C:332:ILE:HD13	1:C:332:ILE:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.73	0.42
1:A:332:ILE:CD1	1:A:349:ALA:HB1	2.50	0.41
1:E:199:SER:HB3	3:E:601:NAP:O1N	2.20	0.41
1:F:366:ASP:OD2	1:F:457:LYS:HE3	2.20	0.41
1:E:259:ILE:HD11	1:E:268:LYS:HB2	2.02	0.41
1:E:326:VAL:HA	1:E:327:PRO:HD3	1.93	0.41
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.50	0.41
1:B:376:THR:O	1:B:377:PRO:C	2.59	0.41
1:E:168:LEU:HB2	1:E:170:ILE:HG12	2.03	0.41
1:C:46:PRO:CB	1:C:52:ARG:HH12	2.32	0.41
1:A:186:LEU:HA	1:A:187:PRO:HD3	1.81	0.41
1:D:376:THR:O	1:D:377:PRO:C	2.57	0.41
1:E:409:LEU:HD23	1:F:68:LYS:HG2	2.02	0.41
1:A:51:THR:HA	4:A:611:HOH:O	2.19	0.41
1:D:215:ASP:OD1	1:D:246:LYS:NZ	2.53	0.41
1:B:397:GLU:O	1:B:397:GLU:HG2	2.20	0.41
1:D:389:LYS:HD2	1:D:389:LYS:HA	1.82	0.41
1:E:186:LEU:HD11	1:E:188:TYR:CZ	2.55	0.41
1:C:332:ILE:HD12	1:C:349:ALA:CB	2.50	0.41
1:A:29:LYS:HZ3	1:B:498:SEC:SE	2.53	0.41
1:B:91:GLU:CD	1:B:92:ASP:N	2.74	0.41
1:E:376:THR:O	1:E:377:PRO:C	2.59	0.41
1:A:29:LYS:HZ2	1:B:498:SEC:SE	2.54	0.41
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.51	0.41
1:A:496:GLY:H	1:A:497:CYS:HB3	1.85	0.41
1:F:12:ASP:HB3	1:F:13:PHE:CD2	2.56	0.40
1:C:46:PRO:HG3	1:C:52:ARG:CZ	2.50	0.40
1:F:322:GLU:HG2	1:F:332:ILE:CD1	2.51	0.40
1:A:474:VAL:O	1:A:477:GLU:HG2	2.22	0.40
1:C:470:GLY:HA2	1:D:450:GLN:OE1	2.21	0.40
1:A:88:TRP:CZ3	1:B:96:HIS:HB2	2.56	0.40
1:E:344:PRO:HG2	1:F:470:GLY:O	2.21	0.40
1:A:259:ILE:CD1	1:A:268:LYS:HB2	2.51	0.40
1:A:322:GLU:HG2	1:A:332:ILE:HD13	2.02	0.40
1:C:34:PHE:C	4:C:614:HOH:O	2.60	0.40
1:B:399:ILE:HA	1:B:399:ILE:HD13	1.91	0.40
1:F:332:ILE:HD13	1:F:332:ILE:HA	1.81	0.40
1:E:80:LEU:HD13	1:E:94:VAL:HG21	2.04	0.40
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.55	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	487/499 (98%)	460 (94%)	26 (5%)	1 (0%)	52 83
1	B	487/499 (98%)	463 (95%)	24 (5%)	0	100 100
1	C	483/499 (97%)	456 (94%)	26 (5%)	1 (0%)	52 83
1	D	488/499 (98%)	461 (94%)	26 (5%)	1 (0%)	52 83
1	E	487/499 (98%)	462 (95%)	24 (5%)	1 (0%)	52 83
1	F	486/499 (97%)	461 (95%)	25 (5%)	0	100 100
All	All	2918/2994 (98%)	2763 (95%)	151 (5%)	4 (0%)	56 86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	497	CYS
1	D	497	CYS
1	E	497	CYS
1	A	497	CYS

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	405/413 (98%)	381 (94%)	24 (6%)	24 53
1	B	405/413 (98%)	382 (94%)	23 (6%)	25 55
1	C	401/413 (97%)	378 (94%)	23 (6%)	25 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	406/413 (98%)	384 (95%)	22 (5%)	27 58
1	E	405/413 (98%)	383 (95%)	22 (5%)	27 58
1	F	404/413 (98%)	384 (95%)	20 (5%)	30 61
All	All	2426/2478 (98%)	2292 (94%)	134 (6%)	27 56

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	29	LYS
1	A	52	ARG
1	A	64	CYS
1	A	67	LYS
1	A	84	ARG
1	A	91	GLU
1	A	93	THR
1	A	107	ASN
1	A	257	GLU
1	A	274	THR
1	A	279	THR
1	A	303	GLU
1	A	305	VAL
1	A	318	VAL
1	A	332	ILE
1	A	372	THR
1	A	397	GLU
1	A	403	HIS
1	A	416	ARG
1	A	424	LYS
1	A	428	ASN
1	A	494	GLN
1	A	497	CYS
1	B	29	LYS
1	B	64	CYS
1	B	91	GLU
1	B	92	ASP
1	B	93	THR
1	B	107	ASN
1	B	199	SER
1	B	257	GLU
1	B	274	THR

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Mol	Chain	Res	Type
1	B	279	THR
1	B	303	GLU
1	B	305	VAL
1	B	318	VAL
1	B	332	ILE
1	B	372	THR
1	B	376	THR
1	B	397	GLU
1	B	403	HIS
1	B	416	ARG
1	B	424	LYS
1	B	428	ASN
1	B	494	GLN
1	B	495	SER
1	C	29	LYS
1	C	64	CYS
1	C	67	LYS
1	C	84	ARG
1	C	91	GLU
1	C	92	ASP
1	C	93	THR
1	C	107	ASN
1	C	274	THR
1	C	279	THR
1	C	303	GLU
1	C	305	VAL
1	C	318	VAL
1	C	332	ILE
1	C	372	THR
1	C	397	GLU
1	C	403	HIS
1	C	416	ARG
1	C	424	LYS
1	C	428	ASN
1	C	494	GLN
1	C	495	SER
1	C	497	CYS
1	D	29	LYS
1	D	64	CYS
1	D	67	LYS
1	D	84	ARG
1	D	91	GLU

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Mol	Chain	Res	Type
1	D	93	THR
1	D	107	ASN
1	D	199	SER
1	D	274	THR
1	D	279	THR
1	D	303	GLU
1	D	318	VAL
1	D	332	ILE
1	D	372	THR
1	D	397	GLU
1	D	403	HIS
1	D	416	ARG
1	D	424	LYS
1	D	428	ASN
1	D	494	GLN
1	D	495	SER
1	D	497	CYS
1	E	29	LYS
1	E	64	CYS
1	E	67	LYS
1	E	84	ARG
1	E	90	LEU
1	E	91	GLU
1	E	92	ASP
1	E	93	THR
1	E	107	ASN
1	E	274	THR
1	E	279	THR
1	E	303	GLU
1	E	318	VAL
1	E	332	ILE
1	E	372	THR
1	E	397	GLU
1	E	403	HIS
1	E	416	ARG
1	E	424	LYS
1	E	428	ASN
1	E	494	GLN
1	E	497	CYS
1	F	12	ASP
1	F	29	LYS
1	F	64	CYS

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Mol	Chain	Res	Type
1	F	91	GLU
1	F	92	ASP
1	F	93	THR
1	F	107	ASN
1	F	274	THR
1	F	279	THR
1	F	303	GLU
1	F	318	VAL
1	F	332	ILE
1	F	372	THR
1	F	397	GLU
1	F	403	HIS
1	F	416	ARG
1	F	424	LYS
1	F	428	ASN
1	F	494	GLN
1	F	495	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	285	ASN
1	A	428	ASN
1	A	439	HIS
1	A	494	GLN
1	B	72	GLN
1	B	285	ASN
1	B	428	ASN
1	B	439	HIS
1	B	494	GLN
1	C	72	GLN
1	C	285	ASN
1	C	428	ASN
1	C	439	HIS
1	C	494	GLN
1	D	72	GLN
1	D	285	ASN
1	D	428	ASN
1	D	439	HIS
1	E	72	GLN
1	E	285	ASN

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Mol	Chain	Res	Type
1	E	428	ASN
1	E	439	HIS
1	E	494	GLN
1	F	72	GLN
1	F	285	ASN
1	F	428	ASN
1	F	439	HIS
1	F	494	GLN

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

12 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	FAD	A	600	-	48,58,58	1.44	6 (12%)	54,89,89	2.22	10 (18%)
3	NAP	A	601	-	27,34,52	1.31	3 (11%)	35,53,80	2.07	4 (11%)
2	FAD	B	600	-	48,58,58	1.78	6 (12%)	54,89,89	2.15	11 (20%)
3	NAP	B	601	-	27,34,52	1.21	4 (14%)	35,53,80	2.23	4 (11%)
2	FAD	C	600	-	48,58,58	1.57	6 (12%)	54,89,89	2.03	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAP	C	601	-	27,34,52	1.21	2 (7%)	35,53,80	1.94	2 (5%)
2	FAD	D	600	-	48,58,58	1.63	7 (14%)	54,89,89	2.13	10 (18%)
3	NAP	D	601	-	27,34,52	1.32	4 (14%)	35,53,80	2.19	3 (8%)
2	FAD	E	600	-	48,58,58	1.64	8 (16%)	54,89,89	2.00	12 (22%)
3	NAP	E	601	-	27,34,52	1.31	3 (11%)	35,53,80	2.00	2 (5%)
2	FAD	F	600	-	48,58,58	1.50	6 (12%)	54,89,89	2.10	10 (18%)
3	NAP	F	601	-	27,34,52	1.22	2 (7%)	35,53,80	1.98	1 (2%)

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	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	NAP	A	601	-	-	0/20/40/67	0/3/3/5
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	NAP	B	601	-	-	0/20/40/67	0/3/3/5
2	FAD	C	600	-	-	0/30/50/50	0/6/6/6
3	NAP	C	601	-	-	0/20/40/67	0/3/3/5
2	FAD	D	600	-	-	0/30/50/50	0/6/6/6
3	NAP	D	601	-	-	0/20/40/67	0/3/3/5
2	FAD	E	600	-	-	0/30/50/50	0/6/6/6
3	NAP	E	601	-	-	0/20/40/67	0/3/3/5
2	FAD	F	600	-	-	0/30/50/50	0/6/6/6
3	NAP	F	601	-	-	0/20/40/67	0/3/3/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAP	P2B-O3X	-2.28	1.46	1.54
3	B	601	NAP	P2B-O3X	-2.11	1.47	1.54
2	D	600	FAD	C4A-N3A	-2.09	1.32	1.35
2	E	600	FAD	C5A-N7A	-2.03	1.32	1.39
2	E	600	FAD	C10-N10	2.00	1.41	1.39
3	A	601	NAP	P2B-O1X	2.05	1.57	1.51
2	E	600	FAD	C9A-N10	2.11	1.41	1.38
2	D	600	FAD	C4-N3	2.28	1.37	1.33
2	D	600	FAD	C10-N1	2.30	1.39	1.35
3	B	601	NAP	O4B-C1B	2.31	1.44	1.41
2	B	600	FAD	C10-N1	2.37	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAP	PN-O5D	2.38	1.68	1.59
3	E	601	NAP	O4B-C1B	2.39	1.44	1.41
2	A	600	FAD	C10-N10	2.41	1.42	1.39
2	F	600	FAD	C9A-N10	2.47	1.42	1.38
2	A	600	FAD	O4B-C1B	2.49	1.44	1.41
3	C	601	NAP	O4B-C1B	2.52	1.44	1.41
3	D	601	NAP	PN-O5D	2.62	1.69	1.59
2	E	600	FAD	C10-N1	2.71	1.40	1.35
3	D	601	NAP	P2B-O1X	2.77	1.60	1.51
2	E	600	FAD	C5X-N5	2.78	1.39	1.35
2	C	600	FAD	C9A-N10	2.79	1.42	1.38
3	F	601	NAP	O4B-C1B	2.80	1.44	1.41
2	C	600	FAD	O4B-C1B	2.88	1.44	1.41
2	A	600	FAD	C4-N3	2.88	1.38	1.33
3	E	601	NAP	P2B-O1X	2.91	1.60	1.51
2	F	600	FAD	O4B-C1B	2.91	1.44	1.41
2	D	600	FAD	C9A-N10	3.04	1.43	1.38
2	B	600	FAD	C9A-N10	3.14	1.43	1.38
2	E	600	FAD	C4-N3	3.16	1.39	1.33
2	A	600	FAD	C10-N1	3.18	1.40	1.35
3	C	601	NAP	P2B-O1X	3.24	1.61	1.51
3	A	601	NAP	PN-O5D	3.25	1.72	1.59
2	C	600	FAD	C10-N1	3.31	1.41	1.35
2	F	600	FAD	C5X-N5	3.37	1.40	1.35
3	B	601	NAP	P2B-O1X	3.46	1.62	1.51
3	F	601	NAP	P2B-O1X	3.53	1.62	1.51
2	B	600	FAD	C4-N3	3.58	1.39	1.33
3	A	601	NAP	O4B-C1B	3.58	1.45	1.41
2	F	600	FAD	C4-N3	3.59	1.39	1.33
3	E	601	NAP	PN-O5D	3.84	1.74	1.59
3	D	601	NAP	O4B-C1B	3.91	1.46	1.41
2	C	600	FAD	C5X-N5	4.00	1.41	1.35
2	F	600	FAD	C10-N1	4.16	1.42	1.35
2	B	600	FAD	C5X-N5	4.21	1.42	1.35
2	A	600	FAD	C5X-N5	4.24	1.42	1.35
2	C	600	FAD	C4-N3	4.31	1.41	1.33
2	D	600	FAD	C5X-N5	4.31	1.42	1.35
2	A	600	FAD	C4X-N5	4.49	1.40	1.33
2	E	600	FAD	O4B-C1B	4.61	1.47	1.41
2	D	600	FAD	O4B-C1B	4.69	1.47	1.41
2	F	600	FAD	C4X-N5	4.98	1.41	1.33
2	C	600	FAD	C4X-N5	5.15	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C4X-N5	5.31	1.41	1.33
2	D	600	FAD	C4X-N5	5.53	1.42	1.33
2	E	600	FAD	C4X-N5	5.96	1.42	1.33
2	B	600	FAD	O4B-C1B	6.62	1.49	1.41

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	NAP	N3A-C2A-N1A	-11.71	119.93	128.89
3	D	601	NAP	N3A-C2A-N1A	-11.27	120.27	128.89
2	A	600	FAD	N3A-C2A-N1A	-10.45	120.89	128.89
3	A	601	NAP	N3A-C2A-N1A	-10.25	121.04	128.89
3	F	601	NAP	N3A-C2A-N1A	-10.25	121.05	128.89
2	D	600	FAD	N3A-C2A-N1A	-10.18	121.10	128.89
3	E	601	NAP	N3A-C2A-N1A	-10.16	121.11	128.89
3	C	601	NAP	N3A-C2A-N1A	-9.87	121.33	128.89
2	F	600	FAD	N3A-C2A-N1A	-9.71	121.46	128.89
2	C	600	FAD	N3A-C2A-N1A	-9.48	121.64	128.89
2	B	600	FAD	N3A-C2A-N1A	-9.27	121.80	128.89
2	E	600	FAD	N3A-C2A-N1A	-8.07	122.72	128.89
2	E	600	FAD	P-O3P-PA	-3.82	122.00	132.73
2	C	600	FAD	P-O3P-PA	-3.33	123.37	132.73
2	F	600	FAD	P-O3P-PA	-3.30	123.47	132.73
2	B	600	FAD	C5B-C4B-C3B	-3.23	102.41	115.21
2	D	600	FAD	O4B-C1B-N9A	-3.21	101.37	108.10
2	B	600	FAD	C4X-C4-N3	-3.14	119.29	123.59
2	C	600	FAD	O4B-C1B-N9A	-3.09	101.62	108.10
2	A	600	FAD	O4B-C1B-N9A	-3.00	101.82	108.10
2	B	600	FAD	P-O3P-PA	-2.94	124.48	132.73
2	F	600	FAD	O4B-C1B-N9A	-2.92	101.99	108.10
2	A	600	FAD	P-O3P-PA	-2.91	124.57	132.73
2	A	600	FAD	C4X-C4-N3	-2.90	119.62	123.59
2	B	600	FAD	O4B-C1B-N9A	-2.86	102.11	108.10
2	D	600	FAD	P-O3P-PA	-2.80	124.88	132.73
2	C	600	FAD	C4X-C4-N3	-2.72	119.86	123.59
3	D	601	NAP	O5B-PA-O1A	-2.56	99.69	109.62
2	B	600	FAD	O3B-C3B-C4B	-2.55	103.40	111.05
2	E	600	FAD	O3'-C3'-C2'	-2.54	102.36	108.75
2	E	600	FAD	O4B-C1B-N9A	-2.52	102.81	108.10
3	A	601	NAP	C1B-N9A-C4A	-2.43	123.27	126.94
3	D	601	NAP	C4B-O4B-C1B	-2.38	107.11	109.72
2	E	600	FAD	C4A-C5A-N7A	-2.33	107.33	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	600	FAD	C4X-C4-N3	-2.32	120.42	123.59
3	A	601	NAP	C4B-O4B-C1B	-2.31	107.18	109.72
2	B	600	FAD	C4B-O4B-C1B	-2.27	107.23	109.72
2	F	600	FAD	C5B-C4B-C3B	-2.18	106.56	115.21
2	E	600	FAD	C4X-C4-N3	-2.15	120.65	123.59
2	D	600	FAD	C9A-C5X-N5	-2.14	119.19	122.36
2	D	600	FAD	C5B-C4B-C3B	-2.10	106.88	115.21
3	B	601	NAP	O5B-PA-O1A	-2.09	101.51	109.62
2	A	600	FAD	C5B-C4B-C3B	-2.07	106.99	115.21
3	C	601	NAP	O5B-PA-O1A	-2.07	101.59	109.62
2	C	600	FAD	C5B-C4B-C3B	-2.06	107.02	115.21
3	B	601	NAP	C1B-N9A-C4A	-2.06	123.83	126.94
2	A	600	FAD	O4'-C4'-C5'	-2.05	105.72	110.19
2	E	600	FAD	O3B-C3B-C4B	-2.03	104.95	111.05
2	F	600	FAD	C4X-C10-N10	-2.02	119.33	120.52
2	D	600	FAD	O3'-C3'-C2'	-2.01	103.68	108.75
2	C	600	FAD	C9A-C5X-N5	-2.01	119.38	122.36
2	C	600	FAD	C2B-C1B-N9A	2.07	117.45	114.29
3	A	601	NAP	O3X-P2B-O2X	2.09	115.32	107.38
2	E	600	FAD	O2'-C2'-C3'	2.12	114.36	109.02
3	E	601	NAP	O3X-P2B-O2X	2.19	115.71	107.38
2	E	600	FAD	O4'-C4'-C3'	2.20	114.54	109.02
2	C	600	FAD	C5X-C9A-N10	2.20	119.29	117.62
2	F	600	FAD	C5X-C9A-N10	2.29	119.36	117.62
2	A	600	FAD	C5X-C9A-N10	2.31	119.37	117.62
2	F	600	FAD	C2B-C1B-N9A	2.58	118.23	114.29
2	B	600	FAD	C5X-C9A-N10	2.58	119.58	117.62
2	C	600	FAD	C1'-N10-C9A	2.60	121.78	118.86
2	A	600	FAD	C2B-C1B-N9A	2.65	118.34	114.29
2	A	600	FAD	O3P-P-O5'	2.70	110.11	102.94
3	B	601	NAP	O3X-P2B-O2X	2.70	117.67	107.38
2	D	600	FAD	C5X-C9A-N10	2.74	119.70	117.62
2	B	600	FAD	C4X-N5-C5X	2.75	119.92	116.76
2	D	600	FAD	C2B-C1B-N9A	2.76	118.50	114.29
2	E	600	FAD	C5X-C9A-N10	2.79	119.74	117.62
2	E	600	FAD	C4X-N5-C5X	2.92	120.12	116.76
2	D	600	FAD	C4X-N5-C5X	3.02	120.24	116.76
2	B	600	FAD	C2B-C1B-N9A	3.10	119.03	114.29
2	C	600	FAD	C4X-N5-C5X	3.27	120.53	116.76
2	F	600	FAD	C4X-N5-C5X	3.34	120.60	116.76
2	E	600	FAD	C4-N3-C2	6.31	120.70	115.25
2	C	600	FAD	C4-N3-C2	6.33	120.72	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	FAD	C4-N3-C2	6.39	120.77	115.25
2	F	600	FAD	C4-N3-C2	7.00	121.30	115.25
2	B	600	FAD	C4-N3-C2	7.40	121.64	115.25
2	A	600	FAD	C4-N3-C2	7.84	122.02	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAP	1	0
3	B	601	NAP	2	0
3	C	601	NAP	1	0
3	D	601	NAP	1	0
3	E	601	NAP	1	0
3	F	601	NAP	1	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, 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	489/499 (97%)	0.71	40 (8%) 14 9	24, 63, 74, 102	0
1	B	489/499 (97%)	0.62	35 (7%) 18 13	24, 63, 74, 102	0
1	C	485/499 (97%)	1.37	125 (25%) 1 0	24, 63, 74, 103	0
1	D	490/499 (98%)	0.94	61 (12%) 5 3	24, 63, 75, 102	0
1	E	489/499 (97%)	0.82	56 (11%) 6 4	24, 63, 74, 101	0
1	F	488/499 (97%)	1.65	171 (35%) 0 0	24, 63, 74, 101	0
All	All	2930/2994 (97%)	1.02	488 (16%) 2 1	24, 63, 74, 103	0

All (488) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	495	SER	8.9
1	D	497	CYS	8.7
1	D	499	GLY	8.6
1	D	496	GLY	7.6
1	F	297	THR	7.4
1	F	272	LYS	6.4
1	A	10	SER	6.2
1	F	294	ASP	6.2
1	F	394	PHE	6.1
1	F	399	ILE	6.1
1	F	137	PRO	6.0
1	C	151	VAL	5.9
1	F	141	MET	5.8
1	F	358	TYR	5.8
1	F	135	ILE	5.8
1	B	10	SER	5.7
1	C	169	GLY	5.4
1	F	143	THR	5.4
1	C	320	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	311	GLU	5.2
1	F	275	ASN	5.2
1	F	279	THR	5.2
1	F	283	GLU	5.1
1	E	92	ASP	5.1
1	D	394	PHE	5.1
1	F	134	PHE	4.9
1	C	296	CYS	4.9
1	F	92	ASP	4.9
1	F	223	ILE	4.9
1	E	497	CYS	4.9
1	B	499	GLY	4.8
1	B	160	ALA	4.8
1	F	278	GLU	4.8
1	F	268	LYS	4.8
1	F	306	GLY	4.8
1	C	154	ALA	4.8
1	F	261	ALA	4.8
1	F	11	TYR	4.8
1	B	496	GLY	4.8
1	F	37	LYS	4.8
1	C	312	LYS	4.8
1	C	281	GLU	4.7
1	F	142	ALA	4.7
1	F	359	GLY	4.7
1	F	298	ARG	4.7
1	F	34	PHE	4.7
1	C	282	ASP	4.7
1	C	365	CYS	4.7
1	E	496	GLY	4.6
1	E	494	GLN	4.6
1	F	487	ARG	4.6
1	F	52	ARG	4.5
1	F	295	SER	4.5
1	F	35	ASP	4.5
1	F	320	ASP	4.5
1	C	35	ASP	4.5
1	E	499	GLY	4.5
1	F	269	VAL	4.4
1	C	495	SER	4.4
1	F	247	PHE	4.4
1	F	277	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	497	CYS	4.4
1	C	338	GLY	4.4
1	A	311	GLU	4.4
1	C	255	LYS	4.4
1	E	396	GLU	4.3
1	F	361	SER	4.3
1	F	131	TYR	4.3
1	D	288	LEU	4.3
1	F	281	GLU	4.3
1	F	151	VAL	4.3
1	F	397	GLU	4.3
1	E	429	LEU	4.3
1	F	313	THR	4.2
1	E	490	GLY	4.2
1	A	92	ASP	4.2
1	F	132	GLY	4.1
1	C	337	GLU	4.1
1	C	361	SER	4.1
1	C	145	ASN	4.1
1	D	397	GLU	4.1
1	D	429	LEU	4.1
1	D	495	SER	4.1
1	F	360	GLY	4.1
1	C	153	SER	4.1
1	E	430	LYS	4.1
1	A	496	GLY	4.1
1	F	146	LYS	4.0
1	F	319	THR	4.0
1	C	146	LYS	4.0
1	F	144	ASN	4.0
1	C	268	LYS	4.0
1	C	37	LYS	4.0
1	E	491	ASP	4.0
1	F	262	GLY	4.0
1	E	398	ASN	4.0
1	F	36	LYS	4.0
1	A	309	ILE	4.0
1	C	335	ILE	4.0
1	F	492	ILE	4.0
1	F	307	VAL	3.9
1	F	284	PHE	3.9
1	C	364	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	495	SER	3.9
1	D	494	GLN	3.9
1	A	499	GLY	3.9
1	A	205	CYS	3.9
1	F	139	LYS	3.9
1	E	277	GLU	3.8
1	A	495	SER	3.8
1	C	137	PRO	3.8
1	C	141	MET	3.8
1	C	157	PHE	3.8
1	C	295	SER	3.8
1	D	272	LYS	3.8
1	D	17	ILE	3.8
1	F	309	ILE	3.7
1	E	463	GLN	3.7
1	F	274	THR	3.7
1	E	159	ILE	3.7
1	C	297	THR	3.7
1	C	175	GLU	3.7
1	E	397	GLU	3.7
1	C	250	GLN	3.7
1	F	305	VAL	3.6
1	C	256	ILE	3.6
1	C	139	LYS	3.6
1	E	91	GLU	3.6
1	D	287	VAL	3.6
1	F	282	ASP	3.6
1	C	122	GLU	3.6
1	C	135	ILE	3.6
1	F	12	ASP	3.6
1	D	9	LYS	3.5
1	C	302	LEU	3.5
1	F	419	ASN	3.5
1	B	17	ILE	3.5
1	C	306	GLY	3.5
1	C	313	THR	3.5
1	F	316	ILE	3.5
1	B	195	VAL	3.5
1	C	266	ARG	3.5
1	B	18	ILE	3.5
1	A	158	LEU	3.5
1	C	270	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	432	ASN	3.5
1	C	131	TYR	3.5
1	C	152	TYR	3.5
1	F	152	TYR	3.5
1	F	331	ALA	3.5
1	A	91	GLU	3.5
1	C	149	GLU	3.4
1	A	312	LYS	3.4
1	F	494	GLN	3.4
1	F	263	THR	3.4
1	F	400	GLU	3.4
1	F	328	TYR	3.4
1	E	487	ARG	3.4
1	F	398	ASN	3.4
1	F	150	LYS	3.4
1	C	48	PRO	3.4
1	D	312	LYS	3.4
1	C	275	ASN	3.4
1	F	431	ASP	3.4
1	C	497	CYS	3.4
1	C	16	ILE	3.4
1	F	251	PHE	3.3
1	A	494	GLN	3.3
1	F	265	GLY	3.3
1	E	428	ASN	3.3
1	C	360	GLY	3.3
1	C	283	GLU	3.3
1	F	340	LEU	3.3
1	C	148	LYS	3.3
1	C	18	ILE	3.3
1	C	147	GLY	3.3
1	F	496	GLY	3.3
1	E	433	GLU	3.3
1	D	40	VAL	3.3
1	A	288	LEU	3.3
1	C	324	THR	3.2
1	F	248	ILE	3.2
1	B	205	CYS	3.2
1	D	276	SER	3.2
1	F	387	GLU	3.2
1	C	143	THR	3.2
1	F	18	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	430	LYS	3.2
1	B	495	SER	3.2
1	C	257	GLU	3.2
1	F	260	GLU	3.2
1	F	148	LYS	3.2
1	E	17	ILE	3.2
1	E	493	LEU	3.2
1	F	334	ASP	3.2
1	C	274	THR	3.2
1	F	324	THR	3.2
1	B	92	ASP	3.1
1	D	195	VAL	3.1
1	F	497	CYS	3.1
1	C	265	GLY	3.1
1	C	359	GLY	3.1
1	F	276	SER	3.1
1	F	155	GLU	3.1
1	C	307	VAL	3.0
1	C	168	LEU	3.0
1	C	261	ALA	3.0
1	C	397	GLU	3.0
1	C	140	ILE	3.0
1	C	170	ILE	3.0
1	F	249	ARG	3.0
1	B	169	GLY	3.0
1	F	266	ARG	3.0
1	D	35	ASP	3.0
1	C	202	ALA	3.0
1	E	362	THR	3.0
1	F	254	THR	3.0
1	F	280	ILE	3.0
1	E	391	VAL	3.0
1	F	436	VAL	3.0
1	B	11	TYR	3.0
1	D	289	LEU	3.0
1	F	499	GLY	3.0
1	D	18	ILE	2.9
1	C	356	ARG	2.9
1	C	267	LEU	2.9
1	D	205	CYS	2.9
1	D	196	VAL	2.9
1	C	322	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	488	SER	2.9
1	A	202	ALA	2.9
1	D	459	GLY	2.9
1	F	169	GLY	2.9
1	B	52	ARG	2.9
1	D	160	ALA	2.9
1	A	317	PRO	2.9
1	F	335	ILE	2.9
1	E	427	CYS	2.9
1	F	308	LYS	2.9
1	E	261	ALA	2.9
1	C	284	PHE	2.9
1	F	140	ILE	2.9
1	F	486	LYS	2.9
1	B	158	LEU	2.9
1	D	28	ALA	2.9
1	E	394	PHE	2.9
1	F	267	LEU	2.8
1	C	354	ALA	2.8
1	C	46	PRO	2.8
1	F	250	GLN	2.8
1	D	27	ALA	2.8
1	C	278	GLU	2.8
1	F	395	GLY	2.8
1	F	149	GLU	2.8
1	D	203	LEU	2.8
1	D	161	THR	2.8
1	F	175	GLU	2.8
1	C	144	ASN	2.8
1	F	176	TYR	2.8
1	A	195	VAL	2.8
1	F	171	PRO	2.8
1	F	167	TYR	2.7
1	F	13	PHE	2.7
1	F	93	THR	2.7
1	C	272	LYS	2.7
1	C	260	GLU	2.7
1	C	317	PRO	2.7
1	D	251	PHE	2.7
1	C	163	GLU	2.7
1	A	147	GLY	2.7
1	C	132	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	339	LYS	2.7
1	D	19	GLY	2.7
1	F	130	ALA	2.7
1	F	337	GLU	2.7
1	E	492	ILE	2.7
1	F	459	GLY	2.7
1	F	293	ARG	2.7
1	E	399	ILE	2.7
1	F	314	GLY	2.7
1	D	202	ALA	2.7
1	F	219	MET	2.7
1	D	91	GLU	2.6
1	F	270	THR	2.6
1	F	45	THR	2.6
1	D	41	LEU	2.6
1	D	92	ASP	2.6
1	C	330	TYR	2.6
1	E	365	CYS	2.6
1	B	19	GLY	2.6
1	F	390	ALA	2.6
1	D	194	LEU	2.6
1	F	362	THR	2.6
1	A	203	LEU	2.6
1	C	328	TYR	2.6
1	E	400	GLU	2.6
1	F	389	LYS	2.6
1	C	259	ILE	2.6
1	A	160	ALA	2.6
1	C	142	ALA	2.6
1	F	428	ASN	2.6
1	F	491	ASP	2.6
1	C	323	GLN	2.6
1	C	303	GLU	2.6
1	A	17	ILE	2.6
1	C	34	PHE	2.6
1	D	201	VAL	2.6
1	D	24	GLY	2.5
1	D	25	LEU	2.5
1	D	277	GLU	2.5
1	E	223	ILE	2.5
1	A	11	TYR	2.5
1	C	276	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	39	MET	2.5
1	C	134	PHE	2.5
1	D	178	ILE	2.5
1	F	145	ASN	2.5
1	C	155	GLU	2.5
1	E	278	GLU	2.5
1	F	252	VAL	2.5
1	C	331	ALA	2.5
1	A	430	LYS	2.5
1	F	256	ILE	2.5
1	F	302	LEU	2.5
1	C	176	TYR	2.5
1	C	15	LEU	2.4
1	E	90	LEU	2.4
1	D	290	ALA	2.4
1	C	45	THR	2.4
1	C	166	ARG	2.4
1	E	434	ARG	2.4
1	C	262	GLY	2.4
1	F	323	GLN	2.4
1	B	194	LEU	2.4
1	F	114	TRP	2.4
1	F	259	ILE	2.4
1	C	334	ASP	2.4
1	F	241	GLU	2.4
1	F	392	GLU	2.4
1	C	332	ILE	2.4
1	E	18	ILE	2.4
1	F	172	GLY	2.4
1	A	432	ASN	2.4
1	D	242	GLU	2.4
1	E	205	CYS	2.4
1	B	206	ALA	2.4
1	C	44	VAL	2.4
1	C	383	CYS	2.4
1	F	22	SER	2.4
1	C	294	ASP	2.4
1	E	364	LYS	2.4
1	D	23	GLY	2.4
1	B	40	VAL	2.4
1	F	322	GLU	2.4
1	F	327	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	360	GLY	2.4
1	D	206	ALA	2.4
1	C	17	ILE	2.4
1	C	304	THR	2.4
1	F	14	ASP	2.4
1	C	43	PHE	2.3
1	F	352	LEU	2.3
1	A	497	CYS	2.3
1	F	296	CYS	2.3
1	A	90	LEU	2.3
1	B	21	GLY	2.3
1	F	354	ALA	2.3
1	C	376	THR	2.3
1	C	123	LYS	2.3
1	C	298	ARG	2.3
1	F	228	PHE	2.3
1	C	160	ALA	2.3
1	E	11	TYR	2.3
1	F	355	GLN	2.3
1	C	263	THR	2.3
1	F	438	PHE	2.3
1	B	159	ILE	2.3
1	C	52	ARG	2.3
1	E	183	LEU	2.3
1	F	157	PHE	2.3
1	A	206	ALA	2.3
1	F	432	ASN	2.3
1	C	248	ILE	2.3
1	E	93	THR	2.3
1	E	366	ASP	2.3
1	F	341	GLU	2.3
1	A	362	THR	2.3
1	F	147	GLY	2.3
1	A	320	ASP	2.3
1	D	16	ILE	2.3
1	C	158	LEU	2.2
1	D	158	LEU	2.2
1	C	121	ARG	2.2
1	D	197	GLY	2.2
1	B	135	ILE	2.2
1	F	15	LEU	2.2
1	A	35	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	226	ARG	2.2
1	B	494	GLN	2.2
1	D	193	THR	2.2
1	F	372	THR	2.2
1	F	41	LEU	2.2
1	D	10	SER	2.2
1	C	362	THR	2.2
1	C	116	TYR	2.2
1	F	365	CYS	2.2
1	A	19	GLY	2.2
1	F	136	GLY	2.2
1	B	161	THR	2.2
1	D	398	ASN	2.2
1	E	202	ALA	2.2
1	A	201	VAL	2.2
1	F	257	GLU	2.2
1	C	19	GLY	2.2
1	F	403	HIS	2.2
1	E	40	VAL	2.2
1	F	42	ASP	2.2
1	F	196	VAL	2.2
1	A	394	PHE	2.2
1	C	367	TYR	2.2
1	D	21	GLY	2.2
1	F	264	PRO	2.2
1	D	26	ALA	2.2
1	F	231	ASP	2.2
1	B	41	LEU	2.1
1	C	21	GLY	2.1
1	B	155	GLU	2.1
1	F	315	LYS	2.1
1	F	348	GLN	2.1
1	F	463	GLN	2.1
1	A	289	LEU	2.1
1	D	399	ILE	2.1
1	F	338	GLY	2.1
1	C	187	PRO	2.1
1	B	396	GLU	2.1
1	A	124	LYS	2.1
1	F	21	GLY	2.1
1	F	273	SER	2.1
1	F	166	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	389	LYS	2.1
1	E	461	THR	2.1
1	A	18	ILE	2.1
1	E	16	ILE	2.1
1	F	405	PHE	2.1
1	B	148	LYS	2.1
1	C	138	HIS	2.1
1	D	127	TYR	2.1
1	C	49	LEU	2.1
1	F	227	GLY	2.1
1	F	493	LEU	2.1
1	A	159	ILE	2.1
1	A	337	GLU	2.1
1	B	311	GLU	2.1
1	E	89	LYS	2.1
1	F	253	PRO	2.1
1	D	402	TYR	2.1
1	C	130	ALA	2.1
1	B	172	GLY	2.1
1	C	220	VAL	2.1
1	C	258	GLN	2.1
1	F	17	ILE	2.1
1	B	20	GLY	2.1
1	C	205	CYS	2.1
1	F	427	CYS	2.1
1	F	161	THR	2.0
1	A	308	LYS	2.0
1	C	316	ILE	2.0
1	D	159	ILE	2.0
1	F	48	PRO	2.0
1	F	95	LYS	2.0
1	E	24	GLY	2.0
1	B	202	ALA	2.0
1	D	22	SER	2.0
1	D	376	THR	2.0
1	C	293	ARG	2.0
1	D	257	GLU	2.0
1	E	469	ILE	2.0
1	E	312	LYS	2.0
1	A	204	GLU	2.0
1	E	363	VAL	2.0
1	F	38	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	16	ILE	2.0
1	C	20	GLY	2.0
1	B	272	LYS	2.0
1	E	288	LEU	2.0
1	B	287	VAL	2.0
1	E	279	THR	2.0
1	D	491	ASP	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAP	F	601	32/48	0.82	0.31	0.19	64,74,99,100	0
2	FAD	F	600	53/53	0.81	0.27	-0.11	60,64,70,71	0
3	NAP	C	601	32/48	0.82	0.26	-0.23	64,74,99,100	0
2	FAD	E	600	53/53	0.95	0.22	-0.30	60,64,70,71	0
2	FAD	C	600	53/53	0.84	0.25	-0.48	60,64,70,71	0
2	FAD	D	600	53/53	0.96	0.24	-0.56	60,64,70,72	0
2	FAD	B	600	53/53	0.95	0.18	-0.82	60,64,70,72	0
3	NAP	E	601	32/48	0.88	0.19	-0.87	64,74,99,100	0
3	NAP	D	601	32/48	0.90	0.20	-0.96	64,74,99,100	0
2	FAD	A	600	53/53	0.95	0.17	-1.12	60,64,70,71	0
3	NAP	B	601	32/48	0.91	0.19	-1.15	64,74,99,100	0
3	NAP	A	601	32/48	0.93	0.16	-1.63	64,74,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.