Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:55 PM GMT

PDB ID	:	4DUG
Title	:	Crystal Structure of Circadian Clock Protein KaiC E318A Mutant
Authors	:	Egli, M.; Mori, T.; Pattanayek, R.; Xu, Y.; Qin, X.; Johnson, C.H.
Deposited on	:	2012-02-21
Resolution	:	3.29 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:

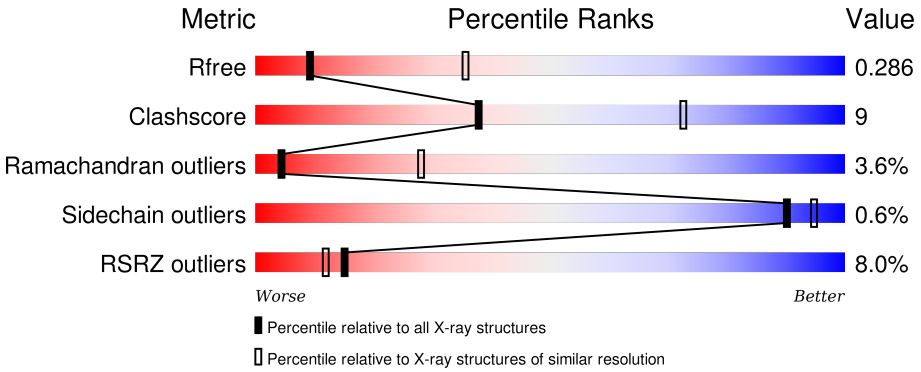
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.29 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	519	11% 74% 23%
1	B	519	7% 67% 28%
1	C	519	8% 74% 21%
1	E	519	6% 69% 27%
1	F	519	8% 69% 27%

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Mol	Chain	Length	Quality of chain
2	D	519	7% 74% 21%

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
3	MG	A	804	-	-	-	X
3	MG	D	601	-	-	-	X
3	MG	F	604	-	-	-	X
5	PO4	C	605	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24157 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 Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3986	2507	701	762	1	15			
1	B	498	Total	C	N	O	P	S	0	0	0
			3925	2471	691	747	1	15			
1	C	497	Total	C	N	O	P	S	0	0	0
			3921	2469	690	746	1	15			
1	E	501	Total	C	N	O	P	S	0	0	0
			3944	2483	692	753	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3986	2507	701	762	1	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4
B	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4
C	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4
E	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4
F	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	500	Total	C	N	O	S	0	0	0
			3937	2481	694	747	15			

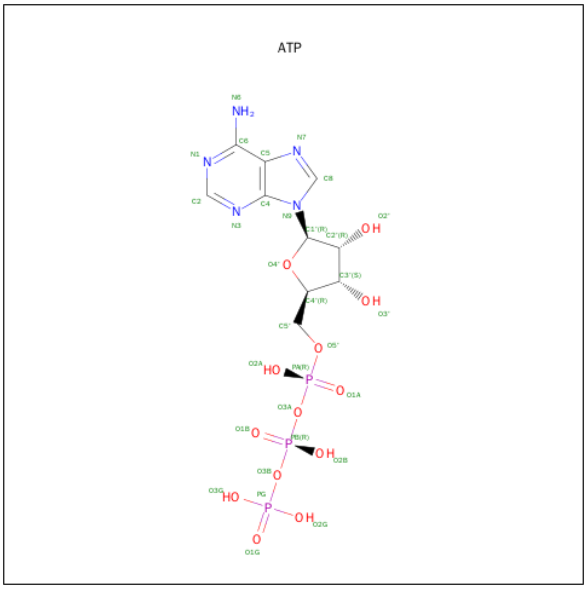
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	318	ALA	GLU	ENGINEERED MUTATION	UNP Q79PF4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	F	2	Total Mg 2 2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0
4	C	1	Total C N O P 31 10 5 13 3	0	0

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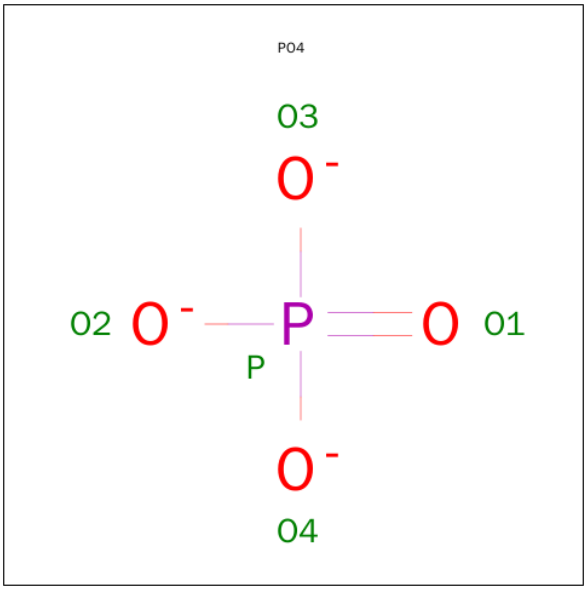
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		

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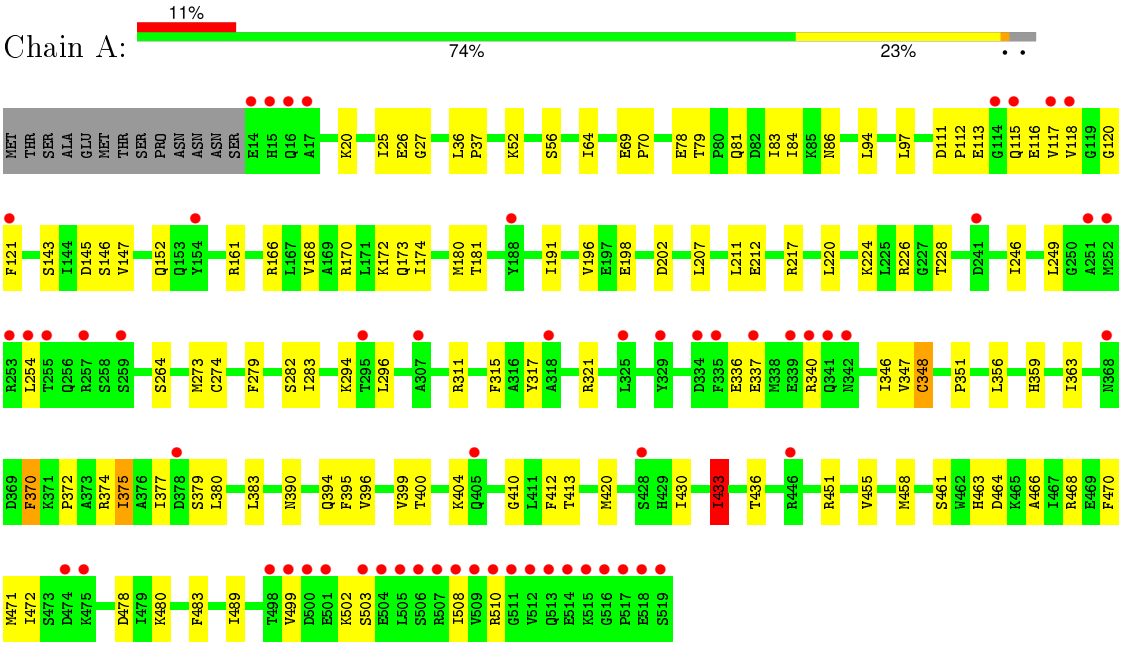
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	11	Total O 11 11	0	0
6	C	12	Total O 12 12	0	0
6	D	14	Total O 14 14	0	0
6	E	15	Total O 15 15	0	0
6	F	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

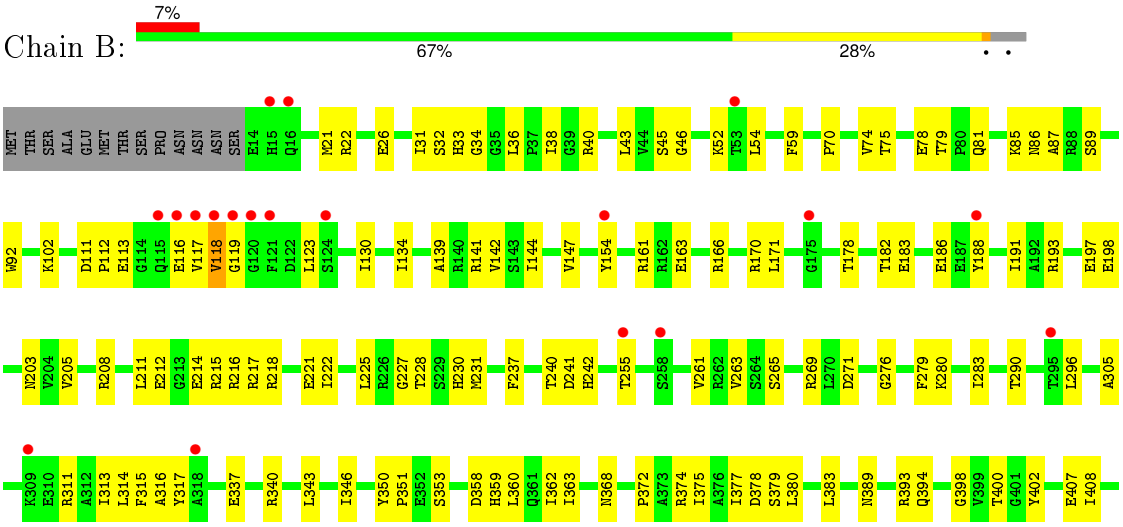
- Molecule 1: Circadian clock protein kinase kaiC

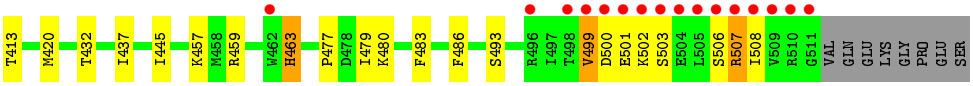
Chain A:



- Molecule 1: Circadian clock protein kinase kaiC

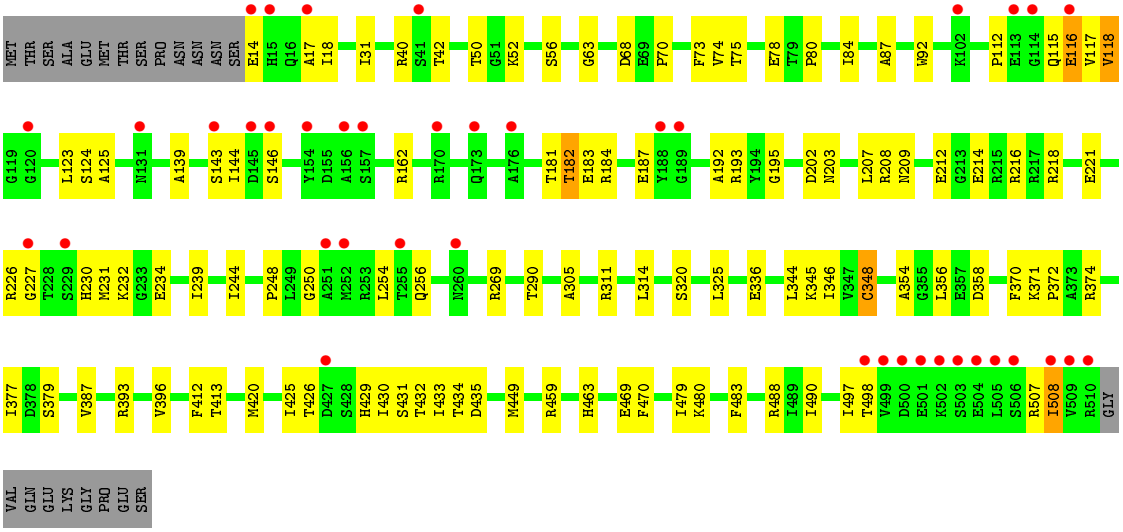
Chain B:





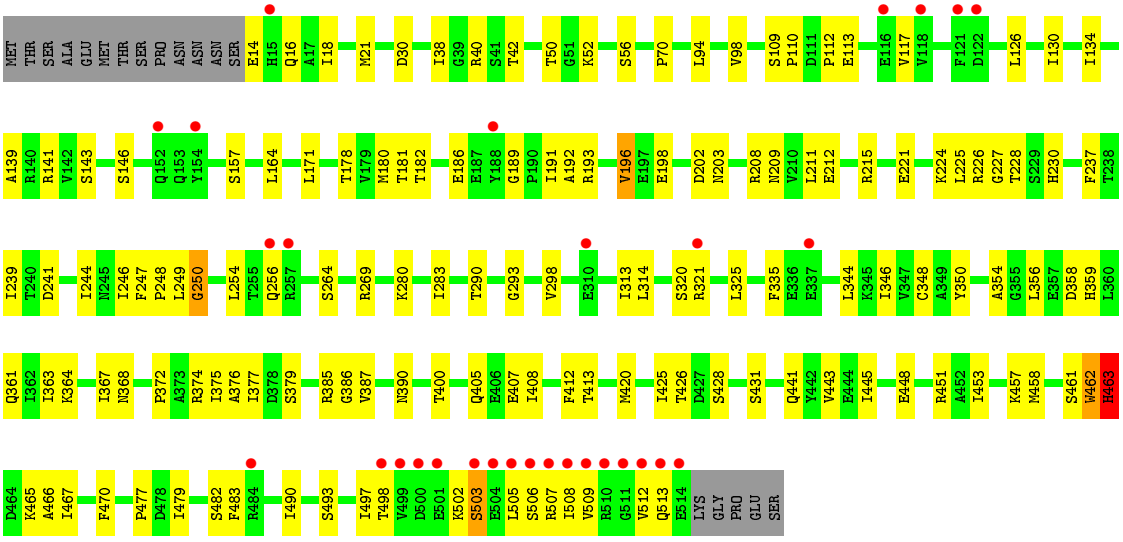
• Molecule 1: Circadian clock protein kinase kaiC

Chain C:



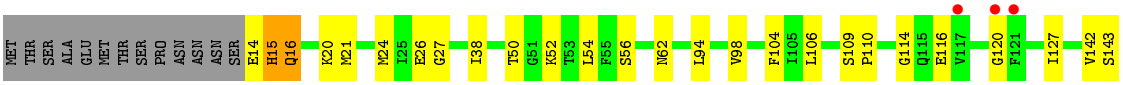
• Molecule 1: Circadian clock protein kinase kaiC

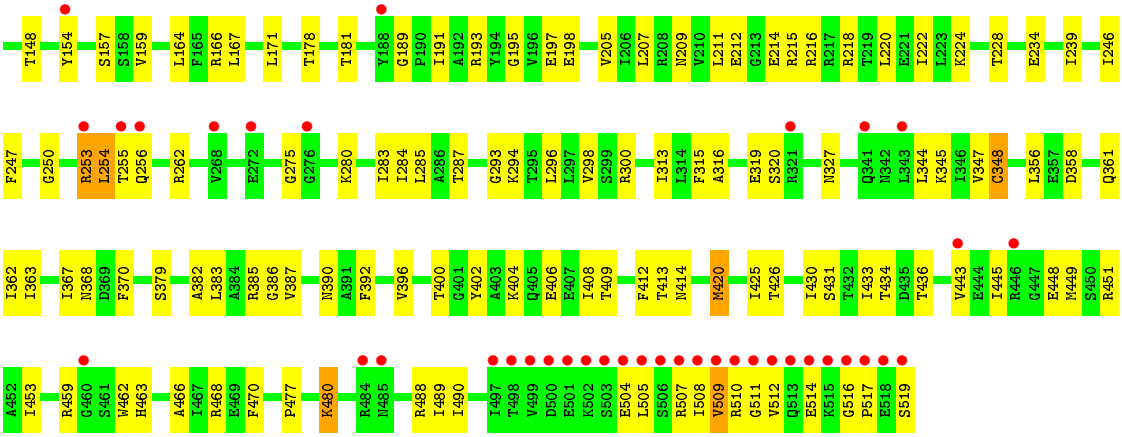
Chain E:



• Molecule 1: Circadian clock protein kinase kaiC

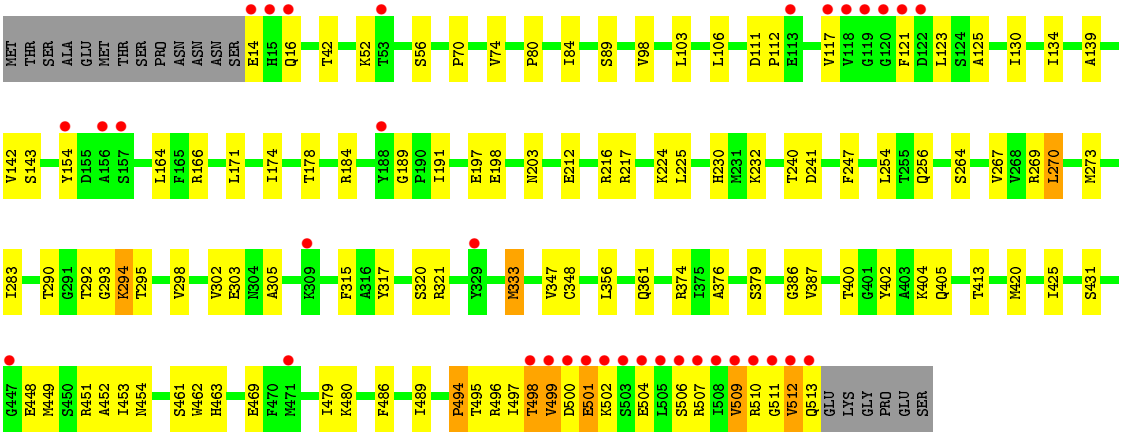
Chain F:





• Molecule 2: Circadian clock protein kinase kaiC

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.71Å 135.06Å 204.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.05 – 3.29 30.05 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.05-3.29) 83.4 (30.05-3.29)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.245 , 0.303 0.230 , 0.286	Depositor DCC
R_{free} test set	2342 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.5	EDS
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 50544 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24157	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: TPO, MG, PO4, ATP

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	0.22	0/4040	0.41	0/5440
1	B	0.22	0/3978	0.41	0/5358
1	C	0.22	0/3974	0.40	0/5353
1	E	0.22	0/3997	0.42	0/5385
1	F	0.22	0/4040	0.42	0/5440
2	D	0.23	0/4002	0.44	0/5393
All	All	0.22	0/24031	0.42	0/32369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3986	0	3982	72	0
1	B	3925	0	3926	97	0
1	C	3921	0	3922	66	0
1	E	3944	0	3937	84	0
1	F	3986	0	3981	89	0
2	D	3937	0	3943	79	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	62	0	24	4	0
4	B	62	0	24	3	0
4	C	62	0	24	1	0
4	D	62	0	24	5	0
4	E	62	0	24	3	0
4	F	62	0	24	5	0
5	C	5	0	0	0	0
6	A	12	0	0	0	0
6	B	11	0	0	0	0
6	C	12	0	0	0	0
6	D	14	0	0	0	0
6	E	15	0	0	0	0
6	F	5	0	0	1	0
All	All	24157	0	23835	442	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 9.

All (442) 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:B:240:THR:HG23	1:B:242:HIS:H	1.12	1.11
1:B:240:THR:HG23	1:B:242:HIS:N	1.88	0.89
2:D:379:SER:H	2:D:413:THR:HB	1.40	0.87
1:E:379:SER:H	1:E:413:THR:HB	1.40	0.86
1:B:502:LYS:H	1:B:503:SER:HA	1.40	0.82
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.66	0.76
1:C:379:SER:H	1:C:413:THR:HB	1.49	0.76
1:E:458:MET:HG2	1:E:461:SER:HB3	1.66	0.76
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.66	0.76
1:E:512:VAL:HA	1:E:513:GLN:HB2	1.69	0.74
1:E:146:SER:H	1:E:181:THR:HB	1.53	0.73
2:D:500:ASP:H	2:D:501:GLU:HA	1.54	0.72
1:B:506:SER:HA	1:B:507:ARG:HB2	1.72	0.71
1:B:171:LEU:HD13	1:B:178:THR:HG21	1.73	0.70
1:F:218:ARG:HH21	1:F:239:ILE:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.74	0.69
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.75	0.68
1:A:321:ARG:HD2	1:B:255:THR:HG23	1.75	0.68
1:F:209:ASN:O	1:F:216:ARG:NH1	2.26	0.68
1:A:466:ALA:HA	1:F:448:GLU:HA	1.74	0.68
1:E:256:GLN:HG3	1:E:405:GLN:HB3	1.76	0.68
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.76	0.67
2:D:321:ARG:NH1	2:D:347:VAL:O	2.28	0.67
1:B:86:ASN:HA	1:C:18:ILE:HD11	1.76	0.67
1:F:142:VAL:HB	1:F:178:THR:HG22	1.77	0.67
1:E:364:LYS:O	1:E:368:ASN:ND2	2.28	0.66
1:C:123:LEU:O	1:C:125:ALA:N	2.28	0.66
1:B:21:MET:HB2	1:B:38:ILE:HG12	1.77	0.66
2:D:495:THR:HG22	2:D:497:ILE:H	1.61	0.65
2:D:290:THR:HG21	1:E:431:SER:HB2	1.77	0.65
2:D:171:LEU:HD13	2:D:178:THR:HG21	1.79	0.65
1:E:208:ARG:NH2	1:E:221:GLU:OE2	2.29	0.65
1:E:40:ARG:NH1	1:E:226:ARG:O	2.30	0.64
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.79	0.64
1:B:379:SER:H	1:B:413:THR:HB	1.62	0.64
1:E:453:ILE:HG21	1:E:479:ILE:HD12	1.80	0.63
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.81	0.63
1:F:287:THR:HG21	1:F:425:ILE:HG23	1.80	0.63
1:A:170:ARG:NH1	1:A:173:GLN:OE1	2.31	0.63
1:B:316:ALA:HA	1:B:378:ASP:HB3	1.81	0.63
1:B:372:PRO:HG2	1:B:408:ILE:HD13	1.80	0.62
2:D:509:VAL:HG22	2:D:510:ARG:HB3	1.81	0.62
1:B:280:LYS:NZ	1:B:407:GLU:OE2	2.32	0.62
1:E:482:SER:OG	1:E:483:PHE:N	2.32	0.62
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.81	0.62
1:C:425:ILE:HG22	1:C:426:THR:HG23	1.82	0.62
1:F:468:ARG:NH1	1:F:480:LYS:O	2.34	0.61
1:C:497:ILE:HG23	1:C:498:THR:H	1.65	0.61
1:F:171:LEU:HD13	1:F:178:THR:HG21	1.81	0.61
1:B:493:SER:HB3	1:C:488:ARG:HG2	1.82	0.61
1:B:315:PHE:HE2	1:B:375:ILE:HD11	1.65	0.61
1:A:20:LYS:HE3	1:A:228:THR:HG21	1.82	0.61
2:D:512:VAL:HA	2:D:513:GLN:HB2	1.82	0.60
2:D:449:MET:HG2	1:E:467:ILE:HD11	1.83	0.60
1:A:283:ILE:HG12	1:A:404:LYS:HE3	1.83	0.60
2:D:451:ARG:NH2	4:D:602:ATP:O2'	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:ILE:HG13	1:F:470:PHE:CD1	2.37	0.59
1:E:14:GLU:HG3	1:E:16:GLN:H	1.68	0.59
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.85	0.59
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.83	0.59
1:C:146:SER:H	1:C:181:THR:HB	1.67	0.59
2:D:500:ASP:H	2:D:502:LYS:HB2	1.68	0.58
1:E:290:THR:HG21	1:F:431:SER:HB2	1.84	0.58
1:F:379:SER:H	1:F:413:THR:HB	1.68	0.58
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.84	0.58
1:B:32:SER:O	1:B:34:GLY:N	2.37	0.57
2:D:501:GLU:HA	2:D:502:LYS:HB2	1.84	0.57
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.36	0.57
1:E:56:SER:HB2	1:E:143:SER:HB3	1.87	0.57
1:C:432:TPO:O	1:C:434:THR:N	2.38	0.57
1:F:294:LYS:N	4:F:602:ATP:O2B	2.38	0.57
1:C:508:ILE:HG21	1:E:512:VAL:HB	1.85	0.57
1:C:396:VAL:HG11	1:C:430:ILE:HG21	1.85	0.57
1:B:368:ASN:ND2	1:B:402:TYR:OH	2.33	0.57
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.70	0.57
1:E:448:GLU:HG2	1:F:466:ALA:HA	1.86	0.56
1:F:256:GLN:HG2	1:F:404:LYS:HB3	1.87	0.56
1:F:14:GLU:N	6:F:702:HOH:O	2.38	0.56
1:F:21:MET:HB2	1:F:38:ILE:HG12	1.86	0.56
1:C:42:THR:HA	1:C:203:ASN:HB2	1.87	0.56
1:A:346:ILE:HG22	1:A:348:CYS:HB2	1.87	0.56
1:F:283:ILE:HG13	1:F:400:THR:HG23	1.88	0.56
1:B:315:PHE:HB2	1:B:377:ILE:HD13	1.87	0.56
1:B:227:GLY:O	1:B:228:THR:HG23	2.05	0.56
1:F:382:ALA:HA	1:F:385:ARG:HE	1.71	0.56
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.88	0.56
1:A:52:LYS:N	4:A:803:ATP:O2B	2.40	0.55
1:B:111:ASP:O	1:B:113:GLU:N	2.40	0.55
2:D:298:VAL:O	2:D:302:VAL:HG23	2.06	0.55
1:C:182:THR:HG22	1:C:183:GLU:H	1.71	0.55
1:E:359:HIS:O	1:E:363:ILE:HG12	2.06	0.55
1:C:344:LEU:HD22	1:C:345:LYS:N	2.22	0.55
1:B:263:VAL:HB	1:B:374:ARG:HH21	1.72	0.55
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.88	0.55
1:A:118:VAL:HG23	1:A:118:VAL:O	2.07	0.55
2:D:142:VAL:HB	2:D:178:THR:HG22	1.89	0.54
2:D:294:LYS:HG2	2:D:413:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:ASP:N	2:D:501:GLU:HA	2.21	0.54
1:C:344:LEU:HD22	1:C:345:LYS:H	1.72	0.54
1:B:87:ALA:HB1	1:B:92:TRP:HE1	1.72	0.54
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.89	0.54
1:A:79:THR:HG22	1:A:81:GLN:HG2	1.89	0.54
1:A:471:MET:HG2	1:A:478:ASP:HB3	1.88	0.54
1:F:20:LYS:HE3	1:F:228:THR:HG21	1.90	0.54
1:E:502:LYS:HG3	1:E:503:SER:H	1.73	0.54
1:B:216:ARG:NE	1:C:221:GLU:OE1	2.36	0.54
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.90	0.54
1:A:146:SER:H	1:A:181:THR:HB	1.73	0.54
1:E:21:MET:HE1	1:E:141:ARG:HG2	1.91	0.54
1:B:240:THR:HG23	1:B:241:ASP:N	2.24	0.53
1:E:375:ILE:HG12	1:E:408:ILE:HG21	1.89	0.53
1:B:290:THR:HG21	1:C:431:SER:HB2	1.90	0.53
4:A:802:ATP:O2'	1:B:463:HIS:NE2	2.42	0.53
1:B:240:THR:CG2	1:B:242:HIS:H	2.02	0.53
1:A:217:ARG:NE	1:F:214:GLU:OE2	2.41	0.53
1:B:502:LYS:N	1:B:503:SER:HA	2.10	0.53
1:E:283:ILE:HG12	1:E:400:THR:HG23	1.90	0.53
2:D:14:GLU:HG3	2:D:16:GLN:H	1.74	0.53
1:A:451:ARG:NH2	4:A:802:ATP:O2'	2.41	0.53
2:D:451:ARG:HH21	1:E:465:LYS:HE3	1.74	0.52
2:D:240:THR:OG1	2:D:241:ASP:N	2.41	0.52
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.92	0.52
1:E:215:ARG:NH2	1:F:234:GLU:O	2.43	0.52
1:F:509:VAL:O	1:F:511:GLY:N	2.43	0.52
1:F:253:ARG:O	1:F:255:THR:N	2.41	0.52
1:B:86:ASN:OD1	1:C:40:ARG:NH2	2.41	0.52
1:C:31:ILE:HG23	1:C:231:MET:HB2	1.91	0.52
1:B:205:VAL:HG22	1:B:222:ILE:HG12	1.91	0.52
1:E:280:LYS:NZ	1:E:407:GLU:OE1	2.40	0.52
1:E:248:PRO:O	1:E:250:GLY:N	2.42	0.52
1:B:337:GLU:HA	1:B:340:ARG:HD2	1.90	0.52
1:E:193:ARG:NH2	1:F:195:GLY:O	2.28	0.52
4:A:802:ATP:O3G	1:B:459:ARG:NH2	2.38	0.52
4:C:603:ATP:O3G	2:D:224:LYS:NZ	2.40	0.52
1:A:436:THR:HG23	1:A:458:MET:HG2	1.92	0.52
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.75	0.52
1:C:214:GLU:OE2	2:D:217:ARG:NH1	2.43	0.51
2:D:452:ALA:HA	2:D:469:GLU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:HB3	1:B:346:ILE:HG22	1.92	0.51
1:B:182:THR:HG22	1:B:183:GLU:H	1.75	0.51
1:F:157:SER:O	1:F:159:VAL:N	2.41	0.51
1:B:85:LYS:HE3	1:C:18:ILE:HG13	1.93	0.51
1:A:86:ASN:OD1	1:B:40:ARG:NH2	2.44	0.51
1:B:393:ARG:NH2	1:B:432:TPO:O2P	2.43	0.51
1:A:254:LEU:HG	1:F:320:SER:HA	1.92	0.51
2:D:121:PHE:HD1	2:D:125:ALA:HB2	1.76	0.51
1:F:430:ILE:HG23	1:F:433:ILE:HD12	1.93	0.51
4:D:602:ATP:HO2'	1:E:463:HIS:CD2	2.29	0.51
1:B:87:ALA:HB1	1:B:92:TRP:NE1	2.26	0.51
2:D:425:ILE:H	2:D:425:ILE:HD12	1.75	0.51
1:A:264:SER:O	1:A:374:ARG:NH2	2.44	0.51
1:E:126:LEU:O	1:E:130:ILE:HG12	2.11	0.51
1:B:225:LEU:HB3	1:B:228:THR:OG1	2.10	0.50
1:B:43:LEU:O	1:B:205:VAL:N	2.38	0.50
2:D:42:THR:HA	2:D:203:ASN:HB2	1.93	0.50
1:F:451:ARG:NH2	4:F:602:ATP:O3'	2.44	0.50
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.77	0.50
1:B:186:GLU:HG3	1:B:188:TYR:H	1.76	0.50
1:E:507:ARG:HG2	1:E:508:ILE:H	1.76	0.50
1:A:27:GLY:HA3	1:A:246:ILE:HB	1.93	0.50
1:A:396:VAL:HG21	1:A:430:ILE:HG21	1.93	0.50
1:E:505:LEU:HB3	1:E:506:SER:HB2	1.94	0.50
2:D:247:PHE:HZ	2:D:361:GLN:HB2	1.76	0.50
1:A:84:ILE:HG12	1:A:94:LEU:HB2	1.94	0.50
1:A:379:SER:H	1:A:413:THR:HB	1.76	0.50
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.94	0.50
1:E:441:GLN:HE22	1:E:490:ILE:HD13	1.77	0.49
2:D:256:GLN:HG3	2:D:404:LYS:HB3	1.93	0.49
1:C:116:GLU:O	1:C:118:VAL:N	2.39	0.49
1:F:54:LEU:HD23	1:F:239:ILE:HD12	1.94	0.49
1:F:283:ILE:HD12	1:F:412:PHE:HE2	1.77	0.49
1:C:230:HIS:CE1	1:C:232:LYS:HG3	2.47	0.49
1:A:315:PHE:HB2	1:A:377:ILE:HG13	1.95	0.49
1:E:320:SER:HA	1:F:254:LEU:HG	1.93	0.49
1:B:360:LEU:HD11	1:B:398:GLY:HA3	1.93	0.49
1:B:89:SER:HB2	4:B:603:ATP:HN61	1.77	0.49
1:A:224:LYS:NZ	4:F:603:ATP:O1G	2.32	0.49
1:F:443:VAL:HG12	1:F:445:ILE:HG13	1.95	0.49
1:E:182:THR:HG21	1:E:192:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:CYS:HB3	2:D:254:LEU:HB2	1.94	0.49
1:B:227:GLY:O	1:B:228:THR:CG2	2.60	0.49
1:E:363:ILE:O	1:E:367:ILE:HG12	2.12	0.49
1:F:262:ARG:NH1	1:F:275:GLY:O	2.46	0.49
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.95	0.49
1:F:396:VAL:HG11	1:F:430:ILE:HG21	1.95	0.49
4:B:602:ATP:O3G	1:C:459:ARG:NH2	2.46	0.49
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.94	0.49
1:E:264:SER:O	1:E:374:ARG:NH2	2.44	0.49
1:A:64:ILE:HD12	1:A:97:LEU:HD13	1.95	0.48
1:B:79:THR:OG1	1:B:81:GLN:OE1	2.31	0.48
1:B:45:SER:HB3	1:B:182:THR:HB	1.94	0.48
2:D:315:PHE:HB3	2:D:317:TYR:HE1	1.77	0.48
2:D:320:SER:HA	1:E:254:LEU:HG	1.94	0.48
4:E:603:ATP:O1G	1:F:224:LYS:NZ	2.46	0.48
1:F:56:SER:HB2	1:F:143:SER:HB3	1.95	0.48
1:E:313:ILE:HG13	1:E:372:PRO:HB3	1.95	0.48
1:F:414:ASN:HD22	1:F:426:THR:HG22	1.79	0.48
1:F:296:LEU:N	4:F:602:ATP:O1A	2.46	0.48
1:F:16:GLN:HB3	1:F:228:THR:HG22	1.95	0.48
1:F:363:ILE:O	1:F:367:ILE:HG12	2.13	0.48
1:C:354:ALA:HB1	1:C:358:ASP:HB2	1.95	0.48
2:D:509:VAL:HG13	2:D:510:ARG:HG2	1.96	0.48
1:F:247:PHE:HZ	1:F:361:GLN:HB2	1.78	0.48
2:D:216:ARG:NE	1:E:221:GLU:OE1	2.34	0.48
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.95	0.48
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.96	0.47
1:E:502:LYS:HD2	1:E:502:LYS:HA	1.72	0.47
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.96	0.47
1:A:56:SER:HB2	1:A:143:SER:HB3	1.95	0.47
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.95	0.47
1:B:437:ILE:HD13	1:B:457:LYS:HD3	1.96	0.47
1:E:377:ILE:HD12	1:E:412:PHE:HE1	1.78	0.47
1:E:241:ASP:OD1	4:E:603:ATP:N6	2.44	0.47
2:D:486:PHE:CE1	2:D:496:ARG:HD3	2.49	0.47
1:C:239:ILE:HG12	1:C:244:ILE:HD13	1.97	0.47
1:B:507:ARG:HG3	1:B:508:ILE:HG12	1.95	0.47
1:E:298:VAL:HG13	1:E:376:ALA:HB1	1.95	0.47
1:C:449:MET:HG3	2:D:454:ASN:HD21	1.79	0.47
1:B:389:ASN:O	1:B:393:ARG:N	2.41	0.47
1:C:325:LEU:HD11	1:C:336:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HE2	1:A:455:VAL:HG23	1.97	0.47
2:D:130:ILE:O	2:D:134:ILE:HG12	2.14	0.47
1:A:152:GLN:HG3	1:B:161:ARG:HH11	1.80	0.47
1:C:56:SER:HB2	1:C:143:SER:HB3	1.97	0.47
1:C:50:THR:HB	1:C:207:LEU:HB3	1.97	0.47
1:C:87:ALA:HB1	1:C:92:TRP:CD1	2.50	0.46
1:F:434:THR:O	1:F:459:ARG:NH2	2.47	0.46
1:A:359:HIS:O	1:A:363:ILE:HG12	2.15	0.46
1:E:18:ILE:HB	1:E:228:THR:HG23	1.96	0.46
1:B:46:GLY:N	1:B:52:LYS:HD3	2.30	0.46
4:E:602:ATP:H2	1:F:462:TRP:HD1	1.62	0.46
1:F:27:GLY:HA3	1:F:246:ILE:HB	1.97	0.46
1:E:325:LEU:HD22	1:E:335:PHE:HB2	1.97	0.46
1:F:316:ALA:HB3	1:F:348:CYS:SG	2.55	0.46
1:B:296:LEU:HD21	1:B:477:PRO:HB3	1.96	0.46
1:B:116:GLU:OE1	1:C:162:ARG:NH2	2.47	0.46
1:E:321:ARG:O	1:E:325:LEU:HG	2.16	0.46
1:B:445:ILE:HD13	1:B:483:PHE:HE2	1.80	0.46
1:B:217:ARG:NH2	1:B:394:GLN:OE1	2.48	0.46
4:D:603:ATP:O3G	1:E:224:LYS:NZ	2.36	0.46
2:D:489:ILE:HD13	2:D:494:PRO:HB3	1.97	0.46
1:A:363:ILE:HG21	1:A:399:VAL:HG13	1.98	0.46
1:A:470:PHE:HE2	1:A:472:ILE:HD11	1.81	0.46
1:E:443:VAL:HG12	1:E:445:ILE:HG12	1.97	0.46
2:D:164:LEU:HD11	2:D:197:GLU:HG3	1.98	0.46
1:E:451:ARG:HB3	1:E:470:PHE:CE1	2.50	0.46
1:B:123:LEU:HG	1:B:163:GLU:HB3	1.97	0.46
1:E:354:ALA:HB1	1:E:358:ASP:HB2	1.96	0.46
1:C:63:GLY:O	1:C:68:ASP:N	2.49	0.46
2:D:273:MET:SD	2:D:479:ILE:HG21	2.56	0.46
2:D:303:GLU:HB2	2:D:333:MET:HE3	1.98	0.46
1:E:426:THR:HG22	1:E:428:SER:H	1.81	0.46
2:D:290:THR:OG1	1:E:457:LYS:NZ	2.41	0.46
1:B:197:GLU:OE2	1:B:197:GLU:N	2.34	0.46
2:D:267:VAL:HB	2:D:270:LEU:HB2	1.98	0.46
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.97	0.46
1:F:396:VAL:HG21	1:F:430:ILE:HD13	1.98	0.45
1:F:358:ASP:O	1:F:362:ILE:HG12	2.17	0.45
1:A:78:GLU:HB3	1:A:83:ILE:HD11	1.98	0.45
1:B:111:ASP:C	1:B:113:GLU:H	2.19	0.45
1:F:284:ILE:HG13	1:F:436:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:NH2	1:C:234:GLU:O	2.49	0.45
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.98	0.45
1:C:470:PHE:HA	1:C:480:LYS:HE2	1.97	0.45
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.99	0.45
1:F:104:PHE:CE2	1:F:106:LEU:HB3	2.51	0.45
1:F:211:LEU:HD12	1:F:215:ARG:O	2.16	0.45
1:B:85:LYS:HZ3	1:C:14:GLU:HG2	1.80	0.45
1:B:313:ILE:HB	1:B:375:ILE:HG13	1.99	0.45
1:A:375:ILE:HG22	1:A:410:GLY:HA2	1.97	0.45
1:E:225:LEU:HD12	1:E:230:HIS:HB3	1.99	0.45
1:F:300:ARG:HH21	1:F:477:PRO:HD2	1.82	0.45
1:A:249:LEU:HD12	1:A:394:GLN:HG3	1.97	0.45
2:D:184:ARG:HH11	2:D:191:ILE:HA	1.81	0.45
1:A:84:ILE:HG23	1:A:94:LEU:H	1.81	0.45
1:E:130:ILE:O	1:E:134:ILE:HG12	2.17	0.45
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.87	0.45
1:F:24:MET:HB2	1:F:62:ASN:HB3	1.99	0.44
1:A:166:ARG:NH2	1:F:114:GLY:O	2.50	0.44
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.98	0.44
1:F:356:LEU:HD11	1:F:387:VAL:HG11	1.99	0.44
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.99	0.44
2:D:386:GLY:HA2	1:E:390:ASN:OD1	2.17	0.44
1:E:344:LEU:HD21	1:E:346:ILE:HD11	1.98	0.44
2:D:283:ILE:HG12	2:D:400:THR:HG23	1.99	0.44
1:A:296:LEU:HD13	1:A:472:ILE:HD12	2.00	0.44
1:B:311:ARG:HG2	1:B:343:LEU:HA	1.98	0.44
1:A:274:CYS:O	1:A:461:SER:OG	2.25	0.44
2:D:56:SER:HB2	2:D:143:SER:HB3	1.99	0.44
1:F:294:LYS:O	1:F:298:VAL:HG23	2.18	0.44
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.53	0.44
2:D:121:PHE:CD1	2:D:125:ALA:HB2	2.51	0.44
1:B:214:GLU:HB3	1:C:234:GLU:HB2	1.99	0.44
1:A:168:VAL:O	1:A:172:LYS:HG3	2.18	0.44
1:B:130:ILE:O	1:B:134:ILE:HG13	2.18	0.44
1:C:75:THR:OG1	1:C:78:GLU:O	2.29	0.44
1:F:514:GLU:N	1:F:514:GLU:OE1	2.50	0.44
1:E:186:GLU:HG3	1:E:189:GLY:N	2.32	0.44
1:B:225:LEU:HD12	1:B:230:HIS:HB3	2.00	0.44
1:F:15:HIS:HB3	1:F:16:GLN:H	1.54	0.44
1:B:265:SER:N	1:B:271:ASP:OD1	2.51	0.44
1:C:490:ILE:HD12	1:C:490:ILE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:PHE:HZ	1:E:361:GLN:HB2	1.83	0.44
1:A:321:ARG:NH2	1:A:347:VAL:O	2.46	0.43
2:D:469:GLU:HG3	2:D:480:LYS:HE3	2.00	0.43
1:E:42:THR:HA	1:E:203:ASN:HB2	2.00	0.43
1:A:483:PHE:HB2	1:A:489:ILE:HD13	2.00	0.43
1:F:280:LYS:O	1:F:409:THR:HB	2.18	0.43
1:A:115:GLN:HB3	1:A:116:GLU:H	1.67	0.43
1:C:314:LEU:HB3	1:C:346:ILE:HD13	2.00	0.43
1:C:356:LEU:HD13	1:C:387:VAL:HG21	2.00	0.43
1:E:506:SER:OG	1:E:507:ARG:N	2.51	0.43
1:F:285:LEU:HB2	1:F:434:THR:HG21	2.00	0.43
1:E:314:LEU:HB3	1:E:346:ILE:HD13	2.00	0.43
1:F:514:GLU:HG3	1:F:519:SER:HB3	2.00	0.43
1:F:368:ASN:OD1	1:F:402:TYR:OH	2.37	0.43
1:C:290:THR:HG21	2:D:431:SER:HB3	2.00	0.43
1:A:464:ASP:OD2	1:A:468:ARG:NH1	2.52	0.43
1:B:358:ASP:O	1:B:362:ILE:HG12	2.19	0.43
1:F:205:VAL:HG22	1:F:222:ILE:HG13	2.01	0.43
1:E:239:ILE:HG12	1:E:244:ILE:HD13	1.99	0.43
1:B:31:ILE:HG23	1:B:231:MET:HB2	2.01	0.43
2:D:264:SER:O	2:D:374:ARG:NH2	2.42	0.43
1:B:87:ALA:HB1	1:B:92:TRP:CD1	2.54	0.43
2:D:80:PRO:O	2:D:84:ILE:HG12	2.18	0.43
1:B:359:HIS:O	1:B:363:ILE:HG12	2.19	0.43
1:C:209:ASN:O	1:C:216:ARG:NH1	2.51	0.43
1:C:182:THR:HG21	1:C:192:ALA:HB1	2.01	0.43
1:F:316:ALA:O	1:F:348:CYS:HA	2.19	0.43
1:E:283:ILE:HG13	1:E:412:PHE:HE2	1.84	0.43
1:B:74:VAL:HB	1:B:144:ILE:HG23	2.01	0.43
1:C:218:ARG:HH12	2:D:232:LYS:HE2	1.84	0.42
1:B:350:TYR:CZ	1:C:254:LEU:HD13	2.54	0.42
1:C:184:ARG:HH22	1:C:208:ARG:HG2	1.84	0.42
1:C:52:LYS:HE3	1:C:52:LYS:HB2	1.76	0.42
1:E:52:LYS:HE3	1:E:52:LYS:HB2	1.86	0.42
1:E:462:TRP:CG	1:E:463:HIS:N	2.87	0.42
1:A:145:ASP:HA	1:A:181:THR:HB	2.01	0.42
2:D:89:SER:HB2	1:E:227:GLY:O	2.18	0.42
2:D:134:ILE:HG21	2:D:174:ILE:HG21	2.01	0.42
1:F:283:ILE:HG23	1:F:412:PHE:HE2	1.84	0.42
1:B:142:VAL:O	1:B:178:THR:HA	2.20	0.42
1:B:54:LEU:N	4:B:603:ATP:O1A	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:THR:HG21	1:A:433:ILE:HG22	2.00	0.42
1:F:109:SER:HA	1:F:110:PRO:HD3	1.90	0.42
2:D:98:VAL:HA	2:D:103:LEU:O	2.19	0.42
1:B:21:MET:SD	1:B:141:ARG:NE	2.92	0.42
1:E:21:MET:HB2	1:E:38:ILE:HG12	2.02	0.42
1:A:468:ARG:HD2	1:A:480:LYS:O	2.20	0.42
2:D:448:GLU:HG2	1:E:466:ALA:HA	2.00	0.42
1:E:237:PHE:HB3	1:E:246:ILE:HG23	2.01	0.42
1:A:294:LYS:HE2	1:A:294:LYS:HB2	1.75	0.42
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.55	0.42
2:D:269:ARG:HG2	2:D:479:ILE:HB	2.00	0.42
1:B:193:ARG:NH2	1:C:195:GLY:O	2.51	0.42
1:E:109:SER:HA	1:E:110:PRO:HD3	1.94	0.42
1:A:273:MET:O	1:A:464:ASP:N	2.41	0.42
1:C:73:PHE:HD1	1:C:143:SER:HB2	1.84	0.42
1:A:337:GLU:OE1	1:A:340:ARG:NH1	2.53	0.42
1:E:164:LEU:HD11	1:E:180:MET:HE1	2.02	0.42
1:A:279:PHE:HB2	1:A:282:SER:HB3	2.01	0.42
2:D:52:LYS:HB2	2:D:52:LYS:HE3	1.84	0.42
1:F:94:LEU:O	1:F:98:VAL:HG23	2.19	0.42
1:C:320:SER:HA	2:D:254:LEU:HB3	2.01	0.42
1:A:470:PHE:CE2	1:A:472:ILE:HD11	2.54	0.42
1:F:420:MET:SD	1:F:449:MET:HE1	2.59	0.42
1:E:493:SER:HB3	1:F:488:ARG:HA	2.00	0.42
1:E:171:LEU:HD13	1:E:178:THR:HG21	2.00	0.42
1:F:313:ILE:HD12	1:F:367:ILE:HD13	2.02	0.42
1:B:116:GLU:C	1:B:118:VAL:H	2.23	0.42
1:F:319:GLU:OE1	1:F:327:ASN:ND2	2.53	0.42
1:C:80:PRO:O	1:C:84:ILE:HG12	2.20	0.42
1:A:207:LEU:HD21	1:A:220:LEU:HD12	2.01	0.42
1:B:203:ASN:HB3	1:B:225:LEU:HD23	2.01	0.41
1:B:483:PHE:HB3	1:B:486:PHE:HB2	2.02	0.41
1:C:202:ASP:HA	1:C:226:ARG:HD2	2.01	0.41
1:A:147:VAL:HG11	1:A:180:MET:HE3	2.02	0.41
1:F:218:ARG:NH2	1:F:239:ILE:H	2.12	0.41
1:A:380:LEU:HD11	1:A:412:PHE:HD2	1.85	0.41
1:C:74:VAL:HB	1:C:144:ILE:HA	2.03	0.41
1:B:36:LEU:HD12	1:B:59:PHE:CE1	2.56	0.41
1:B:218:ARG:HB3	1:B:237:PHE:CZ	2.55	0.41
4:D:602:ATP:HO2'	4:D:602:ATP:HO3'	1.56	0.41
1:E:350:TYR:CE2	1:F:254:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:VAL:HG22	2:D:106:LEU:HD23	2.02	0.41
1:F:164:LEU:HD11	1:F:197:GLU:HG3	2.03	0.41
2:D:512:VAL:HA	2:D:513:GLN:CB	2.46	0.41
1:C:435:ASP:HA	1:C:459:ARG:HH11	1.85	0.41
1:F:191:ILE:HG21	1:F:198:GLU:HG3	2.02	0.41
1:E:112:PRO:O	1:F:166:ARG:HG3	2.20	0.41
1:F:383:LEU:HB2	1:F:392:PHE:HE1	1.85	0.41
1:A:202:ASP:HA	1:A:226:ARG:NH1	2.35	0.41
1:C:254:LEU:HD12	1:C:256:GLN:HE22	1.86	0.41
1:C:184:ARG:NH1	1:C:187:GLU:O	2.53	0.41
1:B:317:TYR:CZ	1:B:383:LEU:HD11	2.55	0.41
2:D:171:LEU:HA	2:D:174:ILE:HD12	2.03	0.41
2:D:511:GLY:HA3	2:D:513:GLN:HG3	2.03	0.41
1:F:382:ALA:HB1	1:F:385:ARG:HH21	1.86	0.41
2:D:298:VAL:HG13	2:D:376:ALA:HB1	2.02	0.41
1:A:25:ILE:O	1:A:27:GLY:N	2.54	0.41
1:F:215:ARG:HA	1:F:215:ARG:HH11	1.86	0.41
1:B:350:TYR:O	1:B:353:SER:OG	2.25	0.41
2:D:111:ASP:HA	2:D:112:PRO:HD3	1.85	0.41
1:F:489:ILE:HG22	1:F:490:ILE:HD13	2.02	0.41
1:E:94:LEU:O	1:E:98:VAL:HG23	2.20	0.41
1:B:75:THR:OG1	1:B:78:GLU:O	2.34	0.41
1:C:311:ARG:HB3	1:C:370:PHE:CE2	2.55	0.41
2:D:498:THR:HB	2:D:499:VAL:HA	2.02	0.41
1:B:22:ARG:O	1:B:141:ARG:NH2	2.54	0.41
1:A:336:GLU:O	1:A:340:ARG:HG3	2.20	0.41
1:A:356:LEU:HD23	1:A:395:PHE:HB2	2.03	0.41
1:F:344:LEU:HD22	1:F:345:LYS:N	2.36	0.41
1:A:69:GLU:HA	1:A:70:PRO:HD3	1.88	0.41
1:F:52:LYS:HB3	1:F:181:THR:HG23	2.03	0.41
1:B:166:ARG:O	1:B:170:ARG:HG2	2.21	0.41
1:B:70:PRO:HG3	1:B:102:LYS:HD2	2.03	0.41
1:F:283:ILE:HG23	1:F:412:PHE:CE2	2.56	0.41
1:A:226:ARG:HH21	4:F:603:ATP:PG	2.44	0.41
2:D:461:SER:OG	2:D:462:TRP:N	2.53	0.41
1:B:351:PRO:HB3	1:B:383:LEU:HD23	2.02	0.40
1:B:499:VAL:C	1:B:501:GLU:H	2.24	0.40
1:A:390:ASN:OD1	1:F:386:GLY:HA3	2.21	0.40
2:D:402:TYR:HA	2:D:405:GLN:HG2	2.03	0.40
2:D:293:GLY:O	2:D:295:THR:N	2.54	0.40
2:D:184:ARG:HD3	2:D:191:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:HG22	1:E:209:ASN:HB2	2.03	0.40
1:A:52:LYS:HE3	1:A:52:LYS:HB2	1.89	0.40
1:B:89:SER:HB3	1:C:227:GLY:O	2.21	0.40
1:F:406:GLU:HB3	1:F:408:ILE:HG12	2.04	0.40
1:A:508:ILE:HG13	1:A:510:ARG:H	1.86	0.40
1:C:377:ILE:HD12	1:C:412:PHE:HE1	1.86	0.40
1:A:170:ARG:O	1:A:174:ILE:HG12	2.22	0.40
1:A:202:ASP:HA	1:A:226:ARG:HH11	1.86	0.40
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.56	0.40
1:B:144:ILE:HG22	1:B:147:VAL:HG12	2.04	0.40
1:C:70:PRO:HB2	1:C:139:ALA:HA	2.04	0.40
1:B:261:VAL:O	1:B:279:PHE:HA	2.20	0.40
2:D:499:VAL:HA	2:D:500:ASP:HA	1.63	0.40
2:D:509:VAL:HA	2:D:510:ARG:HB3	2.03	0.40
4:D:602:ATP:C2	1:E:462:TRP:HA	2.56	0.40
1:E:386:GLY:HA3	1:F:390:ASN:OD1	2.21	0.40
1:A:111:ASP:C	1:A:113:GLU:H	2.25	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	503/519 (97%)	424 (84%)	64 (13%)	15 (3%)	5	33
1	B	495/519 (95%)	425 (86%)	55 (11%)	15 (3%)	5	33
1	C	494/519 (95%)	425 (86%)	51 (10%)	18 (4%)	4	28
1	E	498/519 (96%)	434 (87%)	44 (9%)	20 (4%)	4	24
1	F	503/519 (97%)	427 (85%)	50 (10%)	26 (5%)	2	18
2	D	498/519 (96%)	436 (88%)	47 (9%)	15 (3%)	5	33
All	All	2991/3114 (96%)	2571 (86%)	311 (10%)	109 (4%)	4	28

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LYS
1	B	33	HIS
1	B	117	VAL
1	C	124	SER
1	C	212	GLU
1	C	433	ILE
1	C	507	ARG
1	C	508	ILE
2	D	333	MET
2	D	498	THR
1	E	462	TRP
1	F	254	LEU
1	F	509	VAL
1	F	517	PRO
1	A	26	GLU
1	A	211	LEU
1	A	463	HIS
1	B	112	PRO
1	B	211	LEU
1	B	212	GLU
1	B	420	MET
1	B	463	HIS
1	B	507	ARG
1	C	193	ARG
1	C	463	HIS
2	D	154	TYR
2	D	294	LYS
2	D	463	HIS
2	D	512	VAL
1	E	113	GLU
1	E	211	LEU
1	E	212	GLU
1	E	249	LEU
1	E	463	HIS
1	F	26	GLU
1	F	120	GLY
1	F	154	TYR
1	F	212	GLU
1	F	510	ARG
1	A	420	MET
1	C	17	ALA
1	C	115	GLN

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Mol	Chain	Res	Type
1	C	116	GLU
1	C	250	GLY
1	C	348	CYS
1	C	420	MET
2	D	292	THR
2	D	348	CYS
1	E	348	CYS
1	F	15	HIS
1	F	16	GLN
1	F	250	GLY
1	F	348	CYS
1	F	463	HIS
1	F	507	ARG
1	F	516	GLY
1	A	212	GLU
1	A	348	CYS
1	B	154	TYR
1	B	276	GLY
1	C	118	VAL
2	D	420	MET
2	D	506	SER
1	E	157	SER
1	E	385	ARG
1	E	420	MET
1	E	498	THR
1	F	116	GLU
1	F	189	GLY
1	F	370	PHE
1	F	504	GLU
1	F	508	ILE
1	A	117	VAL
1	A	120	GLY
1	A	370	PHE
1	A	372	PRO
1	A	499	VAL
1	B	480	LYS
1	B	499	VAL
1	C	372	PRO
2	D	212	GLU
2	D	507	ARG
1	E	497	ILE
1	E	503	SER

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Mol	Chain	Res	Type
1	F	253	ARG
1	F	420	MET
1	A	503	SER
1	B	118	VAL
1	B	500	ASP
1	E	117	VAL
1	F	480	LYS
1	F	505	LEU
1	C	371	LYS
1	E	425	ILE
1	E	509	VAL
1	A	112	PRO
1	A	433	ILE
1	C	117	VAL
1	E	250	GLY
1	E	293	GLY
2	D	117	VAL
2	D	189	GLY
1	E	477	PRO
1	B	119	GLY
2	D	494	PRO
1	E	196	VAL
1	F	293	GLY
1	F	512	VAL
1	C	112	PRO

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	430/442 (97%)	427 (99%)	3 (1%)	88 94
1	B	423/442 (96%)	421 (100%)	2 (0%)	92 95
1	C	423/442 (96%)	421 (100%)	2 (0%)	92 95
1	E	425/442 (96%)	422 (99%)	3 (1%)	88 94
1	F	430/442 (97%)	430 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	426/443 (96%)	421 (99%)	5 (1%)	78 90
All	All	2557/2653 (96%)	2542 (99%)	15 (1%)	90 95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	375	ILE
1	A	433	ILE
1	B	26	GLU
1	B	380	LEU
1	C	182	THR
1	C	248	PRO
2	D	270	LEU
2	D	499	VAL
2	D	501	GLU
2	D	504	GLU
2	D	509	VAL
1	E	30	ASP
1	E	196	VAL
1	E	463	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	308	ASN
1	E	368	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	A	432	1	8,10,11	0.69	0	7,14,16	1.56	1 (14%)
1	TPO	B	432	1	8,10,11	0.72	0	7,14,16	1.60	0
1	TPO	C	432	1	8,10,11	0.92	0	7,14,16	1.75	3 (42%)
1	TPO	E	432	1	8,10,11	0.71	0	7,14,16	1.39	0
1	TPO	F	432	1	8,10,11	0.74	0	7,14,16	1.51	1 (14%)

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
1	TPO	A	432	1	-	0/8/11/13	0/0/0/0
1	TPO	B	432	1	-	0/8/11/13	0/0/0/0
1	TPO	C	432	1	-	0/8/11/13	0/0/0/0
1	TPO	E	432	1	-	0/8/11/13	0/0/0/0
1	TPO	F	432	1	-	1/8/11/13	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	432	TPO	CG2-CB-CA	-2.62	107.84	113.17
1	C	432	TPO	O-C-CA	-2.34	119.25	125.44
1	F	432	TPO	O-C-CA	-2.12	119.85	125.44
1	C	432	TPO	C-CA-N	-2.02	105.61	109.83
1	A	432	TPO	C-CA-N	2.41	114.86	109.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	432	TPO	OG1-CB-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	432	TPO	1	0
1	C	432	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ATP	A	802	3	24,33,33	0.98	1 (4%)	31,52,52	1.95	5 (16%)
4	ATP	A	803	3	24,33,33	0.97	1 (4%)	31,52,52	1.87	5 (16%)
4	ATP	B	602	3	24,33,33	1.00	1 (4%)	31,52,52	1.87	4 (12%)
4	ATP	B	603	3	24,33,33	0.98	1 (4%)	31,52,52	1.91	5 (16%)
4	ATP	C	602	3	24,33,33	0.99	1 (4%)	31,52,52	1.96	5 (16%)
4	ATP	C	603	3	24,33,33	0.98	1 (4%)	31,52,52	1.92	5 (16%)
5	PO4	C	605	-	4,4,4	0.47	0	6,6,6	0.27	0
4	ATP	D	602	3	24,33,33	0.98	1 (4%)	31,52,52	1.84	4 (12%)
4	ATP	D	603	3	24,33,33	0.99	1 (4%)	31,52,52	1.89	5 (16%)
4	ATP	E	602	3	24,33,33	0.95	1 (4%)	31,52,52	1.73	4 (12%)
4	ATP	E	603	3	24,33,33	0.97	1 (4%)	31,52,52	1.97	5 (16%)
4	ATP	F	602	3	24,33,33	0.98	1 (4%)	31,52,52	1.87	5 (16%)
4	ATP	F	603	3	24,33,33	0.98	1 (4%)	31,52,52	1.89	6 (19%)

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
4	ATP	A	802	3	-	0/18/38/38	0/3/3/3
4	ATP	A	803	3	-	0/18/38/38	0/3/3/3
4	ATP	B	602	3	-	0/18/38/38	0/3/3/3
4	ATP	B	603	3	-	0/18/38/38	0/3/3/3
4	ATP	C	602	3	-	0/18/38/38	0/3/3/3
4	ATP	C	603	3	-	0/18/38/38	0/3/3/3
5	PO4	C	605	-	-	0/0/0/0	0/0/0/0
4	ATP	D	602	3	-	0/18/38/38	0/3/3/3
4	ATP	D	603	3	-	0/18/38/38	0/3/3/3
4	ATP	E	602	3	-	0/18/38/38	0/3/3/3
4	ATP	E	603	3	-	0/18/38/38	0/3/3/3
4	ATP	F	602	3	-	0/18/38/38	0/3/3/3
4	ATP	F	603	3	-	0/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	603	ATP	C5-C4	3.06	1.47	1.40
4	D	602	ATP	C5-C4	3.08	1.47	1.40
4	F	603	ATP	C5-C4	3.09	1.47	1.40
4	E	602	ATP	C5-C4	3.09	1.47	1.40
4	C	602	ATP	C5-C4	3.09	1.47	1.40
4	A	802	ATP	C5-C4	3.12	1.47	1.40
4	F	602	ATP	C5-C4	3.12	1.47	1.40
4	B	603	ATP	C5-C4	3.13	1.47	1.40
4	C	603	ATP	C5-C4	3.13	1.47	1.40
4	D	603	ATP	C5-C4	3.14	1.47	1.40
4	B	602	ATP	C5-C4	3.15	1.47	1.40
4	A	803	ATP	C5-C4	3.16	1.47	1.40

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	603	ATP	N3-C2-N1	-6.90	123.61	128.89
4	B	603	ATP	N3-C2-N1	-6.76	123.72	128.89
4	D	603	ATP	N3-C2-N1	-6.76	123.72	128.89
4	C	602	ATP	N3-C2-N1	-6.76	123.72	128.89
4	B	602	ATP	N3-C2-N1	-6.75	123.73	128.89
4	A	803	ATP	N3-C2-N1	-6.65	123.80	128.89
4	F	603	ATP	N3-C2-N1	-6.65	123.80	128.89
4	C	603	ATP	N3-C2-N1	-6.61	123.83	128.89
4	F	602	ATP	N3-C2-N1	-6.61	123.83	128.89
4	A	802	ATP	N3-C2-N1	-6.58	123.86	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	602	ATP	N3-C2-N1	-6.55	123.88	128.89
4	E	602	ATP	N3-C2-N1	-6.45	123.95	128.89
4	C	603	ATP	PA-O3A-PB	-4.33	120.58	132.73
4	D	602	ATP	PB-O3B-PG	-4.27	118.34	132.67
4	C	602	ATP	PA-O3A-PB	-4.13	121.12	132.73
4	A	802	ATP	PB-O3B-PG	-3.98	119.33	132.67
4	A	803	ATP	PA-O3A-PB	-3.80	122.05	132.73
4	B	603	ATP	PA-O3A-PB	-3.80	122.06	132.73
4	F	602	ATP	PA-O3A-PB	-3.73	122.24	132.73
4	E	603	ATP	PA-O3A-PB	-3.71	122.30	132.73
4	B	602	ATP	C2'-C1'-N9	-3.55	108.87	114.29
4	C	603	ATP	PB-O3B-PG	-3.48	120.99	132.67
4	C	602	ATP	PB-O3B-PG	-3.41	121.23	132.67
4	F	603	ATP	C4-C5-N7	-3.40	106.35	109.48
4	F	603	ATP	PA-O3A-PB	-3.39	123.22	132.73
4	E	603	ATP	C4-C5-N7	-3.35	106.39	109.48
4	C	602	ATP	C2'-C1'-N9	-3.33	109.20	114.29
4	C	603	ATP	C4-C5-N7	-3.33	106.42	109.48
4	F	602	ATP	C4-C5-N7	-3.31	106.44	109.48
4	A	802	ATP	PA-O3A-PB	-3.30	123.47	132.73
4	D	603	ATP	C4-C5-N7	-3.29	106.46	109.48
4	B	603	ATP	PB-O3B-PG	-3.24	121.81	132.67
4	E	603	ATP	PB-O3B-PG	-3.24	121.81	132.67
4	E	602	ATP	C4-C5-N7	-3.22	106.52	109.48
4	A	802	ATP	C4-C5-N7	-3.20	106.53	109.48
4	A	803	ATP	C4-C5-N7	-3.15	106.58	109.48
4	B	603	ATP	C4-C5-N7	-3.14	106.59	109.48
4	B	602	ATP	C4-C5-N7	-3.14	106.59	109.48
4	A	802	ATP	C2'-C1'-N9	-3.09	109.57	114.29
4	D	603	ATP	C2'-C1'-N9	-3.06	109.61	114.29
4	F	602	ATP	C2'-C1'-N9	-3.06	109.62	114.29
4	D	602	ATP	C4-C5-N7	-3.01	106.71	109.48
4	F	602	ATP	PB-O3B-PG	-2.97	122.70	132.67
4	D	603	ATP	PB-O3B-PG	-2.95	122.77	132.67
4	B	602	ATP	PB-O3B-PG	-2.92	122.88	132.67
4	E	602	ATP	PB-O3B-PG	-2.90	122.95	132.67
4	B	603	ATP	C2'-C1'-N9	-2.87	109.91	114.29
4	A	803	ATP	PB-O3B-PG	-2.86	123.08	132.67
4	A	803	ATP	C2'-C1'-N9	-2.80	110.02	114.29
4	D	603	ATP	PA-O3A-PB	-2.75	125.01	132.73
4	C	602	ATP	C4-C5-N7	-2.75	106.95	109.48
4	E	603	ATP	C2'-C1'-N9	-2.72	110.14	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	603	ATP	PB-O3B-PG	-2.59	123.98	132.67
4	C	603	ATP	C2'-C1'-N9	-2.54	110.41	114.29
4	F	603	ATP	C2'-C1'-N9	-2.50	110.47	114.29
4	E	602	ATP	PA-O3A-PB	-2.26	126.39	132.73
4	D	602	ATP	PA-O3A-PB	-2.21	126.53	132.73
4	F	603	ATP	O4'-C1'-N9	2.12	112.53	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	ATP	3	0
4	A	803	ATP	1	0
4	B	602	ATP	1	0
4	B	603	ATP	2	0
4	C	603	ATP	1	0
4	D	602	ATP	4	0
4	D	603	ATP	1	0
4	E	602	ATP	1	0
4	E	603	ATP	2	0
4	F	602	ATP	3	0
4	F	603	ATP	2	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	505/519 (97%)	0.63	59 (11%) 6 5	66, 113, 156, 183	0
1	B	497/519 (95%)	0.53	35 (7%) 19 16	75, 115, 154, 195	0
1	C	496/519 (95%)	0.31	40 (8%) 15 11	57, 101, 149, 191	0
1	E	500/519 (96%)	0.17	30 (6%) 25 20	41, 87, 140, 176	0
1	F	505/519 (97%)	0.35	42 (8%) 14 11	42, 99, 150, 174	0
2	D	500/519 (96%)	0.15	35 (7%) 19 16	50, 83, 139, 186	0
All	All	3003/3114 (96%)	0.36	241 (8%) 15 12	41, 101, 151, 195	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	8.4
1	A	500	ASP	7.5
2	D	503	SER	7.3
1	A	518	GLU	7.2
1	E	514	GLU	7.1
2	D	509	VAL	6.9
1	A	513	GLN	6.8
2	D	508	ILE	6.8
1	F	518	GLU	6.7
1	B	508	ILE	6.7
1	F	485	ASN	6.7
1	A	516	GLY	6.6
1	A	519	SER	6.5
1	F	517	PRO	6.2
1	A	511	GLY	6.1
1	F	511	GLY	5.9
1	F	500	ASP	5.9
2	D	16	GLN	5.9
1	F	509	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	500	ASP	5.9
1	E	500	ASP	5.7
1	A	257	ARG	5.7
1	A	506	SER	5.7
1	A	507	ARG	5.6
2	D	510	ARG	5.6
1	B	121	PHE	5.5
1	B	117	VAL	5.4
1	B	119	GLY	5.4
1	E	513	GLN	5.4
1	F	506	SER	5.3
1	F	501	GLU	5.3
1	F	516	GLY	5.3
1	B	503	SER	5.3
2	D	117	VAL	5.2
1	A	509	VAL	5.2
1	B	501	GLU	5.2
1	B	15	HIS	5.2
1	E	508	ILE	5.0
2	D	504	GLU	5.0
2	D	499	VAL	5.0
2	D	506	SER	5.0
1	B	511	GLY	4.9
1	E	501	GLU	4.9
1	B	506	SER	4.8
1	B	120	GLY	4.8
2	D	118	VAL	4.8
2	D	119	GLY	4.7
1	A	16	GLN	4.7
1	F	508	ILE	4.7
1	B	116	GLU	4.7
1	A	515	LYS	4.6
1	B	502	LYS	4.6
1	E	509	VAL	4.5
1	C	504	GLU	4.5
1	C	14	GLU	4.5
1	B	498	THR	4.5
2	D	15	HIS	4.5
1	F	503	SER	4.4
1	A	115	GLN	4.3
1	A	503	SER	4.2
1	B	500	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	504	GLU	4.2
1	C	499	VAL	4.1
2	D	505	LEU	4.1
1	E	512	VAL	4.0
1	C	505	LEU	4.0
1	E	506	SER	4.0
1	F	504	GLU	4.0
2	D	121	PHE	3.9
1	E	256	GLN	3.9
1	C	509	VAL	3.9
1	A	405	GLN	3.9
1	C	501	GLU	3.8
1	A	254	LEU	3.8
1	A	508	ILE	3.8
1	A	15	HIS	3.8
2	D	498	THR	3.8
1	C	17	ALA	3.8
1	A	255	THR	3.8
2	D	507	ARG	3.7
2	D	309	LYS	3.7
1	F	507	ARG	3.7
2	D	512	VAL	3.7
1	A	498	THR	3.7
1	B	507	ARG	3.7
1	B	115	GLN	3.7
1	E	503	SER	3.7
2	D	502	LYS	3.6
1	A	505	LEU	3.6
1	F	519	SER	3.5
2	D	120	GLY	3.5
2	D	500	ASP	3.5
1	E	505	LEU	3.5
1	F	510	ARG	3.5
1	B	295	THR	3.5
2	D	122	ASP	3.5
1	F	512	VAL	3.5
1	E	321	ARG	3.5
1	E	504	GLU	3.5
1	A	504	GLU	3.4
1	A	499	VAL	3.4
1	F	484	ARG	3.4
1	A	501	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	3.4
1	A	14	GLU	3.4
1	B	505	LEU	3.3
1	B	255	THR	3.3
1	A	318	ALA	3.3
1	C	251	ALA	3.3
1	C	498	THR	3.3
1	A	251	ALA	3.3
1	C	508	ILE	3.3
1	B	496	ARG	3.2
1	A	17	ALA	3.2
1	C	120	GLY	3.2
1	B	510	ARG	3.2
2	D	511	GLY	3.2
1	B	118	VAL	3.2
1	A	253	ARG	3.2
1	E	499	VAL	3.2
1	F	513	GLN	3.2
1	F	121	PHE	3.2
1	F	255	THR	3.1
1	F	497	ILE	3.1
2	D	513	GLN	3.1
2	D	14	GLU	3.1
1	C	146	SER	3.0
1	F	446	ARG	3.0
1	A	188	TYR	3.0
1	A	510	ARG	3.0
1	C	503	SER	3.0
1	A	514	GLU	3.0
1	F	502	LYS	3.0
1	C	252	MET	3.0
1	E	510	ARG	2.9
1	E	511	GLY	2.9
1	B	258	SER	2.9
1	F	256	GLN	2.9
1	C	113	GLU	2.9
1	F	341	GLN	2.9
1	E	507	ARG	2.9
1	C	427	ASP	2.9
1	C	188	TYR	2.9
1	F	188	TYR	2.9
1	C	173	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	505	LEU	2.8
1	C	116	GLU	2.8
1	F	515	LYS	2.8
1	B	175	GLY	2.8
2	D	156	ALA	2.8
1	C	154	TYR	2.7
1	C	170	ARG	2.7
1	A	117	VAL	2.7
1	A	475	LYS	2.7
2	D	447	GLY	2.7
1	F	154	TYR	2.7
1	A	341	GLN	2.7
1	A	329	TYR	2.7
1	B	154	TYR	2.7
1	E	116	GLU	2.7
1	A	334	ASP	2.7
1	A	512	VAL	2.7
2	D	157	SER	2.6
1	F	253	ARG	2.6
1	C	15	HIS	2.6
1	B	509	VAL	2.6
1	A	342	ASN	2.6
1	C	502	LYS	2.6
1	B	16	GLN	2.6
1	F	268	VAL	2.6
1	A	252	MET	2.6
1	A	295	THR	2.6
1	C	255	THR	2.6
1	A	325	LEU	2.5
1	C	41	SER	2.5
1	B	188	TYR	2.5
1	F	514	GLU	2.5
1	F	499	VAL	2.5
1	A	340	ARG	2.5
1	E	188	TYR	2.5
1	F	321	ARG	2.5
1	C	143	SER	2.5
2	D	471	MET	2.5
2	D	53	THR	2.4
1	E	118	VAL	2.4
1	C	510	ARG	2.4
1	A	474	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	498	THR	2.4
1	B	462	TRP	2.4
1	A	307	ALA	2.4
1	F	343	LEU	2.4
1	A	121	PHE	2.4
2	D	113	GLU	2.4
2	D	501	GLU	2.3
1	A	154	TYR	2.3
2	D	329	TYR	2.3
1	E	310	GLU	2.3
1	C	260	ASN	2.3
1	F	120	GLY	2.3
1	F	443	VAL	2.3
1	F	117	VAL	2.2
1	B	318	ALA	2.2
1	C	156	ALA	2.2
1	B	53	THR	2.2
1	A	368	ASN	2.2
1	C	145	ASP	2.2
1	E	122	ASP	2.2
1	E	498	THR	2.2
1	C	114	GLY	2.2
1	F	276	GLY	2.2
1	F	460	GLY	2.2
1	C	227	GLY	2.2
1	E	484	ARG	2.2
1	E	152	GLN	2.2
1	E	257	ARG	2.2
1	A	337	GLU	2.2
2	D	188	TYR	2.2
1	E	154	TYR	2.1
2	D	154	TYR	2.1
1	E	121	PHE	2.1
1	A	339	GLU	2.1
1	A	428	SER	2.1
1	A	335	PHE	2.1
1	E	15	HIS	2.1
1	B	499	VAL	2.1
1	C	506	SER	2.1
1	A	241	ASP	2.1
1	B	309	LYS	2.1
1	C	102	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	131	ASN	2.1
1	A	259	SER	2.1
1	A	114	GLY	2.0
1	E	337	GLU	2.0
1	C	157	SER	2.0
1	C	229	SER	2.0
1	C	189	GLY	2.0
1	A	446	ARG	2.0
1	F	272	GLU	2.0
1	A	118	VAL	2.0
1	B	124	SER	2.0
1	C	176	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPO	A	432	11/12	0.88	0.24	-	104,112,128,135	0
1	TPO	B	432	11/12	0.91	0.30	-	109,120,131,144	0
1	TPO	C	432	11/12	0.91	0.23	-	83,101,125,141	0
1	TPO	E	432	11/12	0.92	0.23	-	76,87,116,130	0
1	TPO	F	432	11/12	0.69	0.40	-	102,112,126,149	0

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	MG	A	804	1/1	0.96	0.52	6.96	80,80,80,80	0
3	MG	D	601	1/1	0.86	0.51	3.23	112,112,112,112	0
5	PO4	C	605	5/5	0.88	0.50	2.20	104,105,118,130	0
3	MG	F	604	1/1	0.88	0.41	2.17	68,68,68,68	0
4	ATP	F	602	31/31	0.77	0.35	1.15	99,116,132,134	0
4	ATP	D	602	31/31	0.89	0.28	0.62	76,85,93,98	0
4	ATP	E	603	31/31	0.92	0.24	0.47	51,59,75,89	0
4	ATP	E	602	31/31	0.82	0.30	0.43	78,104,118,124	0
4	ATP	D	603	31/31	0.90	0.25	0.33	50,58,75,91	0
4	ATP	A	803	31/31	0.84	0.29	0.29	81,96,117,121	0
4	ATP	C	603	31/31	0.92	0.26	0.24	65,80,96,108	0
4	ATP	F	603	31/31	0.92	0.24	0.23	61,71,80,84	0
4	ATP	C	602	31/31	0.93	0.21	0.22	62,75,86,94	0
4	ATP	B	602	31/31	0.89	0.27	0.22	79,96,105,109	0
3	MG	D	604	1/1	0.83	0.32	0.13	87,87,87,87	0
3	MG	B	601	1/1	0.51	0.33	-0.07	114,114,114,114	0
4	ATP	B	603	31/31	0.87	0.27	-0.42	97,110,121,126	0
4	ATP	A	802	31/31	0.85	0.28	-0.48	96,115,126,130	0
3	MG	F	601	1/1	0.94	0.81	-	100,100,100,100	0
3	MG	C	601	1/1	0.90	0.18	-	77,77,77,77	0
3	MG	C	604	1/1	0.79	0.48	-	101,101,101,101	0
3	MG	E	601	1/1	0.88	0.48	-	85,85,85,85	0
3	MG	B	604	1/1	0.94	0.28	-	114,114,114,114	0
3	MG	E	604	1/1	0.90	0.36	-	71,71,71,71	0
3	MG	A	801	1/1	0.83	0.40	-	110,110,110,110	0

6.5 Other polymers (i)

There are no such residues in this entry.