Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2016 – 12:03 AM GMT

PDB ID	:	8RUC
Title	:	ACTIVATED SPINACH RUBISCO COMPLEXED WITH 2-CARBOXYARABINITOL BISPHOSPHATE
Authors	:	Andersson, I.; Knight, S.; Branden, C.-I.
Deposited on	:	1996-02-22
Resolution	:	1.60 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:

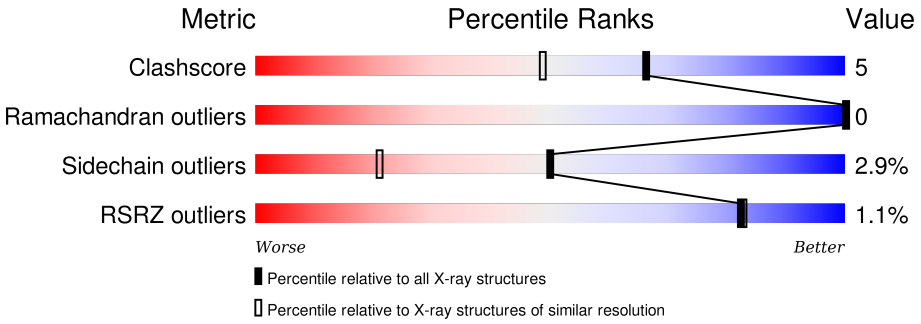
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.60 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	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	475	88% 10%
1	C	475	86% 12%
1	E	475	87% 11%
1	G	475	87% 11%
2	I	123	86% 11%
2	J	123	77% 20%
2	K	123	82% 15%

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Mol	Chain	Length	Quality of chain
2	L	123	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20368 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 RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3657	2319	640	680	18			
1	C	467	Total	C	N	O	S	0	0	0
			3657	2319	640	680	18			
1	E	467	Total	C	N	O	S	0	0	0
			3657	2319	640	680	18			
1	G	467	Total	C	N	O	S	0	0	0
			3657	2319	640	680	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	KCX	LYS	CONFLICT	UNP P00875
C	201	KCX	LYS	CONFLICT	UNP P00875
E	201	KCX	LYS	CONFLICT	UNP P00875
G	201	KCX	LYS	CONFLICT	UNP P00875

- Molecule 2 is a protein called RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	J	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	K	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			
2	L	123	Total	C	N	O	S	0	0	0
			1033	673	167	186	7			

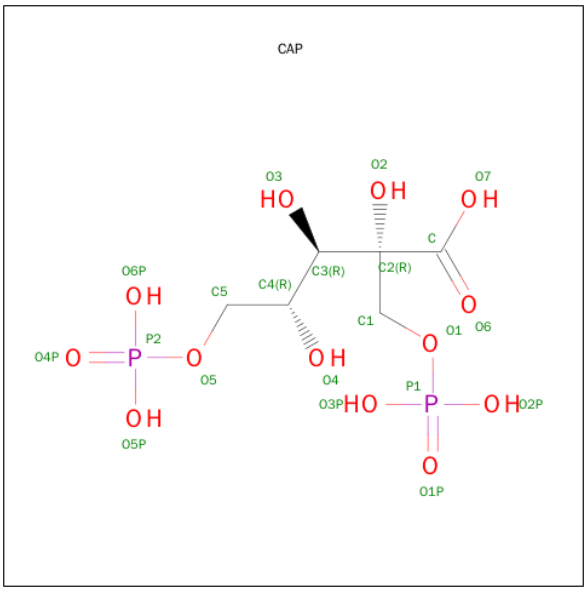
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	2	GLN	LYS	CONFLICT	UNP P00870
I	6	ILE	THR	CONFLICT	UNP P00870
I	7	LEU	GLN	CONFLICT	UNP P00870
I	9	LEU	MET	CONFLICT	UNP P00870
I	11	LYS	ARG	CONFLICT	UNP P00870
I	109	GLU	GLN	CONFLICT	UNP P00870
I	113	ILE	VAL	CONFLICT	UNP P00870
J	2	GLN	LYS	CONFLICT	UNP P00870
J	6	ILE	THR	CONFLICT	UNP P00870
J	7	LEU	GLN	CONFLICT	UNP P00870
J	9	LEU	MET	CONFLICT	UNP P00870
J	11	LYS	ARG	CONFLICT	UNP P00870
J	109	GLU	GLN	CONFLICT	UNP P00870
J	113	ILE	VAL	CONFLICT	UNP P00870
K	2	GLN	LYS	CONFLICT	UNP P00870
K	6	ILE	THR	CONFLICT	UNP P00870
K	7	LEU	GLN	CONFLICT	UNP P00870
K	9	LEU	MET	CONFLICT	UNP P00870
K	11	LYS	ARG	CONFLICT	UNP P00870
K	109	GLU	GLN	CONFLICT	UNP P00870
K	113	ILE	VAL	CONFLICT	UNP P00870
L	2	GLN	LYS	CONFLICT	UNP P00870
L	6	ILE	THR	CONFLICT	UNP P00870
L	7	LEU	GLN	CONFLICT	UNP P00870
L	9	LEU	MET	CONFLICT	UNP P00870
L	11	LYS	ARG	CONFLICT	UNP P00870
L	109	GLU	GLN	CONFLICT	UNP P00870
L	113	ILE	VAL	CONFLICT	UNP P00870

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 21 6 13 2	0	0
4	C	1	Total C O P 21 6 13 2	0	0
4	E	1	Total C O P 21 6 13 2	0	0
4	G	1	Total C O P 21 6 13 2	0	0

- Molecule 5 is water.

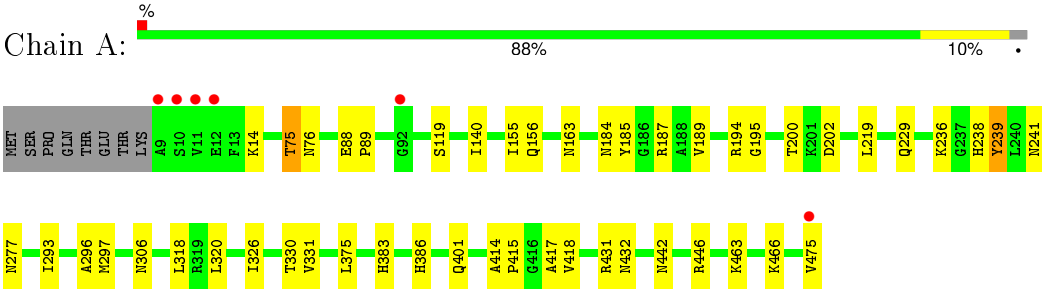
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	314	Total O 314 314	0	0
5	C	297	Total O 297 297	0	0
5	E	280	Total O 280 280	0	0
5	G	308	Total O 308 308	0	0
5	I	84	Total O 84 84	0	0
5	J	78	Total O 78 78	0	0
5	K	77	Total O 77 77	0	0
5	L	82	Total O 82 82	0	0

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.

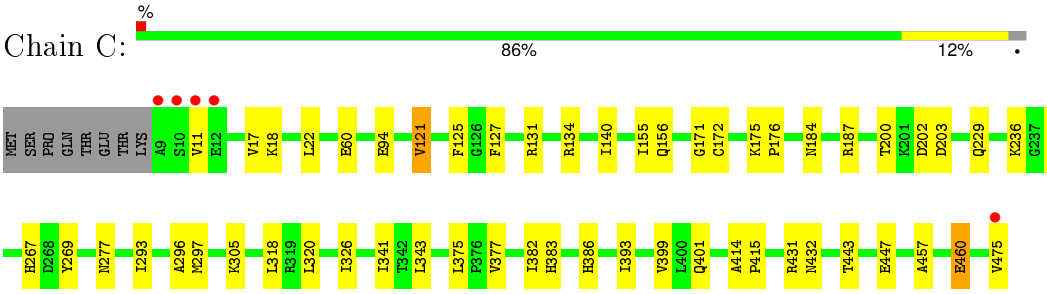
- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain A:



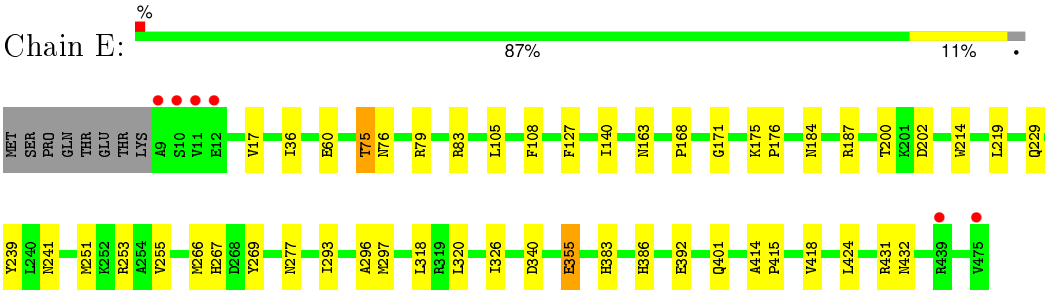
- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain C:



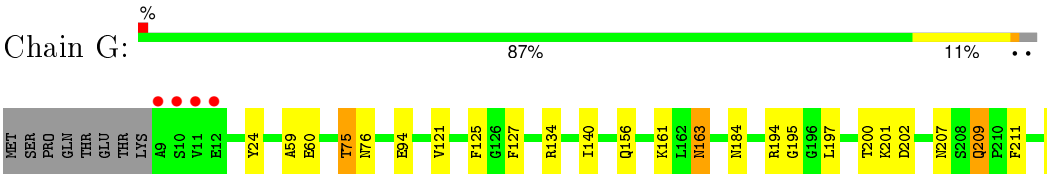
- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

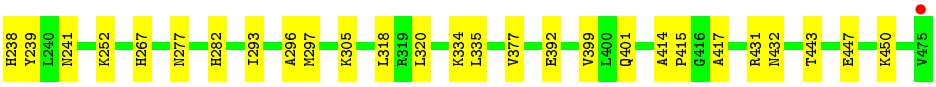
Chain E:



- Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

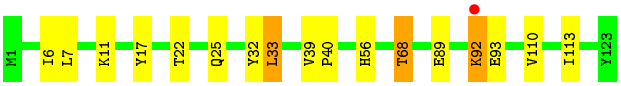
Chain G:





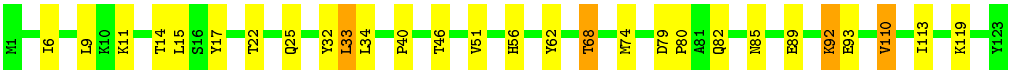
• Molecule 2: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain I:



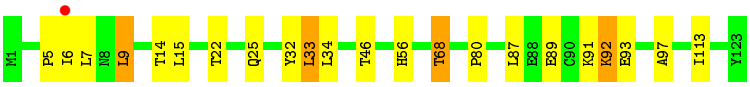
• Molecule 2: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain J:



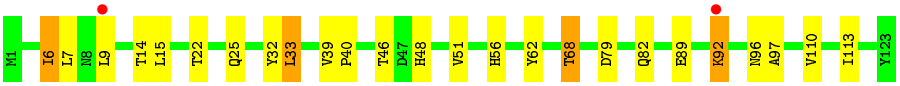
• Molecule 2: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain K:



• Molecule 2: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	157.20Å 157.20Å 201.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.60 97.31 – 1.49	Depositor EDS
% Data completeness (in resolution range)	81.7 (7.00-1.60) 68.8 (97.31-1.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.211 , (Not available) 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	1.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.1	EDS
Estimated twinning fraction	0.065 for -k,-h,-l	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 277449 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20368	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0937e-04.*

[1]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: MG, CAP, KCX

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	0.40	0/3734	0.69	0/5064
1	C	0.39	0/3734	0.69	0/5064
1	E	0.40	0/3734	0.68	0/5064
1	G	0.40	0/3734	0.68	0/5064
2	I	0.39	0/1068	0.65	1/1453 (0.1%)
2	J	0.38	0/1068	0.63	1/1453 (0.1%)
2	K	0.39	0/1068	0.65	1/1453 (0.1%)
2	L	0.39	0/1068	0.62	1/1453 (0.1%)
All	All	0.40	0/19208	0.67	4/26068 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	33	LEU	CA-CB-CG	6.68	130.66	115.30
2	I	33	LEU	CA-CB-CG	6.68	130.66	115.30
2	J	33	LEU	CA-CB-CG	6.04	129.20	115.30
2	L	33	LEU	CA-CB-CG	5.95	128.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3657	0	3565	29	0
1	C	3657	0	3565	33	0
1	E	3657	0	3565	30	0
1	G	3657	0	3565	34	0
2	I	1033	0	990	13	0
2	J	1033	0	990	18	0
2	K	1033	0	990	15	0
2	L	1033	0	990	22	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	21	0	8	0	0
4	C	21	0	9	0	0
4	E	21	0	9	0	0
4	G	21	0	9	0	0
5	A	314	0	0	3	0
5	C	297	0	0	2	0
5	E	280	0	0	2	0
5	G	308	0	0	1	0
5	I	84	0	0	0	0
5	J	78	0	0	0	0
5	K	77	0	0	0	0
5	L	82	0	0	1	0
All	All	20368	0	18255	181	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 5.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.19	0.89
1:G:207:ASN:H	1:G:209:GLN:HE22	1.21	0.88
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.29	0.79
2:L:89:GLU:HG3	2:L:92:LYS:NZ	2.02	0.75
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.35	0.75
2:K:87:LEU:HG	2:K:91:LYS:NZ	2.05	0.72
1:G:209:GLN:HG3	1:G:211:PHE:CE2	2.24	0.72
2:J:89:GLU:HG2	2:J:92:LYS:NZ	2.07	0.69
1:A:475:VAL:HG21	5:A:532:HOH:O	1.93	0.67
1:G:209:GLN:HG3	1:G:211:PHE:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:THR:H	2:J:25:GLN:HE21	1.42	0.67
1:G:450:LYS:HG3	5:G:762:HOH:O	1.93	0.67
1:A:140:ILE:HD13	1:A:320:LEU:HD11	1.79	0.65
1:A:318:LEU:HG	1:A:326:ILE:HD12	1.78	0.65
2:J:92:LYS:HE2	2:J:93:GLU:HB2	1.79	0.64
2:J:68:THR:HG21	2:K:6:ILE:HG12	1.79	0.64
1:C:140:ILE:HD13	1:C:320:LEU:HD11	1.80	0.64
1:A:156:GLN:HG3	2:I:110:VAL:HG12	1.79	0.64
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.80	0.64
1:G:207:ASN:N	1:G:209:GLN:HE22	1.95	0.63
2:J:32:TYR:HE2	2:J:113:ILE:HD11	1.64	0.62
1:C:18:LYS:HE3	5:C:686:HOH:O	1.99	0.62
1:E:267:HIS:CD2	1:E:277:ASN:HD22	2.15	0.62
2:L:89:GLU:O	2:L:92:LYS:HG3	2.00	0.61
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.65	0.61
2:L:6:ILE:HG22	2:L:7:LEU:HG	1.82	0.61
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.49	0.61
1:C:156:GLN:HG3	2:J:110:VAL:HG13	1.84	0.60
1:E:355:GLU:HG3	5:E:546:HOH:O	2.02	0.59
2:L:48:HIS:HE1	5:L:177:HOH:O	1.84	0.59
1:E:383:HIS:H	1:E:386:HIS:HD2	1.51	0.59
2:K:22:THR:H	2:K:25:GLN:HE21	1.51	0.59
1:C:383:HIS:H	1:C:386:HIS:HD2	1.52	0.58
2:K:68:THR:HG21	2:L:6:ILE:HG12	1.84	0.58
1:A:75:THR:HG22	1:A:76:ASN:H	1.69	0.58
2:I:68:THR:HG21	2:J:6:ILE:HG12	1.86	0.57
2:L:89:GLU:HG3	2:L:92:LYS:HZ3	1.69	0.57
2:K:87:LEU:HG	2:K:91:LYS:HZ2	1.70	0.57
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.40	0.57
2:I:92:LYS:HG3	2:I:93:GLU:N	2.20	0.56
2:I:22:THR:H	2:I:25:GLN:HE21	1.52	0.56
2:J:11:LYS:HG3	2:J:17:TYR:CE1	2.40	0.56
2:K:32:TYR:CE2	2:K:113:ILE:HD11	2.40	0.56
1:E:75:THR:HG22	1:E:76:ASN:H	1.70	0.56
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.88	0.56
1:G:60:GLU:HG3	1:G:127:PHE:CZ	2.41	0.56
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.86	0.55
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.89	0.55
1:E:229:GLN:HE21	1:E:236:LYS:H	1.54	0.55
2:J:89:GLU:O	2:J:92:LYS:HG3	2.06	0.55
1:C:229:GLN:HE21	1:C:236:LYS:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.89	0.55
2:K:5:PRO:HG2	2:K:9:LEU:HD11	1.89	0.54
1:C:293:ILE:HG13	1:C:318:LEU:HD21	1.89	0.54
1:G:267:HIS:CD2	1:G:277:ASN:HD22	2.23	0.54
1:E:76:ASN:O	1:E:79:ARG:HG2	2.08	0.54
1:G:140:ILE:HD13	1:G:320:LEU:HD11	1.90	0.54
1:G:229:GLN:HE21	1:G:236:LYS:H	1.56	0.54
2:K:46:THR:HG22	2:K:97:ALA:HB2	1.91	0.53
1:C:267:HIS:CD2	1:C:277:ASN:HD22	2.25	0.53
2:J:40:PRO:HG2	2:J:74:MET:HB2	1.90	0.53
2:K:6:ILE:HG22	2:K:7:LEU:HG	1.91	0.53
1:E:168:PRO:HD2	1:E:424:LEU:HD11	1.91	0.53
1:C:131:ARG:NH1	5:C:557:HOH:O	2.41	0.53
1:A:383:HIS:H	1:A:386:HIS:HD2	1.56	0.53
1:G:431:ARG:HH21	1:G:432:ASN:HD21	1.57	0.53
1:E:293:ILE:HG13	1:E:318:LEU:HD21	1.90	0.52
1:A:184:ASN:ND2	1:A:187:ARG:HH21	2.08	0.52
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.91	0.52
1:C:155:ILE:HG12	1:C:375:LEU:HD13	1.91	0.52
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.57	0.52
1:E:140:ILE:HD13	1:E:320:LEU:HD11	1.91	0.52
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.93	0.52
2:L:79:ASP:HB3	2:L:82:GLN:HG3	1.91	0.52
2:L:32:TYR:CE2	2:L:113:ILE:HD11	2.44	0.52
1:G:75:THR:HG22	1:G:76:ASN:H	1.75	0.51
2:I:6:ILE:HG12	2:L:68:THR:HG21	1.90	0.51
2:K:32:TYR:HE2	2:K:113:ILE:HD11	1.75	0.51
2:L:32:TYR:HE2	2:L:113:ILE:HD11	1.75	0.51
1:G:156:GLN:HG3	2:L:110:VAL:HG12	1.93	0.51
2:J:32:TYR:CE2	2:J:113:ILE:HD11	2.46	0.51
2:L:89:GLU:HG3	2:L:92:LYS:HZ1	1.76	0.50
1:G:194:ARG:NH1	2:L:6:ILE:HD12	2.26	0.50
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.93	0.50
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.94	0.50
1:E:60:GLU:HG3	1:E:127:PHE:CZ	2.47	0.50
2:L:51:VAL:HG13	2:L:62:TYR:HB3	1.93	0.50
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.94	0.50
1:C:121:VAL:HG22	1:C:125:PHE:CE1	2.46	0.50
1:A:442:ASN:HB3	1:A:446:ARG:NH1	2.27	0.50
2:K:87:LEU:HG	2:K:91:LYS:HZ1	1.77	0.49
2:L:22:THR:H	2:L:25:GLN:HE21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ILE:HD11	1:C:475:VAL:HG23	1.94	0.49
2:I:32:TYR:CE2	2:I:113:ILE:HD11	2.47	0.49
2:I:32:TYR:HE2	2:I:113:ILE:HD11	1.75	0.49
1:E:296:ALA:O	1:E:297:MET:HB3	2.13	0.49
1:C:383:HIS:H	1:C:386:HIS:CD2	2.30	0.49
1:G:296:ALA:O	1:G:297:MET:HB3	2.13	0.49
2:J:34:LEU:HD12	2:J:80:PRO:HG3	1.94	0.48
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.59	0.48
1:G:195:GLY:HA3	1:G:417:ALA:HB3	1.95	0.48
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.62	0.48
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.96	0.48
1:C:377:VAL:HG22	1:C:399:VAL:HB	1.95	0.47
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.60	0.47
2:L:51:VAL:CG1	2:L:62:TYR:HB3	2.45	0.47
2:L:46:THR:HG22	2:L:97:ALA:HB2	1.97	0.47
1:A:293:ILE:HG13	1:A:318:LEU:HD21	1.97	0.47
2:J:89:GLU:HG2	2:J:92:LYS:HZ2	1.80	0.46
1:E:383:HIS:H	1:E:386:HIS:CD2	2.32	0.46
1:A:155:ILE:HG12	1:A:375:LEU:HD13	1.97	0.46
1:C:171:GLY:HA3	1:C:401:GLN:HG2	1.95	0.46
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.98	0.46
1:C:296:ALA:O	1:C:297:MET:HB3	2.16	0.46
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.97	0.46
1:A:463:LYS:HE2	5:A:637:HOH:O	2.16	0.46
1:C:457:ALA:O	1:C:460:GLU:HG3	2.15	0.46
1:C:184:ASN:ND2	1:C:187:ARG:HH11	2.13	0.46
2:I:7:LEU:HD11	2:L:96:ASN:HD21	1.80	0.46
1:G:24:TYR:CD2	1:G:59:ALA:HB2	2.50	0.46
1:A:229:GLN:HE21	1:A:236:LYS:H	1.62	0.46
1:A:296:ALA:O	1:A:297:MET:HB3	2.16	0.46
1:C:343:LEU:HD21	1:C:393:ILE:HG23	1.99	0.45
1:C:431:ARG:HH21	1:C:432:ASN:HD21	1.64	0.45
1:G:443:THR:O	1:G:447:GLU:HG3	2.16	0.45
2:I:89:GLU:HG3	2:I:92:LYS:NZ	2.31	0.45
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.64	0.45
2:K:14:THR:HG22	2:K:15:LEU:HG	1.97	0.45
2:L:46:THR:CG2	2:L:97:ALA:HB2	2.47	0.45
1:A:330:THR:O	1:A:331:VAL:HB	2.16	0.45
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.00	0.44
1:A:414:ALA:O	1:A:418:VAL:HG23	2.18	0.44
1:E:184:ASN:ND2	1:E:187:ARG:HH11	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:MET:O	1:E:255:VAL:HG23	2.16	0.44
1:C:382:ILE:HA	1:C:386:HIS:HD2	1.83	0.43
2:I:6:ILE:CD1	2:L:68:THR:HG21	2.48	0.43
1:E:105:LEU:HB3	5:E:599:HOH:O	2.18	0.43
1:C:184:ASN:HD22	1:C:187:ARG:HH11	1.66	0.43
1:G:334:LYS:HG3	1:G:335:LEU:HG	1.99	0.43
2:L:39:VAL:HA	2:L:40:PRO:HD3	1.85	0.43
1:A:185:TYR:O	1:A:189:VAL:HG23	2.18	0.43
1:E:239:TYR:HB3	1:E:266:MET:HB3	2.00	0.43
1:C:18:LYS:HB3	1:C:22:LEU:HD12	2.00	0.42
1:A:88:GLU:HA	1:A:89:PRO:HD3	1.84	0.42
1:E:414:ALA:O	1:E:418:VAL:HG23	2.19	0.42
1:A:442:ASN:HD22	1:A:446:ARG:NH2	2.16	0.42
2:K:92:LYS:HD2	2:K:93:GLU:N	2.34	0.42
1:C:175:LYS:HA	1:C:176:PRO:C	2.40	0.42
1:E:214:TRP:CD2	1:E:253:ARG:HG2	2.55	0.42
1:C:134:ARG:HD2	1:C:305:LYS:O	2.20	0.42
1:G:293:ILE:HG13	1:G:318:LEU:HD21	2.01	0.42
1:E:171:GLY:HA3	1:E:401:GLN:HG2	2.02	0.41
2:L:14:THR:HG22	2:L:15:LEU:HG	2.00	0.41
1:G:377:VAL:HG22	1:G:399:VAL:HB	2.01	0.41
1:C:318:LEU:HG	1:C:326:ILE:HD12	2.02	0.41
1:C:382:ILE:HA	1:C:386:HIS:CD2	2.55	0.41
1:G:134:ARG:HD2	1:G:305:LYS:O	2.19	0.41
1:E:318:LEU:HG	1:E:326:ILE:HD12	2.03	0.41
1:A:219:LEU:HD23	1:G:161:LYS:HE2	2.00	0.41
1:G:252:LYS:HE3	1:G:252:LYS:HB3	1.90	0.41
2:J:46:THR:HG21	2:K:7:LEU:HD11	2.03	0.41
1:G:121:VAL:HG22	1:G:125:PHE:CE1	2.55	0.41
2:J:51:VAL:HG13	2:J:62:TYR:HB3	2.01	0.41
2:J:79:ASP:O	2:J:82:GLN:HB2	2.21	0.41
1:A:239:TYR:HB3	1:A:266:MET:HB3	2.02	0.41
1:A:194:ARG:NH1	2:I:6:ILE:HD12	2.36	0.41
1:E:297:MET:O	1:E:297:MET:HG2	2.21	0.40
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.69	0.40
1:E:175:LYS:HA	1:E:176:PRO:C	2.41	0.40
1:C:443:THR:O	1:C:447:GLU:HG3	2.21	0.40
1:G:184:ASN:HA	1:G:184:ASN:HD22	1.70	0.40
1:A:306:ASN:HB3	5:A:787:HOH:O	2.21	0.40
1:E:36:ILE:HD13	1:E:108:PHE:CE2	2.56	0.40
1:G:201:KCX:HB2	1:G:239:TYR:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ASN:HD22	1:G:163:ASN:HA	1.70	0.40
2:K:34:LEU:HD12	2:K:80:PRO:HG3	2.03	0.40
2:J:92:LYS:HE2	2:J:93:GLU:N	2.37	0.40
1:G:24:TYR:CG	1:G:59:ALA:HB2	2.57	0.40
2:J:14:THR:HG22	2:J:15:LEU:HG	2.02	0.40
2:I:39:VAL:HA	2:I:40:PRO:HD3	1.90	0.40
2:I:11:LYS:HG3	2:I:17:TYR:CZ	2.56	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	464/475 (98%)	448 (97%)	16 (3%)	0	100	100
1	C	464/475 (98%)	450 (97%)	14 (3%)	0	100	100
1	E	464/475 (98%)	446 (96%)	18 (4%)	0	100	100
1	G	464/475 (98%)	448 (97%)	16 (3%)	0	100	100
2	I	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	J	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
2	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
2	L	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
All	All	2340/2392 (98%)	2258 (96%)	82 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	378/386 (98%)	371 (98%)	7 (2%)	65 39
1	C	378/386 (98%)	369 (98%)	9 (2%)	57 27
1	E	378/386 (98%)	368 (97%)	10 (3%)	54 25
1	G	378/386 (98%)	371 (98%)	7 (2%)	65 39
2	I	112/112 (100%)	108 (96%)	4 (4%)	42 15
2	J	112/112 (100%)	104 (93%)	8 (7%)	18 3
2	K	112/112 (100%)	106 (95%)	6 (5%)	27 6
2	L	112/112 (100%)	106 (95%)	6 (5%)	27 6
All	All	1960/1992 (98%)	1903 (97%)	57 (3%)	50 21

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	75	THR
1	A	119	SER
1	A	163	ASN
1	A	239	TYR
1	A	241	ASN
1	A	466	LYS
1	C	11	VAL
1	C	17	VAL
1	C	94	GLU
1	C	121	VAL
1	C	172	CYS
1	C	203	ASP
1	C	241	ASN
1	C	269	TYR
1	C	460	GLU
1	E	17	VAL
1	E	75	THR
1	E	83	ARG
1	E	163	ASN
1	E	219	LEU
1	E	241	ASN
1	E	269	TYR

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Mol	Chain	Res	Type
1	E	340	ASP
1	E	355	GLU
1	E	392	GLU
1	G	75	THR
1	G	94	GLU
1	G	163	ASN
1	G	209	GLN
1	G	241	ASN
1	G	282	HIS
1	G	392	GLU
2	I	33	LEU
2	I	56	HIS
2	I	68	THR
2	I	92	LYS
2	J	9	LEU
2	J	33	LEU
2	J	56	HIS
2	J	68	THR
2	J	85	ASN
2	J	92	LYS
2	J	110	VAL
2	J	119	LYS
2	K	9	LEU
2	K	33	LEU
2	K	56	HIS
2	K	68	THR
2	K	89	GLU
2	K	92	LYS
2	L	6	ILE
2	L	9	LEU
2	L	33	LEU
2	L	56	HIS
2	L	68	THR
2	L	92	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	163	ASN
1	A	184	ASN
1	A	207	ASN

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	A	442	ASN
1	C	156	GLN
1	C	184	ASN
1	C	207	ASN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	386	HIS
1	C	401	GLN
1	C	420	ASN
1	C	432	ASN
1	E	156	GLN
1	E	163	ASN
1	E	184	ASN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	304	GLN
1	E	386	HIS
1	E	401	GLN
1	E	432	ASN
1	E	442	ASN
1	G	156	GLN
1	G	163	ASN
1	G	184	ASN
1	G	207	ASN
1	G	209	GLN
1	G	229	GLN
1	G	238	HIS

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Mol	Chain	Res	Type
1	G	241	ASN
1	G	267	HIS
1	G	304	GLN
1	G	386	HIS
1	G	401	GLN
1	G	420	ASN
1	G	432	ASN
2	I	25	GLN
2	I	29	GLN
2	J	25	GLN
2	J	29	GLN
2	J	48	HIS
2	J	55	HIS
2	K	25	GLN
2	K	29	GLN
2	K	85	ASN
2	L	25	GLN
2	L	29	GLN
2	L	55	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 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	KCX	A	201	1,3	7,11,12	0.44	0	7,12,14	0.89	0
1	KCX	C	201	1,3	7,11,12	0.57	0	7,12,14	0.84	0
1	KCX	E	201	1,3	7,11,12	0.50	0	7,12,14	0.77	0
1	KCX	G	201	1,3	7,11,12	0.64	0	7,12,14	0.80	0

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	KCX	A	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
1	KCX	G	201	1,3	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	201	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	CAP	A	477	3	14,20,20	1.69	3 (21%)	15,31,31	1.10	1 (6%)
4	CAP	C	477	3	14,20,20	1.84	6 (42%)	15,31,31	1.78	4 (26%)
4	CAP	E	477	3	14,20,20	1.40	2 (14%)	15,31,31	1.40	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAP	G	477	3	14,20,20	1.77	2 (14%)	15,31,31	1.83	5 (33%)

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	CAP	A	477	3	-	0/23/29/29	0/0/0/0
4	CAP	C	477	3	-	0/23/29/29	0/0/0/0
4	CAP	E	477	3	-	0/23/29/29	0/0/0/0
4	CAP	G	477	3	-	0/23/29/29	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	477	CAP	O2-C2	-4.13	1.38	1.43
4	A	477	CAP	O2-C2	-4.11	1.38	1.43
4	C	477	CAP	O2-C2	-3.70	1.38	1.43
4	E	477	CAP	O2-C2	-3.43	1.39	1.43
4	A	477	CAP	O4-C4	-3.22	1.36	1.43
4	G	477	CAP	O4-C4	-2.70	1.37	1.43
4	E	477	CAP	O4-C4	-2.41	1.37	1.43
4	A	477	CAP	O3-C3	-2.18	1.38	1.42
4	C	477	CAP	O4-C4	-2.18	1.38	1.43
4	C	477	CAP	P1-O3P	-2.07	1.47	1.54
4	C	477	CAP	P2-O6P	-2.02	1.47	1.54
4	C	477	CAP	C5-C4	2.22	1.55	1.51
4	C	477	CAP	P1-O2P	2.84	1.64	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	477	CAP	O5P-P2-O5	-3.67	96.00	106.56
4	G	477	CAP	O4-C4-C3	-2.77	102.30	109.50
4	G	477	CAP	O5P-P2-O5	-2.07	100.62	106.56
4	G	477	CAP	O6P-P2-O5P	2.48	116.81	107.38
4	A	477	CAP	O3P-P1-O1P	2.49	118.59	110.58
4	C	477	CAP	O6P-P2-O5P	2.62	117.38	107.38
4	C	477	CAP	O3P-P1-O1P	2.76	119.47	110.58
4	G	477	CAP	O3P-P1-O1P	2.79	119.55	110.58
4	E	477	CAP	O6P-P2-O4P	2.85	119.75	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	477	CAP	O6P-P2-O4P	2.88	119.86	110.58
4	G	477	CAP	O6P-P2-O4P	2.96	120.10	110.58
4	E	477	CAP	O3P-P1-O1P	3.10	120.55	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	466/475 (98%)	-0.42	6 (1%) 79 79	4, 11, 27, 44	0
1	C	466/475 (98%)	-0.43	5 (1%) 82 83	5, 11, 26, 45	0
1	E	466/475 (98%)	-0.44	6 (1%) 79 79	5, 11, 26, 44	0
1	G	466/475 (98%)	-0.41	5 (1%) 82 83	5, 11, 27, 47	0
2	I	123/123 (100%)	-0.20	1 (0%) 87 87	7, 19, 31, 40	0
2	J	123/123 (100%)	-0.16	0 100 100	8, 19, 31, 38	0
2	K	123/123 (100%)	-0.22	1 (0%) 87 87	10, 19, 31, 41	0
2	L	123/123 (100%)	-0.17	2 (1%) 74 74	7, 18, 30, 37	0
All	All	2356/2392 (98%)	-0.38	26 (1%) 82 83	4, 12, 29, 47	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	9	ALA	8.0
1	G	10	SER	7.4
1	C	475	VAL	7.3
1	A	9	ALA	7.2
1	A	475	VAL	7.1
1	G	11	VAL	6.4
1	G	9	ALA	6.4
1	E	11	VAL	5.8
1	A	10	SER	5.3
1	G	475	VAL	5.1
1	C	9	ALA	5.1
1	C	11	VAL	4.9
1	E	10	SER	4.9
1	A	11	VAL	4.3
1	E	475	VAL	3.6
1	G	12	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	10	SER	3.2
1	C	12	GLU	3.1
1	A	12	GLU	3.1
1	E	12	GLU	2.8
2	I	92	LYS	2.7
1	A	92	GLY	2.2
1	E	439	ARG	2.1
2	L	9	LEU	2.1
2	K	6	ILE	2.1
2	L	92	LYS	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	KCX	C	201	12/13	0.97	0.06	-	5,8,11,11	0
1	KCX	A	201	12/13	0.97	0.07	-	3,6,12,14	0
1	KCX	G	201	12/13	0.97	0.06	-	4,11,14,14	0
1	KCX	E	201	12/13	0.96	0.08	-	6,8,10,13	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
4	CAP	C	477	21/21	0.98	0.07	0.19	6,11,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CAP	E	477	21/21	0.98	0.06	-0.30	7,12,14,15	0
3	MG	C	476	1/1	0.96	0.07	-0.39	15,15,15,15	0
3	MG	E	476	1/1	0.97	0.06	-0.40	15,15,15,15	0
4	CAP	A	477	21/21	0.98	0.06	-0.49	10,12,15,16	0
4	CAP	G	477	21/21	0.98	0.06	-1.00	4,11,14,17	0
3	MG	G	476	1/1	0.98	0.06	-1.43	14,14,14,14	0
3	MG	A	476	1/1	0.97	0.05	-1.97	15,15,15,15	0

6.5 Other polymers

There are no such residues in this entry.