Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 PM GMT

PDB ID	:	4MKV
Title	:	Structure of Pisum sativum Rubisco with ABA
Authors	:	Loewen, M.C.; Loewen, P.C.; Switala, J.
Deposited on	:	2013-09-05
Resolution	:	2.15 Å(reported)

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

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

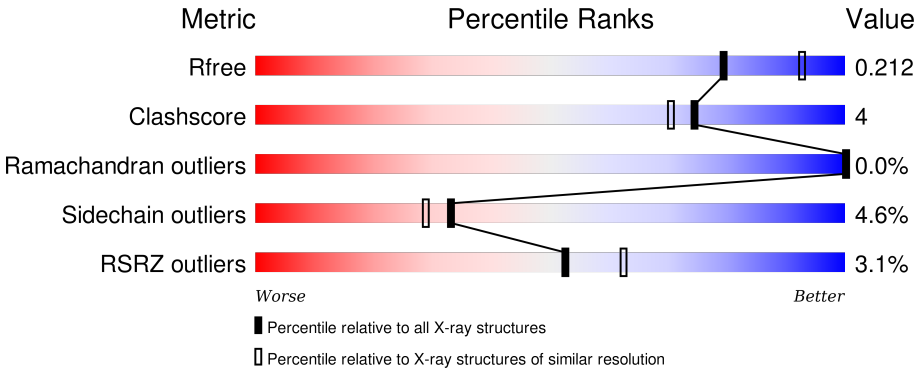
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	458	88% 11%
1	B	458	3% 88% 11%
1	C	458	2% 88% 10%
1	D	458	3% 87% 11%
2	S	123	4% 89% 11%

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Mol	Chain	Length	Quality of chain
2	T	123	3% 94% 5%
2	U	123	13% 91% 9%
2	V	123	6% 88% 11%

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
4	PO4	A	502	-	-	-	X
4	PO4	C	502	-	-	-	X
4	PO4	D	502	-	-	-	X
5	A8S	B	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19725 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 bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	3	0
			3608	2299	632	660	17			
1	B	458	Total	C	N	O	S	0	4	0
			3609	2303	631	658	17			
1	C	458	Total	C	N	O	S	0	5	0
			3621	2309	635	660	17			
1	D	458	Total	C	N	O	S	0	5	0
			3619	2307	633	662	17			

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small chain 3A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1029	678	171	175	5			
2	T	123	Total	C	N	O	S	0	1	0
			1033	682	171	175	5			
2	U	123	Total	C	N	O	S	0	2	0
			1041	686	174	176	5			
2	V	123	Total	C	N	O	S	0	0	0
			1029	678	171	175	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	47	LYS	GLU	CONFLICT	UNP P07689
S	91	LYS	VAL	CONFLICT	UNP P07689
S	92	LYS	ALA	CONFLICT	UNP P07689
S	96	ARG	GLN	CONFLICT	UNP P07689
S	121	ALA	GLU	CONFLICT	UNP P07689
S	122	GLY	SER	CONFLICT	UNP P07689
T	47	LYS	GLU	CONFLICT	UNP P07689
T	91	LYS	VAL	CONFLICT	UNP P07689

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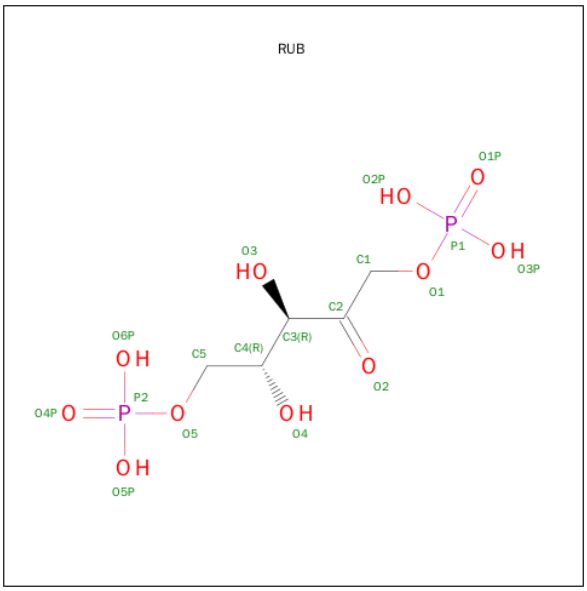
Chain	Residue	Modelled	Actual	Comment	Reference
T	92	LYS	ALA	CONFLICT	UNP P07689
T	96	ARG	GLN	CONFLICT	UNP P07689
T	121	ALA	GLU	CONFLICT	UNP P07689
T	122	GLY	SER	CONFLICT	UNP P07689
U	47	LYS	GLU	CONFLICT	UNP P07689
U	91	LYS	VAL	CONFLICT	UNP P07689
U	92	LYS	ALA	CONFLICT	UNP P07689
U	96	ARG	GLN	CONFLICT	UNP P07689
U	121	ALA	GLU	CONFLICT	UNP P07689
U	122	GLY	SER	CONFLICT	UNP P07689
V	47	LYS	GLU	CONFLICT	UNP P07689
V	91	LYS	VAL	CONFLICT	UNP P07689
V	92	LYS	ALA	CONFLICT	UNP P07689
V	96	ARG	GLN	CONFLICT	UNP P07689
V	121	ALA	GLU	CONFLICT	UNP P07689
V	122	GLY	SER	CONFLICT	UNP P07689

- Molecule 3 is SUGAR (RIBULOSE-1,5-DIPHOSPHATE) (three-letter code: RUB) (formula: $C_5H_{12}O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			18	5	11	2		
3	B	1	Total	C	O	P	0	0
			18	5	11	2		
3	C	1	Total	C	O	P	0	0
			18	5	11	2		

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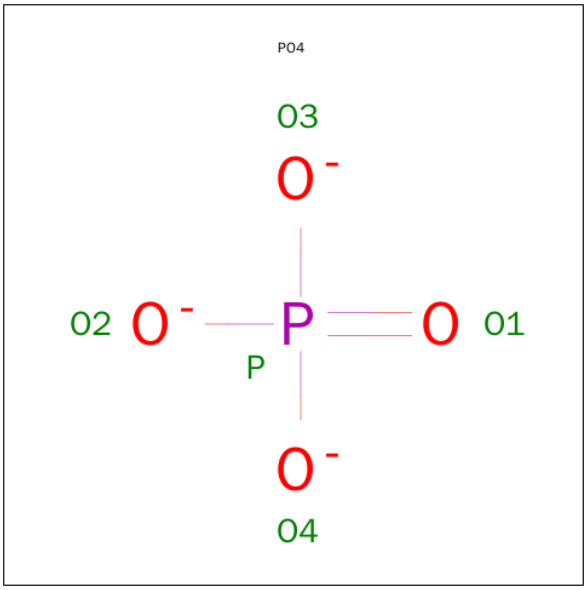
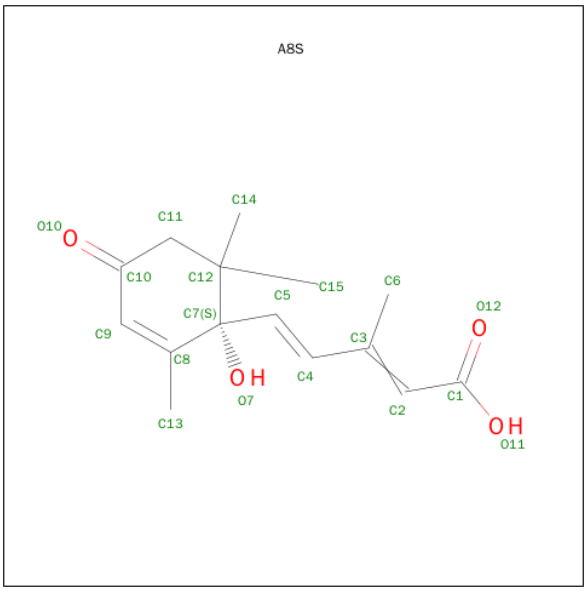
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O P 18 5 11 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is (2Z,4E)-5-[(1S)-1-HYDROXY-2,6,6-TRIMETHYL-4-OXOCYCLOHEX-2-EN-1-YL]-3-METHYLPENTA-2,4-DIENOIC ACID (three-letter code: A8S) (formula: $C_{15}H_{20}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 19 15 4	0	0

- Molecule 6 is water.

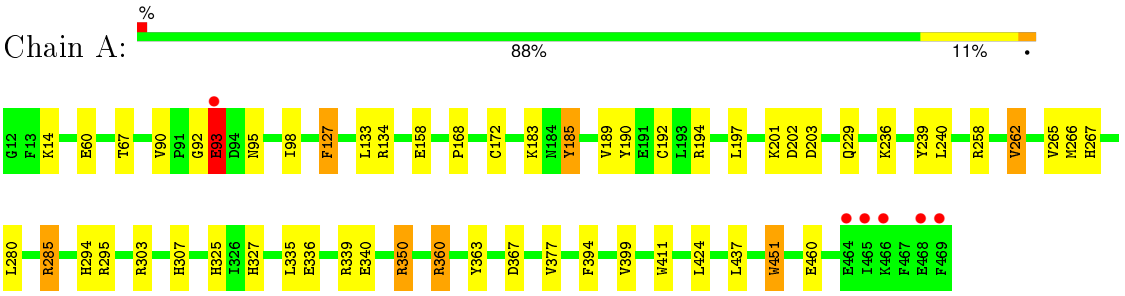
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	215	Total O 215 215	0	0
6	B	208	Total O 208 208	0	0
6	C	174	Total O 174 174	0	0
6	D	201	Total O 201 201	0	0
6	S	67	Total O 67 67	0	0
6	T	77	Total O 77 77	0	0
6	U	36	Total O 36 36	0	0
6	V	52	Total O 52 52	0	0

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.

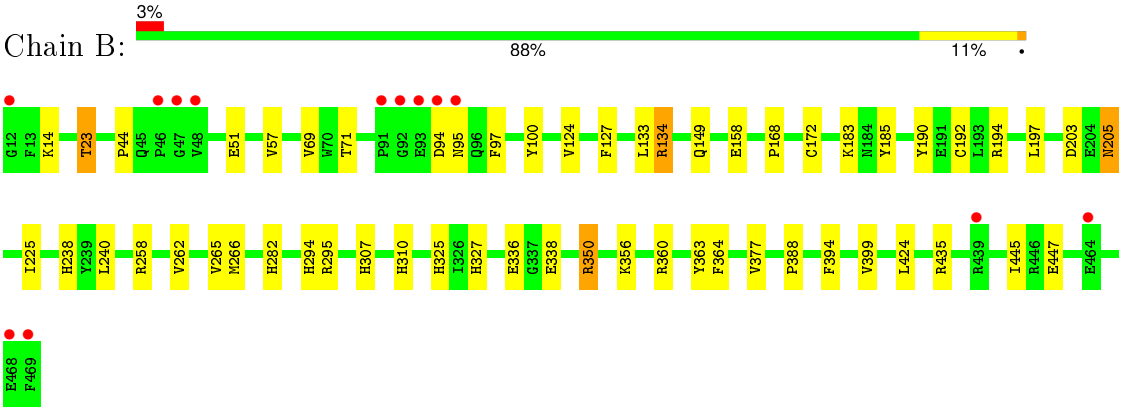
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A:



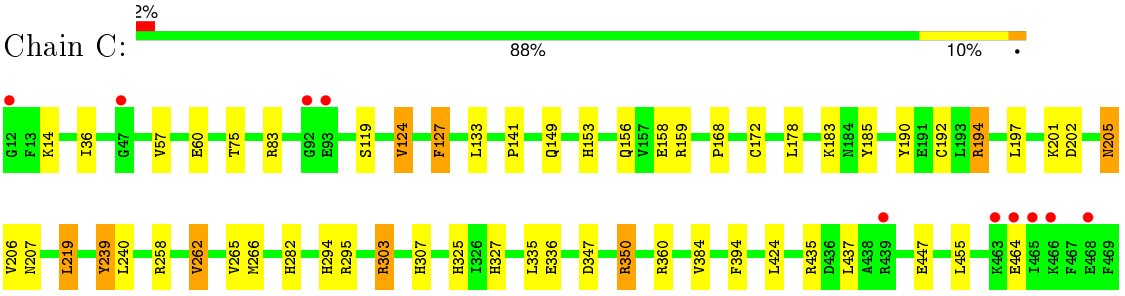
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain B:



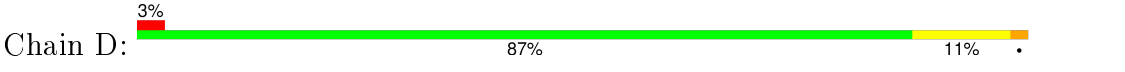
- Molecule 1: Ribulose bisphosphate carboxylase large chain

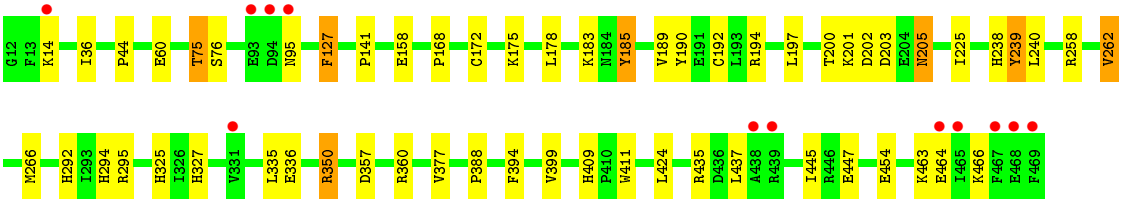
Chain C:



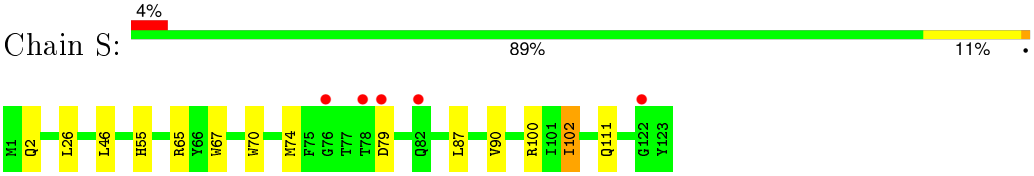
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain D:

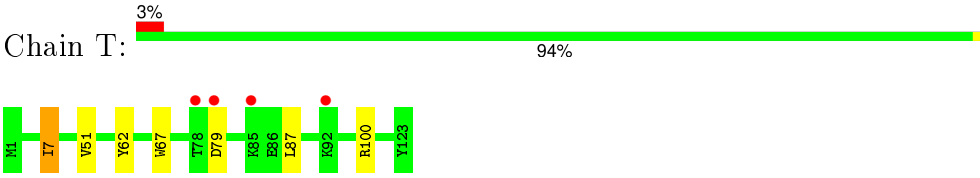




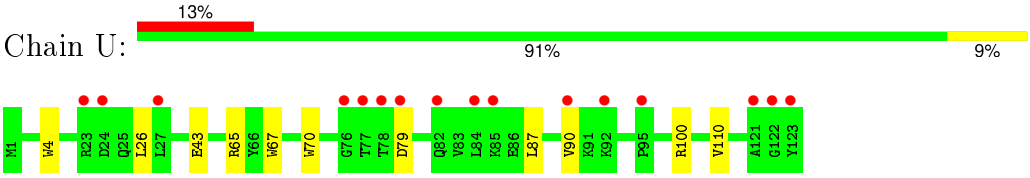
• Molecule 2: Ribulose bisphosphate carboxylase small chain 3A, chloroplastic



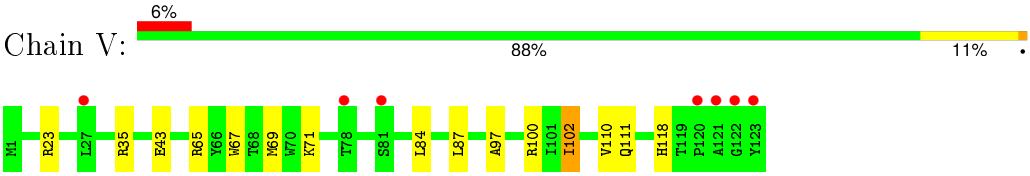
• Molecule 2: Ribulose bisphosphate carboxylase small chain 3A, chloroplastic



• Molecule 2: Ribulose bisphosphate carboxylase small chain 3A, chloroplastic



• Molecule 2: Ribulose bisphosphate carboxylase small chain 3A, chloroplastic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.44Å 110.23Å 203.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.15 48.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.51-2.15) 94.9 (48.51-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.162 , 0.197 0.174 , 0.212	Depositor DCC
R_{free} test set	6458 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.5	EDS
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 128283 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19725	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% 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: RUB, A8S, PO4

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	0.53	0/3704	0.72	1/5021 (0.0%)
1	B	0.52	0/3711	0.69	1/5031 (0.0%)
1	C	0.50	0/3728	0.71	2/5053 (0.0%)
1	D	0.51	0/3723	0.69	1/5047 (0.0%)
2	S	0.50	0/1062	0.68	0/1436
2	T	0.50	0/1069	0.67	0/1446
2	U	0.47	0/1080	0.68	0/1460
2	V	0.49	0/1062	0.72	0/1436
All	All	0.51	0/19139	0.70	5/25930 (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	219	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	350	ARG	CB-CG-CD	-5.08	98.40	111.60
1	A	350	ARG	CB-CG-CD	-5.08	98.40	111.60
1	B	350	ARG	CB-CG-CD	-5.02	98.54	111.60
1	D	350	ARG	CB-CG-CD	-5.02	98.55	111.60

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	3608	0	3545	30	0
1	B	3609	0	3557	36	0
1	C	3621	0	3561	30	1
1	D	3619	0	3552	32	1
2	S	1029	0	1037	8	0
2	T	1033	0	1046	3	0
2	U	1041	0	1057	4	0
2	V	1029	0	1037	9	0
3	A	18	0	8	1	0
3	B	18	0	8	0	0
3	C	18	0	8	1	0
3	D	18	0	8	1	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	B	19	0	19	5	0
6	A	215	0	0	3	0
6	B	208	0	0	1	0
6	C	174	0	0	2	0
6	D	201	0	0	0	0
6	S	67	0	0	3	0
6	T	77	0	0	0	0
6	U	36	0	0	0	0
6	V	52	0	0	2	0
All	All	19725	0	18443	149	1

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 4.

All (149) 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:60:GLU:HG3	1:C:127:PHE:HZ	1.35	0.86
2:S:55:HIS:HD2	6:S:266:HOH:O	1.57	0.86
1:C:60:GLU:HG3	1:C:127:PHE:CZ	2.13	0.82
1:A:60:GLU:HG3	1:A:127:PHE:HZ	1.47	0.79
1:D:409:HIS:HD2	1:D:411:TRP:H	1.30	0.78
1:D:178:LEU:HD21	1:D:205:ASN:HB3	1.67	0.76
1:D:409:HIS:CD2	1:D:411:TRP:H	2.07	0.72
2:T:67:TRP:CZ3	2:T:100:ARG:HG3	2.27	0.70
1:A:367:ASP:OD1	6:A:814:HOH:O	2.10	0.70
1:C:194:ARG:NH2	2:U:4:TRP:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:TYR:HB2	1:D:266:MET:HE1	1.75	0.69
2:U:67:TRP:CZ3	2:U:100:ARG:HG3	2.28	0.68
2:V:67:TRP:CZ3	2:V:100:ARG:HG3	2.27	0.68
1:A:60:GLU:HG3	1:A:127:PHE:CZ	2.27	0.68
2:S:67:TRP:CZ3	2:S:100:ARG:HG3	2.28	0.68
1:A:202:ASP:HB2	1:A:266:MET:HE1	1.75	0.68
1:B:266:MET:CE	1:B:294:HIS:HD2	2.09	0.65
1:C:178:LEU:HD21	1:C:205:ASN:HB3	1.79	0.65
1:B:266:MET:HE3	1:B:294:HIS:HD2	1.61	0.64
1:B:363:TYR:O	5:B:502:A8S:H13A	1.98	0.63
1:B:69[A]:VAL:HG12	1:B:71:THR:OG1	2.00	0.62
1:D:388:PRO:HD3	1:D:445:ILE:HD11	1.82	0.61
1:C:350:ARG:NH2	1:C:394:PHE:O	2.33	0.61
1:D:350:ARG:NH2	1:D:394:PHE:O	2.30	0.61
2:V:43:GLU:OE1	2:V:100:ARG:NH1	2.33	0.61
1:C:57:VAL:HA	1:C:124:VAL:HG21	1.84	0.59
2:U:43:GLU:OE1	2:U:100:ARG:NH1	2.35	0.59
1:A:335:LEU:CD1	3:A:501:RUB:H52	2.33	0.59
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.87	0.58
1:B:57:VAL:HA	1:B:124:VAL:HG21	1.86	0.58
1:A:93:GLU:HA	1:A:95:ASN:H	1.68	0.58
1:B:350:ARG:NH2	1:B:394:PHE:O	2.34	0.57
1:D:335:LEU:CD1	3:D:501:RUB:H52	2.35	0.56
1:B:205:ASN:H	1:B:205:ASN:HD22	1.53	0.56
1:C:57:VAL:HA	1:C:124:VAL:CG2	2.35	0.56
1:D:239:TYR:HB2	1:D:266:MET:CE	2.36	0.56
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.89	0.56
1:A:451:TRP:HD1	6:S:251:HOH:O	1.90	0.55
1:D:201:LYS:HB3	1:D:239:TYR:CD2	2.41	0.55
1:B:100:TYR:CE1	5:B:502:A8S:H13	2.42	0.55
1:A:168:PRO:HD2	1:A:424:LEU:HD11	1.89	0.55
1:B:356:LYS:HD2	5:B:502:A8S:H6	1.88	0.54
2:V:100:ARG:NH2	6:V:224:HOH:O	2.40	0.54
1:A:350:ARG:NH2	1:A:394:PHE:O	2.35	0.54
1:B:266:MET:HE1	1:B:294:HIS:CD2	2.43	0.53
1:C:149:GLN:HE22	1:C:282:HIS:HA	1.72	0.53
1:B:266:MET:CE	1:B:294:HIS:CD2	2.90	0.53
1:B:168:PRO:HD2	1:B:424:LEU:HD11	1.92	0.52
1:B:364:PHE:HE1	5:B:502:A8S:H9	1.75	0.52
2:S:74:MET:HE2	6:S:245:HOH:O	2.10	0.52
1:C:335:LEU:CD1	3:C:501:RUB:H52	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ASP:OD2	1:C:360:ARG:NH2	2.42	0.51
1:C:168:PRO:HD2	1:C:424:LEU:HD11	1.92	0.51
1:C:384:VAL:HG11	1:C:455:LEU:HD11	1.94	0.50
2:T:51[A]:VAL:HG13	2:T:62:TYR:HB3	1.92	0.50
1:D:168:PRO:HD2	1:D:424:LEU:HD11	1.93	0.50
1:A:201:LYS:NZ	1:A:294:HIS:NE2	2.52	0.50
1:C:190:TYR:CZ	1:C:194:ARG:HD2	2.47	0.49
1:A:98:ILE:HD13	1:A:363:TYR:HE2	1.77	0.49
1:B:388:PRO:HD3	1:B:445:ILE:HD11	1.93	0.49
1:C:202:ASP:HB2	1:C:266:MET:HE1	1.93	0.49
1:B:69[A]:VAL:CG1	1:B:71:THR:OG1	2.61	0.49
1:D:292:HIS:HD2	1:D:325:HIS:ND1	2.11	0.48
1:C:435:ARG:NH2	1:C:447:GLU:OE1	2.46	0.48
2:S:100:ARG:HD2	2:S:102:ILE:HD11	1.96	0.47
1:A:201:LYS:HB3	1:A:239:TYR:CD2	2.49	0.47
1:D:158:GLU:CD	1:D:325:HIS:HE2	2.16	0.47
2:U:70:TRP:CE3	2:U:90:VAL:HG13	2.49	0.47
1:C:201:LYS:HB3	1:C:239:TYR:CD2	2.49	0.47
1:C:192:CYS:HB3	1:C:197:LEU:HD12	1.97	0.47
1:B:205:ASN:H	1:B:205:ASN:ND2	2.12	0.47
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.97	0.46
2:V:35:ARG:HD2	6:V:241:HOH:O	2.13	0.46
2:V:100:ARG:HD2	2:V:102:ILE:HD11	1.97	0.46
1:A:192:CYS:HB3	1:A:197:LEU:HD12	1.98	0.46
1:D:185:TYR:OH	1:D:202:ASP:HA	2.15	0.46
1:D:44:PRO:HG2	1:D:95:ASN:HD22	1.81	0.46
2:V:102:ILE:HG12	2:V:111:GLN:NE2	2.31	0.46
1:A:229:GLN:HE21	1:A:236:LYS:H	1.63	0.45
1:C:384:VAL:CG1	1:C:455:LEU:HD11	2.46	0.45
1:D:192:CYS:HB3	1:D:197:LEU:HD12	1.99	0.45
1:B:44:PRO:HG3	1:B:97:PHE:HE1	1.81	0.45
1:B:57:VAL:HA	1:B:124:VAL:CG2	2.46	0.45
1:B:133:LEU:H	1:B:307:HIS:CD2	2.35	0.45
1:D:201:LYS:HB2	1:D:266:MET:HE1	1.99	0.45
2:S:102:ILE:HG12	2:S:111:GLN:NE2	2.32	0.45
1:D:240:LEU:HD12	1:D:262:VAL:HG11	1.98	0.45
1:B:205:ASN:N	1:B:205:ASN:HD22	2.15	0.45
1:B:149:GLN:HE22	1:B:282:HIS:HA	1.81	0.44
1:A:172:CYS:HB3	1:A:197:LEU:HD13	1.98	0.44
1:A:340:GLU:O	1:A:360:ARG:HG2	2.17	0.44
1:C:159:ARG:NH2	6:C:720:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLY:O	1:A:93:GLU:HB2	2.18	0.44
2:S:70:TRP:CD2	2:S:90:VAL:HG22	2.53	0.44
1:A:133:LEU:H	1:A:307:HIS:CD2	2.36	0.44
1:B:94:ASP:HA	1:B:95:ASN:HA	1.67	0.44
1:A:267:HIS:HB2	1:A:280:LEU:HD23	2.00	0.44
1:A:339:ARG:NH1	6:A:753:HOH:O	2.39	0.44
1:A:295:ARG:HG2	1:A:327:HIS:HB2	1.99	0.44
2:V:69:MET:HE3	2:V:71:LYS:O	2.17	0.44
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.20	0.43
1:A:240:LEU:HD12	1:A:262:VAL:HG11	2.00	0.43
1:B:134:ARG:NH2	1:B:310:HIS:HD2	2.15	0.43
1:B:190:TYR:CZ	1:B:194:ARG:HD3	2.53	0.43
2:S:46:LEU:HD13	2:T:7:ILE:HD12	2.00	0.43
1:B:172:CYS:HB3	1:B:197:LEU:HD13	2.00	0.43
1:C:206:VAL:C	1:C:207:ASN:HD22	2.22	0.43
1:B:100:TYR:CE1	5:B:502:A8S:C13	3.02	0.43
1:C:384:VAL:HG11	1:C:455:LEU:CD1	2.49	0.43
1:A:185:TYR:O	1:A:189:VAL:HG23	2.18	0.43
1:B:435:ARG:NH2	1:B:447:GLU:OE1	2.49	0.43
1:C:295:ARG:HG2	1:C:327:HIS:HB2	2.00	0.42
1:D:295:ARG:HG2	1:D:327:HIS:HB2	2.01	0.42
1:A:411:TRP:CZ3	2:S:2:GLN:HB2	2.54	0.42
1:D:75:THR:HG22	1:D:76[A]:SER:H	1.83	0.42
1:D:225:ILE:HD11	1:D:238:HIS:HB3	2.01	0.42
1:A:172:CYS:CB	1:A:197:LEU:HD13	2.49	0.42
1:D:75:THR:HG22	1:D:76[B]:SER:H	1.83	0.42
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.23	0.42
1:C:172:CYS:HB3	1:C:197:LEU:HD13	2.00	0.42
1:B:158:GLU:CD	1:B:325:HIS:HE2	2.19	0.42
1:B:23:THR:CG2	6:B:671:HOH:O	2.68	0.42
1:C:153:HIS:HE1	6:C:612:HOH:O	2.02	0.42
1:C:172:CYS:CB	1:C:197:LEU:HD13	2.50	0.41
1:B:172:CYS:CB	1:B:197:LEU:HD13	2.50	0.41
1:B:240:LEU:HD12	1:B:262:VAL:HG21	2.02	0.41
1:A:133:LEU:H	1:A:307:HIS:HD2	1.68	0.41
1:D:409:HIS:HE1	1:D:454:GLU:O	2.03	0.41
1:C:133:LEU:H	1:C:307:HIS:CD2	2.37	0.41
1:B:377:VAL:HG22	1:B:399:VAL:HB	2.03	0.41
1:D:36:ILE:HG12	1:D:141:PRO:CD	2.50	0.41
1:B:295:ARG:HG2	1:B:327:HIS:HB2	2.01	0.41
1:C:240:LEU:HD12	1:C:262:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:97:ALA:O	2:V:118:HIS:HD2	2.03	0.41
1:B:57:VAL:HG13	1:B:124:VAL:HG21	2.01	0.41
1:D:377:VAL:HG22	1:D:399:VAL:HB	2.02	0.41
1:B:225:ILE:HD11	1:B:238:HIS:HB3	2.03	0.41
1:D:185:TYR:O	1:D:189:VAL:HG23	2.21	0.41
1:D:172:CYS:CB	1:D:197:LEU:HD13	2.52	0.41
1:D:172:CYS:HB3	1:D:197:LEU:HD13	2.01	0.40
1:C:36:ILE:HG12	1:C:141:PRO:CD	2.51	0.40
1:D:435:ARG:NH2	1:D:447:GLU:OE1	2.48	0.40
1:D:357:ASP:OD2	1:D:360:ARG:HD3	2.21	0.40
1:A:285:ARG:NH2	6:A:803:HOH:O	2.53	0.40
1:D:190:TYR:CZ	1:D:194:ARG:HD3	2.56	0.40
1:A:377:VAL:HG22	1:A:399:VAL:HB	2.03	0.40
2:V:23:ARG:HE	2:V:84:LEU:HD13	1.85	0.40
1:A:190:TYR:CZ	1:A:194:ARG:HD3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ARG:NH2	1:D:127:PHE:O[2_555]	2.19	0.01

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	459/458 (100%)	443 (96%)	15 (3%)	1 (0%)	52	51
1	B	460/458 (100%)	441 (96%)	19 (4%)	0	100	100
1	C	461/458 (101%)	445 (96%)	16 (4%)	0	100	100
1	D	461/458 (101%)	444 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
2	T	122/123 (99%)	119 (98%)	3 (2%)	0	100	100
2	U	123/123 (100%)	120 (98%)	3 (2%)	0	100	100
2	V	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
All	All	2328/2324 (100%)	2248 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLU

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	373/370 (101%)	354 (95%)	19 (5%)	29	24
1	B	374/370 (101%)	360 (96%)	14 (4%)	41	38
1	C	375/370 (101%)	353 (94%)	22 (6%)	24	18
1	D	375/370 (101%)	357 (95%)	18 (5%)	31	27
2	S	110/110 (100%)	105 (96%)	5 (4%)	34	30
2	T	111/110 (101%)	108 (97%)	3 (3%)	52	53
2	U	112/110 (102%)	107 (96%)	5 (4%)	34	30
2	V	110/110 (100%)	106 (96%)	4 (4%)	42	40
All	All	1940/1920 (101%)	1850 (95%)	90 (5%)	33	29

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	67	THR
1	A	90	VAL

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Mol	Chain	Res	Type
1	A	93	GLU
1	A	127	PHE
1	A	134	ARG
1	A	183	LYS
1	A	185	TYR
1	A	203	ASP
1	A	258	ARG
1	A	262	VAL
1	A	265	VAL
1	A	285	ARG
1	A	303	ARG
1	A	336	GLU
1	A	360	ARG
1	A	437	LEU
1	A	451	TRP
1	A	460	GLU
1	B	14	LYS
1	B	23	THR
1	B	51	GLU
1	B	127	PHE
1	B	134	ARG
1	B	183	LYS
1	B	185	TYR
1	B	203	ASP
1	B	205	ASN
1	B	258	ARG
1	B	265	VAL
1	B	336	GLU
1	B	338	GLU
1	B	360	ARG
1	C	14	LYS
1	C	75	THR
1	C	83[A]	ARG
1	C	83[B]	ARG
1	C	119[A]	SER
1	C	119[B]	SER
1	C	124	VAL
1	C	127	PHE
1	C	156	GLN
1	C	183	LYS
1	C	185	TYR
1	C	194	ARG

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Mol	Chain	Res	Type
1	C	205	ASN
1	C	219	LEU
1	C	239	TYR
1	C	258	ARG
1	C	262	VAL
1	C	265	VAL
1	C	294	HIS
1	C	303	ARG
1	C	336	GLU
1	C	437	LEU
1	D	14	LYS
1	D	60	GLU
1	D	75	THR
1	D	127	PHE
1	D	175	LYS
1	D	183	LYS
1	D	185	TYR
1	D	203	ASP
1	D	205	ASN
1	D	239	TYR
1	D	258	ARG
1	D	262	VAL
1	D	294	HIS
1	D	336	GLU
1	D	437	LEU
1	D	463	LYS
1	D	464	GLU
1	D	466	LYS
2	S	26	LEU
2	S	65	ARG
2	S	79	ASP
2	S	87	LEU
2	S	102	ILE
2	T	7	ILE
2	T	79	ASP
2	T	87	LEU
2	U	26	LEU
2	U	65	ARG
2	U	79	ASP
2	U	87	LEU
2	U	110	VAL
2	V	65	ARG

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Mol	Chain	Res	Type
2	V	87	LEU
2	V	102	ILE
2	V	110	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	207	ASN
1	A	229	GLN
1	A	292	HIS
1	A	304	GLN
1	A	307	HIS
1	A	401	GLN
1	B	149	GLN
1	B	153	HIS
1	B	205	ASN
1	B	307	HIS
1	C	153	HIS
1	C	207	ASN
1	C	229	GLN
1	C	307	HIS
1	C	401	GLN
1	D	95	ASN
1	D	153	HIS
1	D	156	GLN
1	D	238	HIS
1	D	292	HIS
1	D	307	HIS
1	D	401	GLN
1	D	409	HIS
2	S	55	HIS
2	S	118	HIS
2	U	55	HIS
2	U	118	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	RUB	A	501	-	17,17,17	4.07	6 (35%)	15,25,25	1.67	2 (13%)
4	PO4	A	502	-	4,4,4	0.55	0	6,6,6	0.28	0
3	RUB	B	501	-	17,17,17	3.85	5 (29%)	15,25,25	1.07	1 (6%)
5	A8S	B	502	-	13,19,19	1.76	4 (30%)	12,29,29	1.71	3 (25%)
3	RUB	C	501	-	17,17,17	3.90	6 (35%)	15,25,25	1.76	3 (20%)
4	PO4	C	502	-	4,4,4	0.44	0	6,6,6	0.29	0
3	RUB	D	501	-	17,17,17	4.13	4 (23%)	15,25,25	1.81	2 (13%)
4	PO4	D	502	-	4,4,4	0.42	0	6,6,6	0.27	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
3	RUB	A	501	-	-	0/20/20/20	0/0/0/0
4	PO4	A	502	-	-	0/0/0/0	0/0/0/0
3	RUB	B	501	-	-	0/20/20/20	0/0/0/0
5	A8S	B	502	-	-	0/8/34/34	0/1/1/1
3	RUB	C	501	-	-	0/20/20/20	0/0/0/0
4	PO4	C	502	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RUB	D	501	-	-	0/20/20/20	0/0/0/0
4	PO4	D	502	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	RUB	C4-C3	-4.82	1.49	1.53
3	C	501	RUB	C4-C3	-3.95	1.49	1.53
3	A	501	RUB	C4-C3	-3.80	1.50	1.53
3	D	501	RUB	C4-C3	-3.76	1.50	1.53
3	C	501	RUB	C5-C4	-3.30	1.46	1.51
3	A	501	RUB	C1-C2	-2.69	1.47	1.51
3	D	501	RUB	C1-C2	-2.34	1.47	1.51
3	B	501	RUB	C1-C2	-2.28	1.47	1.51
3	C	501	RUB	C1-C2	-2.19	1.47	1.51
3	A	501	RUB	C5-C4	-2.14	1.48	1.51
3	B	501	RUB	C5-C4	-2.06	1.48	1.51
3	C	501	RUB	P2-O5	2.02	1.67	1.60
5	B	502	A8S	C4-C3	2.16	1.50	1.45
3	A	501	RUB	P2-O5	2.25	1.67	1.60
5	B	502	A8S	C11-C10	2.47	1.53	1.50
5	B	502	A8S	C4-C5	2.97	1.38	1.32
5	B	502	A8S	C7-C12	3.04	1.61	1.57
3	B	501	RUB	O1-C1	5.31	1.46	1.43
3	C	501	RUB	O1-C1	5.65	1.47	1.43
3	D	501	RUB	O1-C1	7.66	1.48	1.43
3	A	501	RUB	O1-C1	8.08	1.48	1.43
3	A	501	RUB	O2-C2	13.13	1.44	1.21
3	C	501	RUB	O2-C2	13.42	1.45	1.21
3	B	501	RUB	O2-C2	13.43	1.45	1.21
3	D	501	RUB	O2-C2	13.87	1.46	1.21

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	502	A8S	C6-C3-C2	-3.70	116.97	125.17
5	B	502	A8S	O7-C7-C12	-2.22	104.89	109.90
3	C	501	RUB	O6P-P2-O5	-2.11	100.49	106.56
3	B	501	RUB	C5-C4-C3	2.30	115.74	111.85
3	D	501	RUB	O5-P2-O4P	2.55	113.64	107.14
3	C	501	RUB	O5-P2-O4P	2.55	113.64	107.14
5	B	502	A8S	C4-C3-C2	2.67	125.68	118.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	RUB	O5-P2-O4P	3.37	115.72	107.14
3	A	501	RUB	C5-C4-C3	3.56	117.88	111.85
3	C	501	RUB	C5-C4-C3	4.59	119.64	111.85
3	D	501	RUB	C5-C4-C3	5.33	120.89	111.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	RUB	1	0
5	B	502	A8S	5	0
3	C	501	RUB	1	0
3	D	501	RUB	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	458/458 (100%)	-0.32	6 (1%) 79 84	11, 22, 46, 79	0
1	B	458/458 (100%)	-0.31	13 (2%) 56 66	12, 23, 48, 87	0
1	C	458/458 (100%)	-0.14	10 (2%) 65 73	14, 28, 54, 85	0
1	D	458/458 (100%)	-0.21	12 (2%) 59 68	13, 27, 52, 88	0
2	S	123/123 (100%)	-0.15	5 (4%) 41 51	17, 28, 52, 65	0
2	T	123/123 (100%)	-0.29	4 (3%) 50 60	18, 30, 53, 58	0
2	U	123/123 (100%)	0.47	16 (13%) 5 8	19, 37, 63, 78	0
2	V	123/123 (100%)	0.04	7 (5%) 27 37	20, 34, 58, 68	0
All	All	2324/2324 (100%)	-0.19	73 (3%) 52 62	11, 27, 53, 88	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	PRO	6.0
1	D	469	PHE	5.3
1	C	468	GLU	5.1
2	V	122	GLY	5.0
1	D	465	ILE	4.8
2	V	121	ALA	4.7
1	B	92	GLY	4.7
1	B	93	GLU	4.6
1	A	465	ILE	4.5
1	C	465	ILE	4.4
1	D	464	GLU	3.8
1	A	468	GLU	3.8
1	A	93	GLU	3.8
1	C	92	GLY	3.7
2	T	92	LYS	3.7
2	U	78	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	U	121	ALA	3.5
1	B	469	PHE	3.5
2	U	84	LEU	3.4
2	V	123	TYR	3.4
1	D	467	PHE	3.3
1	A	469	PHE	3.3
2	V	78	THR	3.2
1	B	468	GLU	3.2
2	U	77	THR	3.2
1	D	94	ASP	3.1
1	B	94	ASP	3.1
1	D	438	ALA	3.1
2	U	123	TYR	3.1
2	U	27	LEU	3.0
2	T	78	THR	3.0
1	A	464	GLU	3.0
2	U	76	GLY	3.0
1	C	466	LYS	3.0
1	D	331	VAL	3.0
1	C	12	GLY	2.9
1	D	468	GLU	2.9
2	U	79	ASP	2.8
2	U	122	GLY	2.8
2	U	23	ARG	2.8
1	B	47	GLY	2.7
1	C	47	GLY	2.7
1	B	95	ASN	2.7
2	U	85	LYS	2.7
1	D	95	ASN	2.7
1	C	464	GLU	2.7
2	S	79	ASP	2.6
1	C	463	LYS	2.6
2	S	82	GLN	2.5
2	U	92	LYS	2.5
2	U	90	VAL	2.5
1	D	93	GLU	2.4
1	B	12	GLY	2.4
2	S	76	GLY	2.4
1	D	14	LYS	2.4
1	B	464	GLU	2.4
1	C	439	ARG	2.4
1	C	93	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	439	ARG	2.3
2	U	82	GLN	2.3
2	T	79	ASP	2.2
2	S	122	GLY	2.2
1	B	439	ARG	2.2
2	U	24	ASP	2.2
2	S	78	THR	2.2
2	T	85	LYS	2.2
2	V	81	SER	2.2
1	B	46	PRO	2.2
2	V	120	PRO	2.1
2	V	27	LEU	2.1
1	A	466	LYS	2.1
1	B	48	VAL	2.0
2	U	95	PRO	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
5	A8S	B	502	19/19	0.65	0.43	26.14	96,102,104,104	0
4	PO4	A	502	5/5	0.92	0.12	6.34	70,73,75,75	0
4	PO4	C	502	5/5	0.96	0.20	4.50	70,70,71,71	0
4	PO4	D	502	5/5	0.92	0.19	4.39	65,65,66,67	0
3	RUB	C	501	18/18	0.98	0.12	0.44	36,41,49,49	0
3	RUB	B	501	18/18	0.98	0.13	0.25	25,35,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	RUB	A	501	18/18	0.97	0.12	0.04	22,35,46,50	0
3	RUB	D	501	18/18	0.96	0.12	-0.20	34,45,57,60	0

6.5 Other polymers (i)

There are no such residues in this entry.