Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2016 – 07:13 PM EDT

PDB ID	:	5AAJ
Title	:	CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-DECANOYL-COA, 3-KETO-DECANOYL-COA AND NADH
Authors	:	Kasaragod, P.; Schmitz, W.; Kalervo Hiltunen, J.; Wierenga, R.K.
Deposited on	:	2015-07-26
Resolution	:	2.49 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:

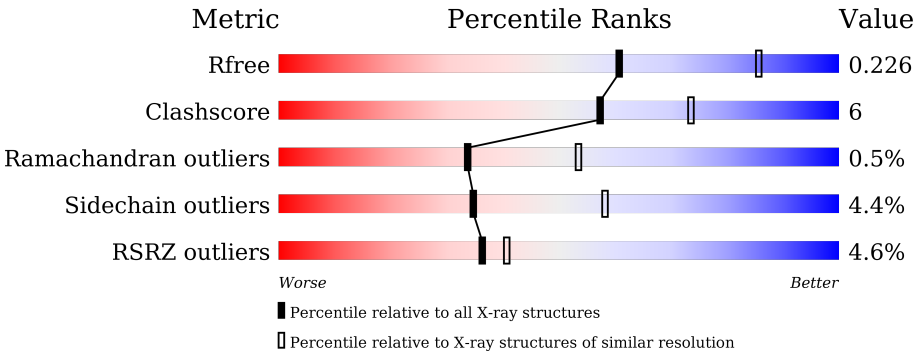
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.49 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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	742	4% 82% 13%
1	B	742	5% 82% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	1721	-	-	-	X
4	NAD	A	1723	-	-	-	X
6	ZOZ	A	1726	-	-	-	X
7	PO4	B	1718	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11729 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5571	3559	977	1012	23			
1	B	718	Total	C	N	O	S	0	1	0
			5518	3528	965	1002	23			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P07896
A	-18	GLY	-	EXPRESSION TAG	UNP P07896
A	-17	SER	-	EXPRESSION TAG	UNP P07896
A	-16	SER	-	EXPRESSION TAG	UNP P07896
A	-15	HIS	-	EXPRESSION TAG	UNP P07896
A	-14	HIS	-	EXPRESSION TAG	UNP P07896
A	-13	HIS	-	EXPRESSION TAG	UNP P07896
A	-12	HIS	-	EXPRESSION TAG	UNP P07896
A	-11	HIS	-	EXPRESSION TAG	UNP P07896
A	-10	HIS	-	EXPRESSION TAG	UNP P07896
A	-9	SER	-	EXPRESSION TAG	UNP P07896
A	-8	SER	-	EXPRESSION TAG	UNP P07896
A	-7	GLY	-	EXPRESSION TAG	UNP P07896
A	-6	LEU	-	EXPRESSION TAG	UNP P07896
A	-5	VAL	-	EXPRESSION TAG	UNP P07896
A	-4	PRO	-	EXPRESSION TAG	UNP P07896
A	-3	ARG	-	EXPRESSION TAG	UNP P07896
A	-2	GLY	-	EXPRESSION TAG	UNP P07896
A	-1	SER	-	EXPRESSION TAG	UNP P07896
A	0	HIS	-	EXPRESSION TAG	UNP P07896
B	-19	MET	-	EXPRESSION TAG	UNP P07896
B	-18	GLY	-	EXPRESSION TAG	UNP P07896
B	-17	SER	-	EXPRESSION TAG	UNP P07896
B	-16	SER	-	EXPRESSION TAG	UNP P07896
B	-15	HIS	-	EXPRESSION TAG	UNP P07896

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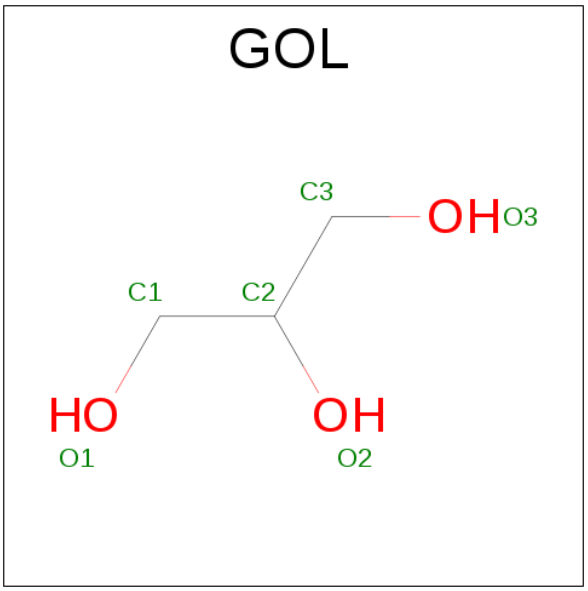
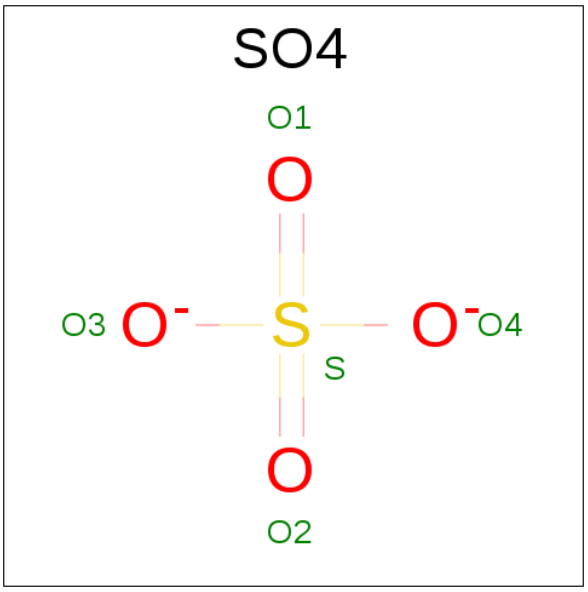
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP P07896
B	-13	HIS	-	EXPRESSION TAG	UNP P07896
B	-12	HIS	-	EXPRESSION TAG	UNP P07896
B	-11	HIS	-	EXPRESSION TAG	UNP P07896
B	-10	HIS	-	EXPRESSION TAG	UNP P07896
B	-9	SER	-	EXPRESSION TAG	UNP P07896
B	-8	SER	-	EXPRESSION TAG	UNP P07896
B	-7	GLY	-	EXPRESSION TAG	UNP P07896
B	-6	LEU	-	EXPRESSION TAG	UNP P07896
B	-5	VAL	-	EXPRESSION TAG	UNP P07896
B	-4	PRO	-	EXPRESSION TAG	UNP P07896
B	-3	ARG	-	EXPRESSION TAG	UNP P07896
B	-2	GLY	-	EXPRESSION TAG	UNP P07896
B	-1	SER	-	EXPRESSION TAG	UNP P07896
B	0	HIS	-	EXPRESSION TAG	UNP P07896

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



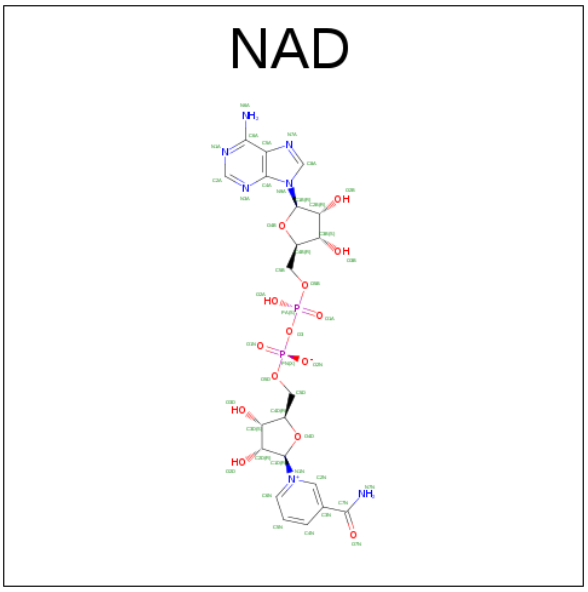
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



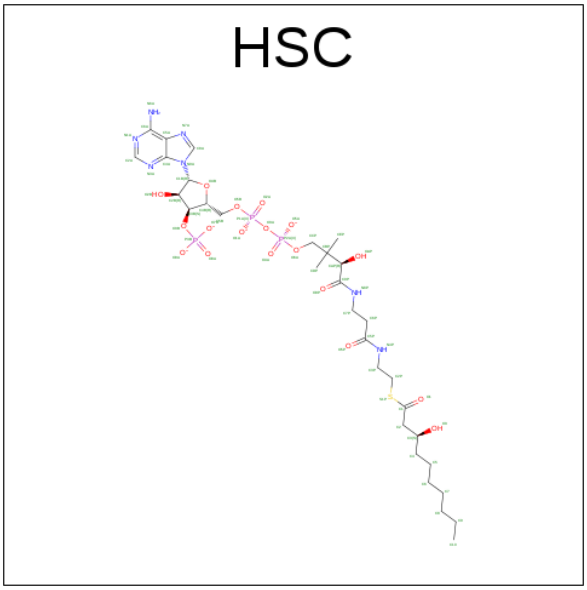
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



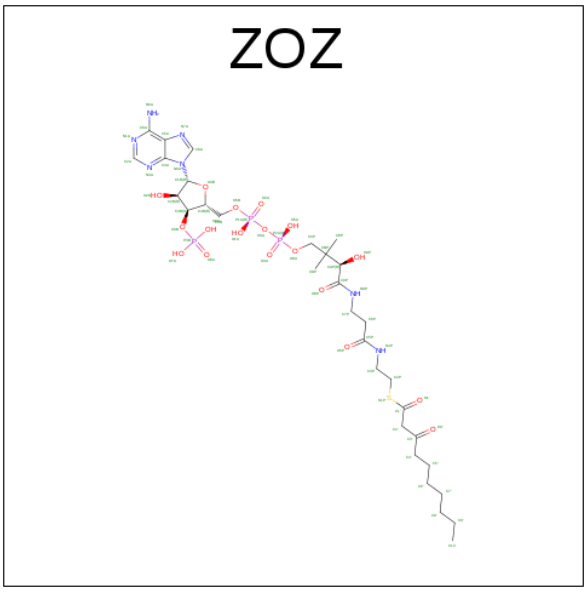
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is (S)-3-HYDROXYDECANOYL-COA (three-letter code: HSC) (formula: $C_{31}H_{50}N_7O_{18}P_3S$).



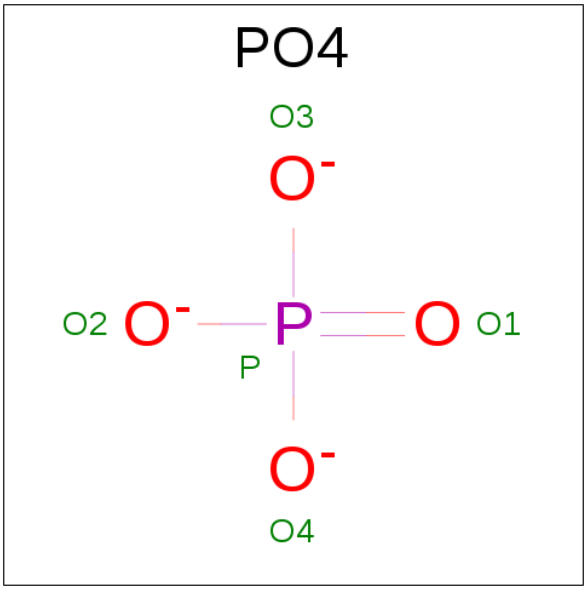
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		

- Molecule 6 is 3-KETO-DECANOYL-COA (three-letter code: ZOZ) (formula: $C_{31}H_{52}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			60	31	7	18	3	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 8 is water.

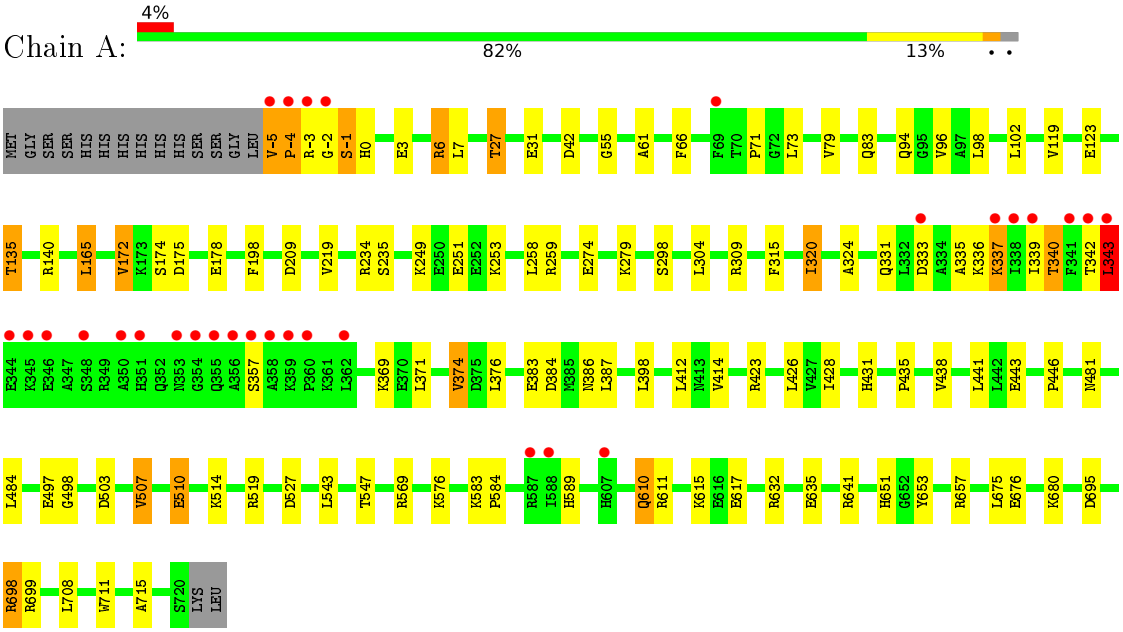
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	244	Total O 244 244	0	0
8	B	135	Total O 135 135	0	0

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.

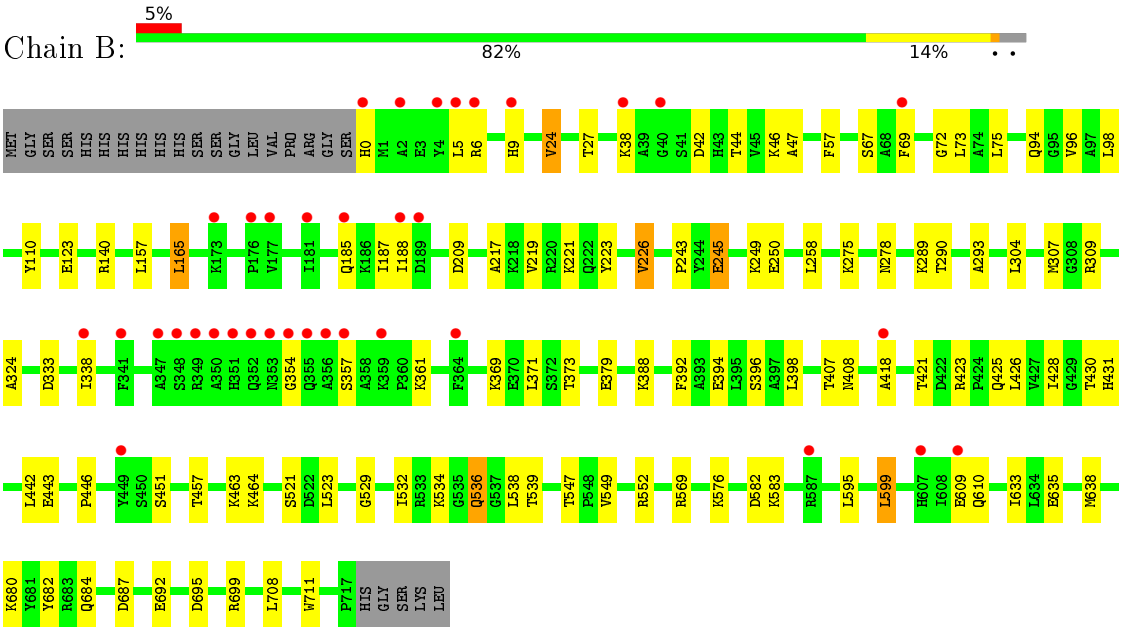
- Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

Chain A:



- Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.96Å 125.08Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.49 47.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.90-2.49) 98.8 (47.90-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.184 , 0.226 0.184 , 0.226	Depositor DCC
R_{free} test set	3206 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11729	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, NAD, HSC, PO4, SO4, ZOZ

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	0.30	0/5704	0.48	1/7728 (0.0%)
1	B	0.27	0/5649	0.44	0/7654
All	All	0.29	0/11353	0.46	1/15382 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	LEU	CA-CB-CG	6.36	129.93	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	5571	0	5677	76	0
1	B	5518	0	5626	57	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	44	0	26	3	0
5	A	60	0	49	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	60	0	48	4	0
6	A	60	0	0	2	0
7	B	5	0	0	1	0
8	A	244	0	0	7	0
8	B	135	0	0	5	1
All	All	11729	0	11442	136	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 6.

All (136) 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:6:ARG:NH2	1:A:42:ASP:OD2	1.87	1.07
1:A:6:ARG:HH11	1:A:6:ARG:CG	1.81	0.93
1:A:-3:ARG:HD3	1:A:27:THR:OG1	1.78	0.82
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.49	0.77
1:A:497:GLU:OE1	1:A:611:ARG:NH1	2.22	0.72
1:A:695:ASP:OD2	1:A:699:ARG:NH1	2.23	0.72
1:B:289:LYS:HG3	1:B:290:THR:HG23	1.71	0.72
1:B:309:ARG:HD3	1:B:338:ILE:HD11	1.71	0.70
1:A:611:ARG:NH2	1:A:617:GLU:OE1	2.25	0.70
1:A:412:LEU:O	8:A:2154:HOH:O	2.10	0.69
1:A:61:ALA:HB2	5:A:1725:HSC:H7A	1.74	0.69
1:A:6:ARG:HH11	1:A:6:ARG:HG3	1.56	0.69
1:B:569:ARG:HG2	1:B:576:LYS:HE3	1.73	0.69
1:B:635:GLU:OE1	1:B:699:ARG:NH2	2.26	0.69
1:A:369:LYS:HA	1:A:398:LEU:HD13	1.76	0.68
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.30	0.67
4:A:1723:NAD:O2N	8:A:2142:HOH:O	2.13	0.66
1:A:172:VAL:HG13	1:A:174:SER:H	1.62	0.64
1:A:431:HIS:HB3	1:A:443:GLU:HB3	1.81	0.62
1:B:6:ARG:NH2	1:B:44:THR:OG1	2.31	0.62
1:A:135:THR:HG21	1:A:235:SER:OG	2.00	0.60
1:A:-1:SER:N	1:A:31:GLU:OE2	2.34	0.60
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.82	0.60
1:A:336:LYS:O	1:A:340:THR:OG1	2.21	0.59
1:A:96:VAL:HG13	1:A:98:LEU:HG	1.86	0.58
1:A:423:ARG:HD3	1:A:426:LEU:HD12	1.85	0.57
1:B:9:HIS:HB3	1:B:185:GLN:HE21	1.68	0.57
1:A:140:ARG:NH2	8:A:2056:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH1	1:A:6:ARG:CG	2.51	0.56
1:B:423:ARG:HB2	1:B:426:LEU:HD12	1.86	0.56
1:B:529:GLY:HA2	1:B:532:ILE:HD12	1.87	0.56
1:A:309:ARG:HD3	1:A:335:ALA:HA	1.85	0.56
1:A:-2:GLY:O	1:A:0:HIS:N	2.38	0.56
1:B:583:LYS:NZ	8:B:2102:HOH:O	2.39	0.55
1:A:71:PRO:O	1:A:259:ARG:NH1	2.35	0.55
1:A:0:HIS:ND1	1:A:3:GLU:OE1	2.40	0.55
1:A:-3:ARG:HD3	1:A:27:THR:HG1	1.72	0.54
1:B:24:VAL:HG11	1:B:75:LEU:HD13	1.89	0.54
1:A:510:GLU:OE2	1:A:615:LYS:NZ	2.39	0.54
1:A:333:ASP:N	1:A:333:ASP:OD1	2.41	0.53
1:A:331:GLN:NE2	4:A:1723:NAD:O3B	2.40	0.53
1:A:6:ARG:NH1	1:A:6:ARG:HG3	2.21	0.53
1:B:521:SER:OG	7:B:1718:PO4:O3	2.22	0.53
1:B:123:GLU:OE2	5:B:1722:HSC:O3	2.26	0.53
1:A:680:LYS:HE2	2:A:1721:GOL:H2	1.92	0.52
1:B:140:ARG:NH2	8:B:2040:HOH:O	2.38	0.52
1:B:595:LEU:HG	1:B:599:LEU:HD22	1.92	0.52
1:A:339:ILE:O	1:A:343:LEU:HD13	2.10	0.51
1:A:611:ARG:HH22	1:A:617:GLU:CD	2.14	0.51
1:A:484:LEU:HD22	1:A:653:TYR:HE1	1.76	0.50
1:B:275:LYS:NZ	5:B:1722:HSC:O2A	2.31	0.50
1:A:315:PHE:HD1	1:A:320:ILE:HD11	1.77	0.50
1:A:123:GLU:OE2	5:A:1725:HSC:O3	2.30	0.50
1:B:9:HIS:HB3	1:B:185:GLN:NE2	2.28	0.48
1:B:418:ALA:O	1:B:421:THR:OG1	2.29	0.48
1:A:583:LYS:HD2	1:A:584:PRO:HD2	1.95	0.48
1:A:498:GLY:HA2	1:A:610:GLN:HE21	1.78	0.48
1:B:431:HIS:HB3	1:B:443:GLU:HB2	1.95	0.48
1:B:695:ASP:HB3	8:B:2129:HOH:O	2.14	0.47
1:B:96:VAL:HG13	1:B:98:LEU:HG	1.96	0.47
1:B:394:GLU:O	1:B:398:LEU:HG	2.15	0.47
4:A:1723:NAD:H2N	4:A:1723:NAD:H2D	1.65	0.47
1:A:102:LEU:HD13	1:A:119:VAL:HB	1.97	0.47
1:A:414:VAL:HG13	8:A:2154:HOH:O	2.13	0.47
1:A:699:ARG:NH2	1:A:715:ALA:O	2.44	0.46
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.50	0.46
1:A:698:ARG:NH1	8:A:2223:HOH:O	2.42	0.46
1:B:425:GLN:HB2	1:B:451:SER:HB3	1.97	0.46
1:B:38:LYS:O	1:B:42:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:HG13	1:A:446:PRO:HA	1.97	0.46
1:A:79:VAL:O	1:A:83:GLN:HG3	2.16	0.46
1:A:484:LEU:HD22	1:A:653:TYR:CE1	2.50	0.46
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.81	0.46
1:B:534:LYS:HG2	1:B:539:THR:HG23	1.98	0.46
1:B:278:ASN:HD22	1:B:463:LYS:CE	2.29	0.45
1:A:135:THR:HG22	1:A:251:GLU:OE1	2.16	0.45
1:A:657:ARG:NH1	8:A:2051:HOH:O	2.28	0.45
1:B:538:LEU:HD22	1:B:552:ARG:HG3	1.98	0.45
1:A:543:LEU:HD11	1:A:547:THR:HG21	1.97	0.45
1:A:569:ARG:HH12	1:A:576:LYS:HE3	1.82	0.45
1:B:307:MET:HG2	1:B:408:ASN:ND2	2.31	0.45
1:A:249:LYS:HA	1:A:249:LYS:HD3	1.79	0.45
1:A:-5:VAL:HG12	1:A:-4:PRO:HD3	1.99	0.45
1:A:519:ARG:HD3	1:A:589:HIS:NE2	2.31	0.45
1:B:582:ASP:OD1	1:B:582:ASP:N	2.49	0.45
1:A:374:VAL:HG13	1:A:376:LEU:H	1.82	0.45
1:B:223:TYR:HB3	1:B:226:VAL:HG13	1.97	0.45
1:A:298:SER:HB2	1:A:374:VAL:HG22	1.99	0.45
1:A:219:VAL:HG13	8:A:2096:HOH:O	2.18	0.44
1:B:217:ALA:O	1:B:221:LYS:HE3	2.17	0.44
1:A:-3:ARG:CD	1:A:27:THR:OG1	2.57	0.44
1:B:278:ASN:HD22	1:B:463:LYS:HE3	1.81	0.44
1:A:-3:ARG:HB3	1:A:27:THR:HG21	1.99	0.44
1:A:369:LYS:HB3	1:A:398:LEU:HD22	1.98	0.44
1:A:66:PHE:CD1	1:A:71:PRO:HD3	2.52	0.44
1:B:46:LYS:HB3	1:B:188:ILE:HD11	2.00	0.44
1:A:-2:GLY:C	1:A:0:HIS:H	2.20	0.44
1:A:514:LYS:HD3	6:A:1726:ZOZ:O9P	2.18	0.43
1:B:249:LYS:HE2	1:B:249:LYS:HB2	1.91	0.43
1:B:569:ARG:NH1	1:B:576:LYS:HD2	2.33	0.43
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.98	0.43
5:B:1722:HSC:H2B	5:B:1722:HSC:H5BA	1.83	0.43
1:B:680:LYS:O	1:B:684:GLN:HG3	2.18	0.43
1:A:279:LYS:HD2	1:A:279:LYS:N	2.33	0.43
1:B:379:GLU:OE2	1:B:388:LYS:NZ	2.47	0.43
1:B:293:ALA:HB1	1:B:457:THR:HA	2.00	0.43
1:A:503:ASP:O	1:A:507:VAL:HG13	2.19	0.43
1:A:384:ASP:HB3	1:A:387:LEU:HB3	2.00	0.43
1:B:47:ALA:HB2	1:B:188:ILE:HD13	2.00	0.42
1:B:67:SER:C	1:B:69:PHE:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.86	0.42
1:A:55:GLY:O	1:A:94:GLN:HG3	2.19	0.42
1:A:632:ARG:O	1:A:635:GLU:HB3	2.19	0.42
1:B:243:PRO:HB2	1:B:245:GLU:OE2	2.19	0.42
1:B:392:PHE:CZ	1:B:407:THR:HB	2.54	0.42
1:B:361:LYS:HE3	1:B:361:LYS:HB2	1.82	0.42
1:B:532:ILE:O	1:B:536:GLN:HG2	2.20	0.42
1:B:430:THR:HB	1:B:442:LEU:HD11	2.02	0.42
1:B:682:TYR:CE1	1:B:692:GLU:HB2	2.55	0.41
1:A:527:ASP:N	1:A:527:ASP:OD1	2.53	0.41
1:A:333:ASP:O	1:A:337:LYS:HE3	2.20	0.41
1:B:428:ILE:HG13	1:B:446:PRO:HA	2.02	0.41
1:B:396:SER:HB2	1:B:421:THR:HG22	2.03	0.41
1:B:110:TYR:CE2	1:B:187:ILE:HD13	2.56	0.41
1:B:708:LEU:HA	1:B:711:TRP:CE2	2.56	0.41
1:A:435:PRO:HG2	1:A:438:VAL:CG2	2.51	0.41
1:B:304:LEU:HD11	1:B:324:ALA:HB1	2.01	0.41
1:B:687:ASP:OD1	1:B:687:ASP:N	2.54	0.41
1:B:5:LEU:HD12	1:B:5:LEU:HA	1.92	0.41
1:B:94:GLN:NE2	8:B:2026:HOH:O	2.54	0.41
1:B:250:GLU:HG2	8:B:2069:HOH:O	2.21	0.40
1:A:340:THR:O	1:A:343:LEU:HD22	2.22	0.40
1:A:175:ASP:HB3	1:A:178:GLU:HG2	2.03	0.40
1:A:481:ASN:HD21	6:A:1726:ZOZ:C3'	2.34	0.40
1:B:72:GLY:HA3	5:B:1722:HSC:H9	2.02	0.40
1:A:274:GLU:OE2	1:A:651:HIS:NE2	2.44	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)
8:B:2011:HOH:O	8:B:2129:HOH:O[1_455]	2.12	0.08

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	725/742 (98%)	690 (95%)	32 (4%)	3 (0%)	39	59
1	B	717/742 (97%)	681 (95%)	32 (4%)	4 (1%)	30	48
All	All	1442/1484 (97%)	1371 (95%)	64 (4%)	7 (0%)	34	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	B	354	GLY
1	B	357	SER
1	B	609	GLU
1	B	57	PHE
1	A	383	GLU
1	A	-4	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	596/609 (98%)	566 (95%)	30 (5%)	30	52
1	B	590/609 (97%)	568 (96%)	22 (4%)	41	67
All	All	1186/1218 (97%)	1134 (96%)	52 (4%)	35	58

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	6	ARG
1	A	7	LEU
1	A	27	THR
1	A	73	LEU
1	A	135	THR

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Mol	Chain	Res	Type
1	A	165	LEU
1	A	172	VAL
1	A	198	PHE
1	A	209	ASP
1	A	234	ARG
1	A	253	LYS
1	A	258	LEU
1	A	320	ILE
1	A	337	LYS
1	A	340	THR
1	A	342	THR
1	A	343	LEU
1	A	357	SER
1	A	371	LEU
1	A	374	VAL
1	A	386	ASN
1	A	441	LEU
1	A	507	VAL
1	A	510	GLU
1	A	610	GLN
1	A	641	ARG
1	A	675	LEU
1	A	676	GLU
1	A	698	ARG
1	B	0	HIS
1	B	24	VAL
1	B	27	THR
1	B	73	LEU
1	B	157	LEU
1	B	165	LEU
1	B	209	ASP
1	B	219	VAL
1	B	226	VAL
1	B	245	GLU
1	B	258	LEU
1	B	333	ASP
1	B	369	LYS
1	B	371	LEU
1	B	373	THR
1	B	464	LYS
1	B	523	LEU
1	B	536	GLN

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Mol	Chain	Res	Type
1	B	547	THR
1	B	549	VAL
1	B	599	LEU
1	B	610	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	610	GLN
1	B	83	GLN
1	B	185	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	1721	-	5,5,5	0.13	0	5,5,5	0.34	0
3	SO4	A	1722	-	4,4,4	0.24	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAD	A	1723	-	42,48,48	1.58	3 (7%)	46,73,73	1.90	3 (6%)
3	SO4	A	1724	-	4,4,4	0.21	0	6,6,6	0.08	0
5	HSC	A	1725	-	53,62,62	1.74	12 (22%)	63,89,89	2.30	14 (22%)
6	ZOZ	A	1726	-	53,62,62	1.76	9 (16%)	61,89,89	2.24	14 (22%)
7	PO4	B	1718	-	4,4,4	0.69	0	6,6,6	0.23	0
2	GOL	B	1719	-	5,5,5	0.30	0	5,5,5	0.32	0
3	SO4	B	1720	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	1721	-	4,4,4	0.24	0	6,6,6	0.10	0
5	HSC	B	1722	-	53,62,62	1.77	12 (22%)	63,89,89	2.26	10 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1721	-	-	0/4/4/4	0/0/0/0
3	SO4	A	1722	-	-	0/0/0/0	0/0/0/0
4	NAD	A	1723	-	-	0/22/62/62	0/5/5/5
3	SO4	A	1724	-	-	0/0/0/0	0/0/0/0
5	HSC	A	1725	-	-	0/57/78/78	0/3/3/3
6	ZOZ	A	1726	-	-	1/57/78/78	0/3/3/3
7	PO4	B	1718	-	-	0/0/0/0	0/0/0/0
2	GOL	B	1719	-	-	0/4/4/4	0/0/0/0
3	SO4	B	1720	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1721	-	-	0/0/0/0	0/0/0/0
5	HSC	B	1722	-	-	0/57/78/78	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1726	ZOZ	C2B-C1B	-5.21	1.45	1.53
5	A	1725	HSC	C2B-C1B	-5.05	1.45	1.53
5	B	1722	HSC	C2B-C1B	-4.57	1.46	1.53
6	A	1726	ZOZ	C2'-C1'	-3.70	1.37	1.50
5	B	1722	HSC	C1-S1P	-3.67	1.71	1.76
6	A	1726	ZOZ	C2B-C3B	-3.37	1.45	1.53
5	B	1722	HSC	C2B-C3B	-3.14	1.46	1.53
5	A	1725	HSC	C2B-C3B	-2.99	1.46	1.53
5	B	1722	HSC	C3B-C4B	-2.97	1.44	1.52
5	B	1722	HSC	OAP-CAP	-2.83	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1726	ZOZ	C3B-C4B	-2.83	1.44	1.52
6	A	1726	ZOZ	OAP-CAP	-2.83	1.36	1.42
5	A	1725	HSC	O3-C3	-2.70	1.35	1.43
5	A	1725	HSC	P3B-O3B	-2.69	1.57	1.62
5	B	1722	HSC	P3B-O3B	-2.68	1.57	1.62
5	A	1725	HSC	OAP-CAP	-2.63	1.37	1.42
5	A	1725	HSC	C1-S1P	-2.62	1.73	1.76
5	A	1725	HSC	C3B-C4B	-2.58	1.45	1.52
5	B	1722	HSC	O3-C3	-2.55	1.36	1.43
5	B	1722	HSC	C2-C3	-2.21	1.45	1.52
5	A	1725	HSC	C2-C3	-2.08	1.46	1.52
5	B	1722	HSC	C4-C3	2.01	1.59	1.52
5	A	1725	HSC	C4-C3	2.01	1.59	1.52
6	A	1726	ZOZ	O1'-C1'	2.18	1.24	1.21
4	A	1723	NAD	C2A-N1A	2.34	1.38	1.33
6	A	1726	ZOZ	C6A-N6A	2.67	1.45	1.34
5	A	1725	HSC	C6A-N6A	2.70	1.45	1.34
5	B	1722	HSC	C6A-N6A	2.76	1.45	1.34
4	A	1723	NAD	C2A-N3A	3.57	1.38	1.32
5	B	1722	HSC	C5P-N4P	4.90	1.45	1.33
5	A	1725	HSC	C5P-N4P	4.91	1.45	1.33
6	A	1726	ZOZ	C5P-N4P	5.06	1.45	1.33
5	B	1722	HSC	C9P-N8P	5.24	1.44	1.33
5	A	1725	HSC	C9P-N8P	5.29	1.44	1.33
6	A	1726	ZOZ	C9P-N8P	5.79	1.45	1.33
4	A	1723	NAD	O7N-C7N	8.06	1.41	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1725	HSC	N3A-C2A-N1A	-11.22	120.06	128.87
6	A	1726	ZOZ	N3A-C2A-N1A	-11.21	120.07	128.87
4	A	1723	NAD	N3A-C2A-N1A	-11.20	120.08	128.87
5	B	1722	HSC	N3A-C2A-N1A	-11.11	120.14	128.87
5	B	1722	HSC	O1-C1-S1P	-4.73	119.08	122.83
5	A	1725	HSC	O1-C1-C2	-4.62	119.49	123.77
5	A	1725	HSC	O1-C1-S1P	-4.08	119.60	122.83
6	A	1726	ZOZ	O1'-C1'-S1P	-3.18	120.31	122.83
6	A	1726	ZOZ	C4B-O4B-C1B	-3.12	106.34	109.64
5	B	1722	HSC	C4B-O4B-C1B	-2.97	106.50	109.64
6	A	1726	ZOZ	O9P-C9P-N8P	-2.96	117.15	123.04
6	A	1726	ZOZ	C2B-C1B-N9A	-2.83	105.90	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1726	ZOZ	P3B-O3B-C3B	-2.82	114.35	121.56
5	A	1725	HSC	C1B-N9A-C4A	-2.81	123.66	126.81
6	A	1726	ZOZ	C1B-N9A-C4A	-2.73	123.75	126.81
5	B	1722	HSC	O1-C1-C2	-2.65	121.31	123.77
6	A	1726	ZOZ	C2B-C3B-C4B	-2.64	98.20	103.25
5	A	1725	HSC	C7P-N8P-C9P	-2.56	117.49	122.62
5	B	1722	HSC	O9P-C9P-N8P	-2.49	118.09	123.04
5	A	1725	HSC	O9P-C9P-N8P	-2.41	118.26	123.04
5	B	1722	HSC	C7P-N8P-C9P	-2.26	118.09	122.62
4	A	1723	NAD	C4B-O4B-C1B	-2.20	107.31	109.64
5	A	1725	HSC	C4B-O4B-C1B	-2.20	107.31	109.64
6	A	1726	ZOZ	C2P-S1P-C1'	2.06	109.43	102.09
5	A	1725	HSC	C6P-C5P-N4P	2.11	120.13	116.46
5	A	1725	HSC	O5B-C5B-C4B	2.11	116.72	109.09
5	A	1725	HSC	C2P-S1P-C1	2.29	110.26	102.09
5	A	1725	HSC	O4B-C1B-N9A	2.34	112.53	108.11
6	A	1726	ZOZ	C6P-C7P-N8P	2.43	117.38	111.94
6	A	1726	ZOZ	C3P-C2P-S1P	2.69	118.63	111.47
4	A	1723	NAD	O4B-C1B-N9A	2.83	113.46	108.11
5	B	1722	HSC	C6P-C7P-N8P	3.08	118.84	111.94
5	B	1722	HSC	O5B-C5B-C4B	3.31	121.03	109.09
5	A	1725	HSC	C6P-C7P-N8P	3.42	119.61	111.94
5	B	1722	HSC	C2P-C3P-N4P	3.51	119.47	112.43
6	A	1726	ZOZ	CAP-C9P-N8P	3.56	124.69	116.31
6	A	1726	ZOZ	C7P-C6P-C5P	3.81	118.75	112.22
5	A	1725	HSC	C2P-C3P-N4P	4.57	121.60	112.43
6	A	1726	ZOZ	C2'-C1'-S1P	5.76	119.13	113.46
5	A	1725	HSC	C2-C1-S1P	6.44	119.14	113.36
5	B	1722	HSC	C2-C1-S1P	6.91	119.58	113.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1726	ZOZ	CAP-C9P-N8P-C7P

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1723	NAD	3	0
5	A	1725	HSC	2	0
6	A	1726	ZOZ	2	0
7	B	1718	PO4	1	0
5	B	1722	HSC	4	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	726/742 (97%)	-0.02	30 (4%)	41	45	18, 43, 95, 164	0
1	B	718/742 (96%)	0.09	36 (5%)	32	36	29, 58, 94, 154	0
All	All	1444/1484 (97%)	0.03	66 (4%)	36	41	18, 51, 95, 164	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	7.2
1	A	357	SER	6.6
1	B	356	ALA	6.6
1	A	355	GLN	5.7
1	A	350	ALA	5.6
1	A	344	GLU	5.0
1	A	338	ILE	4.7
1	B	348	SER	4.6
1	A	-5	VAL	4.6
1	A	354	GLY	4.6
1	B	355	GLN	4.5
1	B	347	ALA	4.5
1	A	353	ASN	4.3
1	A	341	PHE	4.3
1	B	351	HIS	4.1
1	A	337	LYS	4.0
1	A	359	LYS	3.9
1	A	360	PRO	3.9
1	A	358	ALA	3.7
1	B	350	ALA	3.5
1	B	6	ARG	3.5
1	B	353	ASN	3.5
1	A	351	HIS	3.3
1	B	354	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	333	ASP	3.2
1	B	181	ILE	3.1
1	B	357	SER	3.1
1	A	-3	ARG	3.0
1	B	349	ARG	3.0
1	B	4	TYR	2.9
1	B	188	ILE	2.9
1	B	352	GLN	2.8
1	B	359	LYS	2.8
1	B	2	ALA	2.7
1	B	177	VAL	2.7
1	A	588	ILE	2.7
1	B	0	HIS	2.6
1	A	362	LEU	2.6
1	B	449	TYR	2.6
1	A	345	LYS	2.5
1	B	609	GLU	2.5
1	B	9	HIS	2.5
1	A	346	GLU	2.5
1	A	348	SER	2.5
1	B	607	HIS	2.5
1	B	341	PHE	2.5
1	B	364	PHE	2.4
1	A	69	PHE	2.4
1	B	189	ASP	2.4
1	B	176	PRO	2.3
1	A	343	LEU	2.3
1	B	5	LEU	2.3
1	B	185	GLN	2.3
1	B	69	PHE	2.3
1	A	607	HIS	2.2
1	B	418	ALA	2.2
1	A	342	THR	2.2
1	B	173	LYS	2.1
1	B	338	ILE	2.1
1	A	339	ILE	2.1
1	A	-4	PRO	2.1
1	B	38	LYS	2.1
1	A	-2	GLY	2.1
1	B	587	ARG	2.1
1	A	587	ARG	2.0
1	B	40	GLY	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
4	NAD	A	1723	44/44	0.69	0.45	7.34	91,103,117,117	44
6	ZOZ	A	1726	60/60	0.57	0.42	2.79	53,70,144,181	60
2	GOL	A	1721	6/6	0.67	0.23	2.78	85,86,86,86	0
7	PO4	B	1718	5/5	0.95	0.21	2.13	110,110,110,110	0
3	SO4	B	1721	5/5	0.84	0.18	0.97	119,119,119,119	0
5	HSC	A	1725	60/60	0.91	0.15	0.45	31,58,95,95	0
2	GOL	B	1719	6/6	0.90	0.16	0.02	64,64,65,66	0
5	HSC	B	1722	60/60	0.95	0.14	-0.11	41,56,98,121	0
3	SO4	A	1724	5/5	0.99	0.12	-3.45	46,46,49,49	0
3	SO4	B	1720	5/5	0.91	0.17	-	87,87,87,88	0
3	SO4	A	1722	5/5	0.91	0.18	-	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.