Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2016 – 06:55 PM EDT

PDB ID	:	5AAK
Title	:	CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE-1 (RPMFE1) COMPLEXED WITH ACETOACETYL-COA AND NAD
Authors	:	Kasaragod, P.; Schmitz, W.; Kalervo Hiltunen, J.; Wierenga, R.K.
Deposited on	:	2015-07-26
Resolution	:	2.80 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:

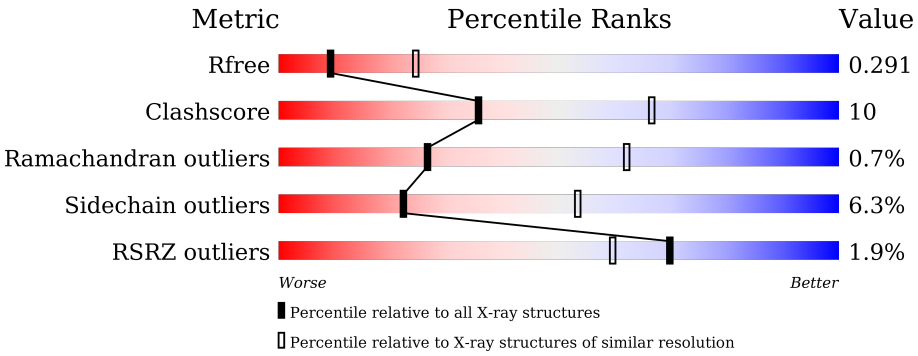
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

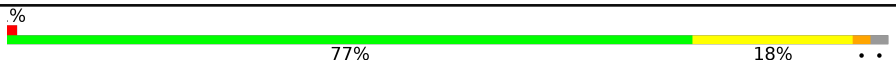
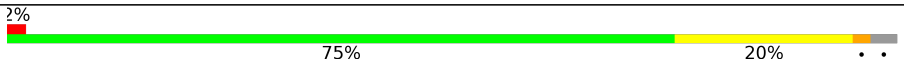
The reported resolution of this entry is 2.80 Å.

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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	
1	B	742	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11498 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	725	Total	C	N	O	S	0	1	0
			5564	3554	976	1011	23			
1	B	721	Total	C	N	O	S	0	1	0
			5538	3539	970	1006	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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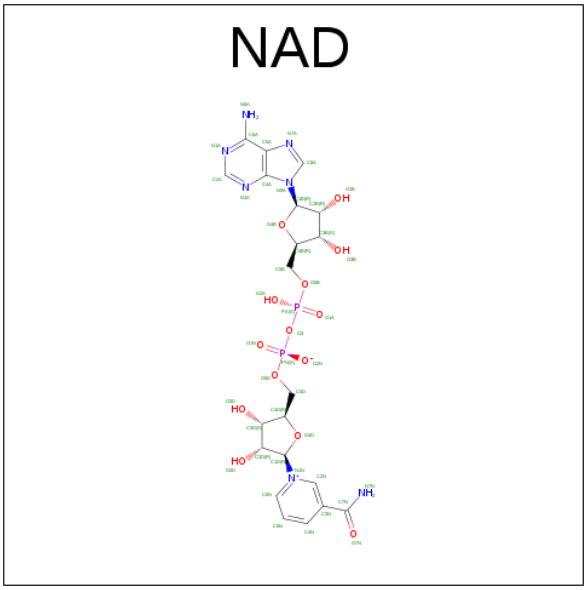
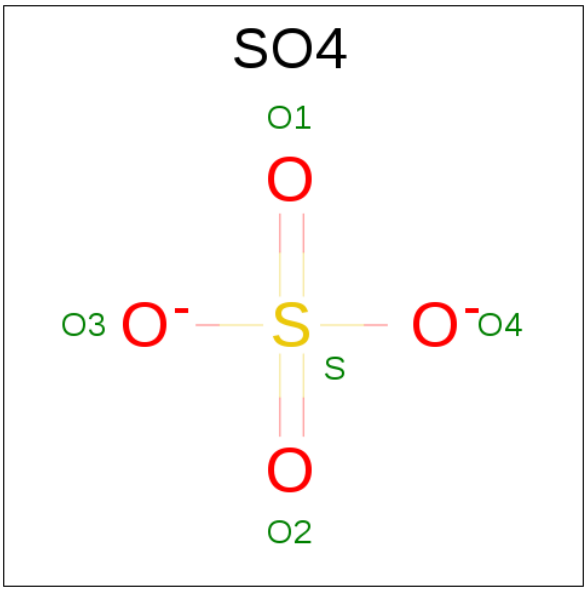
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP P07896
B	-13	HIS	-	EXPRESSION TAG	UNP P07896
B	-12	HIS	-	EXPRESSION TAG	UNP P07896
B	-11	HIS	-	EXPRESSION TAG	UNP P07896
B	-10	HIS	-	EXPRESSION TAG	UNP P07896
B	-9	SER	-	EXPRESSION TAG	UNP P07896
B	-8	SER	-	EXPRESSION TAG	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 NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



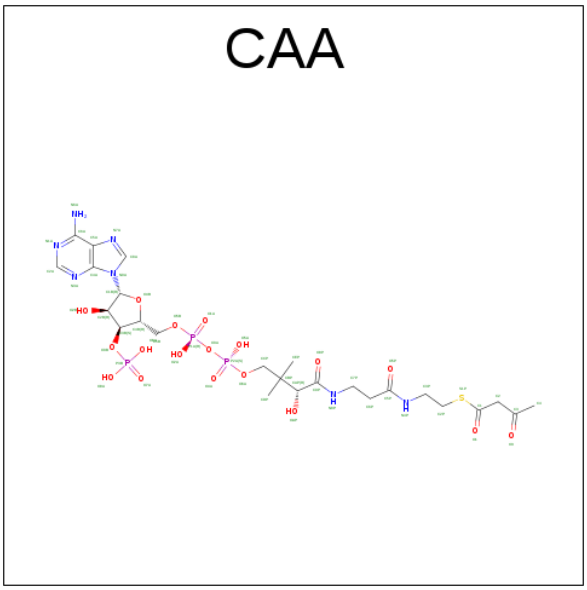
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- 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	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 5 is water.

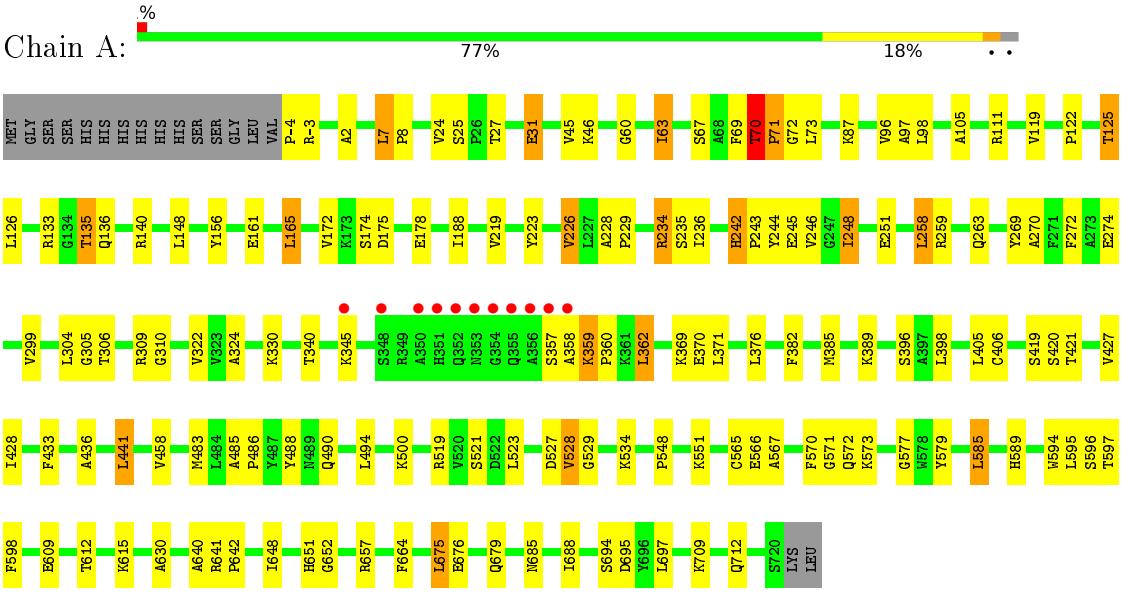
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	86	Total	O	0	0
			86	86		

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.

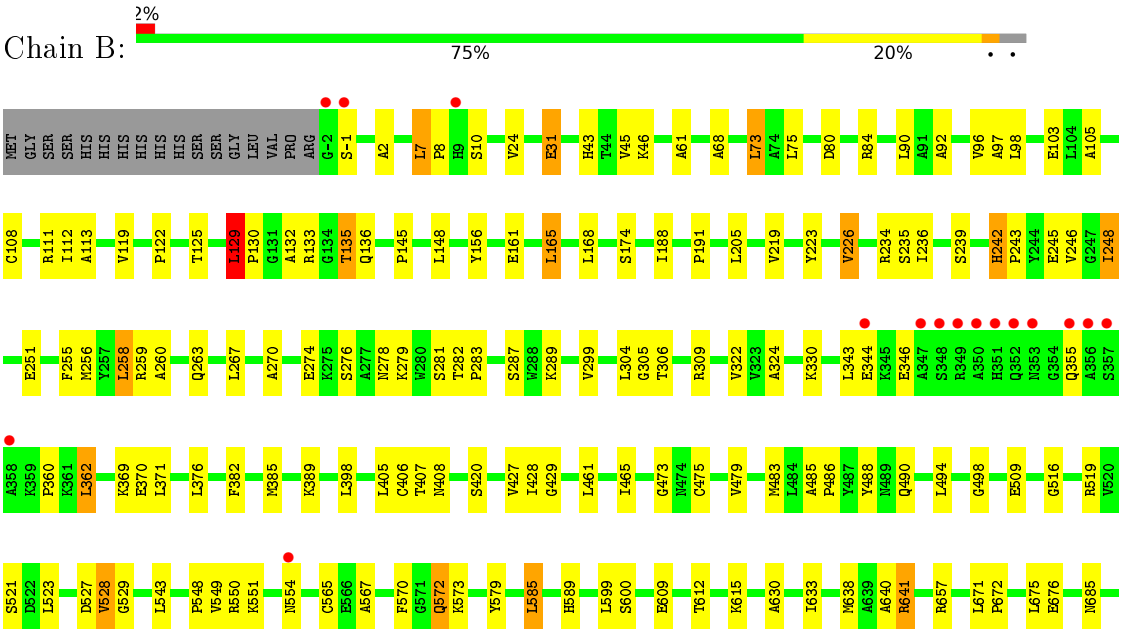
- Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

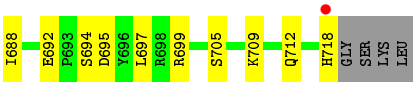
Chain A:



- Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

Chain B:




I688
E692
P693
S694
D695
Y696
L697
R698
R699
S705
K709
Q712
H718
GLY
SER
LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.23Å 125.82Å 223.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.56 – 2.80 32.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (33.56-2.80) 82.5 (32.62-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.300 0.221 , 0.291	Depositor DCC
R_{free} test set	1980 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: CAA, SO4, NAD

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	0.59	0/5697	0.68	3/7717 (0.0%)
1	B	0.58	0/5670	0.67	3/7682 (0.0%)
All	All	0.58	0/11367	0.68	6/15399 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	THR	C-N-CD	-8.91	100.99	120.60
1	B	234	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	234	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	234	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	234	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	129	LEU	CB-CG-CD2	5.05	119.59	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5564	0	5668	109	0
1	B	5538	0	5641	115	0
2	A	44	0	26	4	0
2	B	44	0	26	2	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	54	0	36	3	0
4	B	54	0	36	2	0
5	A	94	0	0	12	0
5	B	86	0	0	21	0
All	All	11498	0	11433	221	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 10.

All (221) 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)
2:A:1721:NAD:H51A	5:A:2048:HOH:O	1.47	1.13
1:B:692:GLU:HG3	5:B:2076:HOH:O	1.60	1.01
1:A:71:PRO:HD3	1:A:259:ARG:HD2	1.47	0.94
1:B:475:CYS:SG	1:B:638:MET:HG3	2.07	0.93
1:B:640:ALA:O	1:B:712:GLN:NE2	2.05	0.90
1:A:597:THR:CG2	1:B:382:PHE:HZ	1.90	0.83
1:A:369:LYS:HA	1:A:398:LEU:HD21	1.61	0.82
1:A:71:PRO:CD	1:A:259:ARG:HD2	2.08	0.82
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.61	0.81
1:B:369:LYS:HA	1:B:398:LEU:HD21	1.61	0.81
1:A:597:THR:HG23	1:B:382:PHE:HZ	1.46	0.81
1:A:597:THR:CG2	1:B:382:PHE:CZ	2.65	0.80
1:B:572:GLN:HG3	5:B:2058:HOH:O	1.82	0.80
1:B:283:PRO:HA	1:B:718:HIS:CE1	2.20	0.75
1:B:657:ARG:NH1	5:B:2014:HOH:O	2.07	0.75
1:A:135:THR:HG21	1:A:235:SER:OG	1.87	0.74
1:B:122:PRO:O	1:B:125:THR:HB	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:THR:HG21	1:B:235:SER:OG	1.87	0.74
1:A:7:LEU:HG	1:A:8:PRO:HD2	1.70	0.72
1:B:73:LEU:HD12	1:B:73:LEU:H	1.54	0.72
1:A:46:LYS:HB2	1:A:188:ILE:HD11	1.73	0.71
1:A:122:PRO:O	1:A:125:THR:HB	1.92	0.69
1:A:148:LEU:HD23	1:A:236:ILE:HD12	1.74	0.69
1:B:7:LEU:HG	1:B:8:PRO:HD2	1.74	0.69
1:A:135:THR:HG22	1:A:251:GLU:OE2	1.92	0.69
1:B:135:THR:HG22	1:B:251:GLU:OE2	1.93	0.68
1:A:67:SER:HB2	1:A:70:THR:OG1	1.94	0.67
1:A:597:THR:HG22	1:B:382:PHE:CZ	2.29	0.67
1:A:597:THR:HG23	1:B:382:PHE:CZ	2.26	0.67
1:B:473:GLY:HA3	1:B:638:MET:SD	2.33	0.67
1:A:97:ALA:HB3	1:A:119:VAL:HG12	1.75	0.67
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.78	0.65
4:A:1725:CAA:H2B	4:A:1725:CAA:O5B	1.96	0.65
1:A:305:GLY:O	1:A:309:ARG:HG3	1.97	0.65
1:B:242:HIS:HB2	1:B:243:PRO:HD2	1.78	0.65
1:B:299:VAL:HG22	1:B:376:LEU:HB3	1.79	0.64
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.34	0.61
1:B:641:ARG:HB3	5:B:2067:HOH:O	1.99	0.61
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.35	0.61
1:A:385:MET:O	1:A:389:LYS:HG3	2.01	0.60
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.82	0.59
1:B:133:ARG:HD2	1:B:248:ILE:HD11	1.83	0.59
1:A:96:VAL:HG13	1:A:98:LEU:HG	1.85	0.59
1:B:259:ARG:NE	5:B:2035:HOH:O	2.36	0.59
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.38	0.58
1:B:205:LEU:O	5:B:2024:HOH:O	2.17	0.58
1:B:346:GLU:N	5:B:2039:HOH:O	2.37	0.58
1:B:305:GLY:O	1:B:309:ARG:HG3	2.04	0.57
1:A:594:TRP:HD1	5:A:2076:HOH:O	1.85	0.57
1:B:276:SER:HA	1:B:279:LYS:HE3	1.87	0.57
1:B:96:VAL:HG13	1:B:98:LEU:HG	1.85	0.57
1:B:46:LYS:CB	1:B:188:ILE:HD11	2.33	0.57
1:B:527:ASP:HB3	1:B:570:PHE:CD1	2.39	0.57
1:B:136:GLN:HG3	1:B:248:ILE:HD12	1.87	0.57
1:B:274:GLU:OE2	1:B:657:ARG:NH2	2.38	0.56
1:B:191:PRO:HG2	5:B:2023:HOH:O	2.05	0.56
1:A:274:GLU:OE2	1:A:657:ARG:NH2	2.39	0.56
1:B:672:PRO:HD3	1:B:705:SER:OG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:PRO:HA	1:B:718:HIS:HE1	1.70	0.56
1:A:274:GLU:OE1	1:A:657:ARG:NH2	2.39	0.55
1:A:419:SER:HA	5:A:2051:HOH:O	2.05	0.55
1:B:483:MET:HE3	1:B:630:ALA:HB2	1.87	0.55
1:B:554:ASN:HB2	5:B:2055:HOH:O	2.05	0.55
4:A:1725:CAA:C2B	4:A:1725:CAA:O5B	2.52	0.55
1:A:299:VAL:HG22	1:A:376:LEU:HB3	1.89	0.55
1:A:640:ALA:O	1:A:712:GLN:NE2	2.29	0.55
1:B:550:ARG:NH1	5:B:2049:HOH:O	2.40	0.55
1:A:46:LYS:CB	1:A:188:ILE:HD11	2.37	0.55
1:A:406:CYS:HA	1:A:428:ILE:O	2.07	0.54
1:B:304:LEU:HD11	1:B:324:ALA:HB1	1.89	0.54
1:B:2:ALA:HB3	1:B:31:GLU:HB3	1.88	0.54
1:A:322:VAL:HB	1:A:362:LEU:HB3	1.90	0.54
1:A:105:ALA:O	1:A:111:ARG:HD3	2.07	0.54
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.89	0.54
1:A:490:GLN:O	1:A:494:LEU:HG	2.08	0.54
1:B:136:GLN:NE2	5:B:2016:HOH:O	2.23	0.53
1:B:108:CYS:O	1:B:111:ARG:NH1	2.41	0.53
1:B:483:MET:CE	1:B:630:ALA:HB2	2.37	0.53
1:A:382:PHE:CE2	2:A:1721:NAD:H8A	2.44	0.53
1:B:148:LEU:HD23	1:B:236:ILE:HD12	1.90	0.52
1:A:405:LEU:HB2	1:A:427:VAL:HG22	1.91	0.52
1:A:310:GLY:HA3	1:A:436:ALA:HB3	1.92	0.52
1:A:242:HIS:HB2	1:A:243:PRO:HD2	1.92	0.52
1:B:344:GLU:C	5:B:2039:HOH:O	2.47	0.52
1:A:-4:PRO:HB2	5:A:2002:HOH:O	2.09	0.52
1:B:509:GLU:OE2	1:B:516:GLY:N	2.38	0.52
1:B:712:GLN:HA	1:B:712:GLN:OE1	2.10	0.52
1:A:244:TYR:CZ	1:A:248:ILE:HD11	2.45	0.51
1:A:675:LEU:HA	1:A:697:LEU:HD21	1.92	0.51
1:B:641:ARG:NE	5:B:2067:HOH:O	2.44	0.51
1:B:281:SER:HA	1:B:287:SER:HA	1.91	0.51
1:B:270:ALA:O	1:B:274:GLU:HG3	2.11	0.50
1:B:322:VAL:HB	1:B:362:LEU:HB3	1.93	0.50
1:A:685:ASN:HB3	1:A:688:ILE:HD12	1.93	0.50
1:B:343:LEU:HD13	1:B:360:PRO:HG2	1.93	0.50
1:A:345:LYS:HE3	5:A:2045:HOH:O	2.12	0.49
1:A:223:TYR:HB3	1:A:226:VAL:CG1	2.42	0.49
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.93	0.49
1:B:519:ARG:HG2	1:B:579:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:GLN:O	1:B:494:LEU:HG	2.12	0.49
1:A:63:ILE:HD11	1:A:126:LEU:HD11	1.94	0.49
1:B:129:LEU:HD13	1:B:258:LEU:CD2	2.43	0.49
1:B:136:GLN:HE22	1:B:239:SER:HA	1.77	0.49
1:B:263:GLN:O	1:B:267:LEU:HD12	2.13	0.49
1:A:269:TYR:O	1:A:270:ALA:C	2.50	0.48
1:A:441:LEU:HD12	1:A:652:GLY:HA3	1.95	0.48
1:B:80:ASP:HB3	1:B:84:ARG:NH1	2.27	0.48
1:A:71:PRO:HD2	1:A:72:GLY:H	1.79	0.48
1:B:528:VAL:CG1	1:B:529:GLY:N	2.76	0.48
1:A:136:GLN:HG3	1:A:248:ILE:HD12	1.94	0.48
1:B:565:CYS:C	1:B:567:ALA:H	2.17	0.48
1:A:305:GLY:HA3	2:A:1721:NAD:O5B	2.13	0.48
1:B:84:ARG:CZ	5:B:2012:HOH:O	2.61	0.48
1:B:699:ARG:HG2	5:B:2079:HOH:O	2.14	0.48
1:B:61:ALA:HB3	4:B:1721:CAA:H2'1	1.94	0.47
1:A:136:GLN:O	1:A:140:ARG:HD2	2.15	0.47
1:A:2:ALA:HB3	1:A:31:GLU:HB3	1.95	0.47
1:A:657:ARG:NH1	5:A:2018:HOH:O	2.46	0.47
1:B:343:LEU:C	5:B:2039:HOH:O	2.52	0.47
1:A:219:VAL:HG13	5:A:2025:HOH:O	2.15	0.47
1:A:597:THR:HG22	1:B:382:PHE:CE1	2.50	0.47
1:B:129:LEU:C	1:B:129:LEU:HD23	2.35	0.47
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.96	0.47
1:A:485:ALA:HB3	1:A:486:PRO:HD3	1.96	0.46
1:B:405:LEU:HB2	1:B:427:VAL:HG22	1.97	0.46
1:A:597:THR:HG21	2:B:1719:NAD:H3B	1.96	0.46
1:B:692:GLU:CG	5:B:2076:HOH:O	2.37	0.46
1:A:-3:ARG:HH22	1:A:25:SER:HB2	1.80	0.46
1:A:71:PRO:HD3	1:A:259:ARG:CD	2.34	0.46
1:B:242:HIS:CB	1:B:243:PRO:HD2	2.43	0.46
1:A:63:ILE:HG23	1:A:272:PHE:HZ	1.81	0.46
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.97	0.46
1:B:408:ASN:CG	1:B:408:ASN:O	2.54	0.46
1:A:488:TYR:HE2	1:A:521:SER:HB2	1.81	0.46
1:A:156:TYR:N	1:A:156:TYR:HD1	2.14	0.45
2:B:1719:NAD:O2N	5:B:2038:HOH:O	2.21	0.45
1:A:528:VAL:CG1	1:A:529:GLY:N	2.79	0.45
1:A:534:LYS:HE2	5:A:2068:HOH:O	2.16	0.45
1:B:129:LEU:HD22	1:B:255:PHE:HD1	1.81	0.45
1:A:263:GLN:HG3	5:A:2031:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:MET:CE	1:A:630:ALA:HB2	2.47	0.45
1:A:527:ASP:HB3	1:A:570:PHE:CD1	2.50	0.45
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.86	0.45
1:A:242:HIS:CD2	1:A:246:VAL:HG12	2.52	0.44
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.80	0.44
1:B:483:MET:O	1:B:486:PRO:HD2	2.17	0.44
1:A:340:THR:HG23	5:A:2042:HOH:O	2.16	0.44
1:B:385:MET:O	1:B:389:LYS:HG3	2.17	0.44
1:B:548:PRO:HG2	1:B:551:LYS:HB3	1.98	0.44
1:A:156:TYR:N	1:A:156:TYR:CD1	2.85	0.44
1:A:369:LYS:HA	1:A:398:LEU:CD2	2.40	0.44
1:A:45:VAL:O	1:A:87:LYS:HD3	2.17	0.44
1:A:642:PRO:HD3	1:A:712:GLN:HG2	1.98	0.44
1:A:382:PHE:CZ	2:A:1721:NAD:H2B	2.51	0.44
1:A:712:GLN:OE1	1:A:712:GLN:HA	2.18	0.44
1:B:461:LEU:O	1:B:465:ILE:HG12	2.17	0.44
1:A:369:LYS:HD3	1:A:398:LEU:HD13	1.99	0.44
1:B:406:CYS:HA	1:B:428:ILE:O	2.17	0.44
1:B:103:GLU:OE1	1:B:132:ALA:HB3	2.18	0.43
1:A:420:SER:HB3	5:A:2052:HOH:O	2.18	0.43
1:A:63:ILE:HG23	1:A:272:PHE:CZ	2.54	0.43
1:A:369:LYS:HG2	1:A:398:LEU:HD22	2.00	0.43
1:B:407:THR:HG23	1:B:429:GLY:HA2	2.00	0.43
1:A:228:ALA:HB3	1:A:229:PRO:HD3	2.00	0.43
1:A:519:ARG:HG2	1:A:579:TYR:CE2	2.54	0.43
1:A:175:ASP:HB3	1:A:178:GLU:HB2	2.01	0.43
1:A:565:CYS:C	1:A:567:ALA:H	2.22	0.43
1:B:675:LEU:HA	1:B:697:LEU:HD21	2.00	0.43
1:A:595:LEU:HA	1:A:598:PHE:HB3	2.01	0.43
1:A:71:PRO:CD	1:A:259:ARG:CD	2.91	0.43
1:B:145:PRO:HD2	5:B:2018:HOH:O	2.18	0.43
1:A:679:GLN:HB2	1:A:679:GLN:HE21	1.65	0.43
1:B:528:VAL:HG13	1:B:529:GLY:N	2.34	0.43
1:B:223:TYR:HB3	1:B:226:VAL:CG1	2.49	0.42
1:B:68:ALA:CB	1:B:260:ALA:HA	2.49	0.42
1:B:369:LYS:HA	1:B:398:LEU:CD2	2.42	0.42
1:B:671:LEU:HB2	1:B:672:PRO:HD3	2.01	0.42
1:A:573:LYS:HA	1:A:585:LEU:HD13	2.01	0.42
1:A:274:GLU:OE2	1:A:651:HIS:NE2	2.43	0.42
1:A:500:LYS:HE2	1:A:596:SER:OG	2.19	0.42
1:A:685:ASN:CB	1:A:688:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HB3	1:B:168:LEU:HD13	2.01	0.42
1:B:156:TYR:N	1:B:156:TYR:CD1	2.87	0.42
1:A:97:ALA:O	1:A:119:VAL:HA	2.19	0.42
1:A:597:THR:CG2	1:B:382:PHE:CE1	3.02	0.42
1:B:242:HIS:CD2	1:B:246:VAL:HG12	2.54	0.42
1:A:133:ARG:HD2	1:A:248:ILE:HD11	2.01	0.42
1:A:357:SER:O	1:A:359:LYS:HD3	2.20	0.42
1:B:572:GLN:NE2	1:B:585:LEU:HD12	2.34	0.42
1:B:573:LYS:HA	1:B:585:LEU:HD13	2.02	0.42
1:B:161:GLU:O	1:B:165:LEU:HB2	2.20	0.42
1:A:223:TYR:HB3	1:A:226:VAL:HG13	2.02	0.41
1:B:488:TYR:HE2	1:B:521:SER:HB2	1.85	0.41
1:B:685:ASN:HB3	1:B:688:ILE:HD12	2.02	0.41
1:A:274:GLU:CD	1:A:657:ARG:NH2	2.73	0.41
1:B:156:TYR:N	1:B:156:TYR:HD1	2.18	0.41
1:A:60:GLY:HA3	4:A:1725:CAA:H21	2.02	0.41
1:B:24:VAL:HG11	1:B:75:LEU:HD13	2.02	0.41
1:A:269:TYR:CE1	1:A:664:PHE:HB2	2.54	0.41
1:A:428:ILE:HG21	1:A:458:VAL:HG21	2.01	0.41
1:B:43:HIS:O	1:B:46:LYS:NZ	2.50	0.41
1:B:483:MET:SD	1:B:630:ALA:HB2	2.60	0.41
1:A:161:GLU:O	1:A:165:LEU:HB2	2.20	0.41
1:A:396:SER:HB2	1:A:421:THR:HG22	2.03	0.41
1:A:441:LEU:HB2	1:A:651:HIS:C	2.41	0.41
1:B:105:ALA:O	1:B:111:ARG:HD3	2.21	0.41
1:B:129:LEU:C	1:B:129:LEU:CD2	2.89	0.41
1:B:191:PRO:CD	5:B:2023:HOH:O	2.67	0.41
1:A:548:PRO:HG2	1:A:551:LYS:HB3	2.02	0.41
1:A:571:GLY:HA2	1:A:577:GLY:HA3	2.03	0.41
1:B:248:ILE:HA	1:B:248:ILE:HD12	1.91	0.41
1:B:61:ALA:CB	4:B:1721:CAA:H2'1	2.51	0.41
1:A:226:VAL:HG22	1:A:229:PRO:HD2	2.03	0.40
1:B:287:SER:OG	1:B:289:LYS:HB2	2.20	0.40
1:A:389:LYS:HD3	5:A:2052:HOH:O	2.20	0.40
1:B:92:ALA:HA	1:B:112:ILE:O	2.21	0.40
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.96	0.40
1:B:692:GLU:CD	5:B:2076:HOH:O	2.60	0.40
1:A:441:LEU:HD11	1:A:648:ILE:HG23	2.04	0.40
1:A:69:PHE:N	1:A:69:PHE:CD1	2.89	0.40
1:B:10:SER:O	1:B:45:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	724/742 (98%)	669 (92%)	50 (7%)	5 (1%)	26	62
1	B	720/742 (97%)	657 (91%)	58 (8%)	5 (1%)	26	62
All	All	1444/1484 (97%)	1326 (92%)	108 (8%)	10 (1%)	26	62

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	B	-1	SER
1	B	355	GLN
1	A	174	SER
1	A	566	GLU
1	A	358	ALA
1	B	130	PRO
1	B	174	SER
1	A	360	PRO
1	B	498	GLY

5.3.2 Protein sidechains

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	595/609 (98%)	558 (94%)	37 (6%)	23	54
1	B	592/609 (97%)	554 (94%)	38 (6%)	22	52
All	All	1187/1218 (98%)	1112 (94%)	75 (6%)	22	53

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	24	VAL
1	A	27	THR
1	A	31	GLU
1	A	63	ILE
1	A	70	THR
1	A	73	LEU
1	A	125	THR
1	A	135	THR
1	A	165	LEU
1	A	172	VAL
1	A	226	VAL
1	A	234	ARG
1	A	242	HIS
1	A	245	GLU
1	A	248	ILE
1	A	258	LEU
1	A	306	THR
1	A	330	LYS
1	A	359	LYS
1	A	362	LEU
1	A	370	GLU
1	A	371	LEU
1	A	441	LEU
1	A	523	LEU
1	A	528	VAL
1	A	572	GLN
1	A	585	LEU
1	A	609	GLU
1	A	612	THR
1	A	615	LYS
1	A	641	ARG
1	A	675	LEU
1	A	676	GLU
1	A	694	SER
1	A	695	ASP
1	A	709	LYS
1	B	7	LEU
1	B	31	GLU
1	B	73	LEU
1	B	90	LEU
1	B	129	LEU

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Mol	Chain	Res	Type
1	B	135	THR
1	B	165	LEU
1	B	219	VAL
1	B	226	VAL
1	B	242	HIS
1	B	245	GLU
1	B	248	ILE
1	B	256	MET
1	B	258	LEU
1	B	278	ASN
1	B	282	THR
1	B	306	THR
1	B	330	LYS
1	B	362	LEU
1	B	370	GLU
1	B	371	LEU
1	B	420	SER
1	B	523	LEU
1	B	528	VAL
1	B	543	LEU
1	B	549	VAL
1	B	572	GLN
1	B	585	LEU
1	B	599	LEU
1	B	600	SER
1	B	609	GLU
1	B	612	THR
1	B	615	LYS
1	B	641	ARG
1	B	676	GLU
1	B	694	SER
1	B	695	ASP
1	B	709	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	242	HIS
1	A	294	GLN
1	A	353	ASN
1	A	572	GLN

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Mol	Chain	Res	Type
1	A	589	HIS
1	A	610	GLN
1	A	679	GLN
1	B	64	HIS
1	B	185	GLN
1	B	242	HIS
1	B	294	GLN
1	B	572	GLN
1	B	589	HIS
1	B	610	GLN
1	B	679	GLN
1	B	718	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	NAD	A	1721	-	42,48,48	1.73	3 (7%)	46,73,73	2.01	2 (4%)
3	SO4	A	1722	-	4,4,4	0.15	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	A	1723	-	4,4,4	0.21	0	6,6,6	0.50	0
3	SO4	A	1724	-	4,4,4	0.09	0	6,6,6	0.11	0
4	CAA	A	1725	-	47,56,56	1.43	7 (14%)	57,83,83	2.50	8 (14%)
2	NAD	B	1719	-	42,48,48	1.76	3 (7%)	46,73,73	1.71	2 (4%)
3	SO4	B	1720	-	4,4,4	0.26	0	6,6,6	0.26	0
4	CAA	B	1721	-	47,56,56	1.28	5 (10%)	57,83,83	1.88	9 (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	NAD	A	1721	-	-	0/22/62/62	0/5/5/5
3	SO4	A	1722	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1723	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1724	-	-	0/0/0/0	0/0/0/0
4	CAA	A	1725	-	-	0/50/71/71	0/3/3/3
2	NAD	B	1719	-	-	0/22/62/62	0/5/5/5
3	SO4	B	1720	-	-	0/0/0/0	0/0/0/0
4	CAA	B	1721	-	-	0/50/71/71	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1721	CAA	C2-C1	-2.76	1.40	1.50
4	A	1725	CAA	C1-S1P	2.30	1.80	1.76
4	A	1725	CAA	O1-C1	2.40	1.24	1.21
4	A	1725	CAA	P3B-O8A	2.56	1.63	1.54
4	B	1721	CAA	P1A-O1A	2.79	1.61	1.51
2	A	1721	NAD	C2A-N1A	2.86	1.39	1.33
2	B	1719	NAD	C2A-N1A	3.11	1.39	1.33
4	A	1725	CAA	P1A-O1A	3.22	1.63	1.51
4	A	1725	CAA	O4B-C1B	3.25	1.45	1.41
4	B	1721	CAA	P2A-O4A	3.27	1.63	1.51
4	B	1721	CAA	O4B-C1B	3.33	1.46	1.41
4	B	1721	CAA	P3B-O7A	3.50	1.61	1.50
4	A	1725	CAA	P2A-O4A	3.58	1.64	1.51
4	A	1725	CAA	P3B-O7A	3.70	1.62	1.50
2	B	1719	NAD	C2A-N3A	4.16	1.39	1.32
2	A	1721	NAD	C2A-N3A	4.19	1.39	1.32
2	A	1721	NAD	O7N-C7N	8.50	1.42	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1719	NAD	O7N-C7N	8.50	1.42	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1721	NAD	N3A-C2A-N1A	-12.20	119.29	128.87
4	A	1725	CAA	N3A-C2A-N1A	-10.52	120.61	128.87
2	B	1719	NAD	N3A-C2A-N1A	-9.92	121.08	128.87
4	B	1721	CAA	N3A-C2A-N1A	-9.42	121.47	128.87
4	A	1725	CAA	O1-C1-S1P	-8.75	115.89	122.83
4	B	1721	CAA	O1-C1-S1P	-3.00	120.45	122.83
4	B	1721	CAA	O8A-P3B-O7A	-2.24	103.33	110.63
4	A	1725	CAA	C5B-C4B-C3B	-2.22	106.14	114.30
4	A	1725	CAA	C1B-N9A-C4A	-2.04	124.53	126.81
2	A	1721	NAD	C2N-C3N-C4N	2.03	120.57	118.27
4	B	1721	CAA	O2A-P1A-O3A	2.08	114.19	105.27
4	A	1725	CAA	O5A-P2A-O3A	2.11	114.32	105.27
4	A	1725	CAA	O2A-P1A-O3A	2.24	114.86	105.27
4	B	1721	CAA	O9A-P3B-O8A	2.25	115.69	107.44
4	B	1721	CAA	C3-C2-C1	2.27	124.43	114.65
4	B	1721	CAA	CEP-CBP-CAP	2.28	113.34	109.17
4	B	1721	CAA	C2B-C1B-N9A	2.29	119.59	113.47
4	A	1725	CAA	C3-C2-C1	2.59	125.80	114.65
2	B	1719	NAD	C4D-O4D-C1D	2.98	112.80	109.64
4	B	1721	CAA	C2-C1-S1P	6.21	119.57	113.46
4	A	1725	CAA	C2-C1-S1P	10.06	123.36	113.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	NAD	4	0
4	A	1725	CAA	3	0
2	B	1719	NAD	2	0
4	B	1721	CAA	2	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	725/742 (97%)	-0.23	11 (1%)	76	68	14, 40, 72, 103	0
1	B	721/742 (97%)	-0.30	17 (2%)	62	50	17, 41, 72, 102	0
All	All	1446/1484 (97%)	-0.26	28 (1%)	70	59	14, 40, 72, 103	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	5.2
1	B	348	SER	4.8
1	B	356	ALA	4.8
1	B	353	ASN	4.7
1	B	-2	GLY	4.5
1	A	354	GLY	4.4
1	A	351	HIS	4.3
1	B	351	HIS	3.6
1	B	718	HIS	3.6
1	B	349	ARG	3.3
1	B	347	ALA	3.3
1	A	355	GLN	3.1
1	A	353	ASN	3.1
1	A	352	GLN	3.1
1	B	352	GLN	3.0
1	B	357	SER	2.9
1	B	355	GLN	2.9
1	A	357	SER	2.9
1	A	358	ALA	2.7
1	B	358	ALA	2.6
1	A	350	ALA	2.5
1	B	554	ASN	2.5
1	A	345	LYS	2.4
1	A	348	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	2.2
1	B	344	GLU	2.2
1	B	-1	SER	2.1
1	B	9	HIS	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	1724	5/5	0.85	0.19	1.75	96,96,97,97	0
3	SO4	B	1720	5/5	0.90	0.16	0.46	87,87,88,88	0
4	CAA	B	1721	54/54	0.95	0.12	-0.65	40,47,51,53	0
4	CAA	A	1725	54/54	0.93	0.14	-0.70	22,56,62,62	0
2	NAD	B	1719	44/44	0.96	0.15	-0.75	42,48,69,71	0
2	NAD	A	1721	44/44	0.94	0.14	-0.84	46,50,62,65	0
3	SO4	A	1722	5/5	0.97	0.10	-1.97	43,43,43,44	0
3	SO4	A	1723	5/5	0.98	0.12	-	38,39,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.