



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 PM GMT

PDB ID : 3ZWC  
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-DECA NOYL-COA  
Authors : Kasaragod, P.; Schmitz, W.; Hiltunen, J.K.; Wierenga, R.K.  
Deposited on : 2011-07-28  
Resolution : 2.30 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](mailto: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.

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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

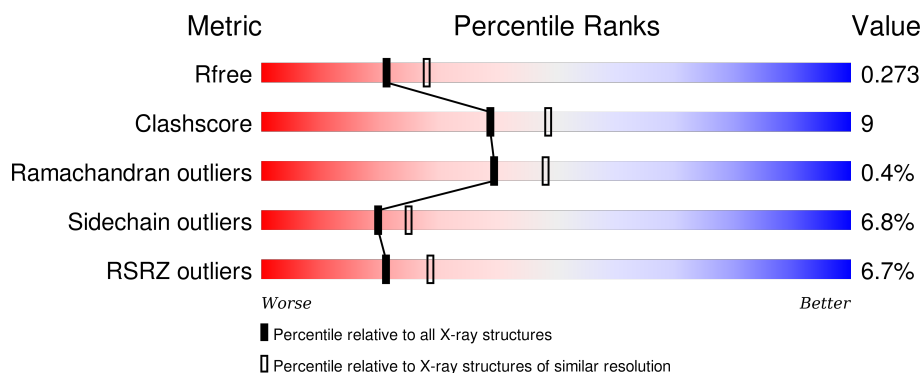
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>5%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	B	742	<div> <div>8%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>

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	HSC	B	1722	-	-	-	X
5	GOL	B	1719	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11720 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	0	0
			5562	3553	976	1010	23			
1	B	719	Total	C	N	O	S	0	0	0
			5524	3532	967	1002	23			

There are 40 discrepancies between the modelled and reference sequences:

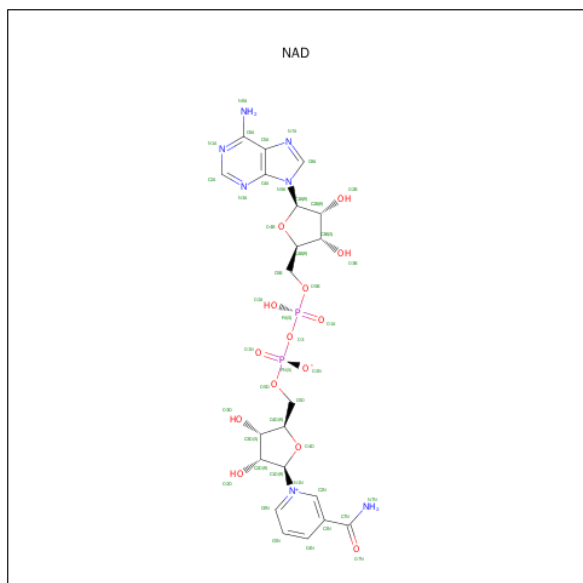
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P07896
A	-18	GLY	-	EXPRESSION TAG	UNP P07896
A	-17	SER	-	EXPRESSION TAG	UNP P07896
A	-16	SER	-	EXPRESSION TAG	UNP P07896
A	-15	HIS	-	EXPRESSION TAG	UNP P07896
A	-14	HIS	-	EXPRESSION TAG	UNP P07896
A	-13	HIS	-	EXPRESSION TAG	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 NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



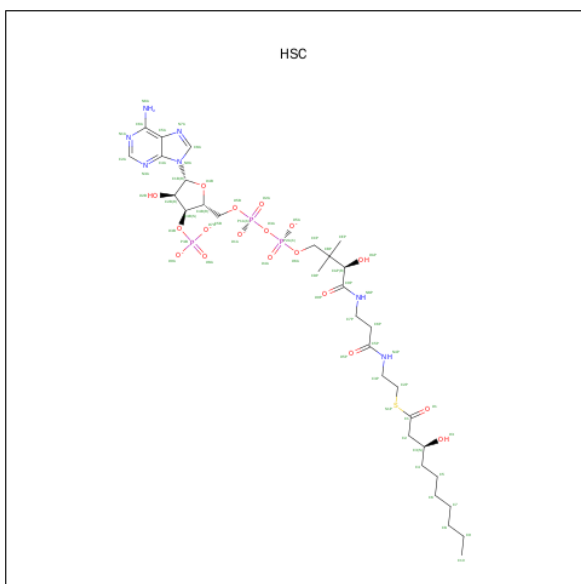
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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



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

- Molecule 4 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
4	A	1	Total	C	N	O	P	S	
			60	31	7	18	3	1	0
4	B	1	Total	C	N	O	P	S	
			60	31	7	18	3	1	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

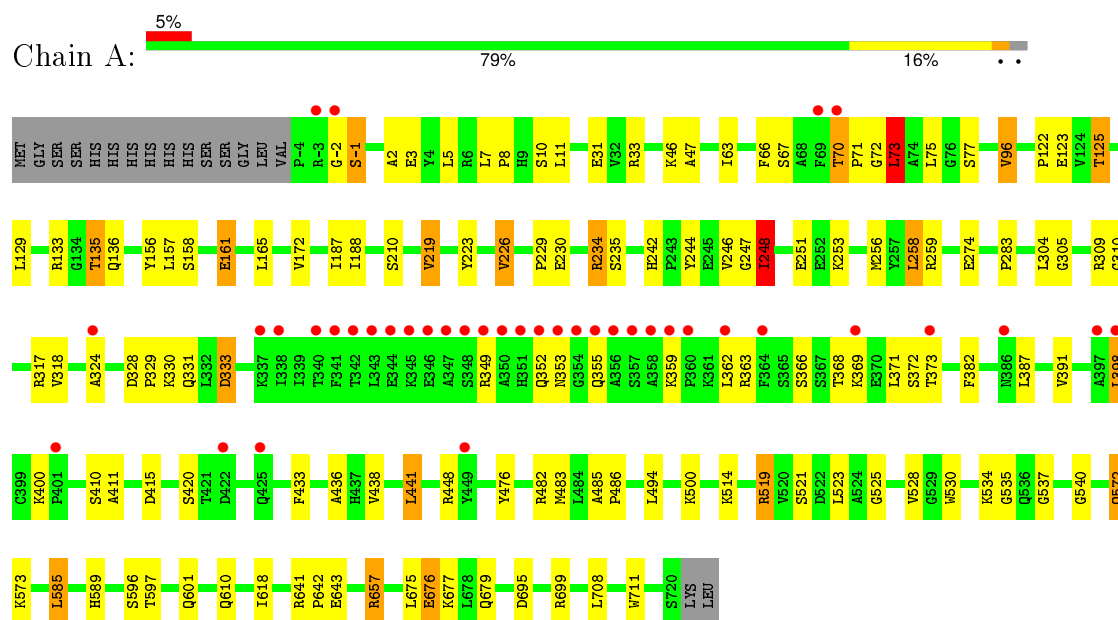
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O		
			231	231	0	0
6	B	174	Total	O		
			174	174	0	0

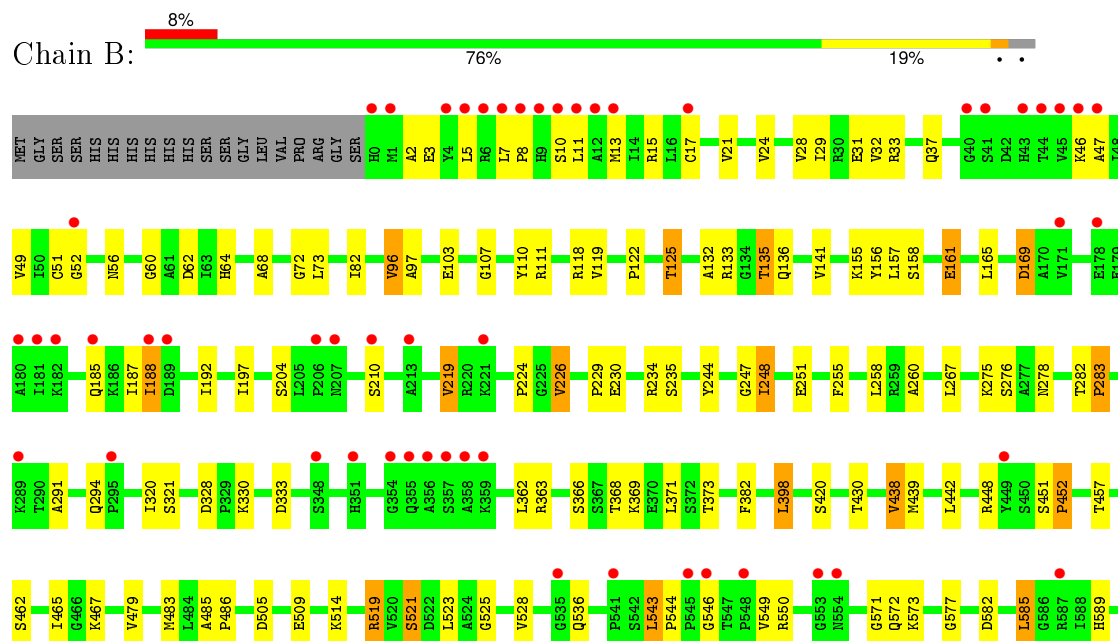
### 3 Residue-property plots

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.

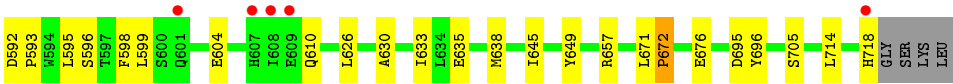
#### • Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME



#### • Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.57Å 126.51Å 224.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.48 – 2.30 44.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (112.48-2.30) 99.6 (44.62-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.231 , 0.280 0.227 , 0.273	Depositor DCC
$R_{free}$ test set	4184 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 83722 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, SO4, NAD, HSC

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	0.92	1/5691 (0.0%)	0.87	11/7709 (0.1%)
1	B	0.95	1/5652 (0.0%)	0.89	7/7658 (0.1%)
All	All	0.93	2/11343 (0.0%)	0.88	18/15367 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17	CYS	CB-SG	7.55	1.95	1.82
1	A	485	ALA	CA-CB	5.13	1.63	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ARG	NE-CZ-NH2	9.49	125.05	120.30
1	A	657	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	A	234	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	234	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	649	TYR	CA-CB-CG	-6.89	100.30	113.40
1	A	258	LEU	CB-CG-CD1	6.84	122.63	111.00
1	B	169	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	B	519	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	626	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	519	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	-2	GLY	N-CA-C	6.00	128.10	113.10
1	A	482	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	248	ILE	CA-CB-CG2	5.88	122.66	110.90
1	A	33	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	519	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	234	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	33	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	5562	0	5667	103	0
1	B	5524	0	5631	103	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
3	A	10	0	0	0	0
3	B	5	0	0	1	0
4	A	60	0	50	9	0
4	B	60	0	50	8	0
5	B	6	0	8	4	0
6	A	231	0	0	12	0
6	B	174	0	0	15	0
All	All	11720	0	11458	205	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (205) 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:73:LEU:HD21	1:A:256:MET:HE2	1.32	1.08
1:A:500:LYS:HD3	6:A:2180:HOH:O	1.54	1.04
1:A:253:LYS:HE2	6:A:2067:HOH:O	1.58	1.03
1:B:514:LYS:HE2	6:B:2111:HOH:O	1.60	1.01
1:A:135:THR:HG21	1:A:235:SER:OG	1.71	0.91
5:B:1719:GOL:O3	5:B:1719:GOL:O1	1.83	0.90
1:B:158:SER:OG	1:B:161:GLU:HG2	1.74	0.88
1:A:73:LEU:HD21	1:A:256:MET:CE	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:CD2	1:A:256:MET:HE2	2.05	0.86
1:A:597:THR:HG23	1:B:382:PHE:HZ	1.42	0.85
1:A:540:GLY:HA3	6:A:2159:HOH:O	1.76	0.84
1:B:135:THR:HG21	1:B:235:SER:OG	1.80	0.81
1:A:73:LEU:CD2	1:A:256:MET:CE	2.59	0.80
1:B:283:PRO:HA	1:B:718:HIS:HE1	1.45	0.80
1:A:597:THR:HG23	1:B:382:PHE:CZ	2.18	0.78
1:A:657:ARG:NH1	6:A:2035:HOH:O	2.12	0.74
1:B:72:GLY:HA3	4:B:1722:HSC:H9A	1.68	0.74
1:B:158:SER:OG	1:B:161:GLU:CG	2.35	0.74
1:A:7:LEU:HG	1:A:8:PRO:HD2	1.68	0.74
1:B:21:VAL:HG12	6:B:2007:HOH:O	1.89	0.72
1:A:67:SER:HB3	1:A:70:THR:OG1	1.90	0.71
1:B:525:GLY:O	1:B:528:VAL:HG22	1.92	0.70
1:B:283:PRO:HA	1:B:718:HIS:CE1	2.27	0.70
1:A:540:GLY:CA	6:A:2159:HOH:O	2.36	0.69
1:A:67:SER:H	1:A:71:PRO:HD3	1.56	0.69
1:B:505:ASP:O	1:B:509:GLU:HG3	1.92	0.69
1:A:679:GLN:HG2	6:A:2219:HOH:O	1.91	0.69
1:B:37:GLN:HB3	6:B:2006:HOH:O	1.93	0.69
1:B:255:PHE:CE2	4:B:1722:HSC:H8	2.27	0.69
1:A:122:PRO:O	1:A:125:THR:HB	1.93	0.68
4:B:1722:HSC:H8A	6:B:2015:HOH:O	1.93	0.68
1:A:96:VAL:HG21	4:A:1724:HSC:HDP	1.74	0.67
1:B:244:TYR:CZ	1:B:248:ILE:HD11	2.29	0.67
1:B:521:SER:HB2	5:B:1719:GOL:H12	1.77	0.67
1:A:158:SER:OG	1:A:161:GLU:HG3	1.94	0.67
1:B:244:TYR:CE1	1:B:248:ILE:HD11	2.29	0.67
1:A:73:LEU:HD22	1:A:256:MET:HE1	1.76	0.67
1:B:133:ARG:HD2	1:B:248:ILE:CG1	2.25	0.67
1:A:72:GLY:C	4:A:1724:HSC:H8	2.17	0.65
1:B:29:ILE:HD12	1:B:73:LEU:HD22	1.78	0.65
1:B:7:LEU:HG	1:B:8:PRO:HD2	1.78	0.65
1:B:122:PRO:O	1:B:125:THR:HB	1.97	0.65
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.32	0.64
1:A:75:LEU:H	4:A:1724:HSC:H8A	1.61	0.64
1:A:123:GLU:CG	4:A:1724:HSC:H2A	2.28	0.64
1:A:73:LEU:N	4:A:1724:HSC:H8	2.14	0.63
1:B:21:VAL:CG1	6:B:2007:HOH:O	2.47	0.62
1:B:155:LYS:NZ	6:B:2039:HOH:O	2.32	0.62
1:A:514:LYS:HD2	6:A:2148:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD22	1:B:47:ALA:HB3	1.83	0.60
1:A:133:ARG:HD2	1:A:248:ILE:CG1	2.32	0.60
1:A:597:THR:CG2	1:B:382:PHE:CZ	2.85	0.60
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.36	0.60
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.33	0.58
1:A:601:GLN:HG3	1:B:382:PHE:CD2	2.39	0.58
1:B:10:SER:HB3	1:B:46:LYS:HG3	1.85	0.58
1:A:597:THR:CG2	1:B:382:PHE:HZ	2.14	0.57
1:B:135:THR:HG22	1:B:251:GLU:OE1	2.03	0.57
1:B:37:GLN:CB	6:B:2006:HOH:O	2.51	0.57
1:A:253:LYS:CE	6:A:2067:HOH:O	2.31	0.57
1:A:135:THR:HB	1:A:251:GLU:OE1	2.05	0.57
1:B:141:VAL:CG2	1:B:197:ILE:HD13	2.34	0.57
1:A:244:TYR:CZ	1:A:248:ILE:HD11	2.40	0.57
1:A:73:LEU:HD22	1:A:256:MET:CE	2.31	0.56
1:A:244:TYR:CZ	1:A:248:ILE:CD1	2.89	0.56
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.86	0.56
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.36	0.56
1:A:641:ARG:HB2	1:A:642:PRO:HD2	1.88	0.56
1:A:411:ALA:HB1	1:A:476:TYR:CE1	2.41	0.55
1:B:118:ARG:HG2	6:B:2044:HOH:O	2.06	0.54
1:A:349:ARG:CG	1:A:352:GLN:HE21	2.21	0.54
1:B:672:PRO:HD3	1:B:705:SER:OG	2.07	0.54
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.89	0.54
1:B:156:TYR:N	1:B:156:TYR:CD1	2.77	0.53
1:A:349:ARG:HG3	1:A:352:GLN:HE21	1.74	0.53
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.90	0.53
1:B:3:GLU:HG2	1:B:5:LEU:HD13	1.90	0.53
1:B:244:TYR:CZ	1:B:248:ILE:CD1	2.92	0.52
1:A:382:PHE:CE2	2:A:1721:NAD:H8A	2.45	0.52
1:B:244:TYR:CE1	1:B:248:ILE:CD1	2.93	0.52
1:A:156:TYR:CD1	1:A:156:TYR:N	2.77	0.52
1:B:369:LYS:HA	1:B:398:LEU:HD13	1.91	0.52
1:A:244:TYR:CE1	1:A:248:ILE:CD1	2.93	0.52
1:A:494:LEU:HD13	1:A:618:ILE:HG12	1.92	0.52
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.92	0.52
1:B:582:ASP:HB2	6:B:2132:HOH:O	2.10	0.52
1:A:525:GLY:O	1:A:528:VAL:HG22	2.10	0.51
1:B:60:GLY:HA3	4:B:1722:HSC:H2PA	1.92	0.51
1:A:369:LYS:HA	1:A:398:LEU:HD13	1.93	0.51
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ALA:HA	6:A:2117:HOH:O	2.10	0.51
1:A:483:MET:O	1:A:486:PRO:HD2	2.10	0.51
1:B:96:VAL:HG11	4:B:1722:HSC:HDP	1.93	0.50
1:A:2:ALA:HB3	1:A:31:GLU:HB3	1.92	0.50
1:B:294:GLN:O	1:B:457:THR:HG23	2.11	0.50
1:B:465:ILE:HG13	1:B:467:LYS:HG3	1.93	0.50
1:A:244:TYR:CE1	1:A:248:ILE:HD11	2.47	0.49
1:B:156:TYR:N	1:B:156:TYR:HD1	2.09	0.49
1:A:310:GLY:HA3	1:A:436:ALA:HB3	1.94	0.49
1:B:543:LEU:HD22	1:B:544:PRO:HD2	1.94	0.49
1:A:70:THR:HB	1:A:71:PRO:HD3	1.93	0.49
1:B:451:SER:O	1:B:452:PRO:C	2.51	0.49
1:A:226:VAL:HG22	1:A:229:PRO:HD2	1.93	0.49
1:B:62:ASP:OD2	1:B:64:HIS:HB2	2.13	0.49
1:A:73:LEU:H	4:A:1724:HSC:H7	1.78	0.49
1:B:546:GLY:N	6:B:2124:HOH:O	2.33	0.49
1:B:111:ARG:N	1:B:169:ASP:OD2	2.40	0.49
1:B:13:MET:HA	1:B:49:VAL:O	2.13	0.49
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.95	0.48
1:A:3:GLU:HG2	1:A:5:LEU:HD13	1.94	0.48
1:A:123:GLU:HG3	4:A:1724:HSC:H2A	1.94	0.48
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.93	0.48
1:A:10:SER:HB3	1:A:46:LYS:HG3	1.95	0.48
1:A:133:ARG:NE	1:A:248:ILE:HG12	2.28	0.48
1:A:573:LYS:HA	1:A:585:LEU:HD13	1.96	0.48
1:B:671:LEU:HB2	1:B:672:PRO:HD3	1.97	0.47
1:B:136:GLN:NE2	1:B:247:GLY:HA3	2.28	0.47
1:B:604:GLU:O	6:B:2134:HOH:O	2.20	0.47
1:B:714:LEU:HD23	6:B:2173:HOH:O	2.15	0.47
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.97	0.47
1:A:382:PHE:CD2	2:A:1721:NAD:H8A	2.49	0.47
1:A:420:SER:OG	1:A:420:SER:O	2.33	0.47
1:B:133:ARG:HD2	1:B:248:ILE:HG13	1.97	0.47
1:B:638:MET:HE3	6:B:2147:HOH:O	2.14	0.47
1:B:192:ILE:N	3:B:1721:SO4:O2	2.42	0.47
1:B:133:ARG:HD2	1:B:248:ILE:HG12	1.94	0.47
1:A:133:ARG:CD	1:A:248:ILE:CG1	2.93	0.47
4:B:1722:HSC:HEP	6:B:2007:HOH:O	2.14	0.47
1:B:226:VAL:HG22	1:B:229:PRO:HD2	1.98	0.46
1:B:2:ALA:HB3	1:B:31:GLU:HB3	1.97	0.46
1:A:382:PHE:CZ	2:A:1721:NAD:H2B	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:LYS:HA	1:B:585:LEU:HD13	1.97	0.46
1:A:96:VAL:HG11	4:A:1724:HSC:HEP	1.98	0.46
1:A:328:ASP:OD1	1:A:330:LYS:HB2	2.15	0.46
1:A:535:GLY:C	1:A:537:GLY:H	2.19	0.46
1:A:305:GLY:HA3	2:A:1721:NAD:O5B	2.16	0.46
1:A:156:TYR:HD1	1:A:156:TYR:N	2.12	0.46
1:B:595:LEU:HA	1:B:598:PHE:HB3	1.97	0.46
1:B:187:ILE:HD12	1:B:187:ILE:C	2.36	0.46
1:A:73:LEU:CD2	1:A:256:MET:HE1	2.36	0.46
1:A:530:TRP:CE2	1:A:534:LYS:HE2	2.51	0.46
1:B:363:ARG:HH22	1:B:373:THR:HG21	1.81	0.46
1:A:158:SER:OG	1:A:161:GLU:CG	2.63	0.45
1:A:329:PRO:O	1:A:333:ASP:HB2	2.16	0.45
1:A:223:TYR:HB3	1:A:226:VAL:HG13	1.98	0.45
1:B:219:VAL:HG11	1:B:230:GLU:HA	1.98	0.45
1:A:11:LEU:HD22	1:A:47:ALA:HB3	1.97	0.45
1:A:676:GLU:HG3	1:A:677:LYS:N	2.32	0.45
1:B:158:SER:HG	1:B:161:GLU:HG2	1.75	0.45
1:B:571:GLY:HA2	1:B:577:GLY:HA3	1.99	0.45
1:B:521:SER:CB	5:B:1719:GOL:H12	2.45	0.44
1:B:110:TYR:HA	1:B:169:ASP:OD2	2.17	0.44
1:A:219:VAL:HG11	1:A:230:GLU:HA	1.99	0.44
1:B:291:ALA:HB2	1:B:452:PRO:HB3	1.99	0.44
1:A:133:ARG:HD2	1:A:248:ILE:HD11	2.00	0.44
1:B:420:SER:OG	1:B:420:SER:O	2.36	0.44
1:A:187:ILE:HD12	1:A:187:ILE:C	2.38	0.44
1:B:224:PRO:HD2	6:B:2058:HOH:O	2.17	0.44
1:B:635:GLU:HB3	1:B:696:TYR:HB2	1.99	0.44
1:A:349:ARG:HG3	1:A:352:GLN:NE2	2.34	0.43
1:B:68:ALA:CB	1:B:260:ALA:HA	2.48	0.43
1:A:400:LYS:HB2	6:A:2115:HOH:O	2.17	0.43
1:A:66:PHE:HA	1:A:71:PRO:HG3	1.99	0.43
1:B:275:LYS:HG3	4:B:1722:HSC:O2B	2.18	0.43
1:A:519:ARG:HD3	1:A:589:HIS:NE2	2.34	0.43
1:A:305:GLY:O	1:A:309:ARG:HG3	2.18	0.43
1:A:382:PHE:HB2	1:A:387:LEU:HD23	2.00	0.43
1:A:363:ARG:HH22	1:A:373:THR:HG21	1.83	0.43
1:B:73:LEU:O	4:B:1722:HSC:H9	2.18	0.43
1:A:244:TYR:CZ	1:A:248:ILE:HD13	2.52	0.43
1:B:438:VAL:CG1	1:B:439:MET:N	2.82	0.43
1:A:641:ARG:HD3	1:A:643:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:OE1	1:A:657:ARG:NH2	2.52	0.42
1:A:572:GLN:HE21	1:A:572:GLN:HB3	1.61	0.42
1:B:103:GLU:OE1	1:B:132:ALA:HB3	2.19	0.42
1:B:438:VAL:HG12	1:B:439:MET:N	2.34	0.42
1:B:82:ILE:HG22	1:B:107:GLY:O	2.19	0.42
1:B:320:ILE:CG2	1:B:321:SER:N	2.82	0.42
1:A:540:GLY:C	6:A:2159:HOH:O	2.57	0.42
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.55	0.42
1:A:353:ASN:HB2	1:A:355:GLN:HG2	2.01	0.42
1:B:430:THR:HB	1:B:442:LEU:HD11	2.02	0.42
1:A:135:THR:CG2	1:A:136:GLN:OE1	2.68	0.42
1:B:244:TYR:CE2	1:B:248:ILE:HD13	2.54	0.42
1:B:462:SER:HA	1:B:465:ILE:HG12	2.02	0.42
1:B:521:SER:HB2	5:B:1719:GOL:C1	2.48	0.41
1:A:136:GLN:NE2	1:A:247:GLY:HA3	2.35	0.41
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.56	0.41
1:A:67:SER:HB3	1:A:70:THR:CB	2.50	0.41
1:B:630:ALA:HB1	1:B:645:ILE:HD13	2.03	0.41
1:B:28:VAL:O	1:B:32:VAL:HG23	2.20	0.41
4:A:1724:HSC:H7A	6:A:2024:HOH:O	2.19	0.41
1:B:135:THR:CG2	1:B:251:GLU:OE1	2.68	0.41
1:A:129:LEU:HD12	1:A:129:LEU:C	2.41	0.41
1:A:317:ARG:HG3	1:A:318:VAL:HG13	2.03	0.41
1:B:52:GLY:HA3	1:B:56:ASN:O	2.20	0.41
1:A:242:HIS:HB3	1:A:246:VAL:HB	2.02	0.40
1:B:328:ASP:OD1	1:B:330:LYS:HB2	2.21	0.40
1:B:15:ARG:HG3	1:B:51:CYS:SG	2.61	0.40
1:B:244:TYR:O	1:B:248:ILE:HB	2.20	0.40
1:B:483:MET:CE	1:B:630:ALA:HB2	2.52	0.40
1:B:479:VAL:HG22	1:B:633:ILE:HG21	2.03	0.40
1:A:387:LEU:O	1:A:391:VAL:HG23	2.21	0.40
1:B:592:ASP:HA	1:B:593:PRO:HD3	1.91	0.40
1:A:415:ASP:OD1	1:A:448:ARG:HB2	2.22	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	723/742 (97%)	691 (96%)	29 (4%)	3 (0%)	39	48
1	B	717/742 (97%)	679 (95%)	35 (5%)	3 (0%)	39	48
All	All	1440/1484 (97%)	1370 (95%)	64 (4%)	6 (0%)	39	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	B	448	ARG
1	B	536	GLN
1	A	73	LEU
1	A	70	THR
1	B	283	PRO

### 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	594/609 (98%)	553 (93%)	41 (7%)	19	24
1	B	590/609 (97%)	551 (93%)	39 (7%)	21	27
All	All	1184/1218 (97%)	1104 (93%)	80 (7%)	20	25

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	63	ILE
1	A	73	LEU
1	A	77	SER
1	A	96	VAL
1	A	125	THR
1	A	135	THR
1	A	157	LEU
1	A	161	GLU
1	A	165	LEU
1	A	172	VAL
1	A	188	ILE
1	A	210	SER
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	248	ILE
1	A	258	LEU
1	A	283	PRO
1	A	331	GLN
1	A	333	ASP
1	A	359	LYS
1	A	362	LEU
1	A	366	SER
1	A	368	THR
1	A	371	LEU
1	A	372	SER
1	A	398	LEU
1	A	410	SER
1	A	438	VAL
1	A	441	LEU
1	A	521	SER
1	A	523	LEU
1	A	572	GLN
1	A	585	LEU
1	A	596	SER
1	A	610	GLN
1	A	675	LEU
1	A	676	GLU
1	A	695	ASP
1	A	699	ARG
1	B	24	VAL
1	B	96	VAL

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Mol	Chain	Res	Type
1	B	125	THR
1	B	135	THR
1	B	157	LEU
1	B	161	GLU
1	B	165	LEU
1	B	185	GLN
1	B	188	ILE
1	B	204	SER
1	B	210	SER
1	B	219	VAL
1	B	226	VAL
1	B	248	ILE
1	B	258	LEU
1	B	276	SER
1	B	278	ASN
1	B	282	THR
1	B	333	ASP
1	B	362	LEU
1	B	366	SER
1	B	368	THR
1	B	371	LEU
1	B	398	LEU
1	B	438	VAL
1	B	452	PRO
1	B	521	SER
1	B	523	LEU
1	B	543	LEU
1	B	549	VAL
1	B	550	ARG
1	B	572	GLN
1	B	585	LEU
1	B	596	SER
1	B	599	LEU
1	B	610	GLN
1	B	672	PRO
1	B	676	GLU
1	B	695	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	572	GLN
1	A	589	HIS
1	A	679	GLN
1	B	294	GLN
1	B	331	GLN
1	B	353	ASN
1	B	572	GLN
1	B	589	HIS
1	B	679	GLN
1	B	718	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
2	NAD	A	1721	-	38,48,48	1.77	4 (10%)	47,73,73	2.18	9 (19%)
3	SO4	A	1722	-	4,4,4	0.62	0	6,6,6	0.39	0
3	SO4	A	1723	-	4,4,4	0.14	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HSC	A	1724	-	52,62,62	2.22	6 (11%)	66,89,89	2.67	18 (27%)
5	GOL	B	1719	-	5,5,5	0.23	0	5,5,5	1.19	1 (20%)
2	NAD	B	1720	-	38,48,48	1.78	4 (10%)	47,73,73	2.21	9 (19%)
3	SO4	B	1721	-	4,4,4	0.14	0	6,6,6	0.87	0
4	HSC	B	1722	-	52,62,62	1.82	5 (9%)	66,89,89	2.31	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	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
4	HSC	A	1724	-	-	0/57/78/78	0/3/3/3
5	GOL	B	1719	-	-	0/4/4/4	0/0/0/0
2	NAD	B	1720	-	-	0/22/62/62	0/5/5/5
3	SO4	B	1721	-	-	0/0/0/0	0/0/0/0
4	HSC	B	1722	-	-	0/57/78/78	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1722	HSC	P3B-O9A	-2.27	1.47	1.51
2	B	1720	NAD	PA-O2A	-2.12	1.45	1.54
4	A	1724	HSC	C1-S1P	2.34	1.81	1.76
2	A	1721	NAD	C2A-N1A	2.39	1.38	1.33
4	A	1724	HSC	O1-C1	2.46	1.24	1.21
2	B	1720	NAD	C2A-N1A	2.73	1.39	1.33
2	A	1721	NAD	O4B-C1B	2.81	1.44	1.41
2	B	1720	NAD	C2A-N3A	3.45	1.38	1.32
2	A	1721	NAD	C2A-N3A	3.76	1.38	1.32
4	B	1722	HSC	O4B-C1B	4.28	1.46	1.41
4	A	1724	HSC	O4B-C1B	4.84	1.47	1.41
4	B	1722	HSC	P3B-O8A	5.46	1.62	1.51
4	B	1722	HSC	C2-C1	6.54	1.60	1.50
4	B	1722	HSC	P3B-O7A	6.61	1.63	1.51
4	A	1724	HSC	P3B-O7A	6.94	1.64	1.51
4	A	1724	HSC	P3B-O8A	8.28	1.67	1.51
4	A	1724	HSC	C2-C1	8.32	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1721	NAD	O7N-C7N	8.40	1.42	1.24
2	B	1720	NAD	O7N-C7N	8.41	1.42	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1721	NAD	N3A-C2A-N1A	-11.93	119.76	128.89
2	B	1720	NAD	N3A-C2A-N1A	-11.37	120.19	128.89
4	A	1724	HSC	N3A-C2A-N1A	-11.02	120.46	128.89
4	A	1724	HSC	O1-C1-S1P	-10.80	114.26	122.83
4	B	1722	HSC	O1-C1-S1P	-10.29	114.67	122.83
4	B	1722	HSC	N3A-C2A-N1A	-9.27	121.79	128.89
2	B	1720	NAD	PN-O3-PA	-3.91	121.75	132.73
4	B	1722	HSC	CDP-CBP-CCP	-3.40	104.09	108.50
4	A	1724	HSC	CDP-CBP-CCP	-3.11	104.47	108.50
2	A	1721	NAD	PN-O3-PA	-2.94	124.48	132.73
4	B	1722	HSC	O7A-P3B-O8A	-2.67	106.55	112.76
2	B	1720	NAD	C1B-N9A-C4A	-2.65	122.94	126.94
4	A	1724	HSC	O7A-P3B-O8A	-2.64	106.63	112.76
4	A	1724	HSC	C3P-C2P-S1P	-2.57	104.48	111.36
2	A	1721	NAD	C4B-O4B-C1B	-2.54	106.93	109.72
5	B	1719	GOL	C3-C2-C1	-2.53	101.21	111.12
4	B	1722	HSC	O3-C3-C4	-2.51	102.15	109.29
4	A	1724	HSC	C7P-C6P-C5P	-2.48	108.22	112.31
4	A	1724	HSC	C6P-C7P-N8P	-2.39	106.64	111.88
2	A	1721	NAD	C1B-N9A-C4A	-2.32	123.44	126.94
2	B	1720	NAD	O3D-C3D-C4D	-2.28	104.20	111.05
4	A	1724	HSC	C4A-C5A-N7A	-2.24	107.42	109.48
4	A	1724	HSC	CEP-CBP-CCP	-2.20	105.65	108.50
4	A	1724	HSC	C6-C5-C4	-2.15	106.01	113.66
2	A	1721	NAD	O7N-C7N-N7N	-2.00	119.78	122.59
2	A	1721	NAD	O5B-PA-O1A	2.01	117.43	109.62
2	A	1721	NAD	C3N-C7N-N7N	2.06	120.07	117.82
2	A	1721	NAD	O4B-C1B-N9A	2.19	112.69	108.10
2	A	1721	NAD	O2A-PA-O3	2.24	115.27	105.09
4	A	1724	HSC	C2A-N1A-C6A	2.25	122.79	118.77
4	B	1722	HSC	O1-C1-C2	2.35	125.99	123.70
4	A	1724	HSC	C2B-C1B-N9A	2.41	117.97	114.29
4	B	1722	HSC	O6A-CCP-CBP	2.47	114.52	110.55
2	B	1720	NAD	O4D-C1D-N1N	2.53	110.91	108.13
2	B	1720	NAD	O2N-PN-O3	2.72	117.41	105.09
2	B	1720	NAD	O3-PA-O5B	2.82	110.41	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1720	NAD	C4D-O4D-C1D	2.88	112.89	109.72
4	A	1724	HSC	C2P-C3P-N4P	2.96	118.29	112.36
4	A	1724	HSC	O6A-CCP-CBP	3.10	115.54	110.55
4	B	1722	HSC	CEP-CBP-CCP	3.34	112.83	108.50
2	B	1720	NAD	C2B-C1B-N9A	3.38	119.45	114.29
4	A	1724	HSC	O3-C3-C2	3.85	119.35	109.42
4	B	1722	HSC	C3-C2-C1	4.40	123.14	112.98
4	A	1724	HSC	C2-C1-S1P	4.45	117.36	113.36
4	A	1724	HSC	O1-C1-C2	4.70	128.29	123.70
4	B	1722	HSC	C2-C1-S1P	6.56	119.26	113.36
4	A	1724	HSC	C3-C2-C1	7.73	130.82	112.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1721	NAD	4	0
4	A	1724	HSC	9	0
5	B	1719	GOL	4	0
3	B	1721	SO4	1	0
4	B	1722	HSC	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	725/742 (97%)	0.35	39 (5%)	29 38	9, 31, 62, 99	0
1	B	719/742 (96%)	0.22	58 (8%)	15 21	10, 32, 62, 96	0
All	All	1444/1484 (97%)	0.28	97 (6%)	21 29	9, 32, 62, 99	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ALA	7.8
1	A	350	ALA	6.9
1	A	354	GLY	5.9
1	A	351	HIS	5.7
1	A	352	GLN	5.7
1	B	43	HIS	5.2
1	B	354	GLY	5.0
1	A	69	PHE	4.9
1	B	0	HIS	4.9
1	A	357	SER	4.9
1	B	358	ALA	4.8
1	B	45	VAL	4.7
1	B	178	GLU	4.7
1	B	718	HIS	4.6
1	A	348	SER	4.6
1	B	449	TYR	4.6
1	B	185	GLN	4.5
1	B	5	LEU	4.4
1	A	341	PHE	4.4
1	B	44	THR	4.4
1	B	8	PRO	4.3
1	A	70	THR	4.3
1	B	541	PRO	4.3
1	B	4	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	4.1
1	B	608	ILE	4.0
1	B	180	ALA	3.9
1	B	535	GLY	3.9
1	B	545	PRO	3.8
1	A	347	ALA	3.7
1	A	355	GLN	3.6
1	A	364	PHE	3.6
1	B	40	GLY	3.6
1	B	207	ASN	3.6
1	B	553	GLY	3.5
1	B	351	HIS	3.4
1	A	349	ARG	3.4
1	A	359	LYS	3.3
1	A	338	ILE	3.3
1	A	-2	GLY	3.3
1	B	10	SER	3.3
1	B	609	GLU	3.3
1	A	337	LYS	3.3
1	B	171	VAL	3.3
1	A	345	LYS	3.2
1	A	398	LEU	3.1
1	A	342	THR	3.1
1	B	13	MET	3.1
1	A	353	ASN	3.0
1	A	362	LEU	3.0
1	B	601	GLN	3.0
1	A	425	GLN	3.0
1	A	360	PRO	2.9
1	B	554	ASN	2.9
1	B	6	ARG	2.9
1	B	7	LEU	2.9
1	B	206	PRO	2.8
1	B	9	HIS	2.8
1	B	188	ILE	2.7
1	A	358	ALA	2.7
1	B	12	ALA	2.7
1	B	181	ILE	2.6
1	B	221	LYS	2.6
1	A	346	GLU	2.6
1	A	369	LYS	2.6
1	B	546	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	397	ALA	2.5
1	A	386	ASN	2.4
1	B	213	ALA	2.4
1	B	1	MET	2.4
1	A	-3	ARG	2.4
1	B	189	ASP	2.4
1	B	607	HIS	2.3
1	A	401	PRO	2.3
1	A	449	TYR	2.3
1	B	11	LEU	2.3
1	A	324	ALA	2.3
1	B	355	GLN	2.3
1	B	210	SER	2.3
1	B	348	SER	2.3
1	B	182	LYS	2.3
1	A	340	THR	2.2
1	B	548	PRO	2.2
1	B	47	ALA	2.2
1	B	41	SER	2.2
1	A	343	LEU	2.2
1	A	422	ASP	2.1
1	A	373	THR	2.1
1	A	344	GLU	2.1
1	B	46	LYS	2.1
1	B	359	LYS	2.1
1	B	289	LYS	2.1
1	B	357	SER	2.1
1	B	587	ARG	2.1
1	B	52	GLY	2.1
1	B	295	PRO	2.0
1	B	17	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	GOL	B	1719	6/6	0.87	0.18	4.00	43,47,48,50	0
4	HSC	B	1722	60/60	0.83	0.19	2.03	56,76,83,83	0
4	HSC	A	1724	60/60	0.84	0.18	1.37	24,62,79,81	0
3	SO4	B	1721	5/5	0.81	0.19	1.07	69,70,74,75	0
2	NAD	A	1721	44/44	0.91	0.14	-0.19	33,42,49,52	0
3	SO4	A	1722	5/5	0.98	0.09	-1.75	27,31,32,35	0
2	NAD	B	1720	44/44	0.97	0.10	-1.94	24,33,41,42	0
3	SO4	A	1723	5/5	0.84	0.25	-	79,82,82,84	0

## 6.5 Other polymers

There are no such residues in this entry.