Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:46 AM GMT

PDB ID	:	2YAU
Title	:	X-ray structure of the Leishmania infantum tryopanothione reductase in complex with auranofin
Authors	:	Baiocco, P.; Ilari, A.; Colotti, G.
Deposited on	:	2011-02-24
Resolution	:	3.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

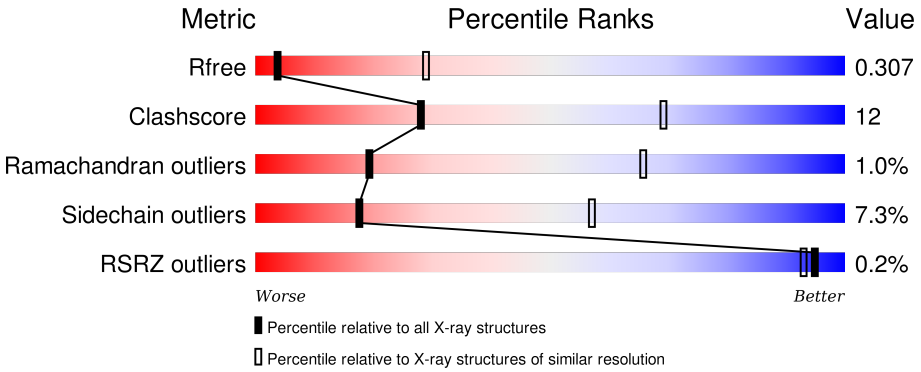
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	511	68% 24% • 5%
1	B	511	68% 25% • 5%

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	AU	B	600	-	-	X	-
7	SO4	A	1490	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7652 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 TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3694	2322	634	711	27			
1	B	488	Total	C	N	O	S	0	0	0
			3694	2322	634	711	27			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP A4HSF7
A	-18	GLY	-	EXPRESSION TAG	UNP A4HSF7
A	-17	SER	-	EXPRESSION TAG	UNP A4HSF7
A	-16	SER	-	EXPRESSION TAG	UNP A4HSF7
A	-15	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-14	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-13	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-12	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-11	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-10	HIS	-	EXPRESSION TAG	UNP A4HSF7
A	-9	SER	-	EXPRESSION TAG	UNP A4HSF7
A	-8	SER	-	EXPRESSION TAG	UNP A4HSF7
A	-7	GLY	-	EXPRESSION TAG	UNP A4HSF7
A	-6	LEU	-	EXPRESSION TAG	UNP A4HSF7
A	-5	VAL	-	EXPRESSION TAG	UNP A4HSF7
A	-4	PRO	-	EXPRESSION TAG	UNP A4HSF7
A	-3	ARG	-	EXPRESSION TAG	UNP A4HSF7
A	-2	GLY	-	EXPRESSION TAG	UNP A4HSF7
A	-1	SER	-	EXPRESSION TAG	UNP A4HSF7
A	0	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-19	MET	-	EXPRESSION TAG	UNP A4HSF7
B	-18	GLY	-	EXPRESSION TAG	UNP A4HSF7
B	-17	SER	-	EXPRESSION TAG	UNP A4HSF7
B	-16	SER	-	EXPRESSION TAG	UNP A4HSF7
B	-15	HIS	-	EXPRESSION TAG	UNP A4HSF7

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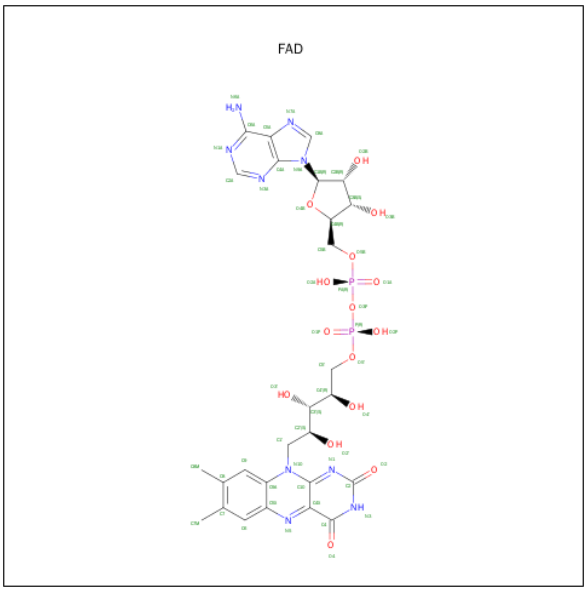
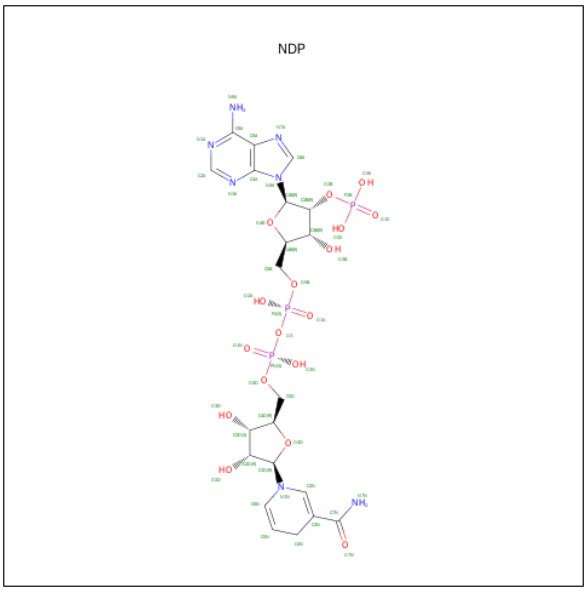
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-13	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-12	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-11	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-10	HIS	-	EXPRESSION TAG	UNP A4HSF7
B	-9	SER	-	EXPRESSION TAG	UNP A4HSF7
B	-8	SER	-	EXPRESSION TAG	UNP A4HSF7
B	-7	GLY	-	EXPRESSION TAG	UNP A4HSF7
B	-6	LEU	-	EXPRESSION TAG	UNP A4HSF7
B	-5	VAL	-	EXPRESSION TAG	UNP A4HSF7
B	-4	PRO	-	EXPRESSION TAG	UNP A4HSF7
B	-3	ARG	-	EXPRESSION TAG	UNP A4HSF7
B	-2	GLY	-	EXPRESSION TAG	UNP A4HSF7
B	-1	SER	-	EXPRESSION TAG	UNP A4HSF7
B	0	HIS	-	EXPRESSION TAG	UNP A4HSF7

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

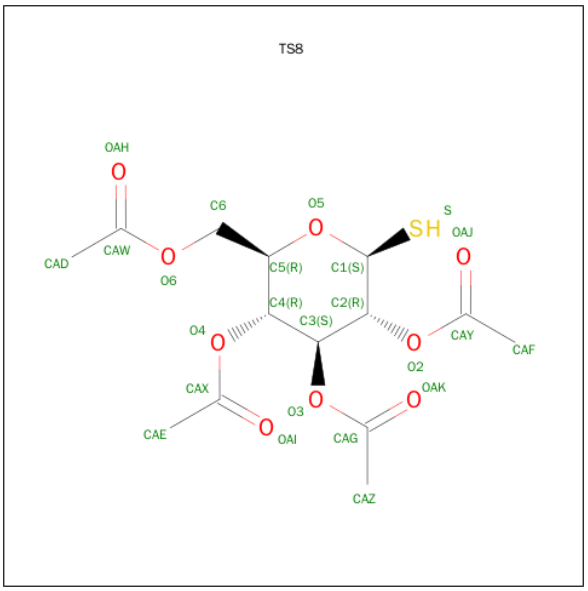


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Au	0	0
			1	1		
4	A	1	Total	Au	0	0
			1	1		

- Molecule 5 is 3,4,5-TRIACETYLOXY-6-(ACETYLOXYMETHYL)OXANE-2-THIOL (three-letter code: TS8) (formula: $C_{14}H_{20}O_9S$).

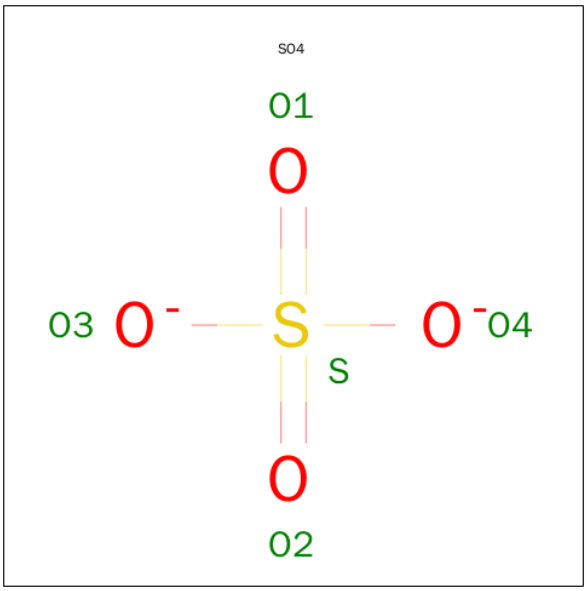


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 24 14 9 1	0	0
5	B	1	Total C O S 24 14 9 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



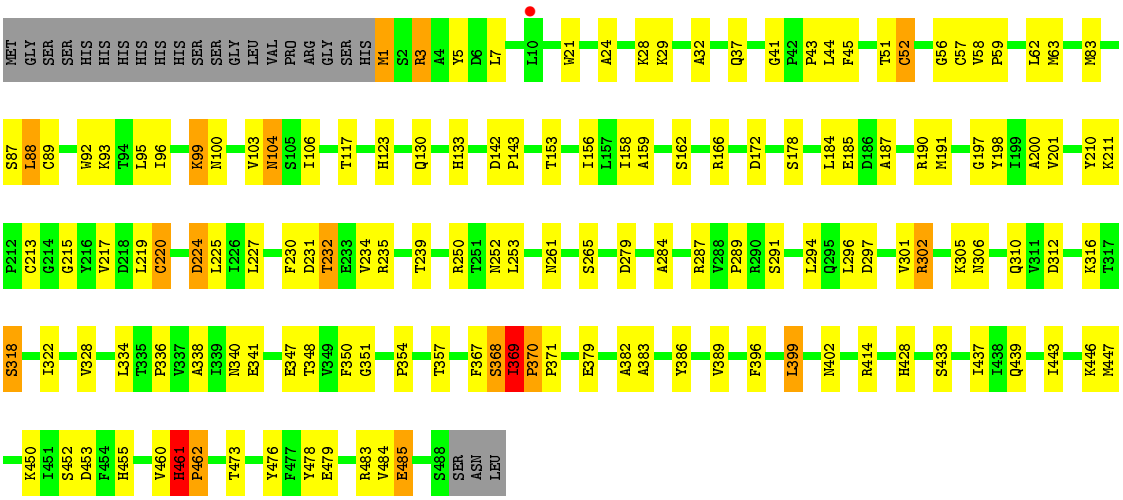
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0

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.

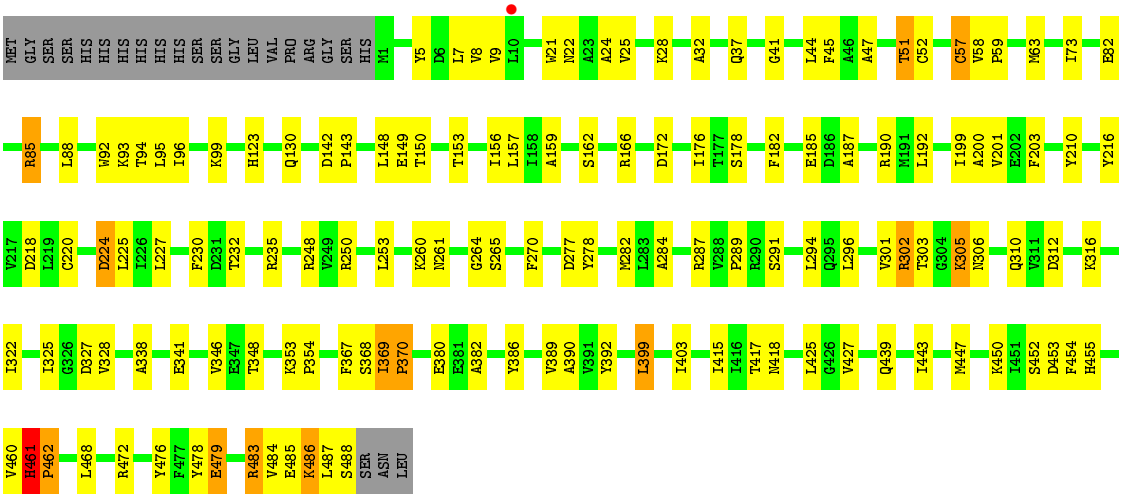
- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	103.06Å 103.06Å 191.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 48.03 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.9 (48.03-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.267 , 0.319 0.259 , 0.307	Depositor DCC
R_{free} test set	1291 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	95.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 18.4	EDS
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 25175 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7652	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: CL, AU, SO4, TS8, NDP, FAD

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	0.45	0/3767	0.59	0/5100
1	B	0.46	0/3767	0.59	0/5100
All	All	0.46	0/7534	0.59	0/10200

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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ILE	Peptide
1	A	461	HIS	Peptide
1	B	461	HIS	Peptide

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	3694	0	3645	89	0
1	B	3694	0	3645	89	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	48	0	26	1	0
3	B	48	0	26	2	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0
5	A	24	0	20	2	0
5	B	24	0	20	3	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	7652	0	7444	172	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 12.

All (172) 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:3:ARG:HH12	1:A:133:HIS:CG	1.77	1.01
1:A:1:MET:SD	1:A:1:MET:N	2.30	0.99
1:B:85:ARG:HG2	1:B:85:ARG:HH11	1.29	0.98
1:B:389:VAL:HG23	1:B:478:TYR:HB2	1.46	0.96
1:A:367:PHE:CE1	1:B:462:PRO:HG2	2.10	0.86
1:B:58:VAL:HB	1:B:59:PRO:HD3	1.57	0.85
1:A:3:ARG:NH1	1:A:133:HIS:CG	2.46	0.82
1:A:479:GLU:HB2	1:A:484:VAL:HG11	1.62	0.81
1:A:162:SER:HB2	1:A:287:ARG:HB3	1.64	0.79
1:A:302:ARG:HB3	1:A:310:GLN:HB2	1.67	0.77
1:A:462:PRO:HG2	1:B:367:PHE:CE1	2.21	0.76
1:B:348:THR:HA	1:B:354:PRO:HA	1.68	0.75
1:A:348:THR:HA	1:A:354:PRO:HA	1.66	0.75
1:A:1:MET:HB2	1:A:3:ARG:HD2	1.67	0.75
1:A:291:SER:HA	1:A:294:LEU:HG	1.68	0.75
1:B:302:ARG:HB3	1:B:310:GLN:HB2	1.69	0.73
1:A:92:TRP:CZ2	1:A:96:ILE:HD11	2.24	0.73
1:A:3:ARG:HH12	1:A:133:HIS:CD2	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ARG:HG2	1:B:85:ARG:NH1	1.93	0.72
1:B:296:LEU:HB3	1:B:301:VAL:HB	1.73	0.69
1:B:57:CYS:HG	4:B:600:AU:AU	1.45	0.69
1:B:162:SER:HB2	1:B:287:ARG:HB3	1.73	0.68
1:A:41:GLY:O	1:A:45:PHE:HA	1.94	0.68
1:A:52:CYS:HG	4:A:600:AU:AU	1.48	0.66
1:B:85:ARG:CG	1:B:85:ARG:HH11	2.06	0.66
1:B:199:ILE:HG13	3:B:550:NDP:O2N	1.96	0.65
1:A:29:LYS:HE3	1:A:350:PHE:HD1	1.61	0.65
1:A:383:ALA:CB	1:A:478:TYR:HD2	2.10	0.65
1:A:389:VAL:HG23	1:A:478:TYR:HB2	1.78	0.65
1:A:452:SER:HA	1:A:455:HIS:CE1	2.33	0.64
1:A:32:ALA:HB1	1:A:123:HIS:CD2	2.32	0.64
1:A:220:CYS:HB2	1:A:253:LEU:HD23	1.79	0.64
1:B:289:PRO:HB3	1:B:328:VAL:HA	1.79	0.64
1:A:92:TRP:HB2	1:A:187:ALA:HB2	1.80	0.63
1:A:201:VAL:HG12	1:A:368:SER:HB3	1.81	0.62
1:B:389:VAL:CG2	1:B:478:TYR:HB2	2.25	0.62
1:B:37:GLN:HE21	1:B:47:ALA:HB2	1.65	0.62
1:A:63:MET:HG2	1:A:95:LEU:HD21	1.80	0.62
1:B:176:ILE:O	1:B:282:MET:HA	1.99	0.62
1:A:383:ALA:HB2	1:A:478:TYR:HD2	1.65	0.62
1:B:291:SER:HA	1:B:294:LEU:HG	1.80	0.62
1:B:479:GLU:HG3	1:B:486:LYS:HG2	1.83	0.61
1:B:190:ARG:HG2	1:B:216:TYR:CE1	2.35	0.60
1:A:52:CYS:HA	1:A:56:GLY:HA3	1.82	0.60
1:A:461:HIS:HE1	5:B:650:TS8:H2	1.67	0.59
1:A:5:TYR:O	1:A:153:THR:HA	2.01	0.59
1:B:52:CYS:HG	4:B:600:AU:AU	1.53	0.59
1:B:487:LEU:HG	1:B:488:SER:N	2.18	0.58
1:A:296:LEU:HB3	1:A:301:VAL:HB	1.84	0.58
1:B:452:SER:HA	1:B:455:HIS:CE1	2.38	0.58
1:B:390:ALA:HB3	1:B:417:THR:OG1	2.04	0.58
1:A:51:THR:HG21	1:A:287:ARG:NH2	2.19	0.58
1:A:21:TRP:HZ3	1:A:117:THR:HG1	1.52	0.57
1:A:219:LEU:O	1:A:250:ARG:N	2.37	0.57
1:A:312:ASP:OD2	1:A:316:LYS:HB3	2.04	0.57
1:A:24:ALA:O	1:A:28:LYS:HA	2.05	0.57
1:B:199:ILE:HG22	1:B:203:PHE:HD2	1.70	0.57
1:B:156:ILE:HB	1:B:322:ILE:HG23	1.86	0.57
1:A:92:TRP:CE2	1:A:96:ILE:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:GLY:O	1:B:45:PHE:HA	2.05	0.56
1:A:231:ASP:HB3	1:A:234:VAL:HG23	1.87	0.56
1:A:261:ASN:HB2	1:A:265:SER:O	2.06	0.56
1:A:3:ARG:NH1	1:A:133:HIS:ND1	2.53	0.56
1:A:58:VAL:HB	1:A:59:PRO:CD	2.36	0.56
1:B:382:ALA:O	1:B:386:TYR:HB2	2.05	0.56
1:A:289:PRO:HB3	1:A:328:VAL:HA	1.88	0.55
1:B:479:GLU:CG	1:B:486:LYS:HG2	2.36	0.55
1:B:312:ASP:OD2	1:B:316:LYS:HB3	2.07	0.55
1:A:224:ASP:HB3	1:A:252:ASN:HD21	1.70	0.55
1:A:305:LYS:H	1:A:305:LYS:HD2	1.72	0.55
1:B:95:LEU:HD13	1:B:210:TYR:OH	2.07	0.54
1:B:201:VAL:HG12	1:B:368:SER:HB3	1.88	0.54
1:B:305:LYS:HD2	1:B:305:LYS:H	1.71	0.54
1:B:52:CYS:SG	1:B:57:CYS:HB3	2.48	0.53
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.43	0.53
1:A:382:ALA:O	1:A:386:TYR:HB2	2.09	0.53
1:B:483:ARG:H	1:B:483:ARG:HD3	1.74	0.53
1:B:148:LEU:HD23	1:B:149:GLU:HG3	1.91	0.52
1:A:479:GLU:HB2	1:A:484:VAL:CG1	2.37	0.52
1:B:443:ILE:O	1:B:447:MET:HB2	2.10	0.52
1:A:450:LYS:O	1:A:453:ASP:HB2	2.10	0.52
1:B:51:THR:HG21	1:B:287:ARG:NH2	2.25	0.51
1:B:9:VAL:HG13	1:B:157:LEU:HD23	1.93	0.51
1:A:433:SER:O	1:A:437:ILE:HG13	2.10	0.51
1:A:1:MET:HB2	1:A:3:ARG:CD	2.39	0.50
1:B:199:ILE:HD12	3:B:550:NDP:O1N	2.11	0.50
1:B:166:ARG:NH1	1:B:172:ASP:O	2.44	0.50
1:B:418:ASN:HB2	1:B:425:LEU:HD21	1.94	0.50
1:A:347:GLU:HA	1:A:351:GLY:HA3	1.93	0.50
5:B:650:TS8:S	6:B:1489:CL:CL	3.07	0.50
1:B:200:ALA:HB2	1:B:284:ALA:HB3	1.93	0.50
1:A:58:VAL:HG13	1:B:399:LEU:HD12	1.94	0.49
1:B:32:ALA:HB1	1:B:123:HIS:CD2	2.48	0.49
1:A:200:ALA:HB2	1:A:284:ALA:HB3	1.94	0.49
5:A:650:TS8:H2	1:B:461:HIS:HE1	1.78	0.49
1:A:369:ILE:HG22	1:A:370:PRO:HD3	1.94	0.49
1:A:439:GLN:OE1	1:B:460:VAL:HG23	2.13	0.48
1:A:190:ARG:HB2	1:A:279:ASP:H	1.78	0.48
1:A:103:VAL:O	1:A:106:ILE:N	2.45	0.48
1:B:8:VAL:HG23	1:B:153:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:HB3	1:A:234:VAL:CG2	2.44	0.48
1:A:462:PRO:HG3	2:B:500:FAD:O4	2.13	0.48
3:A:550:NDP:H6N	3:A:550:NDP:H51N	1.95	0.48
1:A:227:LEU:HB3	1:A:230:PHE:CD1	2.49	0.48
1:B:415:ILE:HG12	1:B:427:VAL:HG22	1.96	0.48
1:A:95:LEU:HD13	1:A:210:TYR:OH	2.14	0.47
1:A:396:PHE:HB2	5:B:650:TS8:HAE	1.96	0.47
2:A:500:FAD:O4	1:B:462:PRO:HG3	2.14	0.47
1:B:227:LEU:HB3	1:B:230:PHE:CD2	2.50	0.47
1:A:156:ILE:HD12	1:A:322:ILE:HG12	1.97	0.47
1:B:392:TYR:HE2	1:B:472:ARG:O	1.98	0.47
1:B:156:ILE:HD12	1:B:322:ILE:HG12	1.97	0.47
1:B:338:ALA:HA	1:B:341:GLU:HB2	1.98	0.46
1:A:159:ALA:O	2:A:500:FAD:H52A	2.15	0.46
1:A:443:ILE:O	1:A:447:MET:HB2	2.14	0.46
1:A:340:ASN:HD22	1:A:357:THR:HG23	1.81	0.46
1:B:261:ASN:HB2	1:B:265:SER:O	2.15	0.46
1:A:32:ALA:HB1	1:A:123:HIS:NE2	2.30	0.46
1:B:224:ASP:OD1	1:B:224:ASP:N	2.46	0.46
1:B:369:ILE:HG22	1:B:370:PRO:HD3	1.98	0.46
1:A:389:VAL:HG23	1:A:478:TYR:CB	2.46	0.46
1:B:92:TRP:HB2	1:B:187:ALA:HB2	1.99	0.45
1:B:353:LYS:HA	1:B:354:PRO:HD3	1.86	0.45
1:A:232:THR:HA	1:A:235:ARG:HD3	1.99	0.45
1:B:253:LEU:HD11	1:B:270:PHE:HB3	1.98	0.45
1:A:62:LEU:HD22	1:B:403:ILE:HD12	1.98	0.45
1:A:83:MET:HE3	1:B:73:ILE:HD13	1.99	0.45
1:B:461:HIS:ND1	1:B:461:HIS:O	2.49	0.45
1:B:5:TYR:O	1:B:153:THR:HA	2.17	0.44
1:A:379:GLU:OE2	1:A:414:ARG:NH2	2.50	0.44
5:A:650:TS8:H2	1:B:461:HIS:CE1	2.52	0.44
1:B:232:THR:HA	1:B:235:ARG:HD3	2.00	0.44
1:B:454:PHE:HE2	1:B:468:LEU:HD22	1.83	0.44
1:B:63:MET:HG2	1:B:95:LEU:HD21	2.00	0.43
1:A:302:ARG:HH11	1:A:318:SER:HB3	1.82	0.43
1:A:399:LEU:O	1:A:402:ASN:ND2	2.50	0.43
1:A:100:ASN:O	1:A:104:ASN:HB3	2.18	0.43
1:A:211:LYS:HD2	1:A:215:GLY:O	2.19	0.43
1:B:24:ALA:O	1:B:28:LYS:HA	2.18	0.43
1:B:415:ILE:HG23	1:B:427:VAL:HG22	2.01	0.43
1:A:460:VAL:HG23	1:B:439:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HB3	1:A:99:LYS:HD3	2.01	0.43
1:B:325:ILE:CG2	1:B:341:GLU:HB3	2.48	0.43
1:B:260:LYS:HE3	1:B:264:GLY:O	2.19	0.43
1:A:291:SER:HB2	1:A:296:LEU:HD21	2.01	0.42
1:A:334:LEU:HB3	1:A:336:PRO:HD2	2.00	0.42
1:B:21:TRP:CE2	1:B:25:VAL:HG21	2.54	0.42
1:B:190:ARG:HD2	1:B:277:ASP:O	2.19	0.42
1:B:22:ASN:HB3	1:B:346:VAL:HG11	2.02	0.42
1:B:450:LYS:O	1:B:453:ASP:HB2	2.20	0.42
1:B:369:ILE:HA	1:B:369:ILE:HD13	1.90	0.41
1:B:380:GLU:H	1:B:380:GLU:CD	2.24	0.41
1:A:191:MET:HB3	1:A:217:VAL:HG22	2.02	0.41
1:A:383:ALA:HB2	1:A:478:TYR:CD2	2.50	0.41
1:B:218:ASP:OD1	1:B:248:ARG:HB3	2.21	0.41
1:B:192:LEU:HD22	1:B:278:TYR:CE2	2.56	0.41
1:A:88:LEU:HD23	1:B:82:GLU:O	2.19	0.41
1:B:159:ALA:O	2:B:500:FAD:H52A	2.21	0.41
1:B:479:GLU:HG3	1:B:484:VAL:HG11	2.01	0.41
1:A:484:VAL:HG22	1:A:485:GLU:N	2.36	0.41
1:A:166:ARG:NH1	1:A:172:ASP:O	2.54	0.41
1:B:59:PRO:HB2	1:B:182:PHE:CE1	2.56	0.41
1:B:190:ARG:HG2	1:B:216:TYR:CZ	2.55	0.41
1:A:231:ASP:HB2	1:A:428:HIS:CG	2.55	0.41
1:B:162:SER:HB3	1:B:327:ASP:HB3	2.02	0.41
1:A:158:ILE:HG22	1:A:328:VAL:HG11	2.02	0.41
1:B:142:ASP:HA	1:B:143:PRO:HD3	1.86	0.41
1:A:89:CYS:SG	1:A:213:CYS:N	2.94	0.40
1:A:197:GLY:O	1:A:198:TYR:C	2.60	0.40
1:A:370:PRO:HA	1:A:371:PRO:HD3	2.01	0.40
1:A:142:ASP:HA	1:A:143:PRO:HD3	1.94	0.40
1:A:338:ALA:HA	1:A:341:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	486/511 (95%)	436 (90%)	45 (9%)	5 (1%)	19 66
1	B	486/511 (95%)	437 (90%)	44 (9%)	5 (1%)	19 66
All	All	972/1022 (95%)	873 (90%)	89 (9%)	10 (1%)	19 66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	B	461	HIS
1	B	462	PRO
1	A	43	PRO
1	B	486	LYS
1	A	232	THR
1	A	370	PRO
1	A	461	HIS
1	B	305	LYS
1	B	370	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	397/417 (95%)	365 (92%)	32 (8%)	15 52
1	B	397/417 (95%)	371 (94%)	26 (6%)	21 62
All	All	794/834 (95%)	736 (93%)	58 (7%)	17 57

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ARG
1	A	7	LEU

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Mol	Chain	Res	Type
1	A	37	GLN
1	A	44	LEU
1	A	52	CYS
1	A	57	CYS
1	A	87	SER
1	A	88	LEU
1	A	93	LYS
1	A	99	LYS
1	A	104	ASN
1	A	130	GLN
1	A	178	SER
1	A	184	LEU
1	A	185	GLU
1	A	220	CYS
1	A	224	ASP
1	A	225	LEU
1	A	239	THR
1	A	297	ASP
1	A	302	ARG
1	A	306	ASN
1	A	318	SER
1	A	368	SER
1	A	369	ILE
1	A	399	LEU
1	A	446	LYS
1	A	473	THR
1	A	476	TYR
1	A	483	ARG
1	A	485	GLU
1	B	7	LEU
1	B	44	LEU
1	B	51	THR
1	B	57	CYS
1	B	85	ARG
1	B	88	LEU
1	B	93	LYS
1	B	94	THR
1	B	99	LYS
1	B	130	GLN
1	B	150	THR
1	B	178	SER
1	B	185	GLU

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Mol	Chain	Res	Type
1	B	220	CYS
1	B	224	ASP
1	B	225	LEU
1	B	250	ARG
1	B	302	ARG
1	B	303	THR
1	B	306	ASN
1	B	369	ILE
1	B	399	LEU
1	B	476	TYR
1	B	479	GLU
1	B	483	ARG
1	B	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	54	ASN
1	A	91	ASN
1	A	252	ASN
1	A	269	HIS
1	A	340	ASN
1	B	37	GLN
1	B	54	ASN
1	B	107	ASN
1	B	269	HIS
1	B	295	GLN
1	B	310	GLN
1	B	340	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	A	1490	-	4,4,4	0.26	0	6,6,6	0.20	0
2	FAD	A	500	-	48,58,58	1.14	5 (10%)	54,89,89	2.18	9 (16%)
3	NDP	A	550	-	42,52,52	1.74	9 (21%)	55,80,80	1.74	6 (10%)
5	TS8	A	650	-	23,24,24	1.94	4 (17%)	31,33,33	1.90	9 (29%)
7	SO4	B	1490	-	4,4,4	0.33	0	6,6,6	0.16	0
2	FAD	B	500	-	48,58,58	1.21	5 (10%)	54,89,89	2.15	9 (16%)
3	NDP	B	550	-	42,52,52	1.74	9 (21%)	55,80,80	1.73	7 (12%)
5	TS8	B	650	-	23,24,24	1.95	4 (17%)	31,33,33	1.94	8 (25%)

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
7	SO4	A	1490	-	-	0/0/0/0	0/0/0/0
2	FAD	A	500	-	-	0/30/50/50	0/6/6/6
3	NDP	A	550	-	-	0/30/77/77	0/5/5/5
5	TS8	A	650	-	-	0/17/37/37	0/1/1/1
7	SO4	B	1490	-	-	0/0/0/0	0/0/0/0
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	NDP	B	550	-	-	0/30/77/77	0/5/5/5
5	TS8	B	650	-	-	0/17/37/37	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	NDP	C4N-C5N	-4.13	1.40	1.49
3	B	550	NDP	C4N-C5N	-3.99	1.40	1.49
2	B	500	FAD	C5X-N5	2.04	1.38	1.35
3	A	550	NDP	C2N-C3N	2.12	1.39	1.34
2	A	500	FAD	C1'-N10	2.14	1.50	1.48
3	A	550	NDP	P2B-O2X	2.20	1.62	1.54
3	B	550	NDP	P2B-O2X	2.24	1.62	1.54
3	B	550	NDP	C2N-C3N	2.30	1.40	1.34
2	A	500	FAD	C4-N3	2.30	1.37	1.33
2	A	500	FAD	C2A-N1A	2.32	1.38	1.33
3	A	550	NDP	O4D-C1D	2.35	1.47	1.42
5	A	650	TS8	O6-CAW	2.37	1.45	1.33
5	B	650	TS8	O6-CAW	2.43	1.46	1.33
2	B	500	FAD	C1'-N10	2.47	1.51	1.48
2	B	500	FAD	C4X-N5	2.49	1.37	1.33
2	A	500	FAD	C4X-N5	2.50	1.37	1.33
3	B	550	NDP	O4D-C1D	2.55	1.48	1.42
2	B	500	FAD	C4-N3	2.90	1.38	1.33
3	A	550	NDP	P2B-O1X	3.18	1.61	1.51
3	B	550	NDP	C6N-C5N	3.34	1.39	1.33
3	A	550	NDP	C6N-C5N	3.44	1.40	1.33
3	B	550	NDP	P2B-O1X	3.45	1.62	1.51
2	A	500	FAD	C2A-N3A	3.55	1.38	1.32
3	A	550	NDP	PA-O1A	3.59	1.64	1.51
3	A	550	NDP	PN-O1N	3.66	1.64	1.51
3	B	550	NDP	PA-O1A	3.78	1.65	1.51
3	B	550	NDP	PN-O1N	3.89	1.65	1.51
2	B	500	FAD	C2A-N3A	4.10	1.39	1.32
3	B	550	NDP	O4B-C1B	4.32	1.46	1.41
5	B	650	TS8	O4-CAX	4.61	1.45	1.35
3	A	550	NDP	O4B-C1B	4.78	1.47	1.41
5	A	650	TS8	O4-CAX	4.83	1.46	1.35
5	A	650	TS8	O2-CAY	4.93	1.46	1.35
5	B	650	TS8	O3-CAG	5.12	1.47	1.35
5	A	650	TS8	O3-CAG	5.17	1.47	1.35
5	B	650	TS8	O2-CAY	5.32	1.47	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FAD	N3A-C2A-N1A	-12.03	119.68	128.89
2	B	500	FAD	N3A-C2A-N1A	-11.95	119.74	128.89
3	A	550	NDP	N3A-C2A-N1A	-9.67	121.49	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	550	NDP	N3A-C2A-N1A	-9.61	121.54	128.89
2	A	500	FAD	P-O3P-PA	-4.22	120.89	132.73
2	B	500	FAD	P-O3P-PA	-4.18	120.99	132.73
5	A	650	TS8	C4-O4-CAX	-2.59	113.69	117.70
3	B	550	NDP	C2D-C1D-N1N	-2.54	106.47	113.34
3	A	550	NDP	C4A-C5A-N7A	-2.45	107.23	109.48
2	B	500	FAD	C4A-C5A-N7A	-2.42	107.25	109.48
3	B	550	NDP	C4A-C5A-N7A	-2.37	107.30	109.48
5	B	650	TS8	C4-O4-CAX	-2.32	114.10	117.70
5	A	650	TS8	O4-CAX-OAI	-2.28	118.36	122.92
5	B	650	TS8	O3-CAG-OAK	-2.28	118.36	122.92
5	B	650	TS8	O4-CAX-OAI	-2.21	118.51	122.92
3	A	550	NDP	PN-O3-PA	-2.19	126.59	132.73
2	A	500	FAD	C4A-C5A-N7A	-2.17	107.48	109.48
2	B	500	FAD	C4X-C10-N10	-2.16	119.25	120.52
2	A	500	FAD	C4X-C10-N10	-2.10	119.28	120.52
2	A	500	FAD	C2B-C1B-N9A	-2.09	111.10	114.29
2	B	500	FAD	C4X-C4-N3	-2.08	120.74	123.59
3	A	550	NDP	C2D-C1D-N1N	-2.07	107.75	113.34
3	B	550	NDP	C5B-C4B-C3B	-2.06	107.05	115.21
3	B	550	NDP	O2B-P2B-O1X	-2.02	102.06	107.11
5	A	650	TS8	C1-O5-C5	2.07	116.65	112.72
3	A	550	NDP	O3-PN-O5D	2.11	108.53	102.94
5	A	650	TS8	O6-C6-C5	2.15	113.16	108.48
5	B	650	TS8	O2-C2-C3	2.33	112.88	108.23
3	B	550	NDP	O3-PN-O5D	2.47	109.50	102.94
2	B	500	FAD	O4B-C1B-N9A	2.50	113.33	108.10
2	A	500	FAD	O4B-C1B-N9A	2.52	113.36	108.10
2	B	500	FAD	C5X-C9A-N10	2.57	119.58	117.62
5	A	650	TS8	O2-C2-C3	2.60	113.42	108.23
2	A	500	FAD	C5X-C9A-N10	2.67	119.65	117.62
5	A	650	TS8	O5-C5-C6	2.72	112.16	106.61
3	A	550	NDP	O4D-C1D-N1N	3.15	114.72	108.07
5	B	650	TS8	C1-O5-C5	3.20	118.80	112.72
5	A	650	TS8	O2-CAY-CAF	3.26	117.26	111.10
3	B	550	NDP	O4D-C1D-N1N	3.33	115.09	108.07
2	A	500	FAD	C4X-N5-C5X	3.40	120.68	116.76
2	B	500	FAD	C4X-N5-C5X	3.69	121.01	116.76
5	B	650	TS8	O4-CAX-CAE	3.82	118.31	111.10
5	B	650	TS8	O2-CAY-CAF	3.86	118.39	111.10
5	A	650	TS8	O4-CAX-CAE	4.62	119.82	111.10
5	A	650	TS8	O3-CAG-CAZ	4.71	119.99	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FAD	C4-N3-C2	4.85	119.44	115.25
2	B	500	FAD	C4-N3-C2	5.00	119.57	115.25
5	B	650	TS8	O3-CAG-CAZ	5.02	120.57	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	2	0
3	A	550	NDP	1	0
5	A	650	TS8	2	0
2	B	500	FAD	2	0
3	B	550	NDP	2	0
5	B	650	TS8	3	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^{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	488/511 (95%)	0.19	1 (0%)	95	93	63, 67, 69, 71	0
1	B	488/511 (95%)	0.16	1 (0%)	95	93	63, 67, 69, 71	0
All	All	976/1022 (95%)	0.17	2 (0%)	95	93	63, 67, 69, 71	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	LEU	2.5
1	B	10	LEU	2.1

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^{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
7	SO4	A	1490	5/5	0.80	0.42	1.35	59,59,59,60	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	SO4	B	1490	5/5	0.83	0.39	0.74	64,64,64,64	5
5	TS8	A	650	24/24	0.70	0.35	0.42	73,76,77,78	24
2	FAD	B	500	53/53	0.95	0.34	0.18	86,89,92,92	0
2	FAD	A	500	53/53	0.95	0.35	0.18	87,90,91,92	0
5	TS8	B	650	24/24	0.74	0.32	-0.09	77,79,80,80	24
3	NDP	A	550	48/48	0.91	0.27	-0.41	60,60,60,60	0
3	NDP	B	550	48/48	0.92	0.25	-0.60	60,60,60,60	0
4	AU	B	600	1/1	0.98	0.24	-0.73	78,78,78,78	1
4	AU	A	600	1/1	0.98	0.23	-0.94	78,78,78,78	1
6	CL	B	1489	1/1	0.96	0.19	-1.35	25,25,25,25	1
6	CL	A	1489	1/1	0.97	0.19	-1.42	30,30,30,30	1

6.5 Other polymers (i)

There are no such residues in this entry.