Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:08 AM GMT

PDB ID	:	3DH9
Title	:	Crystal Structure of Drosophila Thioredoxin Reductase, wild-type
Authors	:	Eckenroth, B.E.; Hondal, R.J.; Everse, SJ.
Deposited on	:	2008-06-17
Resolution	:	2.25 Å(reported)

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

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

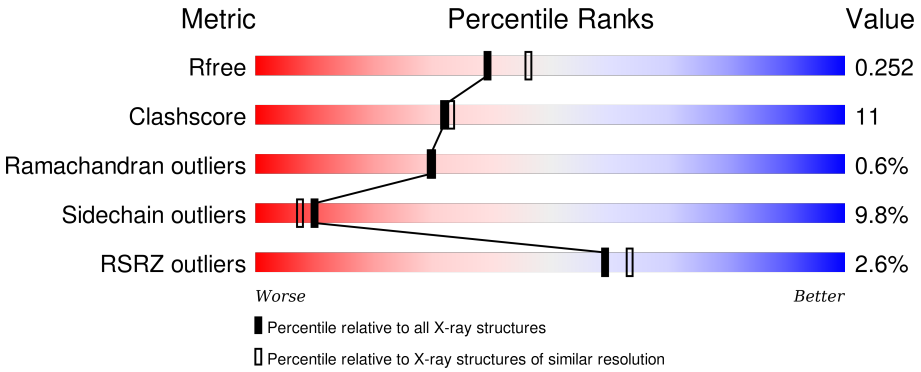
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	482	2% 75% 21% •
1	B	482	3% 76% 19% 5% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8002 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.

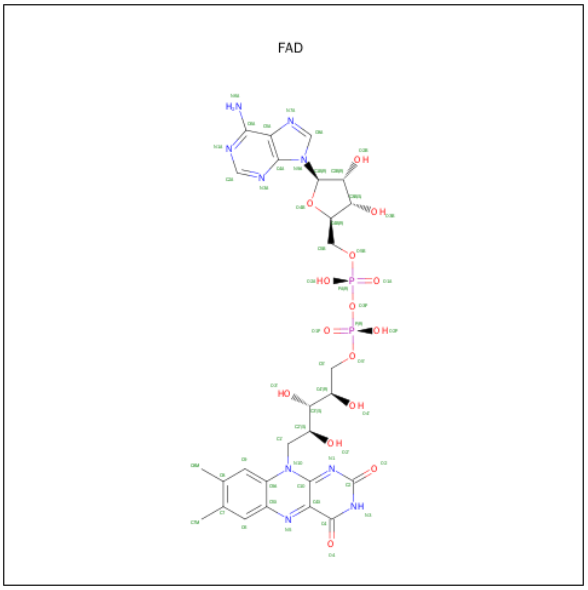
- Molecule 1 is a protein called Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3692	2354	627	699	12			
1	B	482	Total	C	N	O	S	0	0	0
			3692	2354	627	699	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLN	-	EXPRESSION TAG	UNP P91938
A	90	ASP	GLU	ENGINEERED	UNP P91938
A	274	SER	ALA	ENGINEERED	UNP P91938
B	5	GLN	-	EXPRESSION TAG	UNP P91938
B	90	ASP	GLU	ENGINEERED	UNP P91938
B	274	SER	ALA	ENGINEERED	UNP P91938

- 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 water.

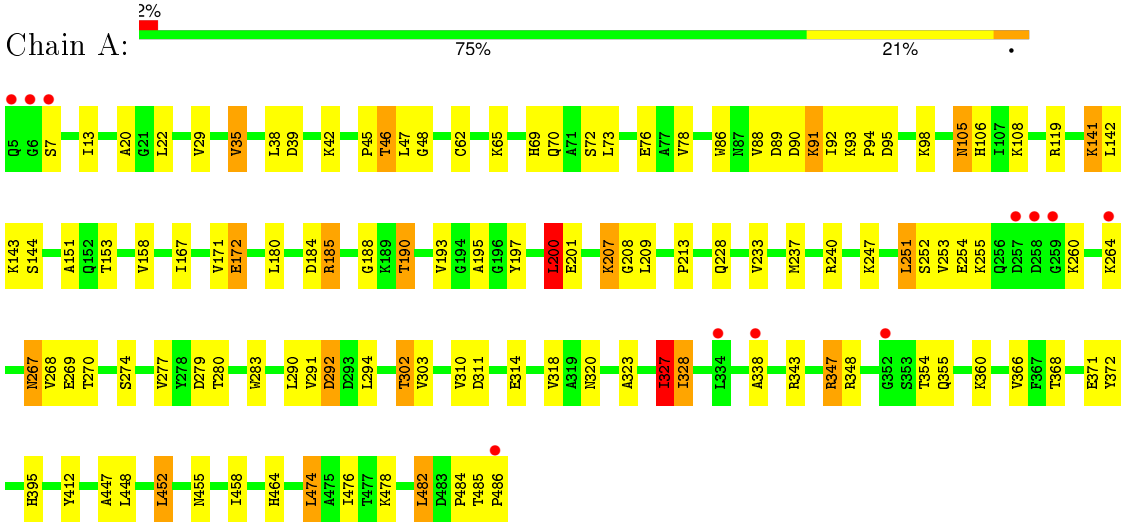
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total	O	0	0
			241	241		
3	B	271	Total	O	0	0
			271	271		

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.

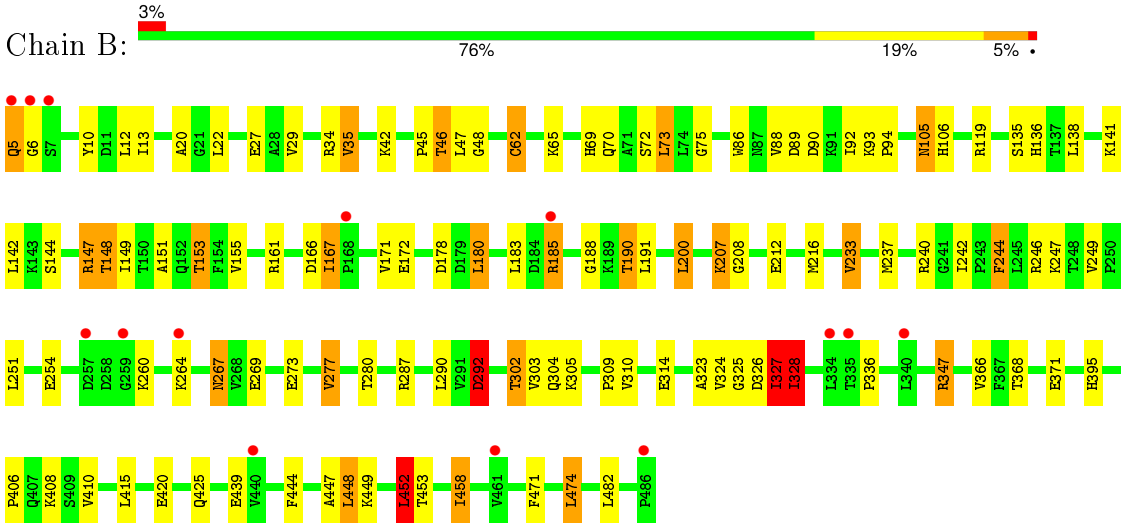
- Molecule 1: Thioredoxin reductase 1

Chain A:



- Molecule 1: Thioredoxin reductase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	150.97Å 150.97Å 267.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.17 – 2.25 31.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.17-2.25) 100.0 (31.18-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.92 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.177 , 0.248 0.186 , 0.252	Depositor DCC
R_{free} test set	5611 reflections (11.20%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 55706 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8002	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.45 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0368e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	1.07	7/3767 (0.2%)	0.98	10/5114 (0.2%)
1	B	1.12	7/3767 (0.2%)	1.01	18/5114 (0.4%)
All	All	1.09	14/7534 (0.2%)	1.00	28/10228 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	ASP	CB-CG	10.81	1.74	1.51
1	A	292	ASP	CB-CG	6.64	1.65	1.51
1	B	444	PHE	CE2-CZ	6.64	1.50	1.37
1	A	76	GLU	CD-OE1	6.37	1.32	1.25
1	A	91	LYS	CE-NZ	6.20	1.64	1.49
1	A	412	TYR	CD2-CE2	6.14	1.48	1.39
1	B	105	ASN	CB-CG	5.92	1.64	1.51
1	B	62	CYS	CB-SG	5.84	1.92	1.82
1	B	233	VAL	CB-CG1	5.76	1.65	1.52
1	B	410	VAL	CB-CG2	5.53	1.64	1.52
1	A	372	TYR	CD2-CE2	-5.52	1.31	1.39
1	A	105	ASN	CB-CG	5.29	1.63	1.51
1	B	439	GLU	CG-CD	5.29	1.59	1.51
1	A	254	GLU	CG-CD	5.09	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	347	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	246	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	B	292	ASP	CB-CG-OD2	8.03	125.52	118.30
1	B	327	ILE	CG1-CB-CG2	7.83	128.63	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	287	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	327	ILE	CB-CA-C	-6.92	97.75	111.60
1	B	327	ILE	CB-CA-C	-6.82	97.96	111.60
1	B	147	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	474	LEU	CB-CG-CD1	6.35	121.79	111.00
1	A	347	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	343	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	B	147	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	326	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	452	LEU	CA-CB-CG	6.19	129.54	115.30
1	B	73	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	328	ILE	CG1-CB-CG2	-6.02	98.15	111.40
1	A	39	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	200	LEU	CB-CG-CD1	5.67	120.65	111.00
1	A	482	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	246	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	180	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	482	LEU	CB-CG-CD1	5.25	119.93	111.00
1	A	184	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	200	LEU	CB-CG-CD1	5.17	119.79	111.00
1	B	178	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	448	LEU	CB-CG-CD1	-5.13	102.27	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3692	0	3710	84	2
1	B	3692	0	3710	79	3
2	A	53	0	31	1	0
2	B	53	0	30	0	0
3	A	241	0	0	15	0
3	B	271	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8002	0	7481	159	4

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 11.

All (159) 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:B:292:ASP:CG	1:B:292:ASP:CB	1.74	1.49
1:B:141:LYS:HB2	3:B:552:HOH:O	1.34	1.23
1:A:141:LYS:HD3	3:A:573:HOH:O	1.36	1.21
1:B:449:LYS:HD3	3:B:752:HOH:O	1.58	1.04
1:B:119:ARG:HD2	3:B:751:HOH:O	1.58	1.02
1:A:105:ASN:HB3	3:A:564:HOH:O	1.62	0.98
1:B:93:LYS:HD3	1:B:94:PRO:HD2	1.44	0.95
1:A:185:ARG:HG2	3:A:516:HOH:O	1.72	0.87
1:A:302:THR:HG22	3:A:700:HOH:O	1.77	0.84
1:A:141:LYS:HB3	1:A:141:LYS:NZ	1.93	0.82
1:B:153:THR:CG2	3:B:591:HOH:O	2.29	0.80
1:A:86:TRP:CE3	1:B:92:ILE:HD12	2.18	0.79
1:B:5:GLN:HG3	1:B:34:ARG:HH21	1.48	0.77
1:B:233:VAL:HG12	1:B:237:MET:HE1	1.67	0.77
1:B:149:ILE:HB	3:B:754:HOH:O	1.85	0.77
1:A:455:ASN:HB3	3:A:552:HOH:O	1.90	0.71
1:B:190:THR:HB	1:B:280:THR:HB	1.73	0.71
1:B:69:HIS:HD2	3:B:509:HOH:O	1.74	0.70
1:A:200:LEU:HG	1:A:237:MET:CE	2.22	0.70
1:A:29:VAL:CG2	1:A:35:VAL:HG13	2.21	0.70
1:A:190:THR:HB	1:A:280:THR:HB	1.72	0.70
1:B:10:TYR:HD1	3:B:754:HOH:O	1.75	0.69
1:B:166:ASP:O	1:B:167:ILE:HD12	1.91	0.69
1:A:233:VAL:HG12	1:A:237:MET:CE	2.24	0.68
1:A:29:VAL:CG2	1:A:35:VAL:CG1	2.71	0.68
1:B:93:LYS:HD3	1:B:94:PRO:CD	2.22	0.67
1:B:45:PRO:O	1:B:46:THR:O	2.12	0.67
1:A:119:ARG:HD2	3:A:710:HOH:O	1.96	0.66
1:B:188:GLY:O	1:B:190:THR:HG22	1.96	0.65
1:B:27:GLU:OE2	1:B:347:ARG:HD3	1.98	0.64
1:A:29:VAL:HG23	1:A:35:VAL:CG1	2.27	0.64
1:A:484:PRO:O	1:A:486:PRO:HD2	1.98	0.64
1:A:318:VAL:HG12	1:A:320:ASN:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HD12	1:B:86:TRP:CE3	2.35	0.62
1:A:323:ALA:O	1:A:328:ILE:HD11	2.00	0.61
1:B:267:ASN:HD22	1:B:269:GLU:H	1.46	0.61
1:A:29:VAL:HG23	1:A:35:VAL:HG11	1.83	0.60
1:B:5:GLN:CG	1:B:34:ARG:HH21	2.13	0.60
1:A:29:VAL:HG22	1:A:35:VAL:HG13	1.83	0.60
1:A:69:HIS:HD2	3:A:528:HOH:O	1.85	0.59
1:A:188:GLY:O	1:A:190:THR:HG22	2.03	0.58
1:B:136:HIS:HD2	1:B:151:ALA:O	1.87	0.58
1:B:147:ARG:HG2	1:B:149:ILE:HG23	1.86	0.58
1:A:233:VAL:HG12	1:A:237:MET:HE2	1.84	0.58
1:B:93:LYS:CD	1:B:94:PRO:HD2	2.27	0.57
1:A:29:VAL:HG22	1:A:35:VAL:CG1	2.34	0.57
1:A:323:ALA:HB1	1:A:327:ILE:HD13	1.85	0.57
1:B:69:HIS:HE1	1:B:371:GLU:OE1	1.88	0.56
1:B:303:VAL:CG1	1:B:305:LYS:O	2.54	0.56
1:B:292:ASP:HB3	3:B:630:HOH:O	2.04	0.56
1:A:46:THR:O	1:A:48:GLY:N	2.38	0.56
1:A:200:LEU:HG	1:A:237:MET:HE3	1.87	0.56
1:B:267:ASN:ND2	1:B:269:GLU:H	2.04	0.56
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.71	0.56
1:A:72:SER:OG	1:A:208:GLY:HA3	2.05	0.55
1:A:78:VAL:HG11	1:A:92:ILE:HD13	1.87	0.55
1:A:197:TYR:O	1:A:201:GLU:HG3	2.07	0.55
1:A:310:VAL:HG21	1:A:328:ILE:CD1	2.37	0.54
1:B:72:SER:OG	1:B:208:GLY:HA3	2.07	0.54
1:A:69:HIS:HE1	1:A:371:GLU:OE1	1.90	0.54
1:A:267:ASN:HD22	1:A:269:GLU:H	1.55	0.54
1:A:46:THR:O	1:A:47:LEU:HB2	2.06	0.54
1:B:327:ILE:HG13	3:B:501:HOH:O	2.06	0.54
1:B:207:LYS:HG3	1:B:242:ILE:HG12	1.90	0.54
1:A:20:ALA:HB2	1:A:338:ALA:HB1	1.90	0.53
1:B:303:VAL:CG1	1:B:304:GLN:N	2.72	0.52
1:A:247:LYS:O	1:A:268:VAL:HG12	2.08	0.52
1:B:323:ALA:HB1	1:B:327:ILE:HD13	1.92	0.52
1:A:185:ARG:HD2	3:A:706:HOH:O	2.10	0.52
1:A:141:LYS:CD	3:A:573:HOH:O	2.16	0.52
1:A:45:PRO:O	1:A:46:THR:CB	2.58	0.51
1:A:267:ASN:ND2	1:A:269:GLU:H	2.07	0.51
1:B:46:THR:O	1:B:48:GLY:N	2.43	0.51
1:B:447:ALA:HB1	1:B:452:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HB3	3:A:706:HOH:O	2.11	0.50
1:B:105:ASN:HB3	3:B:598:HOH:O	2.10	0.50
1:B:260:LYS:HB3	1:B:277:VAL:HG23	1.93	0.50
1:A:200:LEU:HG	1:A:237:MET:HE1	1.92	0.50
1:A:251:LEU:HB3	1:A:264:LYS:HG3	1.94	0.50
1:A:207:LYS:HD2	1:A:240:ARG:O	2.12	0.50
1:A:366:VAL:HG12	1:A:368:THR:HG23	1.93	0.49
1:A:89:ASP:OD2	1:A:90:ASP:N	2.45	0.49
1:A:46:THR:HA	3:A:665:HOH:O	2.12	0.49
1:B:46:THR:O	1:B:47:LEU:HB2	2.13	0.49
1:B:292:ASP:HB3	3:B:620:HOH:O	2.13	0.48
1:A:141:LYS:HB3	1:A:141:LYS:HZ2	1.76	0.48
1:B:147:ARG:O	1:B:148:THR:CB	2.62	0.48
1:A:95:ASP:HB3	1:A:98:LYS:HD2	1.96	0.48
1:B:65:LYS:HD2	1:B:65:LYS:C	2.34	0.48
1:B:191:LEU:HD11	1:B:216:MET:HE3	1.96	0.48
1:B:233:VAL:HG12	1:B:237:MET:CE	2.41	0.48
1:A:233:VAL:HG12	1:A:237:MET:HE1	1.94	0.47
1:A:447:ALA:HB1	1:A:452:LEU:HG	1.97	0.47
1:A:141:LYS:HB3	1:A:141:LYS:HZ1	1.79	0.47
1:A:172:GLU:H	1:A:172:GLU:CD	2.18	0.47
1:A:119:ARG:CD	3:A:710:HOH:O	2.58	0.47
1:B:42:LYS:HE3	3:B:685:HOH:O	2.14	0.46
1:B:240:ARG:NE	3:B:729:HOH:O	2.13	0.46
1:A:94:PRO:HG3	1:A:209:LEU:O	2.15	0.46
1:B:183:LEU:HD13	1:B:185:ARG:HD3	1.97	0.46
1:A:327:ILE:HG13	3:A:529:HOH:O	2.16	0.46
1:B:420:GLU:HB3	1:B:425:GLN:HA	1.97	0.46
1:A:185:ARG:CG	3:A:516:HOH:O	2.45	0.46
1:B:106:HIS:HE1	3:B:619:HOH:O	1.98	0.46
1:A:260:LYS:NZ	1:A:279:ASP:OD1	2.34	0.46
1:A:310:VAL:HG21	1:A:328:ILE:HD11	1.98	0.46
1:B:13:ILE:HD11	3:B:754:HOH:O	2.14	0.45
1:B:302:THR:HG22	3:B:673:HOH:O	2.15	0.45
1:B:89:ASP:OD2	1:B:90:ASP:N	2.49	0.45
1:B:29:VAL:HG22	1:B:35:VAL:HG13	1.99	0.45
1:B:153:THR:HG22	3:B:591:HOH:O	2.07	0.44
1:B:247:LYS:CB	1:B:269:GLU:HG3	2.46	0.44
1:B:20:ALA:HB1	1:B:324:VAL:HG13	1.99	0.44
1:A:484:PRO:O	1:A:486:PRO:CD	2.66	0.44
1:B:70:GLN:HA	1:B:70:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LYS:NZ	1:B:212:GLU:OE2	2.45	0.44
1:A:252:SER:OG	1:A:264:LYS:HG2	2.17	0.44
1:B:292:ASP:H	1:B:292:ASP:CG	2.21	0.44
1:A:464:HIS:HB2	1:B:336:PRO:HG3	2.00	0.44
1:A:158:VAL:HG11	1:A:294:LEU:HD21	2.00	0.43
1:A:38:LEU:N	1:A:38:LEU:HD12	2.33	0.43
1:A:291:VAL:HA	1:A:294:LEU:HD12	1.99	0.43
1:B:161:ARG:HG2	1:B:290:LEU:HD11	1.99	0.43
1:B:12:LEU:HD11	1:B:155:VAL:HG23	2.00	0.43
1:A:13:ILE:HG13	1:A:151:ALA:HB2	2.00	0.43
1:A:106:HIS:HE1	3:B:680:HOH:O	2.02	0.43
1:B:172:GLU:CD	1:B:172:GLU:H	2.22	0.43
1:B:327:ILE:HD12	1:B:328:ILE:N	2.33	0.43
1:B:247:LYS:HB3	1:B:269:GLU:HG3	2.01	0.42
1:B:323:ALA:HB1	1:B:327:ILE:CD1	2.49	0.42
1:A:290:LEU:HD12	2:A:500:FAD:H8A	2.01	0.42
1:B:406:PRO:HG2	1:B:408:LYS:HG3	2.00	0.42
1:A:193:VAL:HG21	1:A:283:TRP:CZ3	2.55	0.42
1:B:327:ILE:HG13	1:B:327:ILE:H	1.62	0.42
1:A:448:LEU:HD12	3:A:707:HOH:O	2.19	0.42
1:B:310:VAL:CG2	1:B:328:ILE:HG12	2.50	0.42
1:A:228:GLN:OE1	1:A:478:LYS:NZ	2.43	0.42
1:B:304:GLN:HB2	1:B:309:PRO:HG3	2.01	0.42
1:B:138:LEU:O	1:B:148:THR:HA	2.19	0.42
1:B:366:VAL:HG12	1:B:368:THR:HG23	2.01	0.42
1:A:311:ASP:C	1:A:311:ASP:OD1	2.59	0.42
1:A:267:ASN:C	1:A:267:ASN:HD22	2.22	0.41
1:B:10:TYR:CD1	3:B:754:HOH:O	2.57	0.41
1:A:267:ASN:HD22	1:A:268:VAL:N	2.19	0.41
1:B:458:ILE:HD11	1:B:474:LEU:O	2.20	0.41
1:A:86:TRP:CZ2	1:B:75:GLY:HA3	2.56	0.41
1:A:190:THR:O	1:A:213:PRO:HA	2.20	0.41
1:A:476:ILE:HD13	1:A:484:PRO:HA	2.03	0.41
1:B:244:PHE:CD2	1:B:244:PHE:N	2.89	0.41
1:A:195:ALA:HA	1:A:200:LEU:HD13	2.02	0.41
1:B:325:GLY:O	1:B:328:ILE:HB	2.21	0.41
1:A:348:ARG:HD3	1:A:355:GLN:O	2.21	0.41
1:A:310:VAL:HG21	1:A:328:ILE:HD13	2.03	0.41
1:A:45:PRO:O	1:A:46:THR:HB	2.21	0.40
1:B:452:LEU:HD22	1:B:453:THR:O	2.21	0.40
1:A:94:PRO:CB	3:B:763:HOH:O	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LEU:HD12	1:B:471:PHE:CD1	2.56	0.40
1:A:65:LYS:HD2	1:A:65:LYS:C	2.41	0.40
1:B:183:LEU:HD22	3:B:595:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:OD1	1:B:105:ASN:OD1[17_675]	1.40	0.80
1:A:105:ASN:OD1	1:A:105:ASN:OD1[12_765]	1.60	0.60
1:B:105:ASN:CG	1:B:105:ASN:OD1[17_675]	1.95	0.25
1:A:270:THR:O	1:B:135:SER:OG[18_765]	2.07	0.13

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	480/482 (100%)	458 (95%)	20 (4%)	2 (0%)	39	43
1	B	480/482 (100%)	461 (96%)	15 (3%)	4 (1%)	24	21
All	All	960/964 (100%)	919 (96%)	35 (4%)	6 (1%)	30	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	THR
1	A	7	SER
1	B	144	SER
1	B	148	THR
1	A	46	THR
1	B	6	GLY

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	392/392 (100%)	349 (89%)	43 (11%)	8 5
1	B	392/392 (100%)	358 (91%)	34 (9%)	13 11
All	All	784/784 (100%)	707 (90%)	77 (10%)	10 7

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	35	VAL
1	A	42	LYS
1	A	62	CYS
1	A	73	LEU
1	A	88	VAL
1	A	91	LYS
1	A	93	LYS
1	A	108	LYS
1	A	141	LYS
1	A	142	LEU
1	A	143	LYS
1	A	144	SER
1	A	153	THR
1	A	167	ILE
1	A	171	VAL
1	A	172	GLU
1	A	180	LEU
1	A	185	ARG
1	A	190	THR
1	A	200	LEU
1	A	207	LYS
1	A	251	LEU
1	A	253	VAL
1	A	255	LYS
1	A	267	ASN
1	A	274	SER

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Mol	Chain	Res	Type
1	A	277	VAL
1	A	292	ASP
1	A	302	THR
1	A	303	VAL
1	A	314	GLU
1	A	327	ILE
1	A	328	ILE
1	A	347	ARG
1	A	354	THR
1	A	360	LYS
1	A	395	HIS
1	A	452	LEU
1	A	458	ILE
1	A	474	LEU
1	A	482	LEU
1	A	485	THR
1	B	5	GLN
1	B	22	LEU
1	B	35	VAL
1	B	62	CYS
1	B	73	LEU
1	B	88	VAL
1	B	142	LEU
1	B	153	THR
1	B	167	ILE
1	B	171	VAL
1	B	180	LEU
1	B	185	ARG
1	B	190	THR
1	B	200	LEU
1	B	207	LYS
1	B	244	PHE
1	B	249	VAL
1	B	251	LEU
1	B	254	GLU
1	B	264	LYS
1	B	267	ASN
1	B	273	GLU
1	B	277	VAL
1	B	292	ASP
1	B	302	THR
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	327	ILE
1	B	328	ILE
1	B	395	HIS
1	B	448	LEU
1	B	452	LEU
1	B	458	ILE
1	B	474	LEU
1	B	482	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	69	HIS
1	A	70	GLN
1	A	106	HIS
1	A	227	GLN
1	A	256	GLN
1	A	267	ASN
1	A	298	ASN
1	A	355	GLN
1	A	425	GLN
1	B	31	ASN
1	B	69	HIS
1	B	70	GLN
1	B	106	HIS
1	B	111	ASN
1	B	136	HIS
1	B	267	ASN
1	B	298	ASN
1	B	355	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	FAD	A	500	-	48,58,58	1.26	4 (8%)	54,89,89	2.30	9 (16%)
2	FAD	B	500	-	48,58,58	1.44	8 (16%)	54,89,89	3.14	17 (31%)

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	FAD	A	500	-	-	0/30/50/50	0/6/6/6
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C3B-C4B	-2.20	1.47	1.53
2	B	500	FAD	O5B-C5B	-2.16	1.36	1.44
2	A	500	FAD	C2A-N3A	2.11	1.35	1.32
2	B	500	FAD	C1'-N10	2.20	1.50	1.48
2	B	500	FAD	C4-N3	2.39	1.37	1.33
2	A	500	FAD	C5X-N5	2.42	1.39	1.35
2	B	500	FAD	C5X-N5	2.78	1.39	1.35
2	B	500	FAD	C9A-N10	3.12	1.43	1.38
2	B	500	FAD	C2A-N3A	3.12	1.37	1.32
2	A	500	FAD	C4-N3	3.90	1.40	1.33
2	A	500	FAD	C4X-N5	3.94	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C4X-N5	4.15	1.39	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	FAD	N3A-C2A-N1A	-14.82	117.55	128.89
2	A	500	FAD	N3A-C2A-N1A	-12.88	119.03	128.89
2	B	500	FAD	C4B-O4B-C1B	-7.73	101.22	109.72
2	B	500	FAD	O3B-C3B-C4B	-5.42	94.79	111.05
2	A	500	FAD	C4X-C4-N3	-3.27	119.12	123.59
2	B	500	FAD	C4X-C4-N3	-3.22	119.19	123.59
2	B	500	FAD	C9A-C5X-N5	-2.94	118.01	122.36
2	B	500	FAD	C4-C4X-C10	-2.90	118.08	119.94
2	B	500	FAD	O5B-PA-O1A	-2.89	98.39	109.62
2	B	500	FAD	C2B-C1B-N9A	-2.76	110.08	114.29
2	B	500	FAD	C4A-C5A-N7A	-2.48	107.20	109.48
2	A	500	FAD	C1B-N9A-C4A	-2.36	123.38	126.94
2	B	500	FAD	C4-C4X-N5	2.04	121.20	118.72
2	A	500	FAD	O2A-PA-O3P	2.06	114.44	105.09
2	B	500	FAD	O5B-C5B-C4B	2.21	117.27	109.12
2	B	500	FAD	C2A-N1A-C6A	2.26	122.81	118.77
2	A	500	FAD	O2'-C2'-C3'	2.32	114.86	109.02
2	A	500	FAD	C4X-N5-C5X	2.79	119.97	116.76
2	A	500	FAD	C4-C4X-N5	3.05	122.42	118.72
2	A	500	FAD	C2A-N1A-C6A	3.36	124.77	118.77
2	B	500	FAD	C4X-N5-C5X	3.64	120.95	116.76
2	B	500	FAD	O2A-PA-O5B	4.16	129.46	108.46
2	B	500	FAD	C5X-C9A-N10	4.59	121.11	117.62
2	B	500	FAD	O4B-C4B-C5B	4.94	127.00	109.32
2	A	500	FAD	C4-N3-C2	5.71	120.18	115.25
2	B	500	FAD	C4-N3-C2	6.99	121.29	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	482/482 (100%)	0.10	11 (2%)	64	68	2, 14, 25, 46	0
1	B	482/482 (100%)	-0.00	14 (2%)	55	60	2, 13, 25, 49	0
All	All	964/964 (100%)	0.05	25 (2%)	59	63	2, 14, 25, 49	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLN	8.1
1	A	6	GLY	6.0
1	A	486	PRO	5.1
1	B	5	GLN	4.8
1	B	6	GLY	4.6
1	A	334	LEU	3.6
1	A	259	GLY	3.6
1	A	7	SER	3.5
1	B	7	SER	3.4
1	B	334	LEU	3.4
1	B	486	PRO	3.2
1	A	338	ALA	3.2
1	A	258	ASP	3.1
1	B	259	GLY	3.0
1	A	257	ASP	2.7
1	B	257	ASP	2.4
1	A	352	GLY	2.4
1	B	264	LYS	2.4
1	A	264	LYS	2.3
1	B	168	PRO	2.2
1	B	440	VAL	2.2
1	B	185	ARG	2.2
1	B	461	VAL	2.1
1	B	335	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	B	500	53/53	0.96	0.19	0.95	2,4,8,11	0
2	FAD	A	500	53/53	0.96	0.16	-0.03	2,5,8,11	0

6.5 Other polymers (i)

There are no such residues in this entry.