



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:38 pm GMT

PDB ID : 2X8C  
Title : THIOREDOXIN GLUTATHIONE REDUCTASE FROM SCHISTOSOMA  
MANSONI WITH THE REDUCED C-TERMINAL END  
Authors : Angelucci, F.; Dimastrogiovanni, D.; Boumis, G.; Brunori, M.; Miele, A.E.;  
Saccoccia, F.; Bellelli, A.  
Deposited on : 2010-03-08  
Resolution : 3.10 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

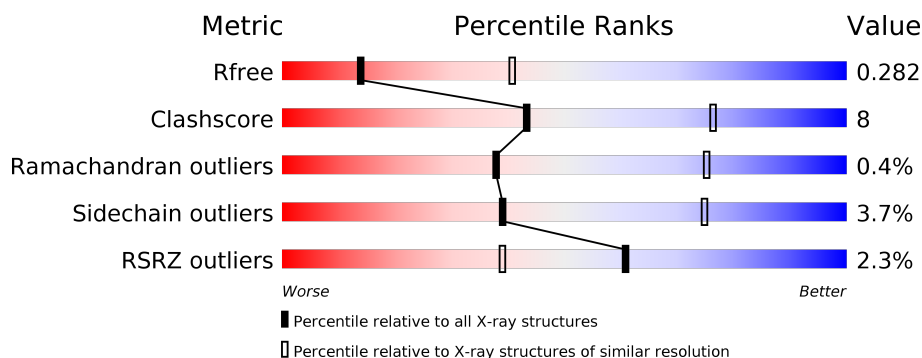
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	598	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	598	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9176 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 GLUTATHIONE REDUCTASE.

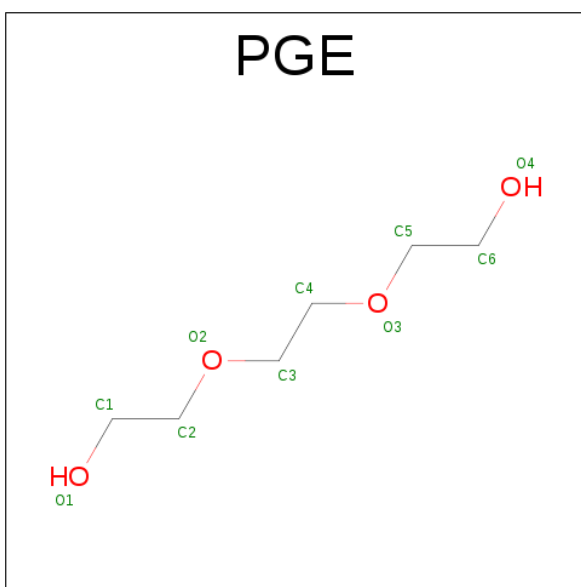
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4503	2859	759	863	22			
1	B	593	Total	C	N	O	S	0	0	0
			4530	2872	764	870	24			

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



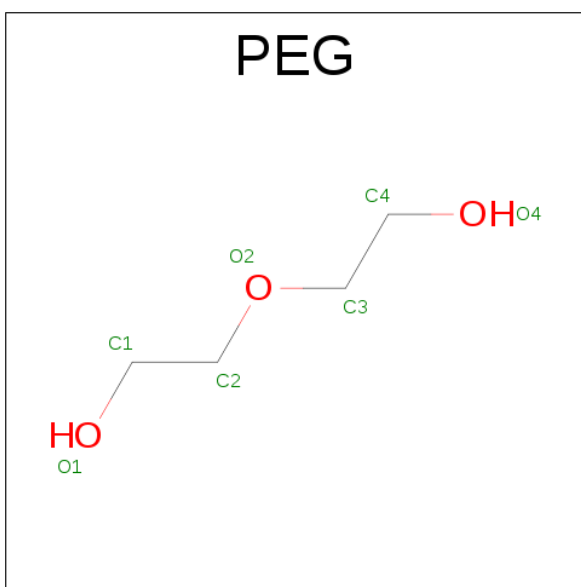
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

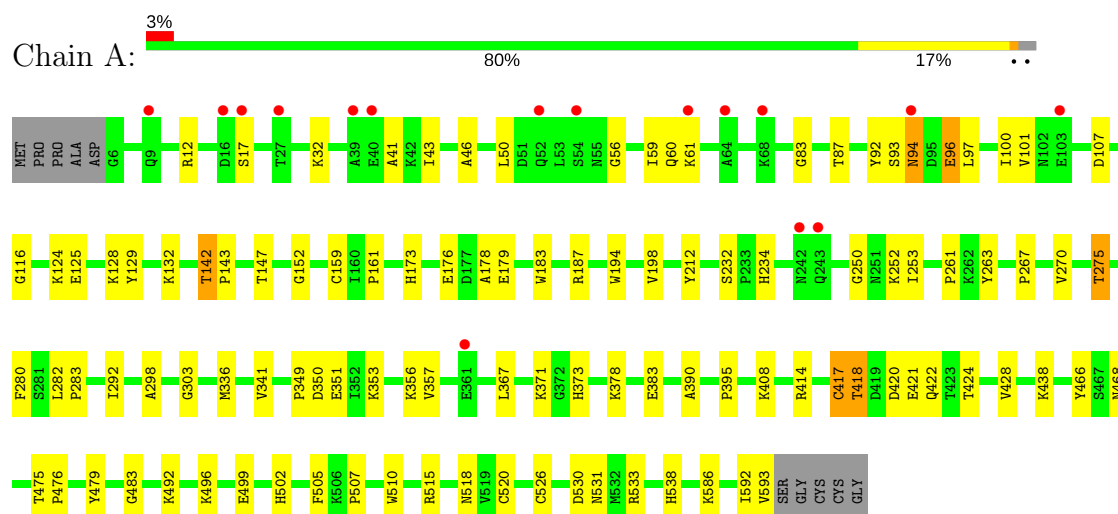


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

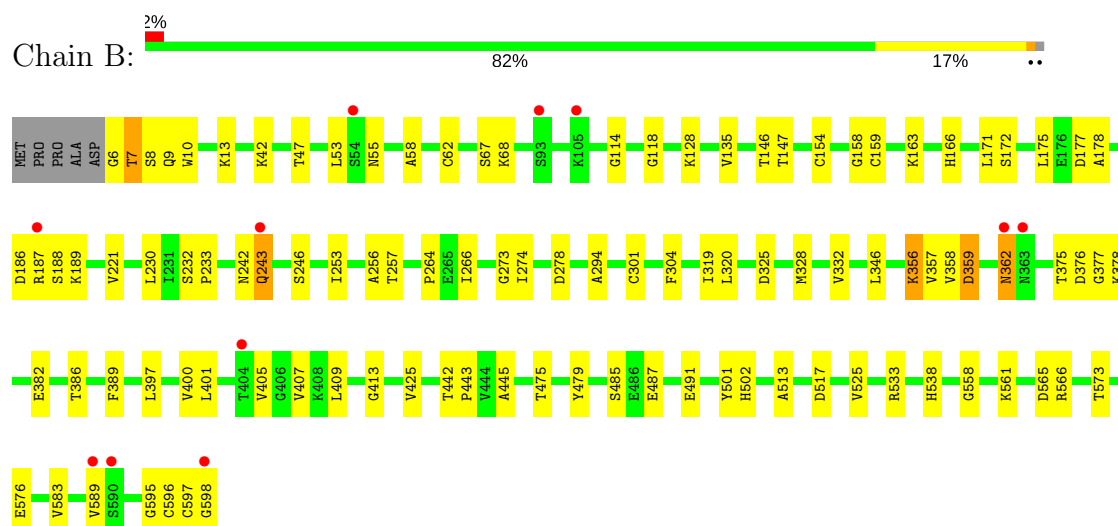
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 GLUTATHIONE REDUCTASE



#### • Molecule 1: THIOREDOXIN GLUTATHIONE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.49Å 87.45Å 185.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.76 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (92.76-3.10) 99.6 (19.97-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.216 , 0.293 0.213 , 0.282	Depositor DCC
$R_{free}$ test set	1298 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, 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	0.50	3/4590 (0.1%)	0.59	0/6218
1	B	0.47	2/4617 (0.0%)	0.60	0/6252
All	All	0.48	5/9207 (0.1%)	0.59	0/12470

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	417	CYS	CB-SG	-8.86	1.67	1.82
1	A	418	THR	C-N	7.95	1.52	1.34
1	B	596	CYS	CB-SG	-6.37	1.71	1.82
1	B	178	ALA	C-N	-5.47	1.21	1.34
1	A	179	GLU	CG-CD	5.22	1.59	1.51

There are no bond angle outliers.

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	4503	0	4520	65	0
1	B	4530	0	4541	84	0
2	A	53	0	31	0	0
2	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	28	0	0
3	B	10	0	14	2	0
4	A	7	0	10	1	0
All	All	9176	0	9175	141	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 8.

All (141) 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:175:LEU:CD1	1:B:187:ARG:NH1	2.21	1.02
1:A:56:GLY:O	1:A:59:ILE:HG13	1.71	0.91
1:B:7:THR:HG23	1:B:55:ASN:HD22	1.36	0.91
1:B:175:LEU:HD13	1:B:187:ARG:NH1	1.85	0.90
1:B:595:GLY:C	1:B:597:CYS:H	1.74	0.89
1:B:175:LEU:HD12	1:B:187:ARG:CZ	2.04	0.88
1:B:175:LEU:HD12	1:B:187:ARG:NH1	1.88	0.87
1:A:50:LEU:HD13	1:A:59:ILE:HD13	1.60	0.83
1:B:189:LYS:NZ	1:B:189:LYS:HB2	1.93	0.83
1:A:59:ILE:HD12	1:A:60:GLN:H	1.41	0.83
1:B:7:THR:HG23	1:B:55:ASN:ND2	1.94	0.81
1:B:533:ARG:NH1	1:B:558:GLY:O	2.13	0.80
1:B:172:SER:HA	1:B:187:ARG:NH2	1.97	0.80
1:B:595:GLY:C	1:B:597:CYS:N	2.39	0.75
1:A:46:ALA:HB2	1:A:129:TYR:HB3	1.70	0.74
1:A:50:LEU:HD22	1:A:59:ILE:HG12	1.70	0.74
1:B:175:LEU:HD13	1:B:187:ARG:HH11	1.52	0.73
1:B:377:GLY:O	1:B:378:LYS:C	2.26	0.73
1:A:420:ASP:C	1:A:421:GLU:OE1	2.30	0.70
1:B:175:LEU:HB3	1:B:187:ARG:HD3	1.75	0.69
1:B:189:LYS:HZ2	1:B:189:LYS:HB2	1.55	0.68
1:A:261:PRO:HB2	1:A:275:THR:HG21	1.76	0.67
1:B:595:GLY:O	1:B:597:CYS:N	2.21	0.67
1:A:59:ILE:HD12	1:A:60:GLN:N	2.10	0.67
1:A:530:ASP:O	1:A:531:ASN:HB2	1.96	0.66
1:B:376:ASP:OD1	1:B:377:GLY:N	2.29	0.66
1:B:397:LEU:HD12	1:B:413:GLY:O	1.96	0.65
1:B:6:GLY:O	1:B:9:GLN:N	2.29	0.65
1:A:499:GLU:OE1	1:A:586:LYS:HE2	1.96	0.65
1:A:176:GLU:HG2	1:A:187:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HD2	1:B:598:GLY:OXT	1.97	0.64
1:A:421:GLU:OE1	1:A:421:GLU:N	2.30	0.64
1:A:183:TRP:CH2	1:B:187:ARG:NH2	2.65	0.63
1:B:172:SER:OG	1:B:187:ARG:NH2	2.31	0.62
1:B:401:LEU:HD21	1:B:407:VAL:HB	1.81	0.62
1:B:189:LYS:NZ	1:B:189:LYS:CB	2.64	0.61
1:A:43:ILE:HD12	1:A:101:VAL:HG21	1.83	0.61
1:A:468:ASN:HD22	1:A:483:GLY:HA2	1.64	0.61
1:B:187:ARG:O	1:B:187:ARG:HG3	1.99	0.61
1:A:395:PRO:HG3	1:A:414:ARG:HG2	1.82	0.60
1:B:175:LEU:CB	1:B:187:ARG:HD3	2.31	0.60
1:B:128:LYS:HE2	1:B:128:LYS:HA	1.82	0.60
1:B:573:THR:O	1:B:576:GLU:HG2	2.01	0.60
1:A:479:TYR:OH	1:A:538:HIS:HD2	1.85	0.60
1:B:320:LEU:HG	3:B:1600:PGE:H32	1.83	0.60
1:A:183:TRP:CZ3	1:B:187:ARG:NH2	2.70	0.60
1:B:301:CYS:HA	1:B:304:PHE:CE1	2.37	0.59
1:A:420:ASP:OD1	1:A:422:GLN:HB3	2.02	0.59
1:A:50:LEU:HD13	1:A:59:ILE:CD1	2.32	0.59
1:B:346:LEU:HB3	1:B:375:THR:HB	1.85	0.58
1:A:183:TRP:CE3	1:B:187:ARG:NH1	2.62	0.58
1:A:142:THR:HG22	1:A:143:PRO:HD2	1.85	0.58
1:A:178:ALA:HA	1:B:171:LEU:HD13	1.85	0.57
1:B:257:THR:HG21	1:B:400:VAL:HG11	1.86	0.57
1:A:356:LYS:HB3	1:A:367:LEU:H	1.69	0.57
1:A:417:CYS:C	1:A:418:THR:O	2.39	0.57
1:B:175:LEU:CD1	1:B:187:ARG:CZ	2.75	0.56
1:B:479:TYR:OH	1:B:538:HIS:HD2	1.88	0.56
1:A:94:ASN:ND2	1:A:96:GLU:HB2	2.20	0.56
1:B:356:LYS:HE2	1:B:357:VAL:H	1.71	0.56
1:B:376:ASP:OD1	1:B:378:LYS:HG3	2.07	0.54
1:B:67:SER:O	1:B:68:LYS:HB2	2.09	0.53
1:B:273:GLY:HA3	1:B:389:PHE:HE2	1.74	0.53
1:A:253:ILE:HB	1:A:428:VAL:HG22	1.91	0.53
1:A:505:PHE:O	1:A:520:CYS:HB2	2.08	0.53
1:A:97:LEU:HA	1:A:100:ILE:HG22	1.91	0.52
1:A:492:LYS:HG2	4:A:1597:PEG:H21	1.90	0.52
1:B:6:GLY:O	1:B:7:THR:C	2.48	0.51
1:B:401:LEU:HD11	1:B:407:VAL:HG21	1.93	0.51
1:B:114:GLY:HA3	1:B:256:ALA:O	2.09	0.51
1:B:325:ASP:HB2	1:B:485:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLY:HA2	1:A:152:GLY:HA3	1.93	0.50
1:B:397:LEU:HD13	1:B:409:LEU:HD22	1.93	0.50
1:A:183:TRP:CZ3	1:B:187:ARG:NH1	2.80	0.50
1:B:10:TRP:O	1:B:13:LYS:N	2.44	0.49
1:B:359:ASP:CG	1:B:362:ASN:HB2	2.33	0.49
1:B:6:GLY:O	1:B:8:SER:N	2.45	0.49
1:A:298:ALA:HB2	1:A:390:ALA:HB3	1.93	0.49
1:B:264:PRO:HB2	1:B:266:ILE:HG12	1.94	0.49
1:A:212:TYR:CD1	1:B:598:GLY:HA2	2.48	0.49
1:B:172:SER:CA	1:B:187:ARG:NH2	2.71	0.49
1:B:442:THR:HB	1:B:443:PRO:HD3	1.93	0.49
1:B:154:CYS:HA	1:B:158:GLY:HA3	1.95	0.48
1:A:418:THR:OG1	1:A:420:ASP:OD1	2.29	0.48
1:A:292:ILE:HG21	1:A:349:PRO:HG3	1.95	0.47
1:B:376:ASP:OD1	1:B:378:LYS:N	2.42	0.47
1:B:294:ALA:HB1	1:B:320:LEU:HA	1.96	0.47
1:A:125:GLU:O	1:A:128:LYS:HB2	2.14	0.47
1:A:234:HIS:HD2	1:A:250:GLY:O	1.96	0.47
1:B:189:LYS:HZ3	1:B:189:LYS:CB	2.28	0.47
1:A:438:LYS:HD2	1:A:466:TYR:CG	2.49	0.47
1:B:501:TYR:CD1	1:B:561:LYS:HE3	2.49	0.47
1:B:230:LEU:HD13	1:B:253:ILE:HG21	1.97	0.46
1:B:42:LYS:HE2	1:B:42:LYS:HA	1.96	0.46
1:A:336:MET:HE2	1:A:341:VAL:HG11	1.97	0.46
1:B:163:LYS:HA	1:B:166:HIS:HB3	1.97	0.45
1:A:267:PRO:HG2	1:A:351:GLU:HB2	1.98	0.45
1:B:135:VAL:HG23	1:B:221:VAL:HG11	1.98	0.45
1:B:405:VAL:HG12	1:B:425:VAL:HG21	1.99	0.45
1:A:232:SER:O	1:A:234:HIS:N	2.50	0.45
1:A:507:PRO:O	1:A:510:TRP:HB2	2.17	0.45
1:A:267:PRO:HG2	1:A:351:GLU:CB	2.47	0.44
1:B:325:ASP:CB	1:B:485:SER:HB2	2.47	0.44
1:B:359:ASP:OD1	1:B:362:ASN:HB2	2.18	0.44
1:A:212:TYR:CE1	1:B:598:GLY:HA2	2.52	0.44
1:A:303:GLY:HA3	1:A:476:PRO:HD3	1.99	0.44
1:B:400:VAL:HG22	2:B:1599:FAD:H61A	1.83	0.44
1:A:356:LYS:HE2	1:A:367:LEU:HD23	2.00	0.44
1:A:173:HIS:HB3	1:A:515:ARG:NH2	2.33	0.44
1:A:263:TYR:CE1	1:A:270:VAL:HA	2.53	0.43
1:B:189:LYS:HZ3	1:B:189:LYS:HB2	1.77	0.43
1:A:518:ASN:OD1	1:A:592:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:HB2	1:A:280:PHE:CD1	2.53	0.43
1:B:58:ALA:O	1:B:62:CYS:HB2	2.19	0.42
1:B:186:ASP:C	1:B:188:SER:N	2.73	0.42
1:A:17:SER:OG	1:A:252:LYS:HE3	2.20	0.42
1:A:350:ASP:OD2	1:A:373:HIS:HD2	2.02	0.42
1:B:561:LYS:NZ	1:B:565:ASP:OD1	2.52	0.42
1:B:118:GLY:HA2	1:B:445:ALA:O	2.19	0.42
1:B:328:MET:O	1:B:332:VAL:HG23	2.18	0.42
1:A:282:LEU:HA	1:A:283:PRO:HD3	1.85	0.42
1:A:420:ASP:OD1	1:A:422:GLN:CB	2.67	0.42
1:A:41:ALA:HB2	1:A:92:TYR:HE1	1.85	0.41
1:A:194:TRP:NE1	1:A:198:VAL:HG21	2.34	0.41
1:A:408:LYS:HB2	1:A:424:THR:HG21	2.03	0.41
1:B:400:VAL:HG22	2:B:1599:FAD:N6A	2.35	0.41
1:B:6:GLY:C	1:B:8:SER:N	2.72	0.41
1:A:526:CYS:HA	1:A:533:ARG:O	2.21	0.41
1:B:377:GLY:O	1:B:378:LYS:O	2.38	0.41
1:B:177:ASP:OD1	1:B:513:ALA:HB1	2.21	0.41
1:A:353:LYS:HE2	1:A:371:LYS:HD2	2.03	0.41
1:B:319:ILE:HA	3:B:1600:PGE:H22	2.02	0.41
1:A:475:THR:HB	1:A:476:PRO:HD2	2.03	0.41
1:A:438:LYS:HD2	1:A:466:TYR:CD2	2.56	0.40
1:A:479:TYR:OH	1:A:538:HIS:CD2	2.70	0.40
1:A:83:GLY:HA3	1:A:87:THR:HB	2.03	0.40
1:B:274:ILE:HB	1:B:278:ASP:HB2	2.03	0.40
1:B:376:ASP:OD2	1:B:378:LYS:HE3	2.21	0.40
1:B:583:VAL:HG13	1:B:589:VAL:HB	2.03	0.40
1:B:346:LEU:HD13	1:B:375:THR:HG21	2.02	0.40
1:B:487:GLU:O	1:B:491:GLU: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	586/598 (98%)	545 (93%)	41 (7%)	0	100	100
1	B	591/598 (99%)	535 (90%)	51 (9%)	5 (1%)	22	62
All	All	1177/1196 (98%)	1080 (92%)	92 (8%)	5 (0%)	38	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	THR
1	B	243	GLN
1	B	233	PRO
1	B	359	ASP
1	B	358	VAL

### 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	489/496 (99%)	471 (96%)	18 (4%)	39	75
1	B	492/496 (99%)	474 (96%)	18 (4%)	39	75
All	All	981/992 (99%)	945 (96%)	36 (4%)	39	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	32	LYS
1	A	61	LYS
1	A	93	SER
1	A	94	ASN
1	A	96	GLU
1	A	107	ASP
1	A	132	LYS
1	A	142	THR
1	A	147	THR
1	A	159	CYS

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Mol	Chain	Res	Type
1	A	275	THR
1	A	357	VAL
1	A	378	LYS
1	A	383	GLU
1	A	496	LYS
1	A	502	HIS
1	A	593	VAL
1	B	47	THR
1	B	53	LEU
1	B	146	THR
1	B	147	THR
1	B	159	CYS
1	B	232	SER
1	B	242	ASN
1	B	243	GLN
1	B	246	SER
1	B	356	LYS
1	B	362	ASN
1	B	382	GLU
1	B	386	THR
1	B	475	THR
1	B	502	HIS
1	B	517	ASP
1	B	525	VAL
1	B	566	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	192	HIS
1	A	209	ASN
1	A	219	ASN
1	A	234	HIS
1	A	326	GLN
1	A	339	HIS
1	A	373	HIS
1	A	468	ASN
1	A	538	HIS
1	B	52	GLN
1	B	94	ASN
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	209	ASN
1	B	243	GLN
1	B	326	GLN
1	B	362	ASN
1	B	373	HIS
1	B	468	ASN
1	B	504	ASN
1	B	538	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](#)

6 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	$\# Z  > 2$
3	PGE	A	1595	-	9,9,9	0.62	0	8,8,8	0.32	0
3	PGE	A	1596	-	9,9,9	0.60	0	8,8,8	0.23	0
4	PEG	A	1597	-	6,6,6	0.52	0	5,5,5	0.28	0
2	FAD	A	1599	-	51,58,58	1.39	6 (11%)	54,89,89	2.04	6 (11%)
2	FAD	B	1599	-	51,58,58	1.38	7 (13%)	54,89,89	1.94	5 (9%)
3	PGE	B	1600	-	9,9,9	0.54	0	8,8,8	0.20	0

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
3	PGE	A	1595	-	-	0/7/7/7	0/0/0/0
3	PGE	A	1596	-	-	0/7/7/7	0/0/0/0
4	PEG	A	1597	-	-	0/4/4/4	0/0/0/0
2	FAD	A	1599	-	-	0/28/50/50	0/6/6/6
2	FAD	B	1599	-	-	0/28/50/50	0/6/6/6
3	PGE	B	1600	-	-	0/7/7/7	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1599	FAD	C1'-N10	2.02	1.50	1.48
2	B	1599	FAD	C5X-N5	2.06	1.38	1.35
2	A	1599	FAD	C2A-N1A	2.63	1.38	1.33
2	B	1599	FAD	C4-N3	2.70	1.37	1.33
2	B	1599	FAD	C2A-N1A	2.70	1.39	1.33
2	A	1599	FAD	C1'-N10	2.89	1.51	1.48
2	A	1599	FAD	C4X-N5	3.07	1.37	1.33
2	A	1599	FAD	C4-N3	3.34	1.39	1.33
2	A	1599	FAD	C2A-N3A	3.57	1.38	1.32
2	B	1599	FAD	C4X-N5	4.01	1.39	1.33
2	B	1599	FAD	C2A-N3A	4.02	1.38	1.32
2	B	1599	FAD	C10-N1	4.43	1.39	1.33
2	A	1599	FAD	C10-N1	4.73	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1599	FAD	N3A-C2A-N1A	-10.54	119.68	128.86
2	A	1599	FAD	N3A-C2A-N1A	-10.05	120.11	128.86
2	A	1599	FAD	C4X-C4-N3	-3.12	119.04	123.48
2	B	1599	FAD	C4X-C4-N3	-2.17	120.39	123.48
2	A	1599	FAD	C1'-N10-C10	2.59	121.16	118.50
2	B	1599	FAD	C5X-C9A-N10	2.95	119.84	117.66
2	A	1599	FAD	C5X-C9A-N10	3.31	120.12	117.66
2	A	1599	FAD	C4X-N5-C5X	3.75	120.72	116.76
2	B	1599	FAD	C4X-N5-C5X	3.90	120.88	116.76
2	B	1599	FAD	C4-N3-C2	5.71	120.15	115.16
2	A	1599	FAD	C4-N3-C2	7.01	121.29	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1597	PEG	1	0
2	B	1599	FAD	2	0
3	B	1600	PGE	2	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	588/598 (98%)	-0.23	16 (2%) 55 30	11, 33, 92, 99	0
1	B	593/598 (99%)	-0.14	11 (1%) 67 46	19, 45, 67, 72	0
All	All	1181/1196 (98%)	-0.18	27 (2%) 61 39	11, 40, 87, 99	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	THR	5.2
1	A	52	GLN	3.5
1	B	404	THR	3.2
1	B	363	ASN	3.1
1	B	187	ARG	3.1
1	A	39	ALA	3.0
1	A	64	ALA	3.0
1	A	94	ASN	2.9
1	B	243	GLN	2.8
1	A	40	GLU	2.8
1	A	61	LYS	2.7
1	B	93	SER	2.7
1	B	105	LYS	2.6
1	B	362	ASN	2.6
1	A	9	GLN	2.5
1	B	54	SER	2.5
1	A	243	GLN	2.4
1	A	242	ASN	2.4
1	A	16	ASP	2.3
1	A	103	GLU	2.2
1	A	17	SER	2.1
1	A	68	LYS	2.1
1	B	590	SER	2.0
1	A	54	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	598	GLY	2.0
1	B	589	VAL	2.0
1	A	361	GLU	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<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
3	PGE	A	1596	10/10	0.91	0.23	1.66	34,38,39,39	0
3	PGE	A	1595	10/10	0.95	0.16	-0.07	17,21,23,23	0
2	FAD	B	1599	53/53	0.95	0.17	-0.33	35,38,51,51	0
2	FAD	A	1599	53/53	0.96	0.14	-0.43	16,22,29,29	0
3	PGE	B	1600	10/10	0.94	0.17	-1.04	39,41,42,43	0
4	PEG	A	1597	7/7	0.86	0.31	-	48,49,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.