



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 PM GMT

PDB ID : 4KPR  
Title : Tetrameric form of rat selenoprotein thioredoxin reductase 1  
Authors : Lindqvist, Y.; Sandalova, T.; Xu, J.; Arner, E.  
Deposited on : 2013-05-14  
Resolution : 2.40 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

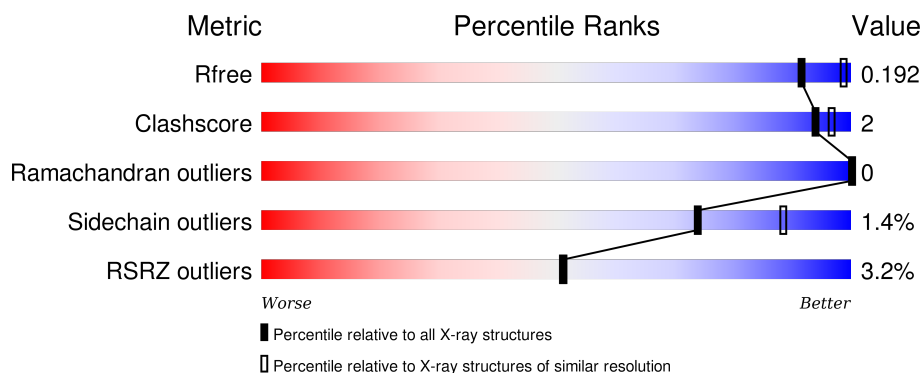
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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	499	<div> <div>12%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	B	499	<div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	E	499	<div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	F	499	<div> <div>89%</div> <div>8%</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
2	SO3	F	501	-	-	-	X
2	SO3	F	502	-	-	-	X
3	MPD	A	501	-	-	-	X
3	MPD	B	501	-	-	-	X
3	MPD	E	502	-	-	-	X
3	MPD	E	504	-	-	-	X
3	MPD	F	503	-	-	-	X
3	MPD	F	504	-	-	-	X
4	FAD	E	505	-	-	-	X
4	FAD	F	505	-	-	-	X

## 2 Entry composition [i](#)

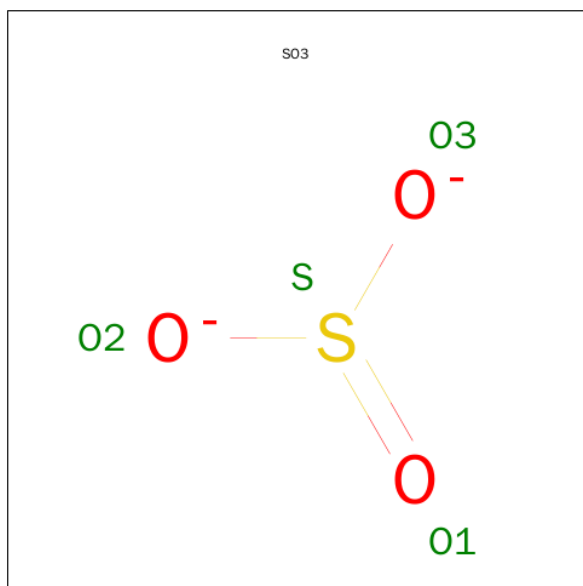
There are 5 unique types of molecules in this entry. The entry contains 15853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	484	Total	C	N	O	S	0	1	0
			3737	2378	631	708	20			
1	F	485	Total	C	N	O	S	0	6	0
			3787	2413	639	715	20			
1	A	484	Total	C	N	O	S	0	1	0
			3741	2381	632	708	20			
1	B	484	Total	C	N	O	S	0	5	0
			3768	2400	636	712	20			

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



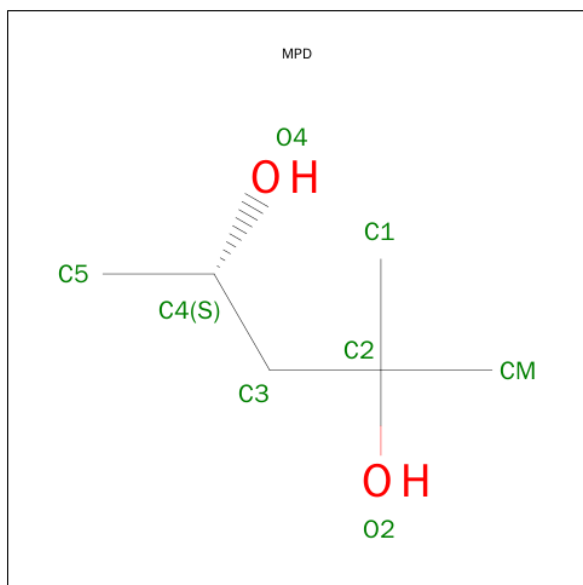
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			4	3	1		
2	F	1	Total	O	S	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			4	3	1		

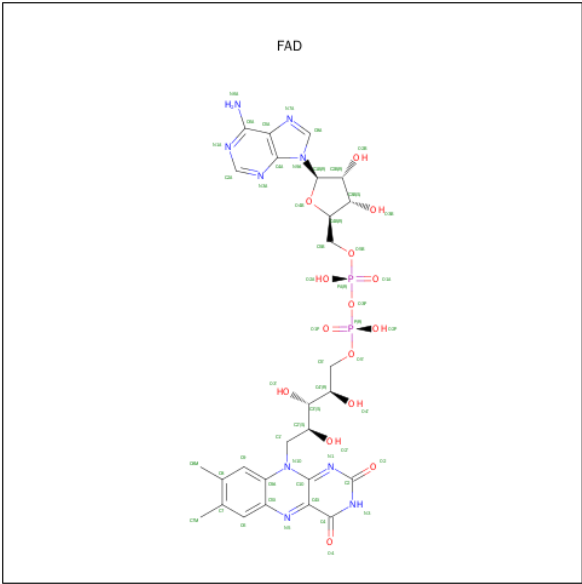
- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

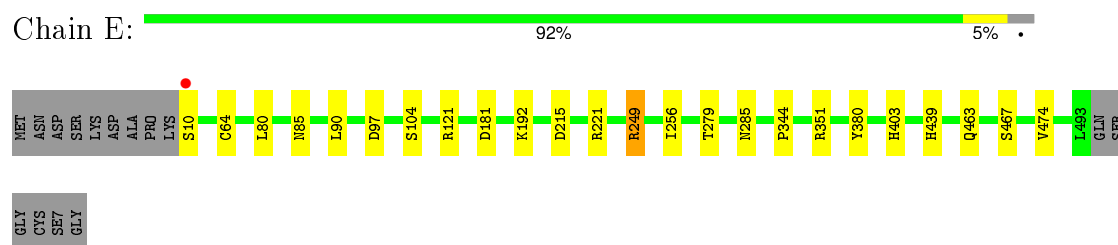
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	173	Total	O	0	0
			173	173		
5	F	191	Total	O	0	0
			191	191		
5	A	34	Total	O	0	0
			34	34		
5	B	126	Total	O	0	0
			126	126		

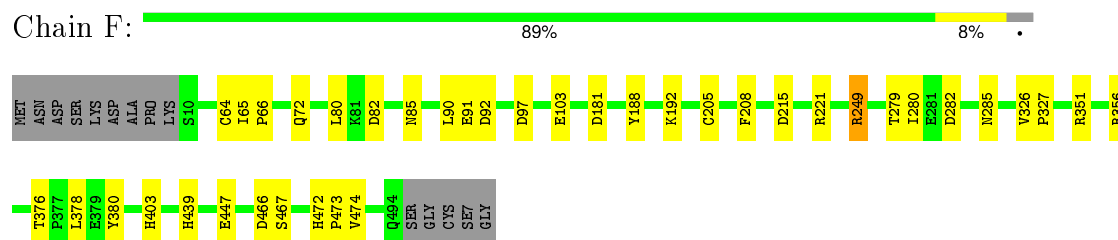
### 3 Residue-property plots

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.

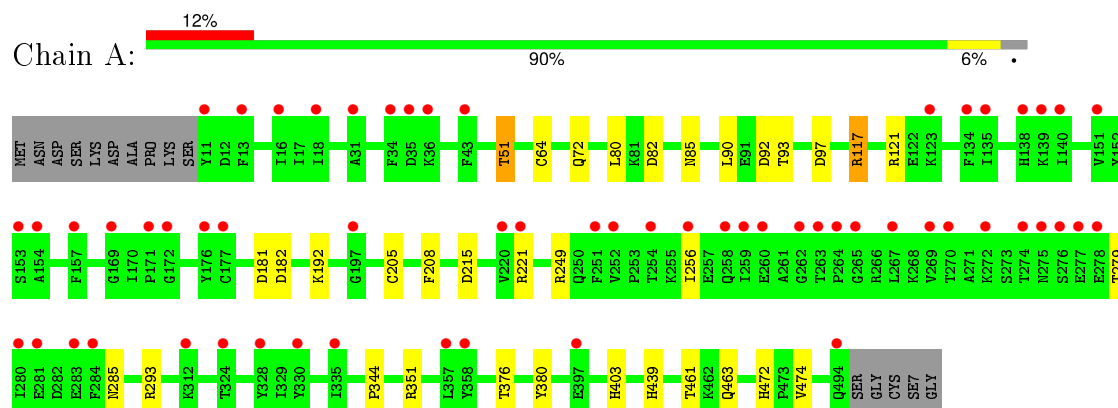
- Molecule 1: Thioredoxin reductase 1, cytoplasmic



- Molecule 1: Thioredoxin reductase 1, cytoplasmic

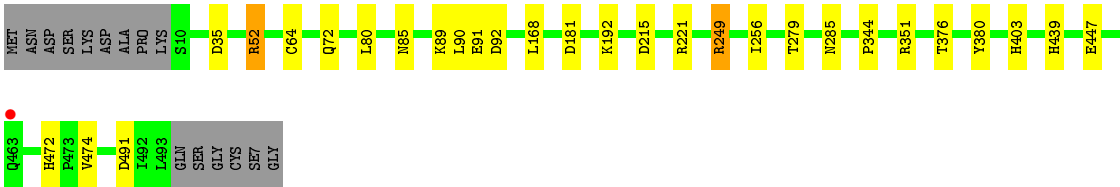


- Molecule 1: Thioredoxin reductase 1, cytoplasmic



- Molecule 1: Thioredoxin reductase 1, cytoplasmic







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.99Å 162.99Å 236.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.67 – 2.40 60.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (60.67-2.40) 99.6 (60.60-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.160 , 0.187 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	7095 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.6	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 141310 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: SO3, MPD, 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	0.80	0/3818	0.86	13/5166 (0.3%)
1	B	0.94	1/3850 (0.0%)	0.94	14/5211 (0.3%)
1	E	0.99	3/3814 (0.1%)	0.92	10/5161 (0.2%)
1	F	1.04	3/3879 (0.1%)	0.93	13/5250 (0.2%)
All	All	0.95	7/15361 (0.0%)	0.92	50/20788 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	447	GLU	CD-OE2	10.17	1.36	1.25
1	F	467	SER	CB-OG	6.82	1.51	1.42
1	E	104	SER	CB-OG	-6.24	1.34	1.42
1	E	463	GLN	CG-CD	5.38	1.63	1.51
1	F	103	GLU	CG-CD	5.28	1.59	1.51
1	B	447	GLU	CD-OE2	5.19	1.31	1.25
1	E	467	SER	CB-OG	5.07	1.48	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	221	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	B	221	ARG	NE-CZ-NH2	8.63	124.61	120.30
1	B	491	ASP	CB-CG-OD1	8.62	126.06	118.30
1	F	221	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	E	221	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	B	221	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	E	249	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	E	181	ASP	CB-CG-OD1	7.25	124.83	118.30
1	B	249	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	221	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	181	ASP	CB-CG-OD1	6.88	124.49	118.30
1	F	215	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	221	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	E	249	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	F	249	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	181	ASP	CB-CG-OD1	6.44	124.10	118.30
1	F	181	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	F	249	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	F	97	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	35	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	117	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	351	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	249	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	215	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	181	ASP	CB-CG-OD1	5.82	123.53	118.30
1	E	351	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	82	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	181	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	E	221	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	491	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	E	97	ASP	CB-CG-OD1	5.58	123.32	118.30
1	E	215	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	117	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	256	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	F	466	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	181	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	F	351	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	F	356	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	A	351	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	F	356	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	168[A]	LEU	N-CA-C	-5.20	96.96	111.00
1	B	168[B]	LEU	N-CA-C	-5.20	96.96	111.00
1	B	351	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	351	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	215	ASP	CB-CG-OD1	5.15	122.94	118.30
1	F	82	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	97	ASP	CB-CG-OD1	5.12	122.91	118.30
1	E	256	ILE	CG1-CB-CG2	-5.07	100.26	111.40
1	A	256	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	A	293	ARG	NE-CZ-NH2	-5.02	117.79	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	3741	0	3753	18	0
1	B	3768	0	3776	16	0
1	E	3737	0	3748	13	0
1	F	3787	0	3797	22	0
2	E	4	0	0	0	0
2	F	8	0	0	0	0
3	A	24	0	42	2	0
3	B	8	0	14	1	0
3	E	24	0	42	2	0
3	F	16	0	28	2	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	E	53	0	31	0	0
4	F	53	0	31	0	0
5	A	34	0	0	1	0
5	B	126	0	0	4	0
5	E	173	0	0	3	0
5	F	191	0	0	1	0
All	All	15853	0	15324	55	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 2.

All (55) 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:85:ASN:HB2	5:A:617:HOH:O	1.79	0.81
1:E:85:ASN:HB2	5:E:643:HOH:O	1.85	0.77
1:B:85:ASN:HB2	5:B:690:HOH:O	1.96	0.66
1:E:90:LEU:HD11	1:F:90:LEU:HD11	1.77	0.66
1:B:249:ARG:HG2	3:B:501:MPD:H53	1.79	0.65
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.83	0.62
1:F:85:ASN:HB2	5:F:610:HOH:O	2.00	0.62
1:B:192:LYS:H	1:B:285:ASN:HD22	1.48	0.61
1:F:282:ASP:OD1	1:A:117:ARG:NH2	2.35	0.60
1:A:90:LEU:HD11	1:B:90:LEU:HD11	1.84	0.59
1:A:51:THR:OG1	1:A:182:ASP:OD1	2.18	0.59
1:F:91:GLU:OE2	1:B:89:LYS:NZ	2.35	0.59
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.86	0.59
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.86	0.59
1:F:280:ILE:HG22	1:A:121:ARG:HD2	1.86	0.58
1:A:192:LYS:H	1:A:285:ASN:HD22	1.51	0.57
1:F:192:LYS:H	1:F:285:ASN:HD22	1.52	0.56
1:E:90:LEU:CD1	1:F:90:LEU:HD11	2.35	0.56
1:E:249:ARG:NH1	3:E:503:MPD:O2	2.39	0.56
1:E:90:LEU:HD11	1:F:90:LEU:CD1	2.36	0.55
1:E:192:LYS:H	1:E:285:ASN:HD22	1.54	0.54
1:E:10:SER:N	5:E:609:HOH:O	2.42	0.52
1:F:249:ARG:HG2	3:F:503:MPD:H53	1.90	0.52
1:B:91:GLU:HG2	1:B:92:ASP:N	2.25	0.52
1:A:461:THR:OG1	1:A:463[A]:GLN:HG2	2.12	0.50
1:F:188:TYR:HE2	3:F:504:MPD:HM2	1.75	0.49
1:A:90:LEU:CD1	1:B:90:LEU:HD11	2.42	0.49
1:A:90:LEU:HD11	1:B:90:LEU:CD1	2.43	0.48
1:A:72:GLN:HE21	1:A:72:GLN:HA	1.78	0.48
1:E:80:LEU:HD23	1:F:80:LEU:HD23	1.96	0.48
1:B:52:ARG:CD	5:B:612:HOH:O	2.61	0.48
1:A:249:ARG:HD3	3:A:502:MPD:O4	2.14	0.48
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.97	0.47
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.97	0.46
1:E:249:ARG:HG2	3:E:503:MPD:H53	1.96	0.46
1:E:10:SER:HA	5:E:609:HOH:O	2.15	0.46
1:F:91:GLU:CG	1:F:92:ASP:N	2.79	0.46
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.98	0.45
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.98	0.45
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.52	0.44
1:F:380:TYR:OH	1:F:439:HIS:CD2	2.68	0.43
1:F:282:ASP:CG	1:A:117:ARG:HH21	2.20	0.43
1:F:472:HIS:HA	1:F:473:PRO:HA	1.86	0.42
1:F:65:ILE:HB	1:F:66:PRO:CD	2.49	0.42
1:F:378:LEU:HA	1:F:378:LEU:HD12	1.94	0.42
1:B:72:GLN:HA	1:B:72:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:TYR:OH	1:B:439:HIS:CD2	2.72	0.42
1:F:205:CYS:HA	1:F:208:PHE:CE2	2.55	0.42
1:F:72:GLN:HA	1:F:72:GLN:HE21	1.85	0.41
1:F:326:VAL:HA	1:F:327:PRO:HD3	1.87	0.41
1:B:52:ARG:HD3	5:B:612:HOH:O	2.19	0.41
1:E:121:ARG:CD	5:B:704:HOH:O	2.69	0.41
1:A:380:TYR:OH	1:A:439:HIS:CD2	2.71	0.41
3:A:503:MPD:HM1	3:A:503:MPD:H52	2.04	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	483/499 (97%)	468 (97%)	15 (3%)	0	100	100
1	B	487/499 (98%)	472 (97%)	15 (3%)	0	100	100
1	E	483/499 (97%)	468 (97%)	15 (3%)	0	100	100
1	F	489/499 (98%)	475 (97%)	14 (3%)	0	100	100
All	All	1942/1996 (97%)	1883 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	403/413 (98%)	395 (98%)	8 (2%)	63	81
1	B	406/413 (98%)	400 (98%)	6 (2%)	72	87
1	E	403/413 (98%)	399 (99%)	4 (1%)	82	93
1	F	409/413 (99%)	404 (99%)	5 (1%)	78	90
All	All	1621/1652 (98%)	1598 (99%)	23 (1%)	74	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	64	CYS
1	E	279	THR
1	E	403	HIS
1	E	474	VAL
1	F	64	CYS
1	F	279	THR
1	F	376	THR
1	F	403	HIS
1	F	474	VAL
1	A	51	THR
1	A	64	CYS
1	A	92	ASP
1	A	93	THR
1	A	279	THR
1	A	376	THR
1	A	403	HIS
1	A	474	VAL
1	B	52	ARG
1	B	64	CYS
1	B	279	THR
1	B	376	THR
1	B	403	HIS
1	B	474	VAL

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

Mol	Chain	Res	Type
1	E	285	ASN
1	E	439	HIS
1	F	72	GLN
1	F	285	ASN

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Mol	Chain	Res	Type
1	F	439	HIS
1	A	72	GLN
1	A	285	ASN
1	A	439	HIS
1	A	494	GLN
1	B	72	GLN
1	B	285	ASN
1	B	439	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](#)

16 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	MPD	A	501	-	6,7,7	0.83	0	7,10,10	0.84	0
3	MPD	A	502	-	6,7,7	0.70	0	7,10,10	1.12	1 (14%)
3	MPD	A	503	-	6,7,7	0.51	0	7,10,10	0.71	0
4	FAD	A	504	-	48,58,58	1.58	10 (20%)	54,89,89	2.45	19 (35%)
3	MPD	B	501	-	6,7,7	0.70	0	7,10,10	1.04	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	B	502	-	48,58,58	1.47	10 (20%)	54,89,89	2.45	17 (31%)
2	SO3	E	501	-	1,3,3	7.74	1 (100%)	0,3,3	0.00	-
3	MPD	E	502	-	6,7,7	0.56	0	7,10,10	1.66	1 (14%)
3	MPD	E	503	-	6,7,7	0.59	0	7,10,10	0.78	0
3	MPD	E	504	-	6,7,7	0.55	0	7,10,10	1.24	1 (14%)
4	FAD	E	505	-	48,58,58	1.81	10 (20%)	54,89,89	2.84	12 (22%)
2	SO3	F	501	-	1,3,3	9.41	1 (100%)	0,3,3	0.00	-
2	SO3	F	502	-	1,3,3	8.30	1 (100%)	0,3,3	0.00	-
3	MPD	F	503	-	6,7,7	0.95	0	7,10,10	1.03	0
3	MPD	F	504	-	6,7,7	0.70	0	7,10,10	2.25	2 (28%)
4	FAD	F	505	-	48,58,58	1.60	12 (25%)	54,89,89	2.49	12 (22%)

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	MPD	A	501	-	-	0/5/5/5	0/0/0/0
3	MPD	A	502	-	-	0/5/5/5	0/0/0/0
3	MPD	A	503	-	-	0/5/5/5	0/0/0/0
4	FAD	A	504	-	-	0/30/50/50	0/6/6/6
3	MPD	B	501	-	-	0/5/5/5	0/0/0/0
4	FAD	B	502	-	-	0/30/50/50	0/6/6/6
2	SO3	E	501	-	-	0/0/0/0	0/0/0/0
3	MPD	E	502	-	-	0/5/5/5	0/0/0/0
3	MPD	E	503	-	-	0/5/5/5	0/0/0/0
3	MPD	E	504	-	-	0/5/5/5	0/0/0/0
4	FAD	E	505	-	-	0/30/50/50	0/6/6/6
2	SO3	F	501	-	-	0/0/0/0	0/0/0/0
2	SO3	F	502	-	-	0/0/0/0	0/0/0/0
3	MPD	F	503	-	-	0/5/5/5	0/0/0/0
3	MPD	F	504	-	-	0/5/5/5	0/0/0/0
4	FAD	F	505	-	-	0/30/50/50	0/6/6/6

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	505	FAD	C2'-C3'	-3.73	1.45	1.53
4	E	505	FAD	C6-C5X	-3.72	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	FAD	C9-C9A	-3.42	1.33	1.40
4	E	505	FAD	C9-C9A	-3.41	1.33	1.40
4	E	505	FAD	C2'-C3'	-3.28	1.46	1.53
4	E	505	FAD	P-O2P	-3.11	1.41	1.54
4	F	505	FAD	C10-N1	-3.04	1.30	1.35
4	B	502	FAD	C10-N10	-2.91	1.35	1.39
4	B	502	FAD	P-O1P	-2.87	1.40	1.51
4	E	505	FAD	C4'-C3'	-2.73	1.47	1.53
4	F	505	FAD	C8A-N7A	-2.57	1.29	1.34
4	F	505	FAD	C4-N3	-2.29	1.28	1.33
4	F	505	FAD	PA-O2A	-2.20	1.45	1.54
4	B	502	FAD	PA-O1A	-2.20	1.43	1.51
4	B	502	FAD	C1'-N10	-2.11	1.46	1.48
4	B	502	FAD	C4-N3	-2.10	1.29	1.33
4	E	505	FAD	C1'-N10	-2.09	1.46	1.48
4	F	505	FAD	C9-C9A	-2.03	1.36	1.40
4	B	502	FAD	C6-C5X	-2.01	1.38	1.41
4	A	504	FAD	C2A-N1A	2.03	1.37	1.33
4	F	505	FAD	C2A-N1A	2.16	1.38	1.33
4	F	505	FAD	C4-C4X	2.16	1.45	1.41
4	B	502	FAD	C8-C7	2.26	1.47	1.41
4	E	505	FAD	C9A-C5X	2.26	1.47	1.42
4	A	504	FAD	C9A-N10	2.28	1.41	1.38
4	B	502	FAD	C4X-C10	2.40	1.45	1.41
4	E	505	FAD	C4X-C10	2.41	1.45	1.41
4	F	505	FAD	C4X-C10	2.41	1.45	1.41
4	F	505	FAD	O4B-C1B	2.70	1.44	1.41
4	B	502	FAD	C4-C4X	2.71	1.46	1.41
4	A	504	FAD	C8-C7	2.78	1.48	1.41
4	A	504	FAD	C2A-N3A	2.86	1.37	1.32
4	F	505	FAD	C8-C7	2.93	1.48	1.41
4	A	504	FAD	O4B-C1B	2.93	1.44	1.41
4	A	504	FAD	C5A-C4A	3.13	1.47	1.40
4	A	504	FAD	C9A-C5X	3.27	1.49	1.42
4	A	504	FAD	C10-N10	3.33	1.43	1.39
4	E	505	FAD	C4-C4X	3.39	1.48	1.41
4	F	505	FAD	C9A-C5X	3.83	1.50	1.42
4	A	504	FAD	C4X-C10	3.84	1.48	1.41
4	A	504	FAD	C4-C4X	4.33	1.49	1.41
4	E	505	FAD	O4B-C1B	7.00	1.50	1.41
2	E	501	SO3	O1-S	7.74	1.77	1.44
2	F	502	SO3	O1-S	8.30	1.80	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	SO3	O1-S	9.41	1.85	1.44

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	505	FAD	N3A-C2A-N1A	-12.84	119.07	128.89
4	F	505	FAD	N3A-C2A-N1A	-9.90	121.32	128.89
4	A	504	FAD	N3A-C2A-N1A	-8.76	122.19	128.89
4	B	502	FAD	N3A-C2A-N1A	-8.04	122.74	128.89
4	B	502	FAD	C4-C4X-C10	-6.47	115.80	119.94
4	F	505	FAD	C4-C4X-C10	-6.12	116.03	119.94
4	E	505	FAD	C4X-C4-N3	-5.73	115.75	123.59
4	F	505	FAD	C4X-C4-N3	-4.29	117.72	123.59
4	A	504	FAD	C4X-C4-N3	-3.99	118.13	123.59
4	A	504	FAD	C1B-N9A-C4A	-3.63	121.46	126.94
4	E	505	FAD	C1B-N9A-C4A	-3.63	121.47	126.94
3	E	502	MPD	CM-C2-C1	-3.40	102.84	110.24
3	F	504	MPD	O2-C2-CM	-3.35	95.82	108.09
4	A	504	FAD	O5B-PA-O1A	-3.29	96.84	109.62
4	A	504	FAD	C4-C4X-C10	-3.27	117.85	119.94
4	A	504	FAD	C4B-O4B-C1B	-3.15	106.26	109.72
4	F	505	FAD	C1B-N9A-C4A	-3.11	122.25	126.94
4	F	505	FAD	C4X-C10-N10	-3.08	118.71	120.52
4	B	502	FAD	C1B-N9A-C4A	-3.06	122.32	126.94
4	B	502	FAD	C4X-C4-N3	-3.05	119.42	123.59
4	A	504	FAD	C1'-C2'-C3'	-2.99	101.27	109.82
4	E	505	FAD	O2'-C2'-C1'	-2.99	102.61	109.94
4	B	502	FAD	C4A-C5A-N7A	-2.91	106.80	109.48
4	A	504	FAD	P-O3P-PA	-2.90	124.57	132.73
4	E	505	FAD	C4-C4X-C10	-2.87	118.11	119.94
4	E	505	FAD	C4X-C10-N10	-2.85	118.84	120.52
4	E	505	FAD	O5B-PA-O1A	-2.83	98.63	109.62
4	A	504	FAD	C4X-C10-N10	-2.70	118.93	120.52
4	B	502	FAD	O2'-C2'-C1'	-2.64	103.45	109.94
4	B	502	FAD	C1'-C2'-C3'	-2.52	102.61	109.82
4	B	502	FAD	C5B-C4B-C3B	-2.35	105.89	115.21
4	A	504	FAD	O2A-PA-O3P	-2.30	94.65	105.09
4	F	505	FAD	O3'-C3'-C2'	-2.24	103.10	108.75
3	A	502	MPD	O2-C2-CM	-2.16	100.18	108.09
4	F	505	FAD	C4A-C5A-N7A	-2.12	107.53	109.48
4	B	502	FAD	O4'-C4'-C5'	-2.11	105.59	110.19
4	E	505	FAD	C9A-C5X-N5	-2.08	119.28	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	505	FAD	C5B-C4B-C3B	-2.06	107.05	115.21
4	B	502	FAD	O3B-C3B-C2B	-2.05	105.17	111.83
4	B	502	FAD	C4X-C10-N10	-2.01	119.34	120.52
4	B	502	FAD	C4-C4X-N5	2.04	121.19	118.72
4	B	502	FAD	C4X-N5-C5X	2.06	119.13	116.76
4	A	504	FAD	N6A-C6A-N1A	2.18	123.89	119.20
4	A	504	FAD	O2A-PA-O5B	2.18	119.48	108.46
4	A	504	FAD	C4-C4X-N5	2.27	121.48	118.72
4	A	504	FAD	O2P-P-O1P	2.29	124.96	112.53
4	F	505	FAD	C5X-C9A-N10	2.31	119.38	117.62
4	A	504	FAD	C1'-N10-C9A	2.40	121.56	118.86
4	F	505	FAD	C2B-C1B-N9A	2.49	118.09	114.29
3	E	504	MPD	O2-C2-CM	2.74	118.12	108.09
4	A	504	FAD	O2A-PA-O1A	2.76	127.50	112.53
4	E	505	FAD	C5X-C9A-N10	2.93	119.84	117.62
4	F	505	FAD	C1'-N10-C9A	3.10	122.34	118.86
4	B	502	FAD	O3P-P-O5'	3.26	111.58	102.94
4	A	504	FAD	O2'-C2'-C3'	3.65	118.20	109.02
4	B	502	FAD	C5X-C9A-N10	3.88	120.56	117.62
4	E	505	FAD	C1'-N10-C9A	3.96	123.31	118.86
4	A	504	FAD	C4X-N5-C5X	4.48	121.92	116.76
3	F	504	MPD	CM-C2-C1	4.62	120.30	110.24
4	E	505	FAD	C4X-N5-C5X	5.03	122.55	116.76
4	B	502	FAD	C1'-N10-C9A	5.78	125.35	118.86
4	A	504	FAD	C4-N3-C2	7.18	121.45	115.25
4	B	502	FAD	C4-N3-C2	7.25	121.51	115.25
4	E	505	FAD	C4-N3-C2	9.24	123.23	115.25
4	F	505	FAD	C4-N3-C2	9.72	123.65	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	MPD	1	0
3	A	503	MPD	1	0
3	B	501	MPD	1	0
3	E	503	MPD	2	0
3	F	503	MPD	1	0
3	F	504	MPD	1	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	484/499 (96%)	0.29	60 (12%) 5 5	39, 86, 133, 151	0
1	B	484/499 (96%)	-0.57	1 (0%) 95 95	34, 50, 83, 129	0
1	E	484/499 (96%)	-0.52	1 (0%) 95 95	32, 48, 78, 106	0
1	F	485/499 (97%)	-0.59	0 100 100	30, 44, 74, 131	0
All	All	1937/1996 (97%)	-0.35	62 (3%) 51 51	30, 52, 114, 151	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	PHE	5.1
1	A	259	ILE	3.9
1	A	135	ILE	3.9
1	A	256	ILE	3.8
1	A	36	LYS	3.8
1	A	176	TYR	3.6
1	A	357	LEU	3.6
1	A	284	PHE	3.6
1	A	34	PHE	3.5
1	A	18	ILE	3.5
1	A	277	GLU	3.5
1	A	169	GLY	3.5
1	A	276	SER	3.4
1	E	10	SER	3.3
1	A	278	GLU	3.1
1	A	13	PHE	3.1
1	A	274	THR	2.9
1	A	35	ASP	2.9
1	A	251	PHE	2.9
1	A	139	LYS	2.8
1	A	358	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	172	GLY	2.8
1	A	154	ALA	2.8
1	A	197	GLY	2.7
1	A	335	ILE	2.7
1	A	275	ASN	2.7
1	A	324	THR	2.7
1	A	11	TYR	2.7
1	A	252	VAL	2.6
1	A	280	ILE	2.6
1	A	134	PHE	2.6
1	A	138	HIS	2.5
1	A	260	GLU	2.5
1	A	328	TYR	2.5
1	A	258	GLN	2.4
1	A	330	TYR	2.4
1	A	397	GLU	2.4
1	A	171	PRO	2.4
1	A	177	CYS	2.4
1	A	264	PRO	2.4
1	A	220	VAL	2.4
1	A	283	GLU	2.4
1	A	254	THR	2.4
1	A	270	THR	2.3
1	A	16	ILE	2.3
1	A	43	PHE	2.3
1	A	151	VAL	2.3
1	A	263	THR	2.3
1	A	140	ILE	2.3
1	A	269	VAL	2.2
1	A	312	LYS	2.2
1	B	463	GLN	2.2
1	A	265	GLY	2.2
1	A	267	LEU	2.1
1	A	494	GLN	2.1
1	A	153	SER	2.1
1	A	123	LYS	2.1
1	A	262	GLY	2.1
1	A	221	ARG	2.1
1	A	272	LYS	2.1
1	A	31	ALA	2.1
1	A	281	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
2	SO3	F	501	4/4	0.95	0.19	17.08	62,68,79,92	4
3	MPD	F	504	8/8	0.90	0.22	8.39	83,102,121,121	0
3	MPD	E	504	8/8	0.94	0.27	8.29	68,73,102,104	0
2	SO3	F	502	4/4	0.94	0.58	6.46	83,86,88,91	4
3	MPD	A	501	8/8	0.97	0.23	5.76	75,79,83,85	0
3	MPD	E	502	8/8	0.94	0.26	5.36	61,66,70,70	0
3	MPD	B	501	8/8	0.94	0.20	3.97	80,90,98,102	0
4	FAD	F	505	53/53	0.98	0.17	3.30	41,48,60,63	0
4	FAD	E	505	53/53	0.98	0.16	2.69	41,54,64,69	0
3	MPD	F	503	8/8	0.92	0.16	2.31	76,81,87,97	0
3	MPD	A	503	8/8	0.87	0.26	1.71	122,133,143,150	8
3	MPD	E	503	8/8	0.92	0.18	1.63	86,93,96,108	0
4	FAD	B	502	53/53	0.98	0.14	1.44	38,46,54,57	0
4	FAD	A	504	53/53	0.95	0.18	0.50	100,118,157,161	0
3	MPD	A	502	8/8	0.91	0.19	-0.11	128,133,149,150	0
2	SO3	E	501	4/4	0.89	0.55	-	75,82,84,91	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.