



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:03 am GMT

PDB ID : 4YSW  
Title : Structure of rat xanthine oxidoreductase, C-terminal deletion protein variant, NADH bound form  
Authors : Nishino, T.; Okamoto, K.; Kawaguchi, Y.; Matsumura, T.; Eger, B.T.; Pai, E.F.  
Deposited on : 2015-03-17  
Resolution : 1.99 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.

---

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

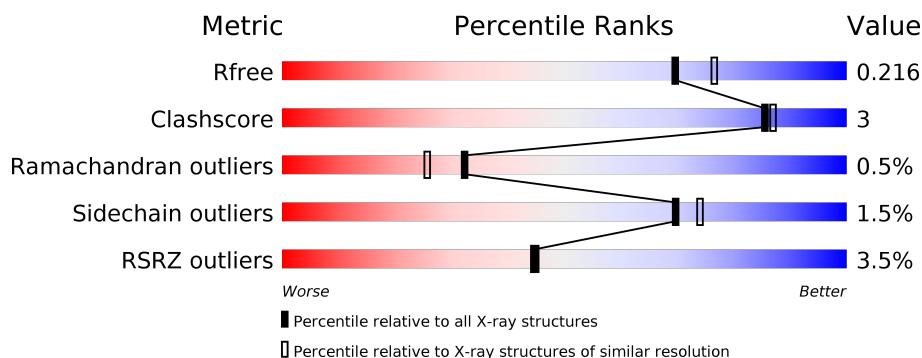
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	1315	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>6% •</div> </div> </div>
1	B	1315	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5% ••</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
8	GOL	B	4008	-	-	-	X

## 2 Entry composition [i](#)

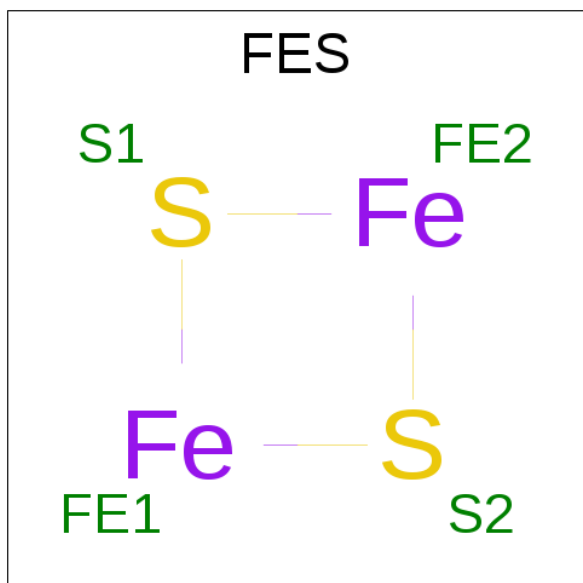
There are 9 unique types of molecules in this entry. The entry contains 21749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1286	Total	C	N	O	S	0	0	0
			9941	6301	1711	1866	63			
1	B	1286	Total	C	N	O	S	0	0	0
			9940	6301	1711	1865	63			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

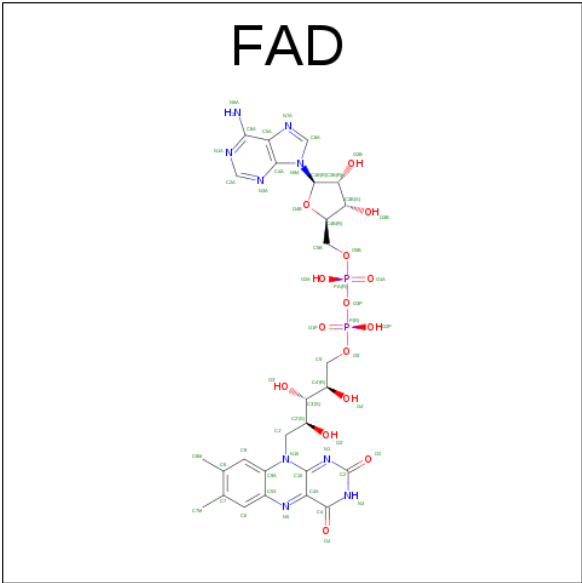


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

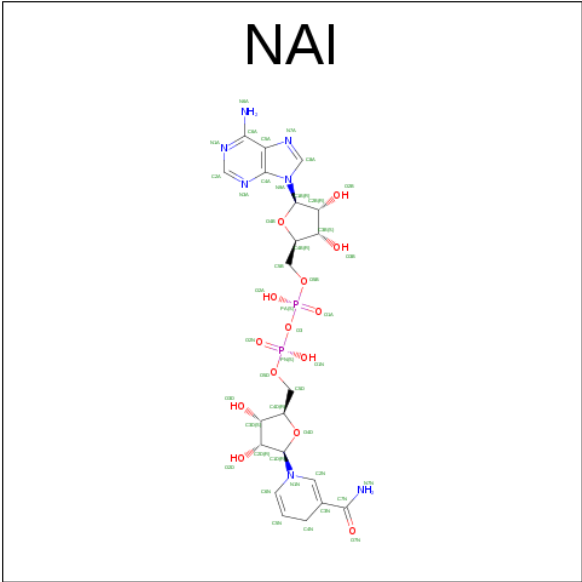
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- 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>).



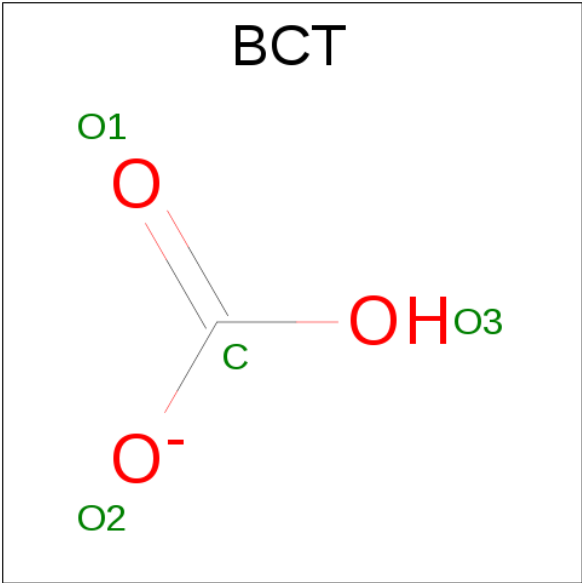
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



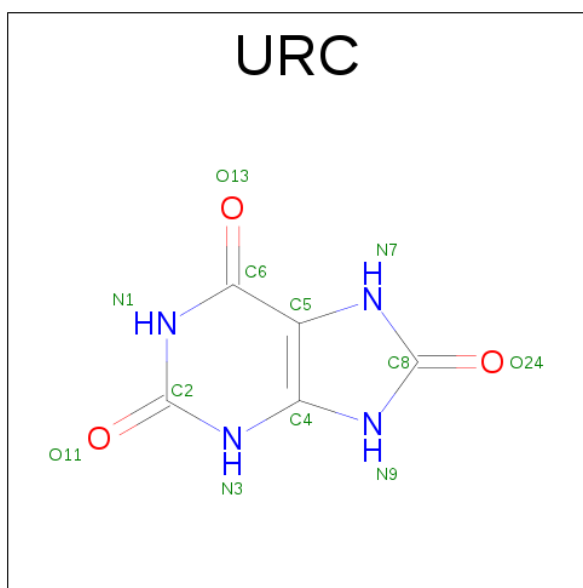
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



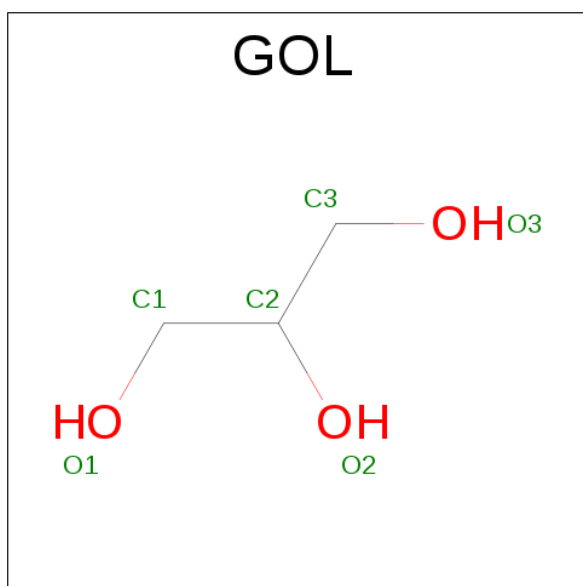
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is URIC ACID (three-letter code: URC) (formula:  $C_5H_4N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	5	4	3		
7	B	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 9 is water.

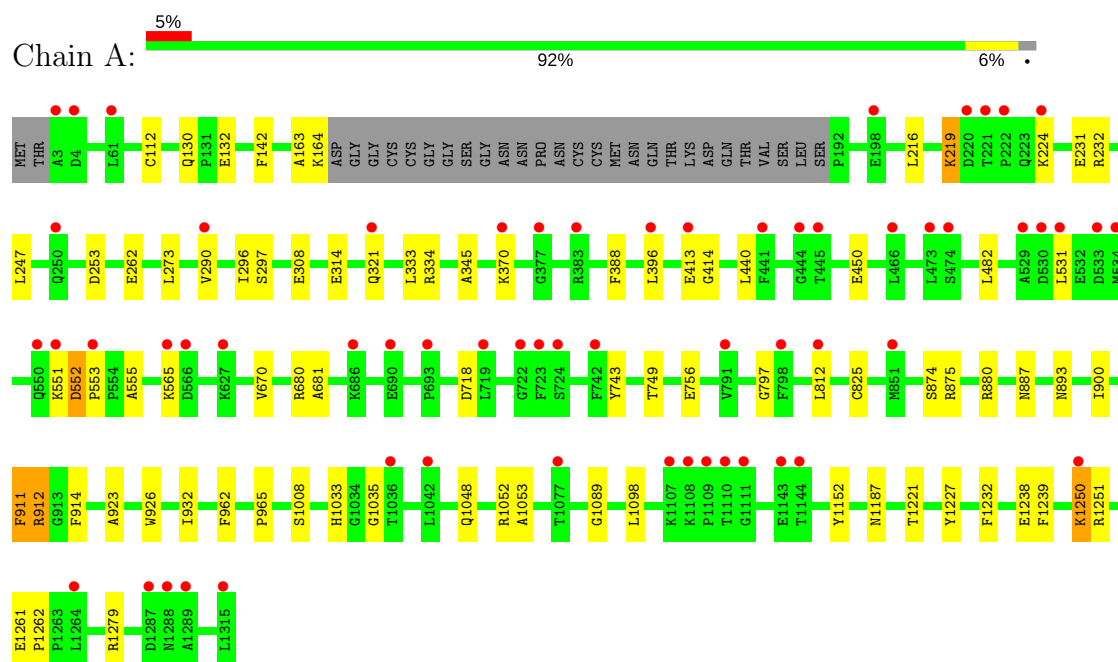
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	698	Total	O	0	0
			698	698		
9	B	914	Total	O	0	0
			914	914		



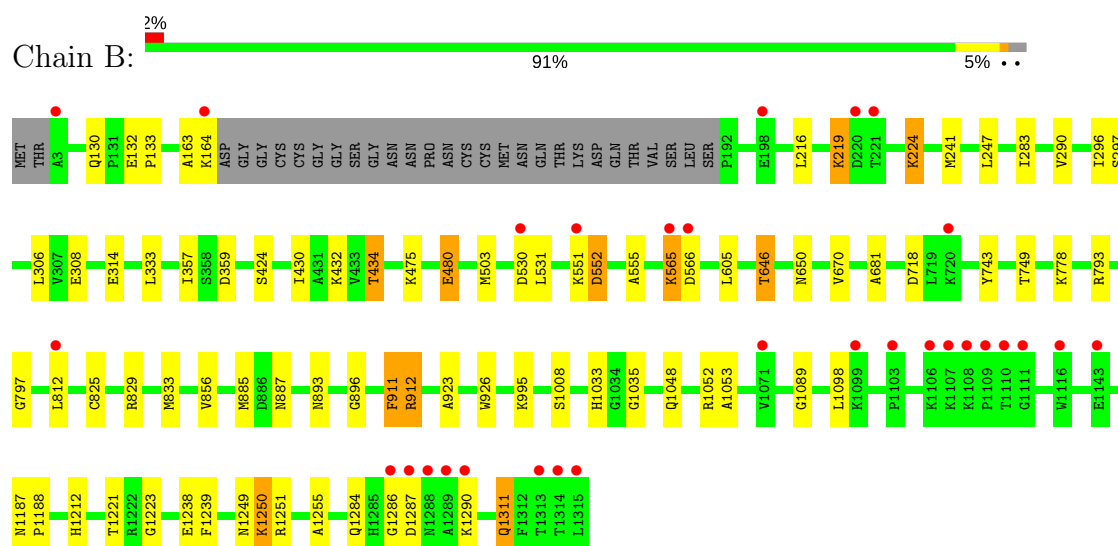
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Xanthine dehydrogenase/oxidase



#### • Molecule 1: Xanthine dehydrogenase/oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.46Å 137.64Å 222.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.41 – 1.99 42.40 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.41-1.99) 94.7 (42.40-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.181 , 0.219 0.180 , 0.216	Depositor DCC
$R_{free}$ test set	9850 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, URC, CA, NAI, FES, BCT, 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	0.43	0/10151	0.55	0/13736
1	B	0.46	0/10150	0.57	0/13734
All	All	0.45	0/20301	0.56	0/27470

There are no bond length outliers.

There are no bond angle outliers.

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	9941	0	9948	47	0
1	B	9940	0	9948	61	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	2	0
4	B	53	0	31	0	0
5	A	44	0	27	0	0
5	B	44	0	27	0	0
6	A	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	0	0
7	A	12	0	4	0	0
7	B	12	0	4	0	0
8	A	6	0	8	0	0
8	B	6	0	8	0	0
9	A	698	0	0	2	0
9	B	914	0	0	6	0
All	All	21749	0	20036	106	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 3.

All (106) 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:1089:GLY:HA3	9:B:4609:HOH:O	1.06	1.22
1:A:1089:GLY:HA3	9:A:3449:HOH:O	1.02	1.17
1:B:749:THR:HB	1:B:812:LEU:HD12	1.37	1.02
1:A:812:LEU:HD11	1:A:825:CYS:HB3	1.44	0.99
1:B:1311:GLN:HE21	1:B:1311:GLN:H	1.16	0.93
1:B:565:LYS:HD3	1:B:565:LYS:H	1.36	0.91
1:B:646:THR:HG23	9:B:4276:HOH:O	1.71	0.90
1:B:812:LEU:HD11	1:B:825:CYS:HB3	1.56	0.87
1:B:565:LYS:CD	1:B:565:LYS:H	1.93	0.81
1:A:812:LEU:HD21	1:A:825:CYS:HB2	1.67	0.76
1:B:565:LYS:HD3	1:B:565:LYS:N	2.00	0.76
1:B:812:LEU:HD21	1:B:825:CYS:HB2	1.70	0.74
1:A:749:THR:HB	1:A:812:LEU:HD12	1.72	0.71
1:B:130:GLN:HE21	1:B:132:GLU:H	1.37	0.71
1:B:829:ARG:HD2	1:B:833:MET:HE2	1.73	0.70
1:A:555:ALA:HB3	1:A:1238:GLU:HG2	1.71	0.70
1:B:551:LYS:O	1:B:552:ASP:HB2	1.92	0.69
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.93	0.66
1:B:359:ASP:OD2	1:B:434:THR:HG21	1.95	0.66
1:A:232:ARG:NH1	1:A:273:LEU:HD13	2.11	0.65
1:B:718:ASP:H	1:B:893:ASN:HD22	1.44	0.65
1:A:130:GLN:HE21	1:A:132:GLU:H	1.47	0.62
1:A:749:THR:HB	1:A:812:LEU:CD1	2.29	0.62
1:B:290:VAL:HG22	1:B:297:SER:HB2	1.81	0.62
1:A:812:LEU:HD21	1:A:825:CYS:CB	2.30	0.61
1:B:749:THR:HB	1:B:812:LEU:CD1	2.24	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ASP:H	1:A:893:ASN:HD22	1.51	0.59
1:B:812:LEU:HD21	1:B:825:CYS:CB	2.33	0.58
1:B:1250:LYS:HG3	9:B:4316:HOH:O	2.05	0.57
1:B:359:ASP:OD2	1:B:434:THR:CG2	2.52	0.57
1:B:241:MET:HE2	1:B:283:ILE:HG21	1.86	0.57
1:B:718:ASP:H	1:B:893:ASN:ND2	2.03	0.56
1:A:232:ARG:HH11	1:A:273:LEU:HD13	1.71	0.55
1:A:718:ASP:H	1:A:893:ASN:ND2	2.04	0.55
1:B:1311:GLN:NE2	1:B:1311:GLN:H	1.96	0.55
1:B:1033:HIS:HD2	1:B:1035:GLY:H	1.53	0.55
1:B:359:ASP:HA	1:B:434:THR:HG21	1.87	0.55
1:B:605:LEU:HD13	1:B:812:LEU:HD23	1.89	0.55
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.54	0.54
1:B:829:ARG:HG3	1:B:833:MET:HE3	1.91	0.52
1:B:833:MET:HE3	1:B:1223:GLY:HA2	1.91	0.52
1:A:1221:THR:HG22	1:A:1227:TYR:HB2	1.91	0.52
1:B:833:MET:CE	1:B:1223:GLY:HA2	2.40	0.52
1:B:670:VAL:HG11	1:B:681:ALA:HB3	1.90	0.52
1:B:432:LYS:HE2	1:B:503:MET:SD	2.50	0.52
1:A:874:SER:HB3	1:A:900:ILE:HG21	1.91	0.52
1:B:216:LEU:O	1:B:219:LYS:HG3	2.09	0.52
1:A:216:LEU:O	1:A:219:LYS:HG3	2.10	0.52
1:A:1033:HIS:HD2	1:A:1035:GLY:H	1.59	0.51
1:A:345:ALA:HB1	4:A:3004:FAD:H4'	1.92	0.51
1:B:1033:HIS:CD2	1:B:1035:GLY:H	2.29	0.50
1:B:224:LYS:HD2	1:B:224:LYS:H	1.76	0.50
1:B:475:LYS:HD3	1:B:480:GLU:OE2	2.12	0.50
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.76	0.49
1:B:1221:THR:HG22	9:B:4952:HOH:O	2.13	0.49
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.27	0.49
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.13	0.49
1:A:932:ILE:HD11	9:A:3689:HOH:O	2.12	0.48
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.14	0.47
1:A:875:ARG:HG2	1:A:900:ILE:HD13	1.97	0.47
1:B:1048:GLN:HE22	1:B:1187:ASN:HB2	1.80	0.47
1:A:932:ILE:HD13	1:A:1279:ARG:NH2	2.30	0.46
1:A:1048:GLN:HE22	1:A:1187:ASN:HB2	1.80	0.46
1:B:308:GLU:HG3	1:B:333:LEU:HD13	1.97	0.46
1:B:296:ILE:HD11	1:B:314:GLU:HG3	1.96	0.46
1:A:756:GLU:OE2	1:B:793:ARG:NH1	2.42	0.45
1:A:308:GLU:HG3	1:A:333:LEU:HD13	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLN:HE21	1:A:414:GLY:H	1.63	0.45
1:A:163:ALA:O	1:A:164:LYS:HB2	2.17	0.45
1:A:1152:TYR:HB3	1:A:1251:ARG:HD2	1.98	0.45
1:A:296:ILE:CD1	1:A:314:GLU:HG3	2.46	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.32	0.45
1:B:1250:LYS:HD2	1:B:1251:ARG:N	2.32	0.44
1:B:164:LYS:HD3	9:B:4891:HOH:O	2.17	0.44
1:B:1212:HIS:HD2	9:B:4967:HOH:O	2.00	0.44
1:B:1250:LYS:HD2	1:B:1251:ARG:H	1.81	0.44
1:B:650:ASN:OD1	1:B:778:LYS:NZ	2.51	0.44
1:A:962:PHE:CE2	1:A:965:PRO:HD3	2.53	0.44
1:A:1033:HIS:CD2	1:A:1035:GLY:H	2.36	0.44
1:B:424:SER:OG	1:B:432:LYS:NZ	2.51	0.43
1:A:555:ALA:O	1:A:1238:GLU:HA	2.18	0.43
1:B:357:ILE:HD13	1:B:430:ILE:HG23	2.00	0.43
1:A:1250:LYS:HD3	1:A:1251:ARG:N	2.34	0.43
1:A:388:PHE:HA	1:A:396:LEU:HG	2.00	0.43
1:A:440:LEU:HB3	1:A:450:GLU:HB2	2.00	0.43
1:B:749:THR:O	1:B:812:LEU:HD13	2.19	0.43
1:A:911:PHE:O	1:A:912:ARG:C	2.57	0.43
1:A:262:GLU:HB2	4:A:3004:FAD:H52A	2.01	0.43
1:A:321:GLN:HG2	1:A:413:GLU:CD	2.39	0.43
1:B:555:ALA:HB3	1:B:1238:GLU:HG2	1.99	0.43
1:B:565:LYS:H	1:B:565:LYS:CE	2.32	0.43
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.19	0.42
1:A:880:ARG:HD2	1:A:914:PHE:HB3	2.02	0.42
1:B:296:ILE:CD1	1:B:314:GLU:HG3	2.50	0.42
1:A:290:VAL:CG2	1:A:297:SER:HB2	2.50	0.42
1:B:885:MET:SD	1:B:896:GLY:HA3	2.59	0.42
1:A:756:GLU:CD	1:B:793:ARG:HH12	2.23	0.41
1:A:142:PHE:HB3	1:A:1232:PHE:CE1	2.55	0.41
1:A:334:ARG:HH21	1:A:551:LYS:NZ	2.18	0.41
1:B:1311:GLN:HE21	1:B:1311:GLN:N	1.98	0.41
1:A:231:GLU:OE2	1:A:680:ARG:NH1	2.54	0.41
1:B:1187:ASN:HA	1:B:1188:PRO:HD2	1.94	0.41
1:B:133:PRO:O	1:B:163:ALA:HA	2.21	0.40
1:B:911:PHE:O	1:B:912:ARG:C	2.59	0.40
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.03	0.40
1:A:552:ASP:HA	1:A:553:PRO:HD3	1.86	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	1282/1315 (98%)	1245 (97%)	32 (2%)	5 (0%)	38	33
1	B	1282/1315 (98%)	1245 (97%)	30 (2%)	7 (0%)	32	26
All	All	2564/2630 (98%)	2490 (97%)	62 (2%)	12 (0%)	32	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	SER
1	B	1008	SER
1	A	912	ARG
1	B	912	ARG
1	A	797	GLY
1	B	552	ASP
1	B	797	GLY
1	B	1290	LYS
1	A	552	ASP
1	A	887	ASN
1	B	887	ASN
1	B	1286	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	1085/1109 (98%)	1071 (99%)	14 (1%)	73	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1085/1109 (98%)	1066 (98%)	19 (2%)	64	68
All	All	2170/2218 (98%)	2137 (98%)	33 (2%)	70	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	CYS
1	A	219	LYS
1	A	224	LYS
1	A	247	LEU
1	A	253	ASP
1	A	370	LYS
1	A	482	LEU
1	A	531	LEU
1	A	565	LYS
1	A	743	TYR
1	A	911	PHE
1	A	1052	ARG
1	A	1239	PHE
1	A	1250	LYS
1	B	219	LYS
1	B	224	LYS
1	B	247	LEU
1	B	306	LEU
1	B	434	THR
1	B	480	GLU
1	B	530	ASP
1	B	531	LEU
1	B	565	LYS
1	B	566	ASP
1	B	646	THR
1	B	743	TYR
1	B	856	VAL
1	B	911	PHE
1	B	1052	ARG
1	B	1239	PHE
1	B	1250	LYS
1	B	1287	ASP
1	B	1311	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	130	GLN
1	A	145	ASN
1	A	250	GLN
1	A	321	GLN
1	A	332	GLN
1	A	449	GLN
1	A	472	GLN
1	A	483	GLN
1	A	550	GLN
1	A	558	GLN
1	A	585	GLN
1	A	642	ASN
1	A	817	HIS
1	A	893	ASN
1	A	1033	HIS
1	A	1048	GLN
1	A	1173	ASN
1	A	1294	GLN
1	B	95	GLN
1	B	130	GLN
1	B	145	ASN
1	B	472	GLN
1	B	585	GLN
1	B	642	ASN
1	B	893	ASN
1	B	1033	HIS
1	B	1048	GLN
1	B	1088	GLN
1	B	1173	ASN
1	B	1284	GLN
1	B	1285	HIS
1	B	1311	GLN

### 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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
2	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	3004	-	51,58,58	1.39	7 (13%)	54,89,89	1.99	7 (12%)
5	NAI	A	3005	-	40,48,48	1.17	2 (5%)	41,73,73	1.82	5 (12%)
6	BCT	A	3006	-	0,3,3	0.00	-	0,3,3	0.00	-
7	URC	A	3007	-	12,13,13	5.07	5 (41%)	12,19,19	7.32	7 (58%)
8	GOL	A	3008	-	5,5,5	0.31	0	5,5,5	0.41	0
2	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
2	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	B	4004	-	51,58,58	1.28	7 (13%)	54,89,89	2.01	6 (11%)
5	NAI	B	4005	-	40,48,48	1.12	2 (5%)	41,73,73	1.70	4 (9%)
6	BCT	B	4006	-	0,3,3	0.00	-	0,3,3	0.00	-
7	URC	B	4007	-	12,13,13	4.98	5 (41%)	12,19,19	7.64	8 (66%)
8	GOL	B	4008	-	5,5,5	0.30	0	5,5,5	0.70	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
2	FES	A	3001	1	-	0/0/4/4	0/1/1/1
2	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	FAD	A	3004	-	-	0/28/50/50	0/6/6/6
5	NAI	A	3005	-	-	0/25/72/72	0/4/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCT	A	3006	-	-	0/0/0/0	0/0/0/0
7	URC	A	3007	-	-	0/0/0/0	0/2/2/2
8	GOL	A	3008	-	-	0/4/4/4	0/0/0/0
2	FES	B	4001	1	-	0/0/4/4	0/1/1/1
2	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	FAD	B	4004	-	-	0/28/50/50	0/6/6/6
5	NAI	B	4005	-	-	0/25/72/72	0/5/5/5
6	BCT	B	4006	-	-	0/0/0/0	0/0/0/0
7	URC	B	4007	-	-	0/0/0/0	0/2/2/2
8	GOL	B	4008	-	-	0/4/4/4	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4007	URC	C4-N3	-9.09	1.36	1.46
7	A	3007	URC	C4-N3	-8.69	1.36	1.46
7	A	3007	URC	C4-N9	-8.02	1.35	1.44
7	B	4007	URC	C4-N9	-7.78	1.35	1.44
7	A	3007	URC	C5-N7	-4.69	1.35	1.45
7	B	4007	URC	C5-N7	-4.41	1.36	1.45
5	A	3005	NAI	C4N-C5N	-4.36	1.39	1.49
5	B	4005	NAI	C4N-C5N	-3.92	1.40	1.49
7	A	3007	URC	C5-C6	-2.48	1.48	1.53
7	B	4007	URC	C5-C6	-2.46	1.48	1.53
4	B	4004	FAD	C5X-N5	2.10	1.38	1.35
4	A	3004	FAD	C5X-N5	2.37	1.38	1.35
4	B	4004	FAD	C2A-N1A	2.38	1.38	1.33
4	A	3004	FAD	C2A-N1A	2.50	1.38	1.33
4	B	4004	FAD	C1'-N10	3.05	1.51	1.48
4	B	4004	FAD	C4-N3	3.08	1.38	1.33
4	A	3004	FAD	C4-N3	3.09	1.38	1.33
4	B	4004	FAD	C2A-N3A	3.28	1.37	1.32
5	A	3005	NAI	C6N-C5N	3.33	1.39	1.33
4	B	4004	FAD	C4X-N5	3.38	1.38	1.33
4	B	4004	FAD	C10-N1	3.50	1.38	1.33
4	A	3004	FAD	C1'-N10	3.53	1.52	1.48
5	B	4005	NAI	C6N-C5N	3.60	1.39	1.33
4	A	3004	FAD	C4X-N5	3.82	1.38	1.33
4	A	3004	FAD	C10-N1	3.88	1.38	1.33
4	A	3004	FAD	C2A-N3A	3.93	1.38	1.32
7	B	4007	URC	O24-C8	11.19	1.47	1.23
7	A	3007	URC	O24-C8	11.67	1.48	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4007	URC	C4-N9-C8	-15.95	102.06	112.89
7	A	3007	URC	C4-N9-C8	-15.27	102.52	112.89
4	B	4004	FAD	N3A-C2A-N1A	-10.57	119.65	128.86
4	A	3004	FAD	N3A-C2A-N1A	-10.41	119.79	128.86
5	B	4005	NAI	N3A-C2A-N1A	-8.98	121.04	128.86
5	A	3005	NAI	N3A-C2A-N1A	-8.79	121.20	128.86
5	A	3005	NAI	C1D-N1N-C6N	-3.39	113.40	120.77
7	B	4007	URC	O24-C8-N7	-3.06	121.70	125.90
7	B	4007	URC	C6-N1-C2	-3.05	121.96	126.23
4	B	4004	FAD	C4X-C4-N3	-3.03	119.17	123.48
4	A	3004	FAD	C4X-C4-N3	-2.97	119.25	123.48
7	B	4007	URC	O24-C8-N9	-2.97	121.83	125.90
7	A	3007	URC	O24-C8-N9	-2.94	121.87	125.90
7	A	3007	URC	C6-N1-C2	-2.91	122.16	126.23
5	B	4005	NAI	O2B-C2B-C1B	-2.66	103.31	111.61
7	A	3007	URC	O24-C8-N7	-2.58	122.36	125.90
5	B	4005	NAI	C1D-N1N-C6N	-2.57	115.19	120.77
5	A	3005	NAI	C1D-N1N-C2N	-2.22	117.32	121.09
7	B	4007	URC	O11-C2-N3	-2.21	118.25	122.89
5	A	3005	NAI	C4A-C5A-N7A	-2.03	107.44	109.41
4	A	3004	FAD	O2'-C2'-C1'	2.16	114.79	109.79
4	B	4004	FAD	C5X-C9A-N10	2.33	119.39	117.66
5	B	4005	NAI	O4D-C1D-N1N	2.46	113.03	108.07
4	A	3004	FAD	C1'-N10-C9A	2.55	120.68	118.35
4	A	3004	FAD	C4X-N5-C5X	2.82	119.74	116.76
4	A	3004	FAD	C5X-C9A-N10	3.02	119.90	117.66
4	B	4004	FAD	C1'-N10-C9A	3.23	121.31	118.35
4	B	4004	FAD	C4X-N5-C5X	3.71	120.68	116.76
5	A	3005	NAI	O4D-C1D-N1N	4.01	116.14	108.07
7	B	4007	URC	N1-C2-N3	5.43	121.79	116.14
7	A	3007	URC	N1-C2-N3	5.49	121.86	116.14
4	B	4004	FAD	C4-N3-C2	6.24	120.61	115.16
4	A	3004	FAD	C4-N3-C2	6.92	121.21	115.16
7	A	3007	URC	N7-C8-N9	8.98	115.77	108.85
7	B	4007	URC	N7-C8-N9	9.88	116.47	108.85
7	A	3007	URC	C5-C4-N9	16.40	110.23	102.64
7	B	4007	URC	C5-C4-N9	16.86	110.44	102.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3004	FAD	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	1286/1315 (97%)	0.28	61 (4%) 32 32	14, 25, 40, 48	0
1	B	1286/1315 (97%)	0.02	30 (2%) 61 60	11, 19, 32, 49	0
All	All	2572/2630 (97%)	0.15	91 (3%) 44 45	11, 22, 38, 49	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1286	GLY	14.0
1	B	1315	LEU	13.1
1	B	1289	ALA	12.5
1	A	1315	LEU	9.1
1	B	1287	ASP	8.2
1	B	1288	ASN	7.1
1	B	1314	THR	5.8
1	A	3	ALA	5.5
1	B	3	ALA	5.1
1	A	1111	GLY	5.1
1	A	1288	ASN	5.0
1	B	1111	GLY	4.4
1	B	1290	LYS	4.3
1	A	396	LEU	4.3
1	B	1107	LYS	4.1
1	A	551	LYS	3.8
1	B	565	LYS	3.7
1	A	1110	THR	3.6
1	A	566	ASP	3.5
1	A	1287	ASP	3.5
1	A	290	VAL	3.5
1	A	198	GLU	3.4
1	B	221	THR	3.4
1	A	531	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1110	THR	3.3
1	B	1106	LYS	3.2
1	B	566	ASP	3.1
1	A	1250	LYS	3.0
1	A	61	LEU	3.0
1	B	551	LYS	3.0
1	A	791	VAL	3.0
1	A	377	GLY	2.9
1	A	222	PRO	2.8
1	A	224	LYS	2.8
1	A	321	GLN	2.8
1	B	530	ASP	2.8
1	A	798	PHE	2.6
1	B	220	ASP	2.6
1	A	1143	GLU	2.6
1	A	1264	LEU	2.6
1	A	530	ASP	2.6
1	A	686	LYS	2.5
1	A	723	PHE	2.5
1	B	1099	LYS	2.5
1	A	812	LEU	2.5
1	A	693	PRO	2.4
1	A	553	PRO	2.4
1	A	1108	LYS	2.4
1	B	1109	PRO	2.4
1	B	1103	PRO	2.4
1	B	1143	GLU	2.4
1	A	445	THR	2.4
1	A	565	LYS	2.4
1	A	724	SER	2.3
1	A	1107	LYS	2.3
1	A	550	GLN	2.3
1	B	1108	LYS	2.3
1	A	722	GLY	2.3
1	A	413	GLU	2.3
1	A	690	GLU	2.3
1	A	529	ALA	2.3
1	A	719	LEU	2.3
1	A	444	GLY	2.3
1	A	370	LYS	2.3
1	A	220	ASP	2.3
1	A	383	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	627	LYS	2.3
1	A	1042	LEU	2.3
1	B	198	GLU	2.2
1	A	473	LEU	2.2
1	A	1289	ALA	2.2
1	A	474	SER	2.2
1	A	441	PHE	2.2
1	A	742	PHE	2.2
1	A	533	ASP	2.2
1	A	221	THR	2.1
1	A	1109	PRO	2.1
1	A	534	MET	2.1
1	A	4	ASP	2.1
1	A	1144	THR	2.1
1	A	250	GLN	2.1
1	A	466	LEU	2.1
1	A	1036	THR	2.1
1	B	720	LYS	2.1
1	B	812	LEU	2.1
1	B	164	LYS	2.1
1	B	1313	THR	2.0
1	B	1071	VAL	2.0
1	A	851	MET	2.0
1	B	1116	TRP	2.0
1	A	1077	THR	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( $\text{\AA}^2$ )	Q<0.9
8	GOL	B	4008	6/6	0.93	0.12	2.92	21,24,25,25	0
8	GOL	A	3008	6/6	0.92	0.13	1.79	24,25,26,26	0
4	FAD	B	4004	53/53	0.98	0.11	0.20	12,14,15,17	0
6	BCT	B	4006	4/4	0.99	0.14	-0.02	17,17,17,18	0
4	FAD	A	3004	53/53	0.97	0.12	-0.04	22,23,25,26	0
5	NAI	A	3005	44/44	0.95	0.11	-0.27	25,31,35,36	0
5	NAI	B	4005	44/44	0.97	0.08	-0.35	17,21,23,24	0
6	BCT	A	3006	4/4	0.98	0.13	-1.25	22,22,22,22	0
7	URC	B	4007	12/12	0.98	0.10	-1.25	19,20,20,20	0
3	CA	A	3003	1/1	0.99	0.05	-1.89	26,26,26,26	0
2	FES	B	4002	4/4	1.00	0.07	-2.05	12,13,13,14	0
2	FES	A	3001	4/4	0.98	0.05	-2.08	26,26,26,28	0
2	FES	A	3002	4/4	0.99	0.07	-2.10	17,18,18,19	0
2	FES	B	4001	4/4	0.98	0.05	-2.91	23,24,24,25	0
7	URC	A	3007	12/12	0.97	0.09	-2.95	23,23,24,24	0
3	CA	B	4003	1/1	1.00	0.04	-3.54	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.