



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:05 AM GMT

PDB ID : 3D9F  
Title : Nitroalkane oxidase: active site mutant S276A crystallized with 1-nitrohexane  
Authors : Heroux, A.; Bozinovski, D.M.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.  
Deposited on : 2008-05-27  
Resolution : 2.20 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 (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

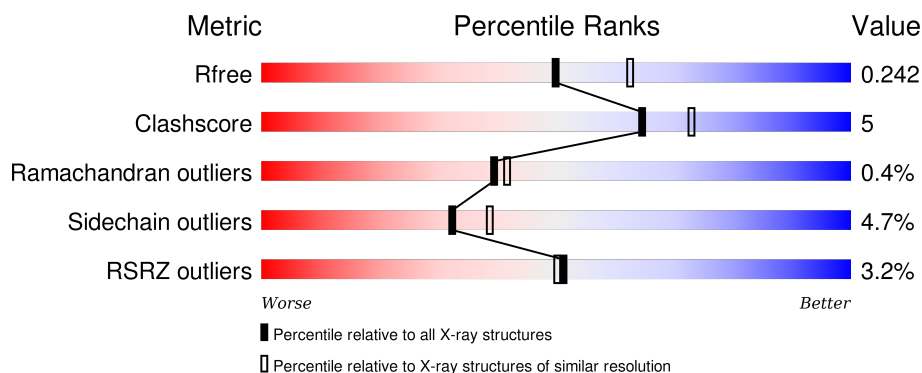
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	438	<div> <div>4%</div> <div>86% 11% ..</div> </div>
1	B	438	<div> <div>5%</div> <div>83% 13% ..</div> </div>
1	C	438	<div> <div>%</div> <div>87% 9% ..</div> </div>
1	D	438	<div> <div>2%</div> <div>84% 12% ..</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
3	N6C	D	600	-	-	-	X
4	GOL	C	701	-	-	-	X
4	GOL	D	701	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13974 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 Nitroalkane oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3305	2095	565	625	20			
1	B	431	Total	C	N	O	S	0	0	0
			3305	2095	565	625	20			
1	C	430	Total	C	N	O	S	0	0	0
			3300	2092	564	624	20			
1	D	430	Total	C	N	O	S	0	0	0
			3300	2092	564	624	20			

There are 4 discrepancies between the modelled and reference sequences:

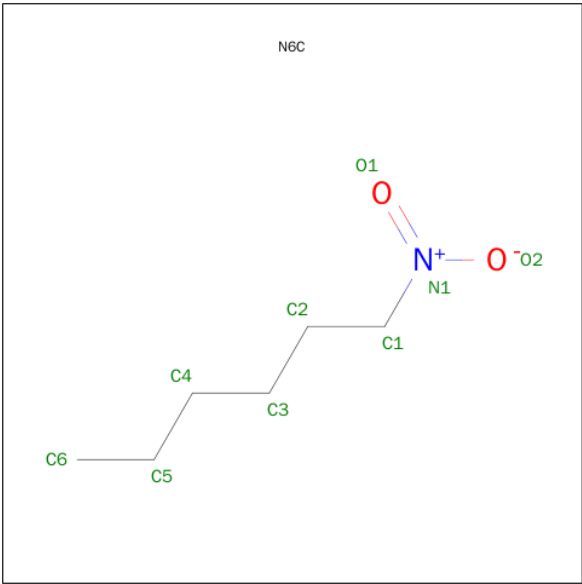
Chain	Residue	Modelled	Actual	Comment	Reference
A	276	ALA	SER	ENGINEERED	UNP Q8X1D8
B	276	ALA	SER	ENGINEERED	UNP Q8X1D8
C	276	ALA	SER	ENGINEERED	UNP Q8X1D8
D	276	ALA	SER	ENGINEERED	UNP Q8X1D8

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 1-NITROHEXANE (three-letter code: N6C) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

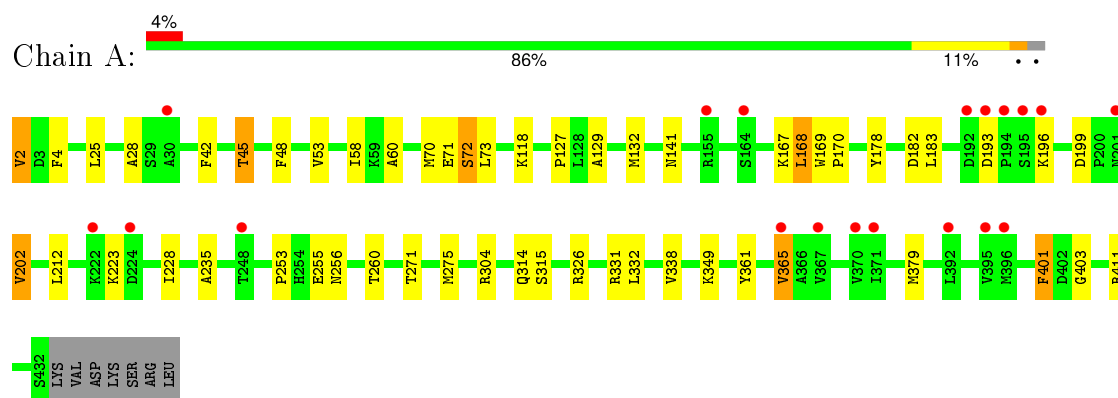
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	B	90	Total 90	O 90	0	0
5	C	138	Total 138	O 138	0	0
5	D	131	Total 131	O 131	0	0

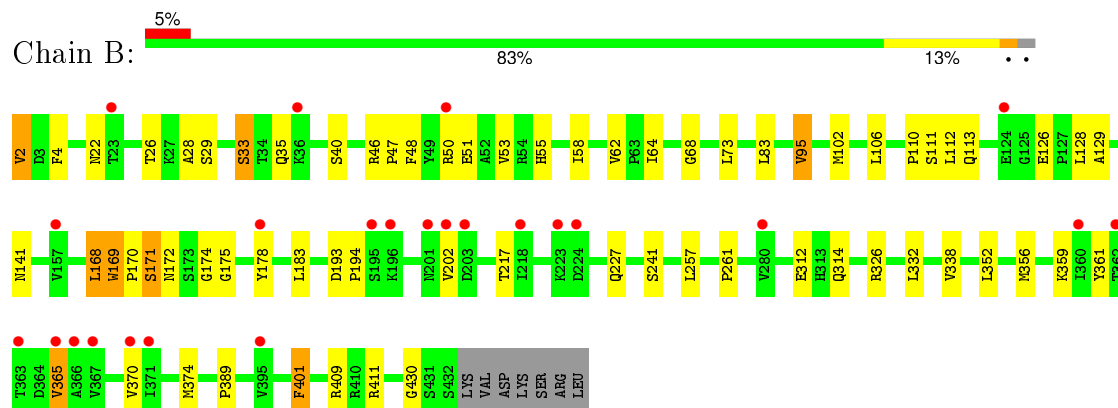
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

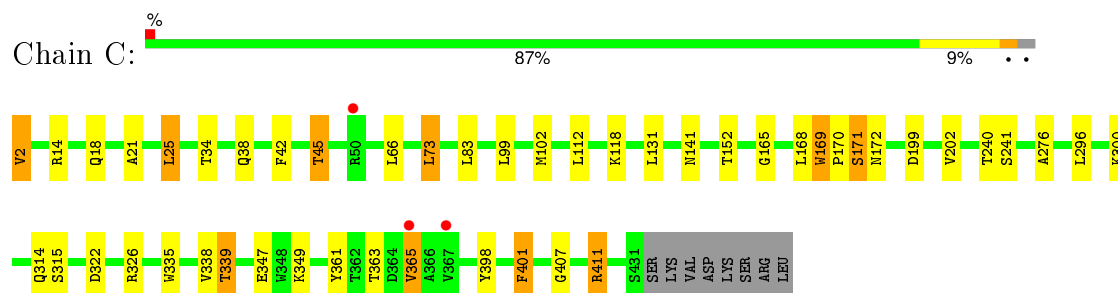
- Molecule 1: Nitroalkane oxidase



- Molecule 1: Nitroalkane oxidase

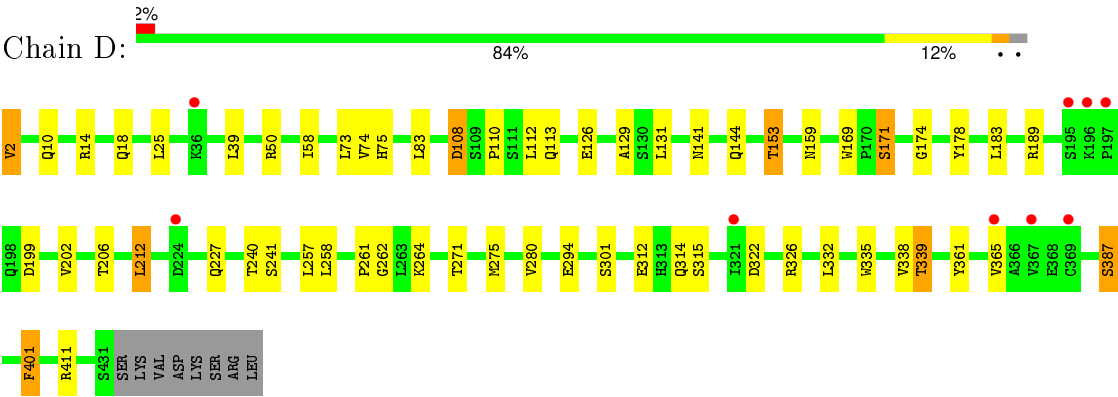


- Molecule 1: Nitroalkane oxidase



- Molecule 1: Nitroalkane oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.33Å 108.33Å 339.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 2.20 48.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.85-2.20) 97.5 (48.85-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.241 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	5789 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.6	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 115212 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13974	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 2.99% 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: GOL, N6C, 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	0.55	0/3374	0.67	2/4580 (0.0%)
1	B	0.55	0/3374	0.63	0/4580
1	C	0.58	0/3369	0.65	0/4573
1	D	0.57	0/3369	0.65	1/4573 (0.0%)
All	All	0.56	0/13486	0.65	3/18306 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH2	-10.97	114.81	120.30
1	A	331	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	D	108	ASP	CB-CA-C	5.94	122.28	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	430	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3305	0	3310	35	1
1	B	3305	0	3310	41	0
1	C	3300	0	3308	31	0
1	D	3300	0	3308	39	1
2	A	53	0	31	3	0
2	B	53	0	31	7	0
2	C	53	0	31	6	0
2	D	53	0	31	3	0
3	A	9	0	13	2	0
3	B	9	0	13	3	0
3	C	9	0	13	4	0
3	D	9	0	13	0	0
4	A	12	0	16	1	0
4	B	12	0	16	1	0
4	C	12	0	16	1	0
4	D	12	0	16	1	0
5	A	109	0	0	0	0
5	B	90	0	0	0	0
5	C	138	0	0	2	0
5	D	131	0	0	1	0
All	All	13974	0	13476	138	1

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 5.

All (138) 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:2:VAL:N	4:C:701:GOL:HO3	1.70	0.89
1:D:141:ASN:HD21	2:D:500:FAD:H61A	1.20	0.87
1:B:29:SER:O	1:B:33:SER:HB2	1.77	0.84
1:A:141:ASN:HD21	2:A:500:FAD:H61A	1.24	0.84
4:B:701:GOL:HO3	1:D:2:VAL:N	1.75	0.84
1:C:73:LEU:HB3	1:C:338:VAL:HB	1.65	0.79
1:B:168:LEU:C	1:B:170:PRO:HD3	2.06	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PHE:HD1	1:C:339:THR:HG21	1.52	0.72
4:A:701:GOL:HO1	1:C:2:VAL:N	1.87	0.72
1:D:199:ASP:HB3	1:D:202:VAL:HG12	1.73	0.69
1:B:141:ASN:HD21	2:B:500:FAD:H61A	1.40	0.69
1:D:326:ARG:HB3	1:D:365:VAL:HG13	1.74	0.69
2:B:500:FAD:N5	3:B:600:N6C:H1	2.07	0.68
1:C:335:TRP:O	1:C:339:THR:HB	1.93	0.67
1:A:53:VAL:HG22	1:A:58:ILE:HG13	1.77	0.65
1:C:141:ASN:HD21	2:C:500:FAD:H61A	1.43	0.65
1:B:35:GLN:HE21	1:B:40:SER:HB3	1.62	0.65
1:A:4:PHE:CD1	1:C:339:THR:HG21	2.31	0.65
1:D:141:ASN:ND2	2:D:500:FAD:H61A	1.95	0.64
1:D:73:LEU:HB3	1:D:338:VAL:HB	1.80	0.63
1:B:50:ARG:HD2	1:B:126:GLU:OE1	1.98	0.63
1:A:271:THR:O	1:A:275:MET:HG3	1.98	0.62
1:D:14:ARG:O	1:D:18:GLN:HG3	1.99	0.62
1:B:359:LYS:HD2	1:B:409:ARG:HG3	1.85	0.59
1:B:73:LEU:HB3	1:B:338:VAL:HB	1.84	0.59
1:B:141:ASN:ND2	2:B:500:FAD:H61A	2.00	0.58
1:B:314:GLN:HE21	1:C:315:SER:H	1.51	0.58
1:A:314:GLN:HE21	1:D:315:SER:H	1.52	0.58
1:B:2:VAL:N	4:D:701:GOL:HO3	2.01	0.57
1:C:326:ARG:NE	5:C:799:HOH:O	2.36	0.57
1:B:4:PHE:HD1	1:D:339:THR:HG21	1.69	0.57
1:A:141:ASN:ND2	2:A:500:FAD:H61A	2.00	0.55
1:B:110:PRO:HA	1:B:113:GLN:HE21	1.71	0.55
1:A:326:ARG:HB3	1:A:365:VAL:HG13	1.87	0.55
1:C:326:ARG:HD3	1:C:365:VAL:HG22	1.89	0.55
1:A:193:ASP:OD1	1:A:196:LYS:HG3	2.06	0.55
1:A:315:SER:H	1:D:314:GLN:HE21	1.55	0.54
1:C:296:LEU:O	1:C:300:LYS:HG3	2.07	0.54
1:C:199:ASP:HB3	1:C:202:VAL:HG13	1.88	0.54
1:A:42:PHE:O	1:A:45:THR:HB	2.07	0.53
1:A:199:ASP:HB3	1:A:202:VAL:HG13	1.90	0.53
1:D:294:GLU:OE1	1:D:387:SER:OG	2.27	0.53
1:B:326:ARG:HB3	1:B:365:VAL:HG13	1.91	0.53
1:B:28:ALA:HA	1:B:48:PHE:CZ	2.43	0.53
1:B:401:PHE:C	1:B:401:PHE:CD2	2.82	0.53
1:C:42:PHE:O	1:C:45:THR:HB	2.09	0.52
1:B:51:GLU:O	1:B:55:HIS:HD2	1.92	0.52
1:B:171:SER:HA	1:B:241:SER:O	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:HB3	1:A:202:VAL:CG1	2.39	0.52
1:B:128:LEU:HD12	1:B:175:GLY:HA2	1.90	0.52
1:A:129:ALA:HA	1:A:183:LEU:O	2.09	0.51
1:C:361:TYR:O	1:C:365:VAL:HB	2.10	0.51
1:A:71:GLU:O	1:A:72:SER:HB3	2.11	0.51
1:D:141:ASN:HB3	1:D:144:GLN:HE21	1.76	0.51
1:A:183:LEU:HD11	1:A:212:LEU:HG	1.92	0.51
1:D:271:THR:O	1:D:275:MET:HG3	2.11	0.51
1:C:152:THR:HA	1:C:165:GLY:HA3	1.94	0.50
1:C:141:ASN:ND2	2:C:500:FAD:H61A	2.08	0.50
2:C:500:FAD:N5	3:C:600:N6C:H1A	2.27	0.50
1:D:58:ILE:N	1:D:58:ILE:HD12	2.27	0.50
1:D:183:LEU:HD11	1:D:212:LEU:HG	1.94	0.49
1:B:95:VAL:HG13	3:B:600:N6C:H5A	1.94	0.49
1:A:304:ARG:HD2	2:B:500:FAD:H51A	1.94	0.49
1:B:169:TRP:N	1:B:170:PRO:HD3	2.27	0.49
1:A:132:MET:O	1:A:167:LYS:HE3	2.13	0.49
1:B:102:MET:HE3	1:B:106:LEU:HG	1.94	0.49
2:A:500:FAD:H52A	2:A:500:FAD:O2P	2.12	0.49
1:C:363:THR:HG22	1:C:398:TYR:HB3	1.94	0.48
1:D:335:TRP:O	1:D:339:THR:HB	2.13	0.48
1:D:171:SER:HA	1:D:241:SER:O	2.13	0.48
1:B:401:PHE:CE1	3:B:600:N6C:H2A	2.49	0.48
1:C:170:PRO:HA	2:C:500:FAD:C4	2.43	0.48
1:B:314:GLN:NE2	1:C:315:SER:H	2.11	0.48
1:A:361:TYR:O	1:A:365:VAL:HB	2.14	0.48
1:C:240:THR:HG21	2:C:500:FAD:HM72	1.95	0.48
1:B:361:TYR:O	1:B:365:VAL:HB	2.14	0.48
1:B:257:LEU:HD21	1:B:261:PRO:HD3	1.95	0.47
1:D:322:ASP:O	1:D:326:ARG:HG3	2.14	0.47
1:B:352:LEU:O	1:B:356:MET:HG2	2.15	0.47
1:D:401:PHE:C	1:D:401:PHE:CD2	2.87	0.47
1:A:379:MET:CE	2:B:500:FAD:HM81	2.44	0.47
1:D:257:LEU:HD21	1:D:261:PRO:HD3	1.96	0.47
1:C:21:ALA:HA	1:C:25:LEU:HB2	1.95	0.47
1:A:314:GLN:NE2	1:D:315:SER:H	2.13	0.46
1:A:127:PRO:HA	1:A:182:ASP:OD1	2.15	0.46
1:A:178:TYR:CE2	1:A:228:ILE:HG21	2.51	0.46
1:A:314:GLN:HB2	1:D:314:GLN:HB2	1.98	0.46
1:A:60:ALA:O	1:A:70:MET:HB2	2.15	0.46
1:C:276:ALA:HB1	3:C:600:N6C:H5	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HA	1:B:183:LEU:O	2.16	0.46
1:A:28:ALA:HA	1:A:48:PHE:CZ	2.51	0.46
1:A:379:MET:HE2	2:B:500:FAD:HM81	1.99	0.45
1:D:10:GLN:HG3	1:D:75:HIS:CE1	2.52	0.45
1:C:407:GLY:O	1:C:411:ARG:HG3	2.17	0.45
1:B:62:VAL:HB	1:B:68:GLY:HA3	1.98	0.45
1:D:159:ASN:H	1:D:159:ASN:ND2	2.15	0.44
1:B:2:VAL:HG11	1:D:74:VAL:HG11	1.98	0.44
1:B:174:GLY:O	1:B:178:TYR:HA	2.17	0.44
1:B:4:PHE:CD1	1:D:339:THR:HG21	2.50	0.44
1:D:361:TYR:O	1:D:365:VAL:HB	2.17	0.44
1:C:322:ASP:O	1:C:326:ARG:HG3	2.16	0.44
1:A:235:ALA:HB2	1:B:389:PRO:HB3	2.00	0.44
1:B:171:SER:O	1:B:172:ASN:HB2	2.18	0.44
1:D:108:ASP:O	1:D:110:PRO:HD3	2.18	0.43
1:B:73:LEU:CB	1:B:338:VAL:HB	2.47	0.43
1:A:304:ARG:CD	2:B:500:FAD:H51A	2.49	0.43
1:D:112:LEU:HD21	1:D:258:LEU:HD12	2.00	0.43
1:C:326:ARG:NH2	5:C:799:HOH:O	2.50	0.43
1:A:401:PHE:CE1	3:A:600:N6C:H1A	2.54	0.43
1:D:129:ALA:HA	1:D:183:LEU:O	2.18	0.43
1:B:314:GLN:HB2	1:C:314:GLN:HB2	2.01	0.42
1:A:73:LEU:HB3	1:A:338:VAL:HB	2.01	0.42
2:C:500:FAD:H52A	2:C:500:FAD:O2P	2.19	0.42
1:D:174:GLY:O	1:D:178:TYR:HA	2.20	0.42
1:C:401:PHE:CE1	3:C:600:N6C:H1	2.55	0.42
1:A:73:LEU:CB	1:A:338:VAL:HB	2.49	0.42
1:D:206:THR:O	1:D:262:GLY:HA2	2.20	0.42
1:D:326:ARG:NE	5:D:748:HOH:O	2.37	0.41
1:C:169:TRP:N	1:C:170:PRO:HD2	2.35	0.41
3:A:600:N6C:H1	3:A:600:N6C:H4	1.60	0.41
1:D:50:ARG:HD2	1:D:126:GLU:OE1	2.20	0.41
1:B:193:ASP:HA	1:B:194:PRO:HD2	1.84	0.41
1:D:240:THR:HG21	2:D:500:FAD:HM72	2.01	0.41
1:C:171:SER:HA	1:C:241:SER:O	2.21	0.41
1:D:153:THR:HA	1:D:189:ARG:O	2.20	0.41
1:C:14:ARG:O	1:C:18:GLN:HG3	2.20	0.41
1:C:171:SER:O	1:C:172:ASN:HB2	2.21	0.41
1:D:199:ASP:HB3	1:D:202:VAL:CG1	2.44	0.41
1:B:64:ILE:HA	1:B:68:GLY:O	2.21	0.41
1:B:46:ARG:HB3	1:B:47:PRO:HD3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:VAL:O	1:B:374:MET:HG3	2.21	0.41
1:C:99:LEU:HD22	3:C:600:N6C:H2A	2.03	0.41
1:A:253:PRO:HB2	1:A:255:GLU:HG2	2.03	0.41
1:B:22:ASN:O	1:B:26:THR:OG1	2.31	0.41
1:D:110:PRO:HA	1:D:113:GLN:HE21	1.85	0.40
1:A:168:LEU:C	1:A:170:PRO:CD	2.90	0.40
1:D:39:LEU:HD13	1:D:178:TYR:CE1	2.57	0.40
1:B:53:VAL:HG22	1:B:58:ILE:HG13	2.03	0.40

All (1) 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:A:260:THR:OG1	1:D:108:ASP:OD2[4_545]	1.86	0.34

## 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	429/438 (98%)	420 (98%)	6 (1%)	3 (1%)	26	25
1	B	429/438 (98%)	418 (97%)	10 (2%)	1 (0%)	52	59
1	C	428/438 (98%)	418 (98%)	9 (2%)	1 (0%)	52	59
1	D	428/438 (98%)	419 (98%)	8 (2%)	1 (0%)	52	59
All	All	1714/1752 (98%)	1675 (98%)	33 (2%)	6 (0%)	39	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	169	TRP
1	D	169	TRP
1	A	72	SER
1	A	403	GLY

### 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	353/362 (98%)	340 (96%)	13 (4%)	41	50
1	B	353/362 (98%)	337 (96%)	16 (4%)	34	41
1	C	353/362 (98%)	333 (94%)	20 (6%)	25	29
1	D	353/362 (98%)	336 (95%)	17 (5%)	31	37
All	All	1412/1448 (98%)	1346 (95%)	66 (5%)	32	39

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	25	LEU
1	A	45	THR
1	A	118	LYS
1	A	168	LEU
1	A	202	VAL
1	A	223	LYS
1	A	256	ASN
1	A	332	LEU
1	A	349	LYS
1	A	365	VAL
1	A	401	PHE
1	A	411	ARG
1	B	2	VAL
1	B	33	SER
1	B	83	LEU
1	B	95	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	111	SER
1	B	112	LEU
1	B	168	LEU
1	B	171	SER
1	B	202	VAL
1	B	217	THR
1	B	227	GLN
1	B	312	GLU
1	B	332	LEU
1	B	365	VAL
1	B	401	PHE
1	B	411	ARG
1	C	2	VAL
1	C	25	LEU
1	C	34	THR
1	C	38	GLN
1	C	45	THR
1	C	66	LEU
1	C	73	LEU
1	C	83	LEU
1	C	102	MET
1	C	112	LEU
1	C	118	LYS
1	C	131	LEU
1	C	168	LEU
1	C	171	SER
1	C	339	THR
1	C	347	GLU
1	C	349	LYS
1	C	365	VAL
1	C	401	PHE
1	C	411	ARG
1	D	2	VAL
1	D	25	LEU
1	D	83	LEU
1	D	131	LEU
1	D	153	THR
1	D	171	SER
1	D	212	LEU
1	D	227	GLN
1	D	264	LYS
1	D	280	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	301	SER
1	D	312	GLU
1	D	332	LEU
1	D	339	THR
1	D	387	SER
1	D	401	PHE
1	D	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	35	GLN
1	A	43	GLN
1	A	113	GLN
1	A	137	ASN
1	A	141	ASN
1	A	159	ASN
1	A	256	ASN
1	A	266	GLN
1	A	314	GLN
1	B	22	ASN
1	B	35	GLN
1	B	38	GLN
1	B	43	GLN
1	B	55	HIS
1	B	113	GLN
1	B	137	ASN
1	B	141	ASN
1	B	144	GLN
1	B	198	GLN
1	B	227	GLN
1	B	256	ASN
1	B	266	GLN
1	B	314	GLN
1	B	357	GLN
1	C	35	GLN
1	C	38	GLN
1	C	43	GLN
1	C	113	GLN
1	C	137	ASN
1	C	141	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	198	GLN
1	C	207	GLN
1	C	256	ASN
1	C	266	GLN
1	C	357	GLN
1	D	18	GLN
1	D	22	ASN
1	D	43	GLN
1	D	113	GLN
1	D	137	ASN
1	D	141	ASN
1	D	144	GLN
1	D	159	ASN
1	D	198	GLN
1	D	227	GLN
1	D	314	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](#)

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
2	FAD	A	500	-	48,58,58	1.20	6 (12%)	54,89,89	2.08	7 (12%)
3	N6C	A	600	-	6,8,8	0.50	0	5,8,8	0.59	0
4	GOL	A	700	-	5,5,5	0.38	0	5,5,5	0.78	0
4	GOL	A	701	-	5,5,5	0.39	0	5,5,5	0.18	0
2	FAD	B	500	-	48,58,58	1.28	6 (12%)	54,89,89	2.06	6 (11%)
3	N6C	B	600	-	6,8,8	0.31	0	5,8,8	0.71	0
4	GOL	B	700	-	5,5,5	0.44	0	5,5,5	0.44	0
4	GOL	B	701	-	5,5,5	0.31	0	5,5,5	0.33	0
2	FAD	C	500	-	48,58,58	1.29	7 (14%)	54,89,89	2.51	7 (12%)
3	N6C	C	600	-	6,8,8	0.27	0	5,8,8	0.63	0
4	GOL	C	700	-	5,5,5	0.29	0	5,5,5	0.34	0
4	GOL	C	701	-	5,5,5	0.35	0	5,5,5	0.50	0
2	FAD	D	500	-	48,58,58	1.23	6 (12%)	54,89,89	2.06	6 (11%)
3	N6C	D	600	-	6,8,8	0.30	0	5,8,8	1.13	1 (20%)
4	GOL	D	700	-	5,5,5	0.32	0	5,5,5	0.42	0
4	GOL	D	701	-	5,5,5	0.29	0	5,5,5	0.45	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	FAD	A	500	-	-	0/30/50/50	0/6/6/6
3	N6C	A	600	-	-	0/5/6/6	0/0/0/0
4	GOL	A	700	-	-	0/4/4/4	0/0/0/0
4	GOL	A	701	-	-	0/4/4/4	0/0/0/0
2	FAD	B	500	-	-	0/30/50/50	0/6/6/6
3	N6C	B	600	-	-	0/5/6/6	0/0/0/0
4	GOL	B	700	-	-	0/4/4/4	0/0/0/0
4	GOL	B	701	-	-	0/4/4/4	0/0/0/0
2	FAD	C	500	-	-	0/30/50/50	0/6/6/6
3	N6C	C	600	-	-	0/5/6/6	0/0/0/0
4	GOL	C	700	-	-	0/4/4/4	0/0/0/0
4	GOL	C	701	-	-	0/4/4/4	0/0/0/0
2	FAD	D	500	-	-	0/30/50/50	0/6/6/6
3	N6C	D	600	-	-	0/5/6/6	0/0/0/0
4	GOL	D	700	-	-	0/4/4/4	0/0/0/0
4	GOL	D	701	-	-	0/4/4/4	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C10-N1	2.07	1.39	1.35
2	C	500	FAD	C2A-N1A	2.13	1.37	1.33
2	D	500	FAD	C5X-N5	2.16	1.38	1.35
2	D	500	FAD	C2A-N1A	2.18	1.38	1.33
2	A	500	FAD	C5X-N5	2.25	1.38	1.35
2	C	500	FAD	C10-N1	2.28	1.39	1.35
2	C	500	FAD	C4-N3	2.33	1.37	1.33
2	C	500	FAD	C5X-N5	2.34	1.39	1.35
2	B	500	FAD	C2A-N1A	2.37	1.38	1.33
2	A	500	FAD	C1'-N10	2.43	1.51	1.48
2	A	500	FAD	C2A-N1A	2.58	1.38	1.33
2	D	500	FAD	C1'-N10	2.69	1.51	1.48
2	B	500	FAD	C1'-N10	2.79	1.51	1.48
2	C	500	FAD	C2A-N3A	2.80	1.37	1.32
2	B	500	FAD	C4-N3	3.01	1.38	1.33
2	A	500	FAD	C4-N3	3.22	1.39	1.33
2	B	500	FAD	C2A-N3A	3.26	1.38	1.32
2	D	500	FAD	C2A-N3A	3.30	1.38	1.32
2	A	500	FAD	C2A-N3A	3.40	1.38	1.32
2	D	500	FAD	C4-N3	3.46	1.39	1.33
2	D	500	FAD	C4X-N5	3.48	1.38	1.33
2	C	500	FAD	C4X-N5	3.75	1.39	1.33
2	A	500	FAD	C4X-N5	3.76	1.39	1.33
2	C	500	FAD	C1'-N10	3.94	1.52	1.48
2	B	500	FAD	C4X-N5	4.08	1.39	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	N3A-C2A-N1A	-14.41	117.86	128.89
2	D	500	FAD	N3A-C2A-N1A	-11.69	119.94	128.89
2	A	500	FAD	N3A-C2A-N1A	-11.65	119.98	128.89
2	B	500	FAD	N3A-C2A-N1A	-11.07	120.42	128.89
2	C	500	FAD	C4X-C4-N3	-3.70	118.53	123.59
2	D	500	FAD	C4X-C4-N3	-3.43	118.89	123.59
2	C	500	FAD	C2B-C1B-N9A	-3.03	109.66	114.29
2	A	500	FAD	C4X-C4-N3	-2.95	119.56	123.59
2	B	500	FAD	C4X-C4-N3	-2.66	119.95	123.59
2	A	500	FAD	C4A-C5A-N7A	-2.24	107.42	109.48
2	B	500	FAD	O4'-C4'-C5'	-2.15	105.51	110.19
2	A	500	FAD	O4'-C4'-C5'	-2.02	105.80	110.19
2	D	500	FAD	C5X-C9A-N10	2.01	119.14	117.62
3	D	600	N6C	O1-N1-C1	2.03	123.39	119.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	C4-C4X-N5	2.12	121.29	118.72
2	A	500	FAD	C5X-C9A-N10	2.20	119.29	117.62
2	C	500	FAD	C5X-C9A-N10	2.31	119.37	117.62
2	A	500	FAD	C1'-N10-C9A	2.56	121.73	118.86
2	D	500	FAD	O2A-PA-O3P	2.68	117.24	105.09
2	C	500	FAD	C4X-N5-C5X	2.84	120.03	116.76
2	B	500	FAD	C4-C4X-N5	3.01	122.38	118.72
2	D	500	FAD	C4X-N5-C5X	3.33	120.60	116.76
2	B	500	FAD	C4X-N5-C5X	3.39	120.66	116.76
2	D	500	FAD	C4-N3-C2	5.31	119.84	115.25
2	B	500	FAD	C4-N3-C2	5.67	120.14	115.25
2	A	500	FAD	C4-N3-C2	5.80	120.26	115.25
2	C	500	FAD	C4-N3-C2	7.45	121.68	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	FAD	3	0
3	A	600	N6C	2	0
4	A	701	GOL	1	0
2	B	500	FAD	7	0
3	B	600	N6C	3	0
4	B	701	GOL	1	0
2	C	500	FAD	6	0
3	C	600	N6C	4	0
4	C	701	GOL	1	0
2	D	500	FAD	3	0
4	D	701	GOL	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	431/438 (98%)	0.04	19 (4%) 38 37	30, 44, 59, 68	1 (0%)
1	B	431/438 (98%)	0.15	24 (5%) 28 27	32, 47, 62, 74	1 (0%)
1	C	430/438 (98%)	-0.21	3 (0%) 89 88	29, 40, 56, 67	1 (0%)
1	D	430/438 (98%)	-0.16	9 (2%) 67 65	31, 40, 54, 62	2 (0%)
All	All	1722/1752 (98%)	-0.04	55 (3%) 51 50	29, 43, 58, 74	5 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	ASP	4.6
1	A	195	SER	4.0
1	B	223	LYS	3.7
1	B	202	VAL	3.5
1	B	36	LYS	3.5
1	A	367	VAL	3.5
1	D	36	LYS	3.5
1	A	196	LYS	3.4
1	B	365	VAL	3.3
1	B	371	ILE	3.3
1	A	371	ILE	3.3
1	B	395	VAL	3.2
1	A	192	ASP	3.1
1	B	370	VAL	3.0
1	B	367	VAL	2.9
1	B	196	LYS	2.8
1	B	203	ASP	2.8
1	B	195	SER	2.8
1	B	366	ALA	2.7
1	A	222	LYS	2.7
1	B	363	THR	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	50	ARG	2.6
1	D	196	LYS	2.6
1	A	155	ARG	2.5
1	A	193	ASP	2.5
1	B	224	ASP	2.5
1	C	367	VAL	2.5
1	D	197	PRO	2.5
1	A	164	SER	2.5
1	A	194	PRO	2.5
1	A	370	VAL	2.5
1	A	396	MET	2.5
1	B	157	VAL	2.5
1	C	50	ARG	2.5
1	D	365	VAL	2.4
1	B	201	ASN	2.4
1	D	369	CYS	2.4
1	B	360	ILE	2.4
1	B	280	VAL	2.3
1	A	201	ASN	2.3
1	B	178	TYR	2.3
1	A	365	VAL	2.3
1	A	392	LEU	2.3
1	D	367	VAL	2.2
1	B	218	ILE	2.2
1	A	395	VAL	2.2
1	B	362	THR	2.2
1	A	30	ALA	2.2
1	B	124	GLU	2.1
1	D	224	ASP	2.1
1	D	195	SER	2.1
1	A	248	THR	2.1
1	D	321	ILE	2.0
1	B	23	THR	2.0
1	C	365	VAL	2.0

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

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

### 6.3 Carbohydrates [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
4	GOL	D	701	6/6	0.94	0.24	4.15	58,61,61,62	0
3	N6C	D	600	9/9	0.91	0.20	2.52	50,52,54,55	0
4	GOL	C	701	6/6	0.92	0.12	2.51	44,47,48,50	0
3	N6C	A	600	9/9	0.90	0.18	1.98	55,57,58,58	0
3	N6C	C	600	9/9	0.89	0.20	1.83	48,51,55,56	0
4	GOL	B	701	6/6	0.86	0.18	1.79	64,66,67,67	0
4	GOL	A	701	6/6	0.96	0.13	1.27	53,56,57,59	0
3	N6C	B	600	9/9	0.92	0.17	0.76	55,56,60,61	0
4	GOL	A	700	6/6	0.92	0.11	0.64	46,48,49,50	0
4	GOL	B	700	6/6	0.97	0.11	0.22	43,44,44,46	0
2	FAD	C	500	53/53	0.98	0.11	-0.69	31,37,39,40	0
2	FAD	D	500	53/53	0.97	0.08	-0.69	33,37,39,39	0
2	FAD	B	500	53/53	0.97	0.08	-0.88	36,41,46,46	0
2	FAD	A	500	53/53	0.97	0.09	-0.99	35,38,40,41	0
4	GOL	D	700	6/6	0.96	0.07	-1.53	42,43,43,44	0
4	GOL	C	700	6/6	0.98	0.07	-1.62	38,39,40,41	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.