



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:12 am GMT

PDB ID : 2VQ7  
Title : BACTERIAL FLAVIN-CONTAINING MONOOXYGENASE IN COMPLEX  
WITH NADP: NATIVE DATA  
Authors : Alfieri, A.; Malito, E.; Orru, R.; Fraaije, M.W.; Mattevi, A.  
Deposited on : 2008-03-12  
Resolution : 2.60 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

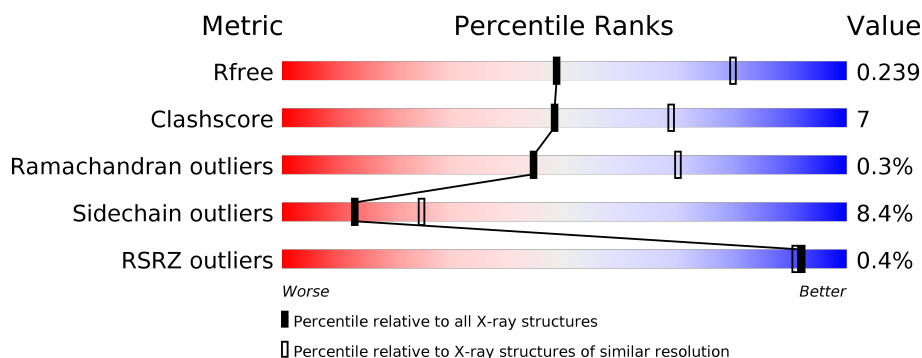
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	461	
1	B	461	
1	C	461	
1	D	461	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EPE	A	1454	-	-	-	X
5	EPE	A	1455	-	-	-	X
5	EPE	C	1456	-	-	X	X
5	EPE	D	1454	-	-	-	X
6	PGE	A	1456	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15184 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 FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			
1	B	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			
1	C	445	Total	C	N	O	S	0	0	0
			3655	2345	606	684	20			
1	D	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			

There are 8 discrepancies between the modelled and reference sequences:

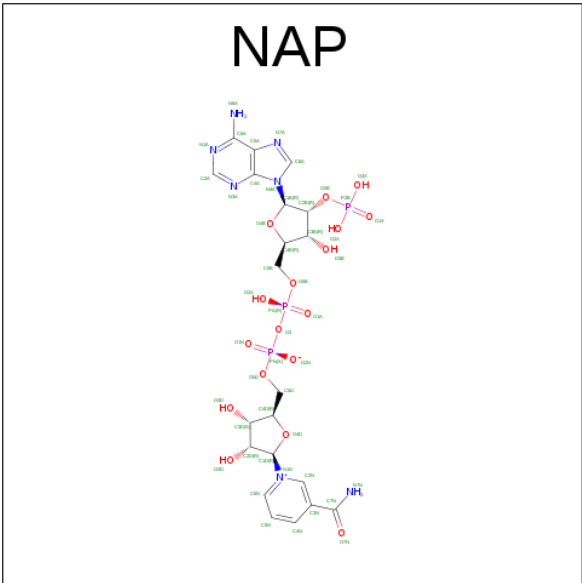
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
A	159	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
B	158	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
B	159	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
C	158	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
C	159	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
D	158	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4
D	159	ALA	GLU	ENGINEERED MUTATION	UNP Q83XK4

- 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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

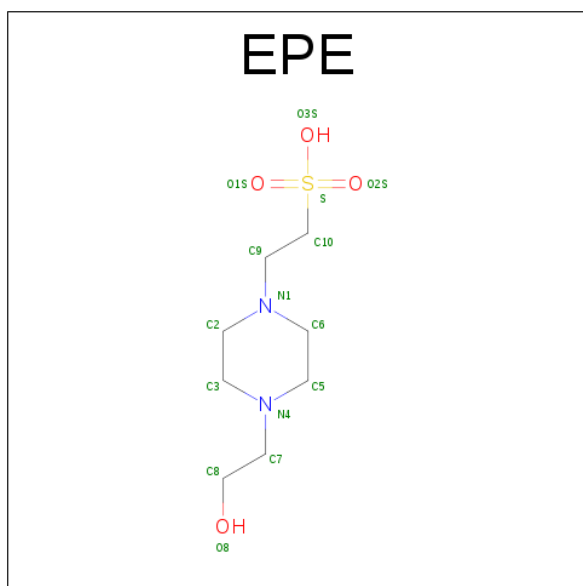


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



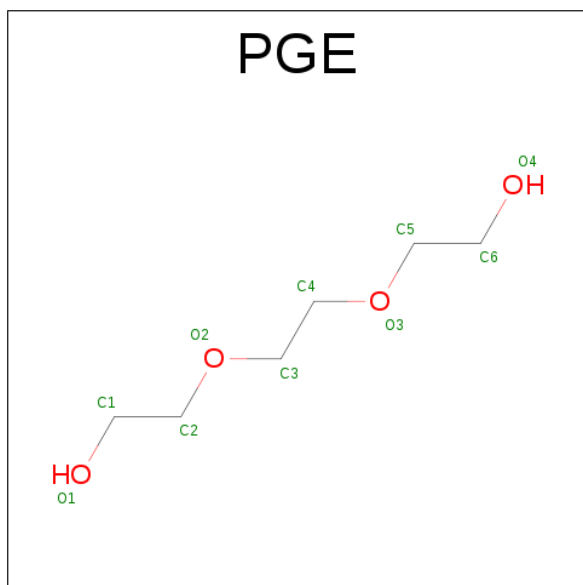
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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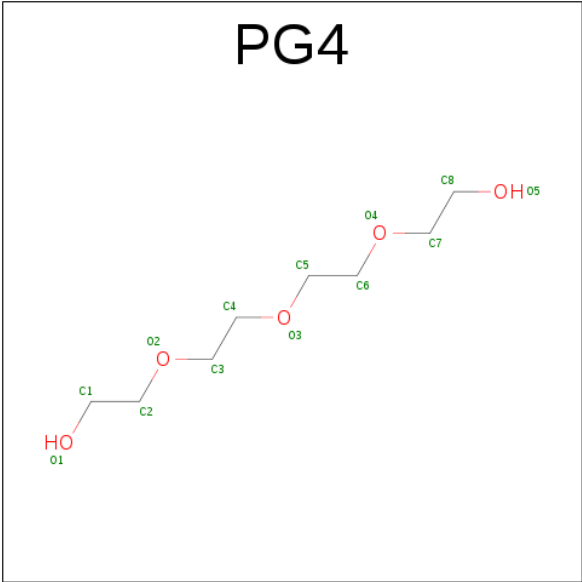
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

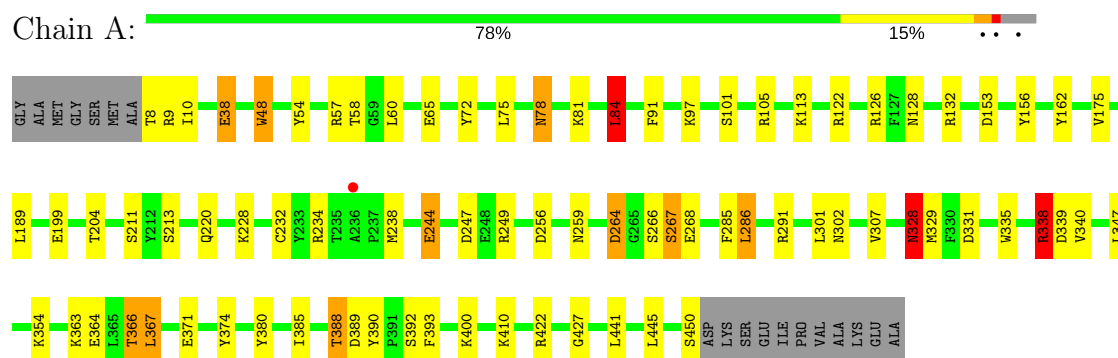
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total	O	0	0
			41	41		
8	B	33	Total	O	0	0
			33	33		
8	C	26	Total	O	0	0
			26	26		
8	D	24	Total	O	0	0
			24	24		



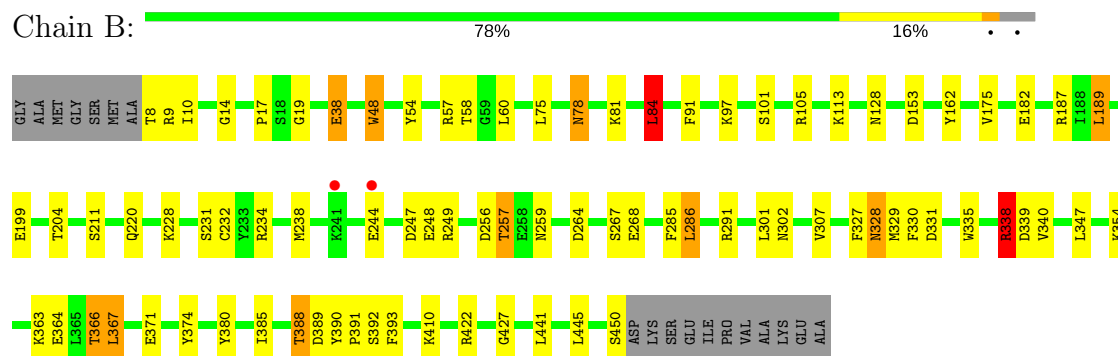
### 3 Residue-property plots [i](#)

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.

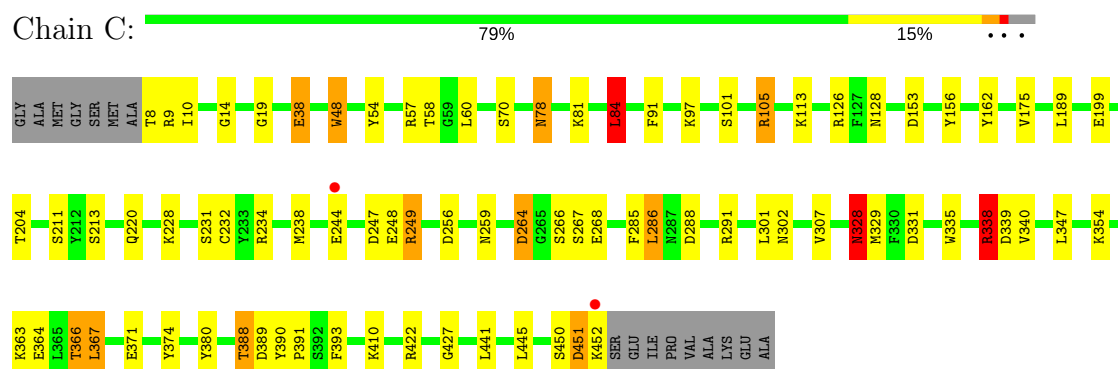
#### • Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



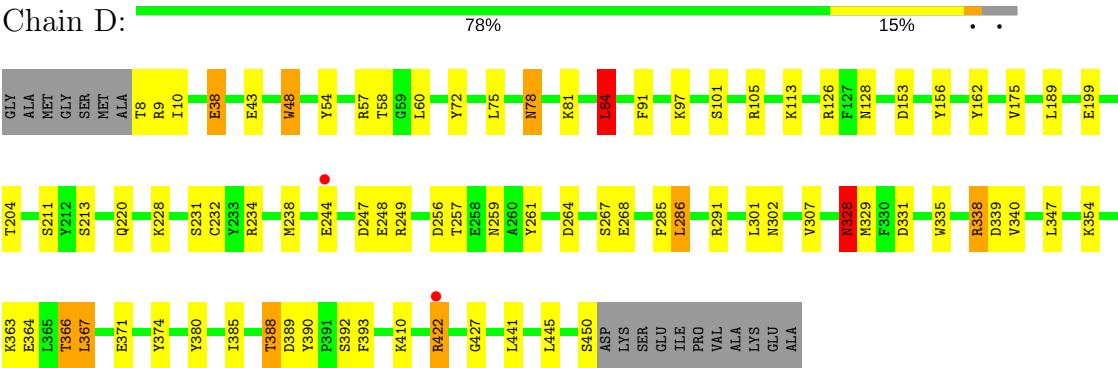
#### • Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



#### • Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



● Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.59Å 219.59Å 133.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	188.98 – 2.60 57.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (188.98-2.60) 98.1 (57.07-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.248 , 0.269 0.226 , 0.239	Depositor DCC
$R_{free}$ test set	5539 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 21.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: PGE, CL, NAP, PG4, EPE, 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	0.60	0/3752	0.68	4/5095 (0.1%)
1	B	0.60	1/3752 (0.0%)	0.68	3/5095 (0.1%)
1	C	0.60	0/3769	0.68	4/5117 (0.1%)
1	D	0.59	0/3752	0.67	3/5095 (0.1%)
All	All	0.59	1/15025 (0.0%)	0.68	14/20402 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLU	CG-CD	5.06	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	338	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	338	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	445	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	84	LEU	CA-CB-CG	5.93	128.94	115.30
1	D	445	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	445	LEU	CA-CB-CG	5.80	128.65	115.30
1	C	445	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	84	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	84	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	338	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	328	ASN	N-CA-CB	-5.37	100.93	110.60
1	A	122	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	328	ASN	N-CA-CB	-5.02	101.56	110.60

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	3638	0	3428	49	0
1	B	3638	0	3428	48	0
1	C	3655	0	3445	53	0
1	D	3638	0	3428	49	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	1	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	30	0	35	10	0
5	C	15	0	17	8	0
5	D	15	0	18	6	0
6	A	10	0	14	0	0
7	B	13	0	18	0	0
8	A	41	0	0	3	0
8	B	33	0	0	1	0
8	C	26	0	0	1	0
8	D	24	0	0	1	0
All	All	15184	0	14055	200	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 7.

All (200) 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)
5:A:1454:EPE:H51	5:A:1454:EPE:O8	1.52	1.08
5:C:1456:EPE:C5	5:C:1456:EPE:O8	2.18	0.90
1:A:388:THR:HG22	1:A:390:TYR:H	1.38	0.88
5:C:1456:EPE:H52	5:C:1456:EPE:O8	1.71	0.88
1:C:388:THR:HG22	1:C:390:TYR:H	1.40	0.86
1:D:388:THR:HG22	1:D:390:TYR:H	1.43	0.81
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.16	0.81
1:A:390:TYR:O	8:A:2035:HOH:O	2.02	0.78
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.20	0.77
1:B:388:THR:HG22	1:B:390:TYR:H	1.48	0.76
1:B:285:PHE:CD1	1:B:286:LEU:HD13	2.22	0.75
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.21	0.75
1:B:390:TYR:O	8:B:2027:HOH:O	2.06	0.74
1:A:388:THR:CG2	1:A:390:TYR:H	2.00	0.72
1:B:57:ARG:NH2	1:C:175:VAL:O	2.22	0.72
1:C:388:THR:CG2	1:C:390:TYR:H	2.03	0.71
1:D:126:ARG:NH1	5:D:1454:EPE:H91	2.06	0.70
1:A:57:ARG:NH2	1:D:175:VAL:O	2.23	0.70
1:A:363:LYS:O	1:A:366:THR:HB	1.93	0.69
1:C:335:TRP:HB3	1:C:388:THR:HG21	1.75	0.69
1:B:175:VAL:O	1:C:57:ARG:NH2	2.26	0.68
1:B:363:LYS:O	1:B:366:THR:HB	1.94	0.67
1:C:390:TYR:O	8:C:2024:HOH:O	2.11	0.67
1:D:363:LYS:O	1:D:366:THR:HB	1.95	0.66
1:D:388:THR:CG2	1:D:390:TYR:H	2.07	0.66
1:B:422:ARG:HD3	1:B:427:GLY:O	1.96	0.66
1:B:335:TRP:HB3	1:B:388:THR:HG21	1.78	0.65
1:B:329:MET:HE2	1:B:380:TYR:HE2	1.61	0.65
1:A:256:ASP:HB3	1:A:259:ASN:H	1.61	0.65
1:C:363:LYS:O	1:C:366:THR:HB	1.96	0.65
1:B:388:THR:CG2	1:B:390:TYR:H	2.09	0.65
1:C:422:ARG:HD3	1:C:427:GLY:O	1.96	0.65
1:D:256:ASP:HB3	1:D:259:ASN:H	1.62	0.64
5:A:1454:EPE:C5	5:A:1454:EPE:O8	2.40	0.64
1:A:175:VAL:O	1:D:57:ARG:NH2	2.30	0.64
1:B:256:ASP:HB3	1:B:259:ASN:H	1.62	0.64
1:C:256:ASP:HB3	1:C:259:ASN:H	1.62	0.64
1:C:301:LEU:O	1:C:302:ASN:HB2	1.98	0.63
1:C:81:LYS:HG2	1:C:91:PHE:CE2	2.34	0.63
1:D:335:TRP:HB3	1:D:388:THR:HG21	1.78	0.63
1:A:335:TRP:HB3	1:A:388:THR:HG21	1.80	0.62
1:A:81:LYS:HG2	1:A:91:PHE:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1455:EPE:H51	5:A:1455:EPE:O8	1.99	0.62
1:D:204:THR:HG23	1:D:228:LYS:HB3	1.81	0.62
1:D:422:ARG:HD3	1:D:427:GLY:O	2.00	0.61
1:B:81:LYS:HG2	1:B:91:PHE:CE2	2.35	0.61
1:A:422:ARG:HD3	1:A:427:GLY:O	2.01	0.61
1:D:81:LYS:HG2	1:D:91:PHE:CE2	2.36	0.61
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.83	0.60
1:D:301:LEU:O	1:D:302:ASN:HB2	2.01	0.60
1:A:329:MET:HE2	1:A:380:TYR:HE2	1.67	0.60
1:A:204:THR:HG23	1:A:228:LYS:HB3	1.83	0.60
1:B:10:ILE:HD12	1:B:162:TYR:HB2	1.83	0.60
1:A:244:GLU:HG3	8:A:2023:HOH:O	2.02	0.60
1:A:301:LEU:O	1:A:302:ASN:HB2	2.02	0.59
1:D:390:TYR:O	8:D:2020:HOH:O	2.17	0.59
1:C:204:THR:HG23	1:C:228:LYS:HB3	1.84	0.58
1:D:338:ARG:NH1	1:D:339:ASP:OD1	2.37	0.58
1:B:328:ASN:OD1	1:B:393:PHE:CZ	2.57	0.57
1:C:10:ILE:HD12	1:C:162:TYR:HB2	1.86	0.57
5:C:1456:EPE:O8	5:C:1456:EPE:H51	2.02	0.56
1:A:328:ASN:OD1	1:A:393:PHE:CZ	2.58	0.56
1:A:10:ILE:HD12	1:A:162:TYR:HB2	1.87	0.56
1:B:328:ASN:OD1	1:B:393:PHE:HZ	1.89	0.56
1:B:204:THR:HG23	1:B:228:LYS:HB3	1.87	0.56
1:B:329:MET:HE2	1:B:380:TYR:CE2	2.40	0.56
1:A:338:ARG:NH1	1:A:339:ASP:OD1	2.39	0.55
1:C:451:ASP:O	1:C:452:LYS:HD2	2.06	0.55
5:A:1455:EPE:O3S	1:B:9:ARG:NH2	2.40	0.55
1:D:329:MET:HE2	1:D:380:TYR:HE2	1.71	0.55
5:A:1455:EPE:C5	5:A:1455:EPE:O8	2.55	0.55
1:C:329:MET:HE2	1:C:380:TYR:HE2	1.71	0.54
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.66	0.54
5:A:1454:EPE:H51	5:A:1454:EPE:HO8	1.65	0.54
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.71	0.54
5:D:1454:EPE:O8	5:D:1454:EPE:C5	2.55	0.54
1:B:285:PHE:HD1	1:B:286:LEU:HD13	1.68	0.54
1:A:328:ASN:OD1	1:A:393:PHE:HZ	1.89	0.54
1:B:301:LEU:O	1:B:302:ASN:HB2	2.07	0.53
1:B:338:ARG:NH1	1:B:339:ASP:OD1	2.41	0.53
1:C:328:ASN:OD1	1:C:393:PHE:CZ	2.61	0.53
1:C:126:ARG:NH1	5:C:1456:EPE:H91	2.23	0.53
1:D:328:ASN:OD1	1:D:393:PHE:CZ	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ARG:HH12	5:D:1454:EPE:H91	1.75	0.51
1:C:232:CYS:HA	1:C:249:ARG:O	2.11	0.51
1:C:48:TRP:NE1	1:C:113:LYS:HG2	2.26	0.50
1:B:231:SER:HB2	1:B:248:GLU:HG2	1.93	0.50
1:D:81:LYS:HG2	1:D:91:PHE:CZ	2.47	0.50
1:B:291:ARG:NH2	1:C:153:ASP:OD1	2.41	0.50
1:D:78:ASN:H	1:D:78:ASN:HD22	1.60	0.50
1:A:329:MET:HE2	1:A:380:TYR:CE2	2.46	0.50
1:A:48:TRP:NE1	1:A:113:LYS:HG2	2.27	0.50
1:C:328:ASN:OD1	1:C:393:PHE:HZ	1.92	0.50
1:D:364:GLU:HA	1:D:367:LEU:HD22	1.93	0.50
1:B:81:LYS:HG2	1:B:91:PHE:CZ	2.46	0.50
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.71	0.50
1:D:231:SER:HB2	1:D:248:GLU:HG2	1.94	0.49
1:D:328:ASN:OD1	1:D:393:PHE:HZ	1.94	0.49
1:C:126:ARG:CZ	5:C:1456:EPE:H91	2.43	0.49
1:D:48:TRP:NE1	1:D:113:LYS:HG2	2.28	0.48
1:C:156:TYR:CE1	5:C:1456:EPE:H61	2.49	0.48
1:B:175:VAL:HB	1:C:57:ARG:HH21	1.78	0.48
1:D:81:LYS:O	1:D:84:LEU:HD22	2.12	0.48
1:B:371:GLU:HA	1:B:374:TYR:CZ	2.48	0.48
1:A:81:LYS:HG2	1:A:91:PHE:CZ	2.48	0.48
1:B:422:ARG:CD	1:B:427:GLY:O	2.62	0.48
1:D:81:LYS:HB2	1:D:101:SER:O	2.14	0.48
1:D:211:SER:HB3	3:D:1452:NAP:O1N	2.14	0.47
1:A:156:TYR:CE1	5:A:1454:EPE:H52	2.49	0.47
1:D:385:ILE:HD12	1:D:392:SER:HA	1.96	0.47
1:C:81:LYS:HG2	1:C:91:PHE:CZ	2.48	0.47
1:C:338:ARG:NH1	1:C:339:ASP:OD1	2.44	0.47
1:C:371:GLU:HA	1:C:374:TYR:CZ	2.49	0.47
1:C:231:SER:HB2	1:C:248:GLU:HG2	1.97	0.47
1:A:57:ARG:HH21	1:D:175:VAL:HB	1.80	0.47
1:B:81:LYS:HB2	1:B:101:SER:O	2.15	0.46
5:D:1454:EPE:O8	5:D:1454:EPE:H52	2.15	0.46
1:B:48:TRP:NE1	1:B:113:LYS:HG2	2.31	0.46
1:B:81:LYS:O	1:B:84:LEU:HD22	2.15	0.46
1:B:78:ASN:HD22	1:B:78:ASN:H	1.63	0.46
1:D:156:TYR:CE1	5:D:1454:EPE:H61	2.51	0.46
1:A:81:LYS:HB2	1:A:101:SER:O	2.16	0.46
1:B:153:ASP:OD1	1:C:291:ARG:NH2	2.48	0.46
1:C:267:SER:O	1:C:268:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ARG:HG3	1:D:38:GLU:HB2	1.98	0.46
1:B:267:SER:O	1:B:268:GLU:HG2	2.15	0.45
1:B:57:ARG:HH21	1:C:175:VAL:HB	1.82	0.45
1:A:156:TYR:CD1	5:A:1454:EPE:H52	2.52	0.45
1:A:211:SER:HB3	3:A:1452:NAP:O1N	2.16	0.45
1:C:422:ARG:CD	1:C:427:GLY:O	2.64	0.45
5:D:1454:EPE:O1S	5:D:1454:EPE:H62	2.17	0.45
1:B:75:LEU:HD11	2:B:1451:FAD:H6	1.98	0.45
1:C:331:ASP:HB3	1:C:390:TYR:CE1	2.52	0.45
1:D:267:SER:O	1:D:268:GLU:HG2	2.17	0.45
1:A:153:ASP:OD1	1:D:291:ARG:NH2	2.47	0.45
1:C:329:MET:HE3	1:C:380:TYR:HD2	1.82	0.45
1:C:81:LYS:O	1:C:84:LEU:HD22	2.17	0.44
1:A:232:CYS:HA	1:A:249:ARG:O	2.18	0.44
1:A:371:GLU:HA	1:A:374:TYR:CZ	2.52	0.44
1:A:78:ASN:HD22	1:A:78:ASN:H	1.64	0.44
1:B:338:ARG:HG3	1:B:339:ASP:N	2.31	0.44
1:B:54:TYR:HB2	1:B:105:ARG:CZ	2.47	0.44
1:C:211:SER:HB3	3:C:1454:NAP:O1N	2.17	0.44
1:C:329:MET:HE2	1:C:380:TYR:CE2	2.51	0.44
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.53	0.44
1:B:232:CYS:HA	1:B:249:ARG:O	2.18	0.44
1:B:364:GLU:HA	1:B:367:LEU:HD22	1.99	0.44
1:D:72:TYR:OH	3:D:1452:NAP:H4N	2.17	0.44
1:A:385:ILE:HD12	1:A:392:SER:HA	2.00	0.43
1:C:329:MET:HE3	1:C:380:TYR:CD2	2.53	0.43
1:D:331:ASP:HB3	1:D:390:TYR:CE1	2.54	0.43
1:B:211:SER:HB3	3:B:1452:NAP:O1N	2.18	0.43
1:B:385:ILE:HD12	1:B:392:SER:HA	1.99	0.43
1:C:126:ARG:NH2	5:C:1456:EPE:H91	2.34	0.43
1:C:78:ASN:H	1:C:78:ASN:HD22	1.65	0.43
1:D:329:MET:HE3	1:D:380:TYR:HD2	1.84	0.43
1:D:371:GLU:HA	1:D:374:TYR:CZ	2.53	0.43
1:C:9:ARG:HG3	1:C:38:GLU:HB2	2.00	0.43
1:D:75:LEU:HD11	2:D:1451:FAD:H6	2.00	0.43
1:C:81:LYS:HB2	1:C:101:SER:O	2.19	0.43
1:A:75:LEU:HD11	2:A:1451:FAD:H6	2.01	0.43
1:D:329:MET:HE2	1:D:380:TYR:CE2	2.52	0.43
1:C:338:ARG:HG3	1:C:339:ASP:N	2.33	0.43
1:A:65:GLU:OE2	1:A:132:ARG:NH2	2.52	0.42
1:D:232:CYS:HA	1:D:249:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:O	1:A:84:LEU:HD22	2.19	0.42
1:A:126:ARG:NH1	5:A:1454:EPE:H91	2.34	0.42
1:A:213:SER:HA	3:A:1452:NAP:H5N	2.02	0.42
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.94	0.42
1:C:54:TYR:HB2	1:C:105:ARG:CZ	2.50	0.42
1:B:187:ARG:HD3	1:B:189:LEU:HD22	2.00	0.42
1:C:70:SER:HB2	2:C:1453:FAD:HM82	2.02	0.42
1:D:213:SER:HA	3:D:1452:NAP:H5N	2.02	0.42
1:A:364:GLU:HA	1:A:367:LEU:HD22	2.02	0.42
1:A:175:VAL:HB	1:D:57:ARG:HH21	1.85	0.42
1:A:385:ILE:O	8:A:2035:HOH:O	2.21	0.41
1:C:264:ASP:HB3	1:C:266:SER:H	1.85	0.41
1:A:267:SER:O	1:A:268:GLU:HG2	2.20	0.41
1:A:9:ARG:HG3	1:A:38:GLU:HB2	2.03	0.41
5:C:1456:EPE:S	5:C:1456:EPE:H62	2.59	0.41
1:A:264:ASP:HB3	1:A:266:SER:H	1.85	0.41
1:D:54:TYR:HB2	1:D:105:ARG:CZ	2.50	0.41
5:A:1455:EPE:H62	5:A:1455:EPE:H102	1.84	0.41
1:D:329:MET:HE3	1:D:380:TYR:CD2	2.54	0.41
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.56	0.41
1:B:9:ARG:HG3	1:B:38:GLU:HB2	2.02	0.41
1:C:288:ASP:OD1	1:C:291:ARG:NH1	2.53	0.41
1:C:390:TYR:HA	1:C:391:PRO:HD3	1.94	0.41
1:D:43:GLU:OE2	2:D:1451:FAD:O2B	2.34	0.41
1:A:291:ARG:NH2	1:D:153:ASP:OD1	2.51	0.41
1:C:14:GLY:O	1:C:19:GLY:HA3	2.20	0.41
1:C:364:GLU:HA	1:C:367:LEU:HD22	2.02	0.41
1:A:54:TYR:HB2	1:A:105:ARG:CZ	2.51	0.40
1:B:256:ASP:OD1	1:B:257:THR:N	2.53	0.40
1:B:327:PHE:HA	1:B:330:PHE:CD2	2.55	0.40
1:C:213:SER:HA	3:C:1454:NAP:H5N	2.02	0.40
1:A:422:ARG:CD	1:A:427:GLY:O	2.69	0.40
1:A:72:TYR:OH	3:A:1452:NAP:H4N	2.21	0.40
1:D:256:ASP:HB2	1:D:261:TYR:HE1	1.87	0.40
1:B:14:GLY:O	1:B:19:GLY:HA3	2.22	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	441/461 (96%)	414 (94%)	25 (6%)	2 (0%)	32	58
1	B	441/461 (96%)	415 (94%)	25 (6%)	1 (0%)	51	76
1	C	443/461 (96%)	421 (95%)	20 (4%)	2 (0%)	32	58
1	D	441/461 (96%)	416 (94%)	24 (5%)	1 (0%)	51	76
All	All	1766/1844 (96%)	1666 (94%)	94 (5%)	6 (0%)	44	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ASP
1	B	389	ASP
1	C	389	ASP
1	D	389	ASP
1	C	328	ASN
1	A	328	ASN

### 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	385/397 (97%)	353 (92%)	32 (8%)	13	25
1	B	385/397 (97%)	353 (92%)	32 (8%)	13	25
1	C	387/397 (98%)	354 (92%)	33 (8%)	12	24
1	D	385/397 (97%)	353 (92%)	32 (8%)	13	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1542/1588 (97%)	1413 (92%)	129 (8%)	13	25

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	38	GLU
1	A	48	TRP
1	A	58	THR
1	A	60	LEU
1	A	78	ASN
1	A	84	LEU
1	A	97	LYS
1	A	128	ASN
1	A	189	LEU
1	A	199	GLU
1	A	220	GLN
1	A	234	ARG
1	A	238	MET
1	A	244	GLU
1	A	247	ASP
1	A	264	ASP
1	A	267	SER
1	A	286	LEU
1	A	307	VAL
1	A	328	ASN
1	A	338	ARG
1	A	340	VAL
1	A	347	LEU
1	A	354	LYS
1	A	366	THR
1	A	367	LEU
1	A	388	THR
1	A	400	LYS
1	A	410	LYS
1	A	441	LEU
1	A	450	SER
1	B	8	THR
1	B	17	PRO
1	B	38	GLU
1	B	48	TRP
1	B	58	THR

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	78	ASN
1	B	84	LEU
1	B	97	LYS
1	B	128	ASN
1	B	189	LEU
1	B	199	GLU
1	B	220	GLN
1	B	234	ARG
1	B	238	MET
1	B	244	GLU
1	B	247	ASP
1	B	257	THR
1	B	264	ASP
1	B	286	LEU
1	B	307	VAL
1	B	328	ASN
1	B	338	ARG
1	B	340	VAL
1	B	347	LEU
1	B	354	LYS
1	B	366	THR
1	B	367	LEU
1	B	388	THR
1	B	410	LYS
1	B	441	LEU
1	B	450	SER
1	C	8	THR
1	C	38	GLU
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	78	ASN
1	C	84	LEU
1	C	97	LYS
1	C	105	ARG
1	C	128	ASN
1	C	189	LEU
1	C	199	GLU
1	C	220	GLN
1	C	234	ARG
1	C	238	MET

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Mol	Chain	Res	Type
1	C	244	GLU
1	C	247	ASP
1	C	249	ARG
1	C	264	ASP
1	C	286	LEU
1	C	307	VAL
1	C	328	ASN
1	C	338	ARG
1	C	340	VAL
1	C	347	LEU
1	C	354	LYS
1	C	366	THR
1	C	367	LEU
1	C	388	THR
1	C	410	LYS
1	C	441	LEU
1	C	450	SER
1	C	451	ASP
1	D	8	THR
1	D	38	GLU
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	78	ASN
1	D	84	LEU
1	D	97	LYS
1	D	128	ASN
1	D	189	LEU
1	D	199	GLU
1	D	220	GLN
1	D	234	ARG
1	D	238	MET
1	D	244	GLU
1	D	247	ASP
1	D	257	THR
1	D	264	ASP
1	D	286	LEU
1	D	307	VAL
1	D	328	ASN
1	D	338	ARG
1	D	340	VAL
1	D	347	LEU

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Mol	Chain	Res	Type
1	D	354	LYS
1	D	366	THR
1	D	367	LEU
1	D	388	THR
1	D	410	LYS
1	D	422	ARG
1	D	441	LEU
1	D	450	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	128	ASN
1	A	148	GLN
1	A	328	ASN
1	B	63	ASN
1	B	128	ASN
1	B	148	GLN
1	B	328	ASN
1	C	63	ASN
1	C	78	ASN
1	C	128	ASN
1	C	148	GLN
1	C	328	ASN
1	D	63	ASN
1	D	78	ASN
1	D	128	ASN
1	D	148	GLN
1	D	328	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 4 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	FAD	A	1451	-	51,58,58	1.31	7 (13%)	54,89,89	1.90	7 (12%)
3	NAP	A	1452	-	44,52,52	1.43	6 (13%)	51,80,80	1.78	9 (17%)
5	EPE	A	1454	-	15,15,15	1.25	1 (6%)	18,20,20	2.47	6 (33%)
5	EPE	A	1455	-	15,15,15	1.09	1 (6%)	18,20,20	2.79	8 (44%)
6	PGE	A	1456	-	9,9,9	0.55	0	8,8,8	0.16	0
2	FAD	B	1451	-	51,58,58	1.33	5 (9%)	54,89,89	2.04	8 (14%)
3	NAP	B	1452	-	44,52,52	1.41	4 (9%)	51,80,80	1.88	9 (17%)
7	PG4	B	1453	-	12,12,12	0.63	0	11,11,11	0.23	0
2	FAD	C	1453	-	51,58,58	1.28	5 (9%)	54,89,89	2.21	8 (14%)
3	NAP	C	1454	-	44,52,52	1.37	6 (13%)	51,80,80	1.72	7 (13%)
5	EPE	C	1456	-	15,15,15	1.17	1 (6%)	18,20,20	2.48	5 (27%)
2	FAD	D	1451	-	51,58,58	1.33	6 (11%)	54,89,89	2.09	8 (14%)
3	NAP	D	1452	-	44,52,52	1.28	5 (11%)	51,80,80	1.79	9 (17%)
5	EPE	D	1454	-	15,15,15	1.17	1 (6%)	18,20,20	2.61	6 (33%)

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	1451	-	-	0/28/50/50	0/6/6/6
3	NAP	A	1452	-	-	0/27/67/67	0/5/5/5
5	EPE	A	1454	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	A	1455	-	-	0/9/19/19	0/1/1/1
6	PGE	A	1456	-	-	0/7/7/7	0/0/0/0
2	FAD	B	1451	-	-	0/28/50/50	0/6/6/6
3	NAP	B	1452	-	-	0/27/67/67	0/5/5/5
7	PG4	B	1453	-	-	0/10/10/10	0/0/0/0
2	FAD	C	1453	-	-	0/28/50/50	0/6/6/6
3	NAP	C	1454	-	-	0/27/67/67	0/5/5/5
5	EPE	C	1456	-	-	0/9/19/19	0/1/1/1
2	FAD	D	1451	-	-	0/28/50/50	0/6/6/6
3	NAP	D	1452	-	-	0/27/67/67	0/5/5/5
5	EPE	D	1454	-	-	0/9/19/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1451	FAD	O4B-C4B	-2.01	1.40	1.45
3	C	1454	NAP	C4N-C3N	2.02	1.42	1.39
3	B	1452	NAP	P2B-O2X	2.04	1.63	1.54
3	C	1454	NAP	C7N-N7N	2.06	1.37	1.33
3	C	1454	NAP	C2N-C3N	2.07	1.42	1.39
3	D	1452	NAP	P2B-O2X	2.09	1.63	1.54
2	A	1451	FAD	C2A-N1A	2.17	1.38	1.33
3	B	1452	NAP	P2B-O1X	2.18	1.58	1.50
3	A	1452	NAP	P2B-O3X	2.19	1.63	1.54
3	C	1454	NAP	P2B-O2X	2.23	1.64	1.54
2	D	1451	FAD	C2A-N1A	2.27	1.38	1.33
2	A	1451	FAD	C4-N3	2.27	1.37	1.33
3	A	1452	NAP	P2B-O2B	2.40	1.63	1.59
3	A	1452	NAP	C7N-N7N	2.47	1.37	1.33
3	D	1452	NAP	C2N-C3N	2.56	1.42	1.39
2	D	1451	FAD	C4-N3	2.57	1.37	1.33
2	C	1453	FAD	C5X-N5	2.60	1.39	1.35
3	D	1452	NAP	P2B-O2B	2.68	1.64	1.59
2	D	1451	FAD	C1'-N10	2.70	1.51	1.48
2	B	1451	FAD	C1'-N10	2.85	1.51	1.48
3	D	1452	NAP	O4D-C1D	2.92	1.45	1.41
2	C	1453	FAD	C4-N3	3.01	1.38	1.33
2	C	1453	FAD	C4X-N5	3.09	1.37	1.33
2	C	1453	FAD	C10-N1	3.13	1.37	1.33
3	D	1452	NAP	O4B-C1B	3.15	1.45	1.41
2	B	1451	FAD	C4X-N5	3.18	1.37	1.33
2	A	1451	FAD	C10-N1	3.20	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1451	FAD	C4-N3	3.24	1.38	1.33
2	A	1451	FAD	C4X-N5	3.38	1.38	1.33
2	D	1451	FAD	C4X-N5	3.39	1.38	1.33
2	A	1451	FAD	C1'-N10	3.40	1.51	1.48
2	A	1451	FAD	C2A-N3A	3.48	1.38	1.32
2	B	1451	FAD	C2A-N3A	3.63	1.38	1.32
3	A	1452	NAP	O4B-C1B	3.63	1.46	1.41
3	C	1454	NAP	O4B-C1B	3.69	1.46	1.41
3	B	1452	NAP	O4D-C1D	3.71	1.46	1.41
3	A	1452	NAP	O4D-C1D	3.73	1.46	1.41
5	A	1455	EPE	C10-S	3.75	1.83	1.77
3	C	1454	NAP	O4D-C1D	3.79	1.46	1.41
5	D	1454	EPE	C10-S	3.88	1.83	1.77
2	B	1451	FAD	C10-N1	3.91	1.38	1.33
3	A	1452	NAP	P2B-O1X	3.93	1.64	1.50
5	C	1456	EPE	C10-S	3.98	1.83	1.77
2	D	1451	FAD	C10-N1	4.02	1.38	1.33
2	C	1453	FAD	C2A-N3A	4.11	1.39	1.32
5	A	1454	EPE	C10-S	4.14	1.83	1.77
2	D	1451	FAD	C2A-N3A	4.21	1.39	1.32
3	B	1452	NAP	O4B-C1B	5.27	1.48	1.41

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1453	FAD	N3A-C2A-N1A	-11.02	119.26	128.86
2	D	1451	FAD	N3A-C2A-N1A	-10.05	120.10	128.86
2	B	1451	FAD	N3A-C2A-N1A	-10.05	120.11	128.86
2	A	1451	FAD	N3A-C2A-N1A	-9.02	121.00	128.86
3	B	1452	NAP	N3A-C2A-N1A	-8.60	121.37	128.86
3	C	1454	NAP	N3A-C2A-N1A	-8.03	121.86	128.86
3	D	1452	NAP	N3A-C2A-N1A	-7.76	122.10	128.86
3	A	1452	NAP	N3A-C2A-N1A	-7.23	122.56	128.86
3	D	1452	NAP	C4B-O4B-C1B	-4.88	104.57	109.77
3	B	1452	NAP	C4B-O4B-C1B	-3.73	105.80	109.77
3	C	1454	NAP	C4B-O4B-C1B	-3.71	105.83	109.77
3	A	1452	NAP	C4B-O4B-C1B	-3.49	106.05	109.77
3	C	1454	NAP	C3B-C2B-C1B	-3.30	96.29	102.75
2	A	1451	FAD	C4A-C5A-N7A	-3.19	106.33	109.41
3	A	1452	NAP	C3B-C2B-C1B	-2.98	96.92	102.75
3	B	1452	NAP	O7N-C7N-N7N	-2.88	118.48	122.58
3	D	1452	NAP	C3B-C2B-C1B	-2.87	97.14	102.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1452	NAP	C3B-C2B-C1B	-2.86	97.16	102.75
3	B	1452	NAP	O3D-C3D-C2D	-2.83	102.77	111.83
2	B	1451	FAD	C4A-C5A-N7A	-2.83	106.68	109.41
2	C	1453	FAD	C4A-C5A-N7A	-2.77	106.73	109.41
2	C	1453	FAD	C4X-C4-N3	-2.66	119.70	123.48
3	D	1452	NAP	O7N-C7N-N7N	-2.49	119.04	122.58
3	D	1452	NAP	C4A-C5A-N7A	-2.46	107.03	109.41
3	B	1452	NAP	C4A-C5A-N7A	-2.44	107.05	109.41
3	C	1454	NAP	C4A-C5A-N7A	-2.40	107.09	109.41
3	D	1452	NAP	O2D-C2D-C1D	-2.40	104.10	111.61
2	D	1451	FAD	C4A-C5A-N7A	-2.39	107.10	109.41
3	A	1452	NAP	C4A-C5A-N7A	-2.32	107.17	109.41
3	A	1452	NAP	O7N-C7N-N7N	-2.29	119.32	122.58
3	B	1452	NAP	O2D-C2D-C1D	-2.29	104.46	111.61
3	C	1454	NAP	O3D-C3D-C2D	-2.28	104.53	111.83
3	A	1452	NAP	O3D-C3D-C2D	-2.28	104.53	111.83
2	B	1451	FAD	C4X-C4-N3	-2.28	120.24	123.48
2	D	1451	FAD	C4X-C4-N3	-2.22	120.32	123.48
2	A	1451	FAD	C4X-C4-N3	-2.14	120.44	123.48
3	A	1452	NAP	O7N-C7N-C3N	-2.10	117.17	119.62
3	A	1452	NAP	C1B-N9A-C4A	-2.10	123.02	126.64
3	C	1454	NAP	O2D-C2D-C1D	-2.09	105.07	111.61
2	C	1453	FAD	C1'-N10-C10	-2.03	116.42	118.50
3	D	1452	NAP	O3D-C3D-C2D	-2.02	105.37	111.83
3	B	1452	NAP	C2A-N1A-C6A	2.01	122.30	118.77
3	D	1452	NAP	C2A-N1A-C6A	2.18	122.58	118.77
2	B	1451	FAD	C4-C4X-N5	2.18	121.07	118.68
2	D	1451	FAD	C4-C4X-N5	2.25	121.15	118.68
5	A	1455	EPE	C7-N4-C3	2.26	117.06	111.26
2	A	1451	FAD	C5X-C9A-N10	2.41	119.45	117.66
5	A	1455	EPE	C2-C3-N4	2.54	115.78	110.63
2	C	1453	FAD	C5X-C9A-N10	2.63	119.61	117.66
5	A	1455	EPE	C7-N4-C5	2.66	118.09	111.26
5	D	1454	EPE	C7-N4-C5	2.67	118.11	111.26
5	C	1456	EPE	C2-C3-N4	2.75	116.19	110.63
5	D	1454	EPE	C7-N4-C3	2.78	118.38	111.26
5	A	1454	EPE	C7-N4-C5	2.87	118.61	111.26
2	D	1451	FAD	C5X-C9A-N10	2.88	119.80	117.66
2	B	1451	FAD	C5X-C9A-N10	2.93	119.83	117.66
5	A	1455	EPE	C6-C5-N4	2.95	116.59	110.63
5	C	1456	EPE	O2S-S-C10	2.99	109.36	106.79
2	C	1453	FAD	C4X-N5-C5X	3.13	120.06	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1455	EPE	C6-N1-C2	3.13	115.96	108.87
2	A	1451	FAD	C4X-N5-C5X	3.31	120.26	116.76
5	C	1456	EPE	C7-N4-C3	3.36	119.87	111.26
2	B	1451	FAD	C4X-N5-C5X	3.37	120.32	116.76
5	D	1454	EPE	C2-C3-N4	3.37	117.45	110.63
3	D	1452	NAP	C3N-C7N-N7N	3.45	121.72	117.77
3	C	1454	NAP	C3N-C7N-N7N	3.58	121.87	117.77
2	D	1451	FAD	C4X-N5-C5X	3.60	120.56	116.76
5	A	1454	EPE	C7-N4-C3	3.61	120.52	111.26
5	D	1454	EPE	O2S-S-C10	3.73	110.00	106.79
5	A	1454	EPE	O1S-S-C10	4.05	110.27	106.79
5	A	1454	EPE	C6-N1-C2	4.28	118.57	108.87
2	A	1451	FAD	C1'-N10-C9A	4.30	122.28	118.35
5	A	1454	EPE	O2S-S-C10	4.31	110.49	106.79
3	B	1452	NAP	C3N-C7N-N7N	4.35	122.74	117.77
5	A	1454	EPE	C5-N4-C3	4.85	119.86	108.87
5	A	1455	EPE	O2S-S-C10	4.93	111.03	106.79
3	A	1452	NAP	C3N-C7N-N7N	5.01	123.49	117.77
2	B	1451	FAD	C1'-N10-C9A	5.08	123.01	118.35
2	B	1451	FAD	C4-N3-C2	5.34	119.83	115.16
5	A	1455	EPE	O1S-S-C10	5.35	111.39	106.79
5	C	1456	EPE	O1S-S-C10	5.58	111.58	106.79
5	D	1454	EPE	O1S-S-C10	5.62	111.62	106.79
2	D	1451	FAD	C1'-N10-C9A	5.63	123.51	118.35
2	A	1451	FAD	C4-N3-C2	5.70	120.14	115.16
2	C	1453	FAD	C1'-N10-C9A	5.84	123.69	118.35
2	D	1451	FAD	C4-N3-C2	5.85	120.27	115.16
5	C	1456	EPE	C5-N4-C3	6.10	122.69	108.87
2	C	1453	FAD	C4-N3-C2	6.16	120.55	115.16
5	D	1454	EPE	C5-N4-C3	6.29	123.11	108.87
5	A	1455	EPE	C5-N4-C3	6.37	123.30	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1451	FAD	1	0
3	A	1452	NAP	3	0
5	A	1454	EPE	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1455	EPE	4	0
2	B	1451	FAD	1	0
3	B	1452	NAP	1	0
2	C	1453	FAD	1	0
3	C	1454	NAP	2	0
5	C	1456	EPE	8	0
2	D	1451	FAD	2	0
3	D	1452	NAP	3	0
5	D	1454	EPE	6	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	443/461 (96%)	-0.33	1 (0%) 94 95	41, 51, 64, 73	0
1	B	443/461 (96%)	-0.30	2 (0%) 90 89	41, 51, 65, 73	0
1	C	445/461 (96%)	-0.26	2 (0%) 92 91	41, 51, 65, 73	0
1	D	443/461 (96%)	-0.19	2 (0%) 90 89	41, 51, 65, 73	0
All	All	1774/1844 (96%)	-0.27	7 (0%) 92 91	41, 51, 65, 73	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	ARG	2.6
1	C	452	LYS	2.5
1	B	241	LYS	2.4
1	B	244	GLU	2.3
1	C	244	GLU	2.1
1	D	244	GLU	2.1
1	A	236	ALA	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
5	EPE	A	1455	15/15	0.74	0.25	9.69	86,88,100,100	0
5	EPE	D	1454	15/15	0.73	0.26	5.10	93,95,106,106	0
5	EPE	C	1456	15/15	0.67	0.29	4.57	87,93,105,105	0
6	PGE	A	1456	10/10	0.73	0.24	4.44	99,101,103,104	0
5	EPE	A	1454	15/15	0.76	0.22	2.06	82,85,99,99	0
7	PG4	B	1453	13/13	0.87	0.16	1.14	60,64,72,72	0
3	NAP	B	1452	48/48	0.96	0.15	0.58	32,36,44,47	0
2	FAD	C	1453	53/53	0.97	0.18	0.45	38,44,46,47	0
3	NAP	D	1452	48/48	0.94	0.16	0.20	32,36,44,47	0
2	FAD	B	1451	53/53	0.97	0.16	0.11	37,45,46,47	0
2	FAD	A	1451	53/53	0.97	0.15	0.11	37,45,46,47	0
3	NAP	A	1452	48/48	0.95	0.15	-0.01	32,36,44,48	0
2	FAD	D	1451	53/53	0.97	0.16	-0.08	38,44,46,47	0
3	NAP	C	1454	48/48	0.96	0.13	-0.47	32,36,44,47	0
4	CL	A	1453	1/1	0.95	0.31	-	58,58,58,58	0
4	CL	B	1454	1/1	0.99	0.35	-	58,58,58,58	0
4	CL	D	1453	1/1	0.97	0.27	-	64,64,64,64	0
4	CL	C	1455	1/1	0.98	0.23	-	56,56,56,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.