



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:53 AM GMT

PDB ID : 2C12
Title : Crystal Structure of Nitroalkane Oxidase in Complex with Spermine, a Competitive Inhibitor
Authors : Nagpal, A.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.
Deposited on : 2005-09-10
Resolution : 2.07 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
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

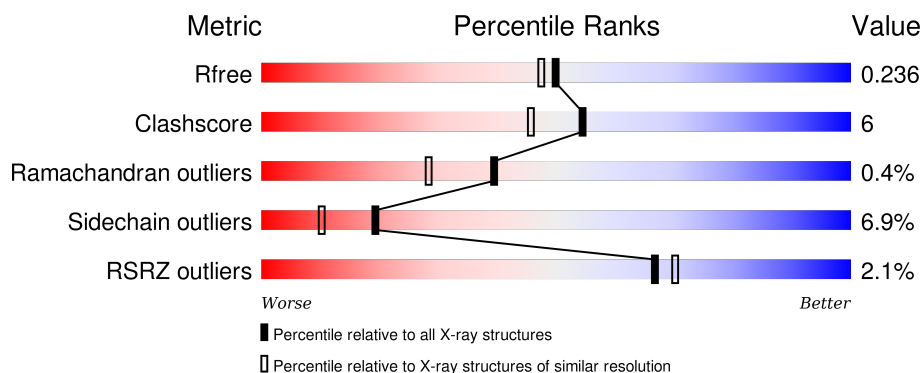
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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 ≥ 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	439	<div> <div>2%</div> <div>82% 13% ..</div> </div>
1	B	439	<div> <div>79% 16% ..</div> </div>
1	C	439	<div> <div>3%</div> <div>81% 14% ..</div> </div>
1	D	439	<div> <div>2%</div> <div>82% 14% ..</div> </div>
1	E	439	<div> <div>2%</div> <div>85% 11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	439	

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	GOL	A	1433	-	-	-	X
3	GOL	B	1434	-	-	-	X
3	GOL	C	1432	-	-	-	X
3	GOL	C	1435	-	-	-	X
3	GOL	C	1437	-	-	-	X
3	GOL	D	1432	-	-	-	X
3	GOL	D	1435	-	-	-	X
3	GOL	D	1437	-	-	-	X
3	GOL	E	1433	-	-	-	X
3	GOL	E	1434	-	-	-	X
3	GOL	E	1435	-	-	-	X
3	GOL	F	1434	-	-	-	X
4	SPM	C	1434	-	-	X	X
4	SPM	D	1434	-	-	-	X
4	SPM	F	1433	-	-	-	X
5	PE4	B	1436	-	-	X	-
5	PE4	F	1435	-	-	X	-

2 Entry composition [i](#)

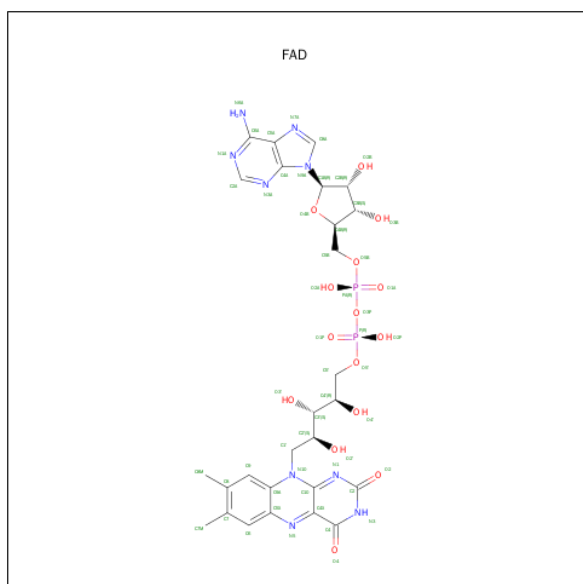
There are 6 unique types of molecules in this entry. The entry contains 21487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

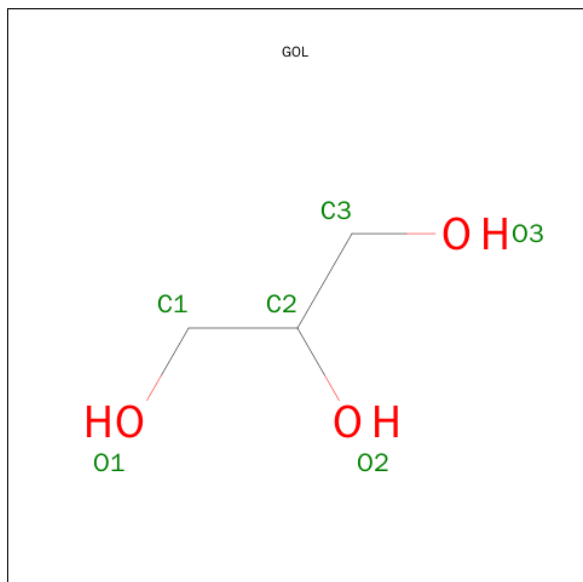
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	B	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	C	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	D	430	Total	C	N	O	S	0	3	0
			3313	2097	568	627	21			
1	E	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	F	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



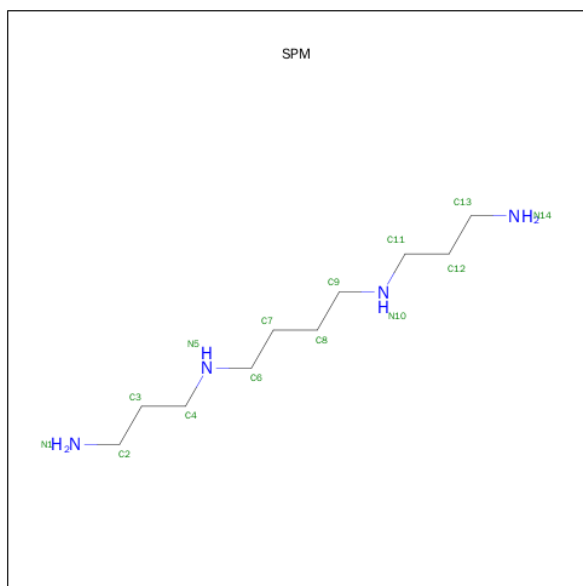
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



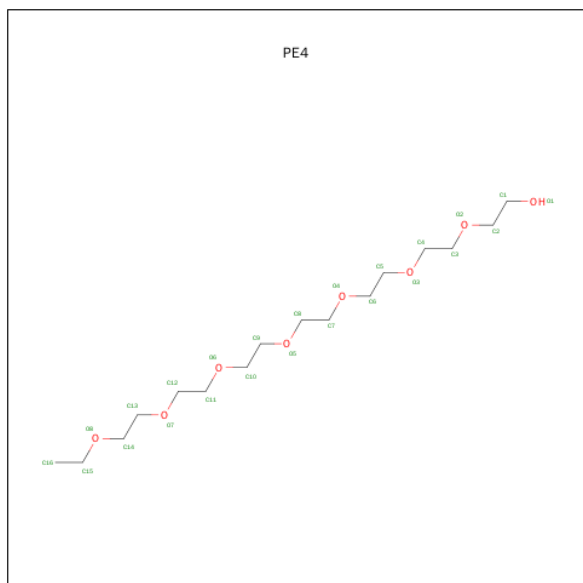
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			14	10	4		
4	C	1	Total	C	N	0	0
			14	10	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	N	0	0
			14	10	4		
4	F	1	Total	C	N	0	0
			14	10	4		

- Molecule 5 is 2-{2-[2-(2-{2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			24	16	8		
5	F	1	Total	C	O	0	0
			24	16	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	207	Total	O	0	0
			207	207		
6	C	164	Total	O	0	0
			164	164		
6	D	159	Total	O	0	0
			159	159		
6	E	187	Total	O	0	0
			187	187		

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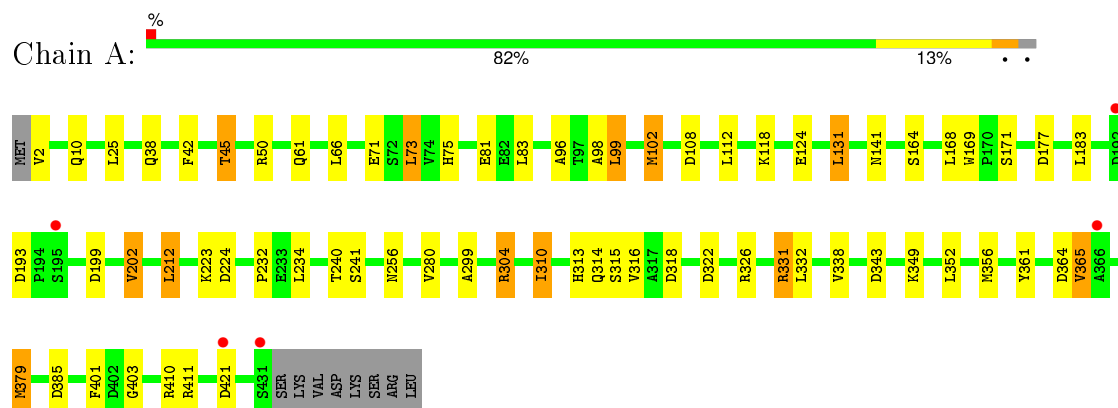
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	205	Total 205	O 205	0	0

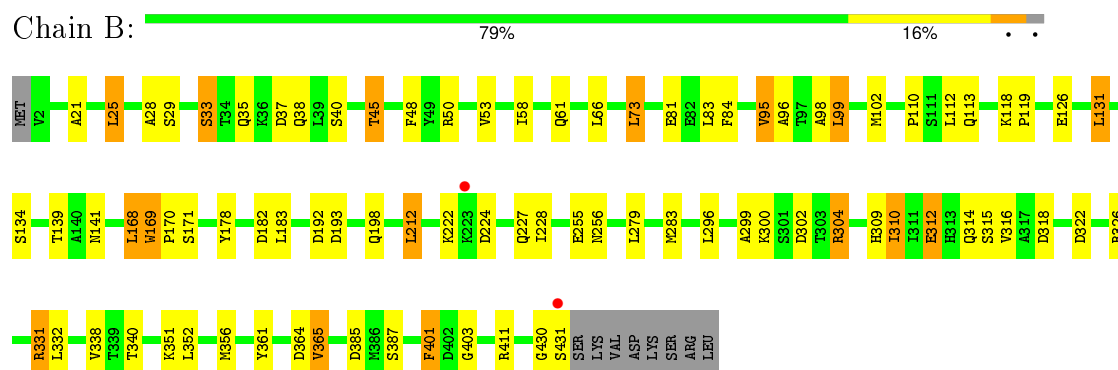
3 Residue-property plots [i](#)

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.

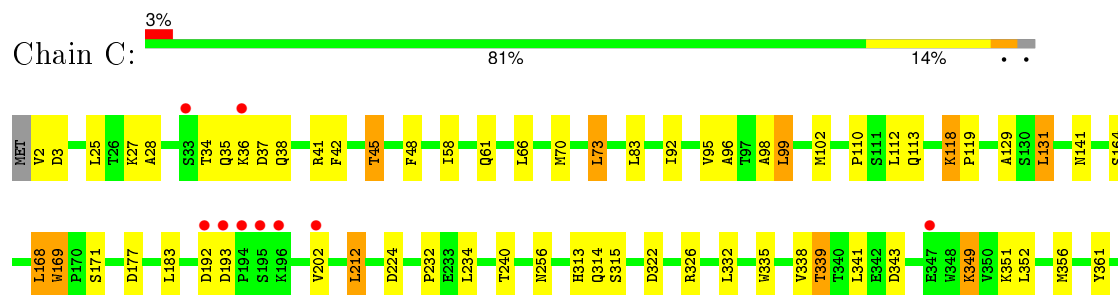
• Molecule 1: NITROALKANE OXIDASE



• Molecule 1: NITROALKANE OXIDASE

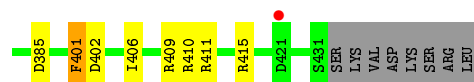
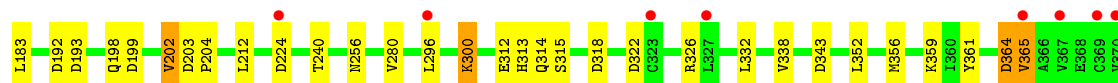
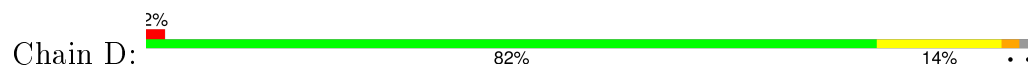


• Molecule 1: NITROALKANE OXIDASE

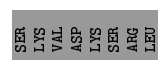
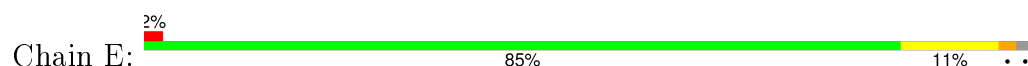




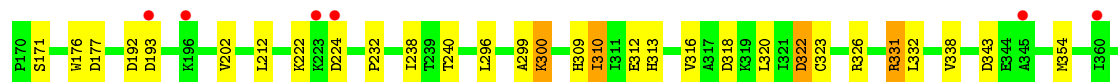
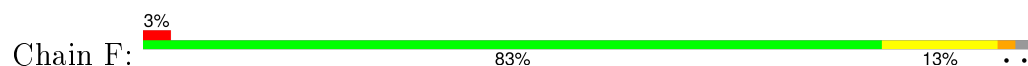
• Molecule 1: NITROALKANE OXIDASE



• 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, α , β , γ	103.39Å 103.39Å 485.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.07 49.24 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.07) 97.8 (49.24-2.07)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.71 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.225 0.199 , 0.236	Depositor DCC
R_{free} test set	9048 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.4	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 180532 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21487	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PE4, GOL, SPM, 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	1/3384 (0.0%)	0.79	13/4592 (0.3%)
1	B	0.53	0/3384	0.80	11/4592 (0.2%)
1	C	0.52	0/3384	0.77	9/4592 (0.2%)
1	D	0.52	0/3398	0.78	15/4611 (0.3%)
1	E	0.53	0/3384	0.75	7/4592 (0.2%)
1	F	0.54	1/3384 (0.0%)	0.80	11/4592 (0.2%)
All	All	0.53	2/20318 (0.0%)	0.78	66/27571 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	MET	SD-CE	-9.42	1.25	1.77
1	F	95	VAL	CB-CG1	-5.23	1.41	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	331	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	D	410	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	F	331	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	D	410	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	331	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	410	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	A	410	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	B	364	ASP	CB-CG-OD2	7.31	124.88	118.30
1	F	224	ASP	CB-CG-OD2	7.25	124.82	118.30
1	B	37	ASP	CB-CG-OD2	7.24	124.82	118.30
1	D	224	ASP	CB-CG-OD2	7.09	124.69	118.30
1	B	331	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	385	ASP	CB-CG-OD2	6.95	124.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	318	ASP	CB-CG-OD2	6.83	124.45	118.30
1	C	224	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	224	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	302	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	364	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	331	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	318	ASP	CB-CG-OD2	6.52	124.17	118.30
1	E	224	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	385	ASP	CB-CG-OD2	6.44	124.09	118.30
1	F	385	ASP	CB-CG-OD2	6.32	123.99	118.30
1	D	322	ASP	CB-CG-OD2	6.13	123.82	118.30
1	E	193	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	385	ASP	CB-CG-OD2	6.11	123.80	118.30
1	F	193	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	193	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	193	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	224	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	318	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	177	ASP	CB-CG-OD2	5.91	123.62	118.30
1	E	385	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	331	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	322	ASP	CB-CG-OD2	5.77	123.50	118.30
1	E	177	ASP	CB-CG-OD2	5.70	123.42	118.30
1	D	343	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	364	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	177	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	108	ASP	CB-CG-OD2	5.63	123.37	118.30
1	F	343	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	3	ASP	CB-CG-OD2	5.60	123.34	118.30
1	D	402	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	343	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	193	ASP	CB-CG-OD2	5.55	123.30	118.30
1	F	318	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	37	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	182	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	203	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	385	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	364	ASP	CB-CG-OD2	5.37	123.13	118.30
1	F	177	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	37	ASP	CB-CG-OD2	5.35	123.12	118.30
1	F	411	ARG	CG-CD-NE	5.33	123.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	37	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	322	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	322	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	203	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	411	ARG	CB-CG-CD	5.21	125.15	111.60
1	A	343	ASP	CB-CG-OD2	5.21	122.98	118.30
1	D	415	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	177	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	182	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	343	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3309	0	3320	45	0
1	B	3309	0	3320	58	0
1	C	3309	0	3320	45	0
1	D	3313	0	3323	34	0
1	E	3309	0	3320	28	0
1	F	3309	0	3320	36	0
2	A	53	0	31	6	0
2	B	53	0	31	8	0
2	C	53	0	31	4	0
2	D	53	0	31	3	0
2	E	53	0	31	3	0
2	F	53	0	31	5	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
3	C	24	0	32	2	0
3	D	24	0	32	2	0
3	E	18	0	24	1	0
3	F	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	26	4	0
4	C	14	0	26	9	0
4	D	14	0	26	0	0
4	F	14	0	26	5	0
5	B	24	0	34	17	0
5	F	24	0	34	9	0
6	A	195	0	0	4	0
6	B	207	0	0	14	0
6	C	164	0	0	7	0
6	D	159	0	0	5	0
6	E	187	0	0	5	0
6	F	205	0	0	14	0
All	All	21487	0	20401	261	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 6.

All (261) 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:B:1436:PE4:H141	6:B:2206:HOH:O	1.29	1.27
6:A:2191:HOH:O	1:B:310:ILE:HG21	1.35	1.23
1:C:141:ASN:HD21	2:C:1433:FAD:H61A	1.19	0.91
1:A:379:MET:HE2	1:B:401:PHE:HA	1.56	0.88
5:F:1435:PE4:H142	6:F:2203:HOH:O	1.75	0.87
1:A:10:GLN:HG3	1:A:75:HIS:CE1	2.09	0.87
1:F:354:MET:SD	6:F:2152:HOH:O	2.34	0.86
1:B:141:ASN:HD21	2:B:1432:FAD:H61A	1.21	0.85
1:D:141:ASN:HD21	2:D:1433:FAD:H61A	1.25	0.83
4:C:1434:SPM:H41	6:C:2164:HOH:O	1.77	0.82
1:A:141:ASN:HD21	2:A:1432:FAD:H61A	1.27	0.81
1:E:141:ASN:HD21	2:E:1432:FAD:H61A	1.31	0.76
1:C:102[A]:MET:HE3	4:C:1434:SPM:C11	2.16	0.76
1:F:137:ASN:OD1	1:F:151:GLN:OE1	2.05	0.74
1:E:73:LEU:HB3	1:E:338:VAL:HB	1.69	0.73
1:F:141:ASN:HD21	2:F:1432:FAD:H61A	1.34	0.73
1:B:29:SER:O	1:B:33:SER:HB2	1.90	0.72
1:C:73:LEU:HB3	1:C:338:VAL:HB	1.73	0.70
1:D:45:THR:HG23	6:D:2031:HOH:O	1.91	0.69
5:B:1436:PE4:H163	6:B:2204:HOH:O	1.93	0.68
1:B:141:ASN:ND2	2:B:1432:FAD:H61A	1.90	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102[A]:MET:HE3	4:C:1434:SPM:H111	1.77	0.66
1:F:81:GLU:OE2	1:F:331:ARG:HD3	1.96	0.65
1:F:73:LEU:HB3	1:F:338:VAL:HB	1.79	0.65
1:A:314:GLN:HE21	1:D:315:SER:H	1.44	0.65
1:A:99:LEU:HD22	1:A:131:LEU:HD23	1.79	0.65
1:C:102[A]:MET:HE3	4:C:1434:SPM:H112	1.79	0.64
1:A:73:LEU:HB3	1:A:338:VAL:HB	1.80	0.64
1:F:99:LEU:HD22	1:F:131:LEU:HD23	1.78	0.64
1:B:73:LEU:HB3	1:B:338:VAL:HB	1.79	0.64
1:F:151:GLN:HG3	6:F:2073:HOH:O	1.99	0.63
1:B:296:LEU:O	1:B:300:LYS:HG3	1.98	0.63
1:E:35:GLN:HE21	1:E:40:SER:HB3	1.63	0.63
1:F:96:ALA:HB1	1:F:171:SER:HB2	1.79	0.63
1:D:141:ASN:ND2	2:D:1433:FAD:H61A	1.95	0.63
1:A:61:GLN:HE21	1:A:98:ALA:HB2	1.63	0.62
1:C:45:THR:CG2	6:C:2040:HOH:O	2.46	0.62
1:A:45:THR:HG23	6:A:2044:HOH:O	2.00	0.62
1:F:95:VAL:HG13	4:F:1433:SPM:C8	2.29	0.61
1:A:379:MET:HE3	2:B:1432:FAD:H2'	1.81	0.61
1:A:326:ARG:HB3	1:A:365:VAL:HG13	1.81	0.61
1:F:38:GLN:HG3	1:F:232:PRO:O	1.99	0.61
1:C:27:LYS:HE2	6:C:2009:HOH:O	2.00	0.61
1:D:99:LEU:HD22	1:D:131:LEU:HD23	1.83	0.60
1:C:38:GLN:HG3	1:C:232:PRO:O	2.02	0.60
1:A:71:GLU:HB2	1:A:75:HIS:CD2	2.37	0.60
1:D:73:LEU:HB3	1:D:338:VAL:HB	1.82	0.60
1:B:96:ALA:HB1	1:B:171:SER:HB2	1.83	0.59
5:F:1435:PE4:C11	6:F:2204:HOH:O	2.49	0.59
1:D:96:ALA:HB1	1:D:171:SER:HB2	1.85	0.59
5:B:1436:PE4:C11	6:B:2206:HOH:O	2.51	0.59
1:C:141:ASN:ND2	2:C:1433:FAD:H61A	1.94	0.59
1:A:379:MET:CE	1:B:401:PHE:HA	2.28	0.59
1:B:351:LYS:HZ2	5:B:1436:PE4:H131	1.68	0.59
1:C:96:ALA:HB1	1:C:171:SER:HB2	1.84	0.59
1:B:315:SER:H	1:C:314:GLN:HE21	1.51	0.58
1:F:110:PRO:HA	1:F:113:GLN:HE21	1.67	0.58
1:B:222:LYS:HD2	6:B:2103:HOH:O	2.03	0.58
1:B:314:GLN:HE21	1:C:315:SER:H	1.50	0.58
1:B:351:LYS:NZ	5:B:1436:PE4:H122	2.17	0.58
1:F:35:GLN:HE21	1:F:40:SER:HB3	1.69	0.58
1:C:99:LEU:HD22	1:C:131:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1432:FAD:O5B	1:B:304:ARG:HG2	2.04	0.58
5:B:1436:PE4:C12	6:B:2206:HOH:O	2.51	0.57
2:B:1432:FAD:O2'	4:B:1433:SPM:N1	2.35	0.57
1:C:326:ARG:HB3	1:C:365:VAL:HG13	1.85	0.57
1:A:45:THR:CG2	6:A:2044:HOH:O	2.51	0.57
1:B:351:LYS:NZ	5:B:1436:PE4:H131	2.19	0.57
1:E:96:ALA:HB1	1:E:171:SER:HB2	1.86	0.57
1:B:299:ALA:HA	1:B:310:ILE:HG22	1.85	0.57
5:F:1435:PE4:H111	6:F:2204:HOH:O	2.04	0.57
5:B:1436:PE4:H52	6:B:2207:HOH:O	2.04	0.57
1:B:310:ILE:HG23	1:B:316:VAL:HG11	1.85	0.57
1:A:379:MET:CE	2:B:1432:FAD:H2'	2.36	0.56
1:A:379:MET:HE1	1:B:401:PHE:CB	2.35	0.56
1:E:326:ARG:NE	6:E:2137:HOH:O	2.39	0.56
1:A:299:ALA:HA	1:A:310:ILE:HG22	1.88	0.56
1:C:38:GLN:NE2	1:C:41:ARG:HH21	2.04	0.55
1:A:10:GLN:CG	1:A:75:HIS:CE1	2.88	0.55
1:E:240:THR:HG21	2:E:1432:FAD:HM72	1.89	0.55
1:B:45:THR:HG23	6:B:2046:HOH:O	2.06	0.55
1:A:322:ASP:O	1:A:326:ARG:HG3	2.07	0.55
1:B:95:VAL:HG13	4:B:1433:SPM:H62	1.89	0.55
1:E:141:ASN:ND2	2:E:1432:FAD:H61A	2.04	0.55
1:E:98:ALA:O	1:E:102[A]:MET:HG3	2.06	0.55
1:C:102[A]:MET:CE	4:C:1434:SPM:H112	2.38	0.54
1:C:352:LEU:O	1:C:356:MET:HG2	2.07	0.54
1:E:313:HIS:HD2	6:E:2128:HOH:O	1.90	0.54
1:A:81:GLU:OE2	1:A:331:ARG:HD3	2.07	0.54
1:A:310:ILE:HG23	1:A:316:VAL:HG11	1.88	0.54
1:A:315:SER:H	1:D:314:GLN:HE21	1.56	0.54
1:F:299:ALA:HA	1:F:310:ILE:HG22	1.89	0.54
1:C:371:ILE:HG21	3:C:1437:GOL:H2	1.90	0.54
1:F:95:VAL:HG13	4:F:1433:SPM:H82	1.88	0.54
1:B:326:ARG:HB3	1:B:365:VAL:HG13	1.89	0.54
1:F:326:ARG:HB3	1:F:365:VAL:HG13	1.88	0.54
1:A:96:ALA:HB1	1:A:171:SER:HB2	1.90	0.54
1:E:361:TYR:O	1:E:365:VAL:HB	2.09	0.53
1:E:61:GLN:HE21	1:E:98:ALA:HB2	1.73	0.53
1:B:326:ARG:NH1	6:B:2151:HOH:O	2.40	0.53
1:A:38:GLN:NE2	1:A:234:LEU:H	2.06	0.53
3:F:1434:GOL:C2	6:F:2201:HOH:O	2.56	0.53
1:E:326:ARG:HB3	1:E:365:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HD3	1:A:365:VAL:HG22	1.90	0.53
1:F:310:ILE:HG23	1:F:316:VAL:HG11	1.91	0.53
1:F:141:ASN:ND2	2:F:1432:FAD:H61A	2.06	0.52
1:B:304:ARG:HB2	1:B:310:ILE:HD13	1.90	0.52
1:E:99:LEU:HD22	1:E:131:LEU:HD23	1.92	0.52
5:B:1436:PE4:H41	5:B:1436:PE4:H101	1.92	0.52
1:C:45:THR:HG23	6:C:2040:HOH:O	2.09	0.52
1:A:310:ILE:HA	1:A:313:HIS:HD2	1.75	0.52
1:E:168:LEU:HD13	1:E:169:TRP:NE1	2.25	0.52
1:C:402:ASP:HA	4:C:1434:SPM:N1	2.24	0.51
1:A:38:GLN:HG3	1:A:232:PRO:O	2.10	0.51
1:A:141:ASN:ND2	2:A:1432:FAD:H61A	2.02	0.51
1:B:309:HIS:O	1:B:312:GLU:HB2	2.11	0.51
1:C:326:ARG:HD3	1:C:365:VAL:HG22	1.91	0.51
1:B:99:LEU:HD22	1:B:131:LEU:HD23	1.92	0.51
1:B:95:VAL:HG13	4:B:1433:SPM:C6	2.40	0.51
1:B:110:PRO:HA	1:B:113:GLN:HE21	1.76	0.51
4:C:1434:SPM:C4	6:C:2164:HOH:O	2.47	0.51
5:F:1435:PE4:H101	5:F:1435:PE4:H62	1.93	0.50
1:A:304:ARG:HB2	1:A:310:ILE:HD13	1.92	0.50
1:B:45:THR:CG2	6:B:2046:HOH:O	2.58	0.50
1:D:129:ALA:HA	1:D:183:LEU:O	2.11	0.50
5:B:1436:PE4:H121	6:B:2206:HOH:O	2.11	0.50
5:F:1435:PE4:C14	6:F:2203:HOH:O	2.45	0.50
1:C:110:PRO:HA	1:C:113:GLN:HE21	1.77	0.50
1:C:35:GLN:HA	1:C:35:GLN:HE21	1.76	0.50
5:B:1436:PE4:C16	6:B:2204:HOH:O	2.57	0.49
1:E:199:ASP:HB3	1:E:202:VAL:CG1	2.42	0.49
1:B:361:TYR:O	1:B:365:VAL:HB	2.13	0.49
1:F:326:ARG:NH1	1:F:368:GLU:OE1	2.45	0.49
2:A:1432:FAD:H51A	1:B:304:ARG:HD3	1.94	0.49
1:C:183:LEU:HD11	1:C:212:LEU:HG	1.95	0.49
5:B:1436:PE4:C6	5:B:1436:PE4:H101	2.42	0.48
1:D:45:THR:CG2	6:D:2031:HOH:O	2.57	0.48
1:D:16:HIS:HE1	6:D:2020:HOH:O	1.96	0.48
1:B:314:GLN:HE22	1:C:313:HIS:HB3	1.78	0.48
1:F:300:LYS:O	1:F:309:HIS:ND1	2.47	0.48
1:F:38:GLN:HE22	1:F:238:ILE:HA	1.78	0.47
1:B:35:GLN:HE21	1:B:40:SER:HB3	1.78	0.47
1:F:21:ALA:HA	1:F:25:LEU:HB2	1.96	0.47
1:C:42:PHE:O	1:C:45:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:VAL:CG1	4:F:1433:SPM:C6	2.92	0.47
5:B:1436:PE4:H62	5:B:1436:PE4:H101	1.96	0.47
1:A:171:SER:HA	1:A:241:SER:O	2.14	0.47
1:D:29:SER:O	1:D:33[B]:SER:HB3	2.15	0.47
1:A:379:MET:HE1	1:B:401:PHE:HB2	1.95	0.47
1:F:296:LEU:O	1:F:300:LYS:HG2	2.14	0.47
1:D:199:ASP:HB3	1:D:202:VAL:HG13	1.97	0.47
1:D:361:TYR:O	1:D:365:VAL:HB	2.15	0.47
1:F:407:GLY:O	1:F:411:ARG:HG2	2.16	0.46
1:D:202:VAL:HG22	6:D:2068:HOH:O	2.14	0.46
1:B:50:ARG:HD2	1:B:126:GLU:OE1	2.15	0.46
1:E:45:THR:HG23	6:E:2036:HOH:O	2.14	0.46
1:C:129:ALA:HA	1:C:183:LEU:O	2.16	0.46
1:C:349:LYS:HD3	6:C:2151:HOH:O	2.15	0.46
1:E:45:THR:CG2	6:E:2036:HOH:O	2.64	0.46
1:D:406:ILE:N	1:D:406:ILE:HD12	2.31	0.46
1:B:351:LYS:HZ3	5:B:1436:PE4:H122	1.80	0.46
1:F:240:THR:HG21	2:F:1432:FAD:HM72	1.97	0.46
1:A:199:ASP:HB3	1:A:202:VAL:CG1	2.46	0.46
1:D:16:HIS:CD2	3:D:1437:GOL:H11	2.51	0.46
5:F:1435:PE4:H122	5:F:1435:PE4:H102	1.43	0.45
1:D:53:VAL:HG22	1:D:58:ILE:CG1	2.46	0.45
1:D:169:TRP:N	1:D:170:PRO:HD2	2.31	0.45
1:A:183:LEU:HD11	1:A:212:LEU:HG	1.99	0.45
1:E:322:ASP:O	1:E:326:ARG:HG3	2.16	0.45
1:D:22[A]:ASN:OD1	6:D:2006:HOH:O	2.21	0.45
5:F:1435:PE4:H121	5:F:1435:PE4:H141	1.37	0.45
1:D:118:LYS:HB3	1:D:119:PRO:HD3	1.98	0.45
1:B:84:PHE:CE1	1:B:283:MET:HG2	2.51	0.45
1:F:151:GLN:CG	6:F:2073:HOH:O	2.59	0.45
1:F:320:LEU:HD23	6:F:2167:HOH:O	2.15	0.45
1:E:21:ALA:HA	1:E:25:LEU:HB2	1.99	0.45
1:E:304:ARG:CD	2:F:1432:FAD:H51A	2.47	0.45
1:A:42:PHE:O	1:A:45:THR:HB	2.16	0.45
1:F:102[B]:MET:HE3	6:F:2199:HOH:O	2.15	0.45
1:A:304:ARG:HG2	2:B:1432:FAD:O5B	2.17	0.45
1:F:310:ILE:HA	1:F:313:HIS:HD2	1.82	0.45
1:A:2:VAL:N	3:C:1436:GOL:HO3	2.15	0.45
5:F:1435:PE4:C6	5:F:1435:PE4:H101	2.47	0.44
1:B:61:GLN:HE21	1:B:98:ALA:HB2	1.81	0.44
6:A:2191:HOH:O	1:B:310:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1433:FAD:H52A	2:C:1433:FAD:O2P	2.17	0.44
1:A:314:GLN:NE2	1:D:315:SER:H	2.14	0.44
1:B:315:SER:H	1:C:314:GLN:NE2	2.14	0.44
1:B:314:GLN:NE2	1:C:315:SER:H	2.15	0.44
1:C:92:ILE:HG21	1:C:240:THR:HG22	1.99	0.44
1:E:153:THR:HA	1:E:189:ARG:O	2.18	0.44
1:B:81:GLU:OE2	1:B:331:ARG:HD3	2.17	0.44
1:D:364:ASP:OD1	3:D:1436:GOL:O2	2.35	0.44
1:A:240:THR:HG21	2:A:1432:FAD:HM72	1.98	0.44
2:A:1432:FAD:C8A	1:B:310:ILE:HD11	2.49	0.43
1:D:326:ARG:HB3	1:D:365:VAL:HG13	2.00	0.43
1:B:169:TRP:N	1:B:170:PRO:CD	2.80	0.43
1:F:128:LEU:HD11	1:F:176:TRP:CE2	2.53	0.43
1:D:198:GLN:HE22	1:D:204:PRO:HB3	1.84	0.43
5:B:1436:PE4:C10	6:B:2206:HOH:O	2.66	0.43
1:E:98:ALA:O	1:E:102[B]:MET:HG2	2.19	0.43
1:D:296:LEU:O	1:D:300:LYS:HG2	2.19	0.43
1:C:335:TRP:O	1:C:339:THR:HB	2.19	0.43
2:C:1433:FAD:H9	2:C:1433:FAD:H1'2	1.82	0.43
1:D:240:THR:HG21	2:D:1433:FAD:HM72	1.99	0.43
1:A:352:LEU:O	1:A:356:MET:HG2	2.19	0.43
1:E:110:PRO:HA	1:E:113:GLN:HE21	1.83	0.43
1:E:237:HIS:HD2	6:E:2034:HOH:O	2.02	0.43
3:F:1434:GOL:C3	6:F:2201:HOH:O	2.66	0.43
1:A:98:ALA:O	1:A:102[B]:MET:HG3	2.19	0.42
1:A:314:GLN:HE22	1:D:313:HIS:HB3	1.84	0.42
3:F:1434:GOL:H2	6:F:2201:HOH:O	2.19	0.42
1:D:35:GLN:HE21	1:D:40:SER:HB3	1.84	0.42
1:B:134:SER:HA	1:B:139:THR:HG21	2.01	0.42
1:B:21:ALA:HA	1:B:25:LEU:HB2	2.01	0.42
1:A:315:SER:H	1:D:314:GLN:NE2	2.15	0.42
1:D:359:LYS:HD2	1:D:409:ARG:HG3	2.00	0.42
1:A:304:ARG:HG2	2:B:1432:FAD:C5B	2.50	0.42
1:B:45:THR:HG21	6:B:2113:HOH:O	2.19	0.42
1:B:168:LEU:C	1:B:170:PRO:HD3	2.40	0.42
1:C:61:GLN:HE21	1:C:98:ALA:HB2	1.84	0.42
1:F:95:VAL:CG1	4:F:1433:SPM:H62	2.50	0.42
1:C:118:LYS:HB3	1:C:119:PRO:HD3	2.01	0.42
1:C:168:LEU:O	1:C:169:TRP:HB2	2.19	0.42
1:B:198:GLN:NE2	6:B:2087:HOH:O	2.50	0.42
1:F:380:LYS:NZ	6:F:2169:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1436:PE4:H91	5:B:1436:PE4:H71	1.36	0.42
1:C:45:THR:HG21	6:C:2039:HOH:O	2.19	0.42
1:B:168:LEU:C	1:B:170:PRO:CD	2.88	0.42
1:E:319:LYS:NZ	3:E:1435:GOL:O2	2.53	0.42
1:C:38:GLN:NE2	1:C:234:LEU:H	2.18	0.42
1:C:58:ILE:N	1:C:58:ILE:HD12	2.34	0.42
1:F:46:ARG:HB3	1:F:47:PRO:HD3	2.01	0.42
1:E:304:ARG:HD2	2:F:1432:FAD:H51A	2.02	0.41
1:B:178:TYR:CE2	1:B:228:ILE:HG21	2.55	0.41
5:B:1436:PE4:C10	5:B:1436:PE4:H62	2.50	0.41
1:C:95:VAL:HB	4:C:1434:SPM:H82	2.01	0.41
1:B:183:LEU:HD11	1:B:212:LEU:HG	2.01	0.41
1:D:352:LEU:O	1:D:356:MET:HG2	2.20	0.41
1:B:118:LYS:HB3	1:B:119:PRO:HD3	2.02	0.41
5:F:1435:PE4:H41	5:F:1435:PE4:H62	1.47	0.41
1:C:28:ALA:HA	1:C:48:PHE:CZ	2.56	0.41
1:B:28:ALA:HA	1:B:48:PHE:CZ	2.55	0.41
1:B:352:LEU:O	1:B:356:MET:HG2	2.21	0.41
1:C:361:TYR:O	1:C:365:VAL:HB	2.21	0.41
1:C:401:PHE:C	1:C:401:PHE:CD2	2.93	0.41
1:B:340:THR:O	1:B:351:LYS:HE2	2.21	0.41
1:F:95:VAL:CG1	4:F:1433:SPM:H61	2.50	0.41
1:A:361:TYR:O	1:A:365:VAL:HB	2.21	0.41
1:F:322:ASP:O	1:F:326:ARG:HG3	2.21	0.41
1:C:341:LEU:HD23	1:C:351:LYS:HB3	2.03	0.41
1:B:53:VAL:HG22	1:B:58:ILE:HG13	2.02	0.41
1:A:314:GLN:HB2	1:D:314:GLN:HB2	2.03	0.41
1:C:70:MET:CE	4:C:1434:SPM:N14	2.85	0.40
1:E:183:LEU:HD11	1:E:212:LEU:HG	2.03	0.40
1:A:310:ILE:HD11	2:B:1432:FAD:C8A	2.52	0.40
1:F:323:CYS:SG	6:F:2167:HOH:O	2.62	0.40
1:C:38:GLN:HE21	1:C:41:ARG:HH21	1.68	0.40
1:E:99:LEU:HA	1:E:102[B]:MET:HG3	2.03	0.40
1:D:401:PHE:C	1:D:401:PHE:CD2	2.94	0.40
1:B:279:LEU:HD13	4:B:1433:SPM:H112	2.03	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	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	34	22
1	B	429/439 (98%)	421 (98%)	5 (1%)	3 (1%)	26	14
1	C	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	34	22
1	D	431/439 (98%)	425 (99%)	5 (1%)	1 (0%)	52	43
1	E	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	34	22
1	F	429/439 (98%)	422 (98%)	6 (1%)	1 (0%)	52	43
All	All	2576/2634 (98%)	2537 (98%)	28 (1%)	11 (0%)	39	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP
1	B	430	GLY
1	C	169	TRP
1	D	169	TRP
1	E	169	TRP
1	F	169	TRP
1	A	403	GLY
1	B	403	GLY
1	C	403	GLY
1	E	403	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	356/364 (98%)	329 (92%)	27 (8%)	16	7
1	B	356/364 (98%)	328 (92%)	28 (8%)	15	7
1	C	356/364 (98%)	331 (93%)	25 (7%)	19	10
1	D	358/364 (98%)	335 (94%)	23 (6%)	22	12
1	E	356/364 (98%)	332 (93%)	24 (7%)	20	11
1	F	356/364 (98%)	333 (94%)	23 (6%)	21	12
All	All	2138/2184 (98%)	1988 (93%)	150 (7%)	19	10

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	45	THR
1	A	50	ARG
1	A	66	LEU
1	A	73	LEU
1	A	83	LEU
1	A	99	LEU
1	A	102[A]	MET
1	A	102[B]	MET
1	A	112	LEU
1	A	118	LYS
1	A	124	GLU
1	A	131	LEU
1	A	164	SER
1	A	168	LEU
1	A	202	VAL
1	A	212	LEU
1	A	223	LYS
1	A	256	ASN
1	A	280	VAL
1	A	304	ARG
1	A	310	ILE
1	A	332	LEU
1	A	349	LYS
1	A	365	VAL
1	A	401	PHE
1	A	411	ARG
1	B	25	LEU
1	B	33	SER
1	B	38	GLN

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Mol	Chain	Res	Type
1	B	45	THR
1	B	66	LEU
1	B	73	LEU
1	B	83	LEU
1	B	95	VAL
1	B	99	LEU
1	B	102[A]	MET
1	B	102[B]	MET
1	B	112	LEU
1	B	131	LEU
1	B	168	LEU
1	B	192	ASP
1	B	212	LEU
1	B	227	GLN
1	B	255	GLU
1	B	256	ASN
1	B	304	ARG
1	B	310	ILE
1	B	312	GLU
1	B	332	LEU
1	B	365	VAL
1	B	387	SER
1	B	401	PHE
1	B	411	ARG
1	B	431	SER
1	C	2	VAL
1	C	25	LEU
1	C	34	THR
1	C	36	LYS
1	C	45	THR
1	C	66	LEU
1	C	73	LEU
1	C	83	LEU
1	C	99	LEU
1	C	112	LEU
1	C	118	LYS
1	C	131	LEU
1	C	164	SER
1	C	168	LEU
1	C	192	ASP
1	C	202	VAL
1	C	212	LEU

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Mol	Chain	Res	Type
1	C	256	ASN
1	C	332	LEU
1	C	339	THR
1	C	349	LYS
1	C	365	VAL
1	C	401	PHE
1	C	411	ARG
1	C	420	GLU
1	D	2	VAL
1	D	3	ASP
1	D	25	LEU
1	D	45	THR
1	D	50	ARG
1	D	66	LEU
1	D	83	LEU
1	D	99	LEU
1	D	112	LEU
1	D	131	LEU
1	D	160	GLU
1	D	168	LEU
1	D	192	ASP
1	D	202	VAL
1	D	212	LEU
1	D	256	ASN
1	D	280	VAL
1	D	300	LYS
1	D	312	GLU
1	D	332	LEU
1	D	365	VAL
1	D	401	PHE
1	D	411	ARG
1	E	2	VAL
1	E	25	LEU
1	E	45	THR
1	E	50	ARG
1	E	66	LEU
1	E	73	LEU
1	E	83	LEU
1	E	99	LEU
1	E	112	LEU
1	E	124	GLU
1	E	131	LEU

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Mol	Chain	Res	Type
1	E	164	SER
1	E	168	LEU
1	E	202	VAL
1	E	212	LEU
1	E	256	ASN
1	E	280	VAL
1	E	312	GLU
1	E	332	LEU
1	E	349	LYS
1	E	365	VAL
1	E	401	PHE
1	E	411	ARG
1	E	431	SER
1	F	2	VAL
1	F	11	LEU
1	F	25	LEU
1	F	50	ARG
1	F	59	LYS
1	F	66	LEU
1	F	73	LEU
1	F	99	LEU
1	F	112	LEU
1	F	124	GLU
1	F	168	LEU
1	F	192	ASP
1	F	202	VAL
1	F	212	LEU
1	F	222	LYS
1	F	300	LYS
1	F	310	ILE
1	F	312	GLU
1	F	332	LEU
1	F	365	VAL
1	F	401	PHE
1	F	409	ARG
1	F	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	38	GLN
1	A	43	GLN
1	A	61	GLN
1	A	113	GLN
1	A	137	ASN
1	A	141	ASN
1	A	198	GLN
1	A	256	ASN
1	A	266	GLN
1	A	309	HIS
1	A	314	GLN
1	A	357	GLN
1	B	16	HIS
1	B	35	GLN
1	B	38	GLN
1	B	43	GLN
1	B	113	GLN
1	B	137	ASN
1	B	141	ASN
1	B	198	GLN
1	B	207	GLN
1	B	227	GLN
1	B	256	ASN
1	B	266	GLN
1	B	314	GLN
1	C	16	HIS
1	C	18	GLN
1	C	22	ASN
1	C	35	GLN
1	C	38	GLN
1	C	43	GLN
1	C	113	GLN
1	C	137	ASN
1	C	141	ASN
1	C	198	GLN
1	C	256	ASN
1	C	266	GLN
1	C	309	HIS
1	C	314	GLN
1	D	16	HIS
1	D	18	GLN
1	D	35	GLN

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Mol	Chain	Res	Type
1	D	43	GLN
1	D	113	GLN
1	D	137	ASN
1	D	141	ASN
1	D	198	GLN
1	D	227	GLN
1	D	256	ASN
1	D	314	GLN
1	D	357	GLN
1	E	16	HIS
1	E	22	ASN
1	E	35	GLN
1	E	43	GLN
1	E	55	HIS
1	E	61	GLN
1	E	113	GLN
1	E	137	ASN
1	E	141	ASN
1	E	151	GLN
1	E	198	GLN
1	E	237	HIS
1	E	256	ASN
1	E	266	GLN
1	E	309	HIS
1	E	313	HIS
1	E	314	GLN
1	F	35	GLN
1	F	38	GLN
1	F	43	GLN
1	F	113	GLN
1	F	141	ASN
1	F	198	GLN
1	F	207	GLN
1	F	256	ASN
1	F	266	GLN
1	F	314	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

27 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	1432	-	48,58,58	1.56	8 (16%)	54,89,89	2.09	8 (14%)
3	GOL	A	1433	-	5,5,5	0.37	0	5,5,5	0.34	0
2	FAD	B	1432	-	48,58,58	1.72	8 (16%)	54,89,89	1.98	7 (12%)
4	SPM	B	1433	-	13,13,13	0.53	0	12,12,12	1.22	1 (8%)
3	GOL	B	1434	-	5,5,5	0.34	0	5,5,5	0.32	0
3	GOL	B	1435	-	5,5,5	0.40	0	5,5,5	0.50	0
5	PE4	B	1436	-	23,23,23	0.65	0	22,22,22	1.01	2 (9%)
3	GOL	C	1432	-	5,5,5	0.35	0	5,5,5	0.66	0
2	FAD	C	1433	-	48,58,58	1.72	8 (16%)	54,89,89	2.01	10 (18%)
4	SPM	C	1434	-	13,13,13	0.34	0	12,12,12	1.26	2 (16%)
3	GOL	C	1435	-	5,5,5	0.32	0	5,5,5	0.38	0
3	GOL	C	1436	-	5,5,5	0.45	0	5,5,5	0.75	0
3	GOL	C	1437	-	5,5,5	0.54	0	5,5,5	1.20	1 (20%)
3	GOL	D	1432	-	5,5,5	0.38	0	5,5,5	0.57	0
2	FAD	D	1433	-	48,58,58	1.59	7 (14%)	54,89,89	2.16	12 (22%)
4	SPM	D	1434	-	13,13,13	0.36	0	12,12,12	0.92	1 (8%)
3	GOL	D	1435	-	5,5,5	0.55	0	5,5,5	0.40	0
3	GOL	D	1436	-	5,5,5	0.43	0	5,5,5	0.30	0
3	GOL	D	1437	-	5,5,5	0.43	0	5,5,5	0.49	0
2	FAD	E	1432	-	48,58,58	1.85	8 (16%)	54,89,89	2.09	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	1433	-	5,5,5	0.27	0	5,5,5	0.45	0
3	GOL	E	1434	-	5,5,5	0.44	0	5,5,5	0.91	0
3	GOL	E	1435	-	5,5,5	0.43	0	5,5,5	0.20	0
2	FAD	F	1432	-	48,58,58	1.55	7 (14%)	54,89,89	2.23	10 (18%)
4	SPM	F	1433	-	13,13,13	0.42	0	12,12,12	1.00	0
3	GOL	F	1434	-	5,5,5	0.47	0	5,5,5	0.46	0
5	PE4	F	1435	-	23,23,23	0.86	0	22,22,22	1.10	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	1432	-	-	0/30/50/50	0/6/6/6
3	GOL	A	1433	-	-	0/4/4/4	0/0/0/0
2	FAD	B	1432	-	-	0/30/50/50	0/6/6/6
4	SPM	B	1433	-	-	0/11/11/11	0/0/0/0
3	GOL	B	1434	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1435	-	-	0/4/4/4	0/0/0/0
5	PE4	B	1436	-	-	0/21/21/21	0/0/0/0
3	GOL	C	1432	-	-	0/4/4/4	0/0/0/0
2	FAD	C	1433	-	-	0/30/50/50	0/6/6/6
4	SPM	C	1434	-	-	0/11/11/11	0/0/0/0
3	GOL	C	1435	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1436	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1437	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1432	-	-	0/4/4/4	0/0/0/0
2	FAD	D	1433	-	-	0/30/50/50	0/6/6/6
4	SPM	D	1434	-	-	0/11/11/11	0/0/0/0
3	GOL	D	1435	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1436	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1437	-	-	0/4/4/4	0/0/0/0
2	FAD	E	1432	-	-	0/30/50/50	0/6/6/6
3	GOL	E	1433	-	-	0/4/4/4	0/0/0/0
3	GOL	E	1434	-	-	0/4/4/4	0/0/0/0
3	GOL	E	1435	-	-	0/4/4/4	0/0/0/0
2	FAD	F	1432	-	-	0/30/50/50	0/6/6/6
4	SPM	F	1433	-	-	0/11/11/11	0/0/0/0
3	GOL	F	1434	-	-	0/4/4/4	0/0/0/0
5	PE4	F	1435	-	-	0/21/21/21	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1432	FAD	C4'-C3'	-5.50	1.42	1.53
2	B	1432	FAD	C4'-C3'	-5.13	1.43	1.53
2	C	1433	FAD	C4'-C3'	-5.10	1.43	1.53
2	A	1432	FAD	C4'-C3'	-5.01	1.43	1.53
2	D	1433	FAD	C4'-C3'	-4.96	1.43	1.53
2	F	1432	FAD	C4'-C3'	-4.79	1.43	1.53
2	B	1432	FAD	O5'-C5'	-2.47	1.34	1.44
2	E	1432	FAD	O5'-C5'	-2.36	1.35	1.44
2	D	1433	FAD	C6-C5X	-2.30	1.38	1.41
2	C	1433	FAD	C5A-N7A	-2.20	1.31	1.39
2	A	1432	FAD	C1'-N10	-2.19	1.46	1.48
2	E	1432	FAD	P-O2P	-2.13	1.45	1.54
2	B	1432	FAD	C9A-C5X	-2.04	1.38	1.42
2	D	1433	FAD	O5'-C5'	-2.04	1.36	1.44
2	A	1432	FAD	C10-N10	-2.01	1.36	1.39
2	A	1432	FAD	C4X-C10	-2.01	1.37	1.41
2	C	1433	FAD	C9A-N10	2.06	1.41	1.38
2	B	1432	FAD	O3'-C3'	2.07	1.47	1.43
2	A	1432	FAD	C7M-C7	2.15	1.55	1.51
2	F	1432	FAD	C7M-C7	2.31	1.55	1.51
2	C	1433	FAD	C5X-N5	2.40	1.39	1.35
2	E	1432	FAD	C5X-N5	2.49	1.39	1.35
2	F	1432	FAD	C9A-N10	2.54	1.42	1.38
2	F	1432	FAD	C4X-N5	2.57	1.37	1.33
2	C	1433	FAD	O3'-C3'	2.59	1.49	1.43
2	F	1432	FAD	O3'-C3'	2.61	1.49	1.43
2	A	1432	FAD	C4X-N5	2.62	1.37	1.33
2	B	1432	FAD	C5X-N5	2.76	1.39	1.35
2	A	1432	FAD	C5X-N5	2.79	1.39	1.35
2	C	1433	FAD	C4-N3	3.09	1.38	1.33
2	E	1432	FAD	C4-N3	3.11	1.38	1.33
2	F	1432	FAD	C5X-N5	3.16	1.40	1.35
2	E	1432	FAD	C10-N1	3.22	1.41	1.35
2	D	1433	FAD	C5X-N5	3.28	1.40	1.35
2	D	1433	FAD	C4-N3	3.33	1.39	1.33
2	D	1433	FAD	O4B-C1B	3.66	1.45	1.41
2	F	1432	FAD	C4-N3	3.69	1.39	1.33
2	A	1432	FAD	C4-N3	3.92	1.40	1.33
2	C	1433	FAD	C4X-N5	4.20	1.39	1.33
2	B	1432	FAD	C4-N3	4.22	1.40	1.33
2	B	1432	FAD	O4B-C1B	4.23	1.46	1.41
2	D	1433	FAD	C4X-N5	4.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1432	FAD	C4X-N5	4.49	1.40	1.33
2	E	1432	FAD	C4X-N5	4.65	1.40	1.33
2	C	1433	FAD	O4B-C1B	5.09	1.47	1.41
2	E	1432	FAD	O4B-C1B	6.07	1.48	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1432	FAD	N3A-C2A-N1A	-9.31	121.76	128.89
2	D	1433	FAD	N3A-C2A-N1A	-9.08	121.94	128.89
2	A	1432	FAD	N3A-C2A-N1A	-8.69	122.24	128.89
2	B	1432	FAD	N3A-C2A-N1A	-8.03	122.74	128.89
2	C	1433	FAD	N3A-C2A-N1A	-8.01	122.76	128.89
2	E	1432	FAD	N3A-C2A-N1A	-7.57	123.10	128.89
2	B	1432	FAD	C4X-C4-N3	-3.58	118.69	123.59
2	F	1432	FAD	C4X-C4-N3	-3.54	118.74	123.59
2	D	1433	FAD	C4X-C4-N3	-3.51	118.79	123.59
2	C	1433	FAD	O3'-C3'-C4'	-3.19	100.71	108.75
2	E	1432	FAD	C4X-C4-N3	-3.18	119.23	123.59
2	D	1433	FAD	C4A-C5A-N7A	-3.16	106.57	109.48
2	E	1432	FAD	O3'-C3'-C4'	-3.11	100.91	108.75
2	A	1432	FAD	C4X-C4-N3	-2.88	119.65	123.59
4	B	1433	SPM	C3-C4-N5	-2.84	104.86	111.96
2	A	1432	FAD	O3P-P-O5'	-2.83	95.43	102.94
2	C	1433	FAD	C4X-C4-N3	-2.81	119.75	123.59
2	C	1433	FAD	C4B-O4B-C1B	-2.68	106.77	109.72
2	D	1433	FAD	O3'-C3'-C4'	-2.68	102.01	108.75
2	B	1432	FAD	O3P-P-O5'	-2.67	95.85	102.94
5	B	1436	PE4	O6-C10-C9	-2.64	98.64	110.36
2	A	1432	FAD	C4A-C5A-N7A	-2.60	107.09	109.48
2	C	1433	FAD	C4A-C5A-N7A	-2.54	107.14	109.48
2	D	1433	FAD	O3P-P-O5'	-2.30	96.83	102.94
5	B	1436	PE4	O6-C11-C12	-2.09	101.10	110.36
2	E	1432	FAD	C4B-O4B-C1B	-2.08	107.44	109.72
2	C	1433	FAD	C9A-C5X-N5	-2.06	119.31	122.36
2	F	1432	FAD	C4A-C5A-N7A	-2.04	107.60	109.48
3	C	1437	GOL	O3-C3-C2	2.00	119.90	110.18
2	F	1432	FAD	C6-C5X-C9A	2.02	121.64	118.98
2	D	1433	FAD	O2A-PA-O3P	2.07	114.48	105.09
2	F	1432	FAD	O2P-P-O3P	2.10	114.62	105.09
4	C	1434	SPM	C6-N5-C4	2.17	121.05	113.35
4	D	1434	SPM	C11-N10-C9	2.25	121.34	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1433	FAD	C5X-C9A-N10	2.51	119.52	117.62
2	D	1433	FAD	C1'-N10-C9A	2.52	121.69	118.86
2	C	1433	FAD	C5X-C9A-N10	2.56	119.56	117.62
2	F	1432	FAD	C1'-N10-C9A	2.58	121.76	118.86
2	E	1432	FAD	C5X-C9A-N10	2.59	119.59	117.62
2	D	1433	FAD	C4-C4X-N5	2.61	121.89	118.72
2	B	1432	FAD	O4'-C4'-C5'	2.79	116.28	110.19
4	C	1434	SPM	C12-C11-N10	2.82	119.00	111.96
2	F	1432	FAD	C4X-N5-C5X	2.90	120.10	116.76
2	D	1433	FAD	O4'-C4'-C5'	3.04	116.81	110.19
2	E	1432	FAD	O4'-C4'-C5'	3.04	116.81	110.19
2	B	1432	FAD	C5X-C9A-N10	3.04	119.93	117.62
2	A	1432	FAD	C1'-N10-C9A	3.23	122.49	118.86
2	C	1433	FAD	O4'-C4'-C5'	3.67	118.19	110.19
2	A	1432	FAD	O4'-C4'-C5'	3.79	118.46	110.19
2	F	1432	FAD	O4'-C4'-C5'	3.90	118.69	110.19
2	A	1432	FAD	O3'-C3'-C2'	4.70	120.59	108.75
2	D	1433	FAD	O3'-C3'-C2'	4.77	120.78	108.75
2	B	1432	FAD	O3'-C3'-C2'	5.01	121.38	108.75
2	F	1432	FAD	O3'-C3'-C2'	5.05	121.47	108.75
2	C	1433	FAD	O3'-C3'-C2'	5.08	121.55	108.75
2	E	1432	FAD	O3'-C3'-C2'	5.13	121.67	108.75
2	C	1433	FAD	C4-N3-C2	5.87	120.32	115.25
2	A	1432	FAD	C4-N3-C2	5.91	120.36	115.25
2	B	1432	FAD	C4-N3-C2	6.67	121.01	115.25
2	D	1433	FAD	C4-N3-C2	6.91	121.22	115.25
2	F	1432	FAD	C4-N3-C2	7.11	121.40	115.25
2	E	1432	FAD	C4-N3-C2	7.91	122.09	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1432	FAD	6	0
2	B	1432	FAD	8	0
4	B	1433	SPM	4	0
5	B	1436	PE4	17	0
2	C	1433	FAD	4	0
4	C	1434	SPM	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1436	GOL	1	0
3	C	1437	GOL	1	0
2	D	1433	FAD	3	0
3	D	1436	GOL	1	0
3	D	1437	GOL	1	0
2	E	1432	FAD	3	0
3	E	1435	GOL	1	0
2	F	1432	FAD	5	0
4	F	1433	SPM	5	0
3	F	1434	GOL	3	0
5	F	1435	PE4	9	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, 95th 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 ²)	Q<0.9
1	A	430/439 (97%)	-0.14	5 (1%)	81 83	17, 25, 36, 45	0
1	B	430/439 (97%)	-0.19	2 (0%)	91 93	16, 24, 36, 49	0
1	C	430/439 (97%)	-0.06	13 (3%)	54 59	18, 27, 42, 54	0
1	D	430/439 (97%)	-0.02	10 (2%)	64 67	18, 27, 42, 49	0
1	E	430/439 (97%)	-0.19	10 (2%)	64 67	16, 24, 38, 46	0
1	F	430/439 (97%)	0.01	15 (3%)	48 53	16, 25, 39, 49	0
All	All	2580/2634 (97%)	-0.10	55 (2%)	67 70	16, 25, 39, 54	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	SER	5.0
1	F	151	GLN	4.6
1	C	196	LYS	4.6
1	F	431	SER	4.4
1	E	192	ASP	4.1
1	E	431	SER	4.1
1	C	193	ASP	4.0
1	C	202	VAL	3.4
1	E	195	SER	3.4
1	C	36	LYS	3.1
1	E	193	ASP	3.0
1	A	421	ASP	3.0
1	A	192	ASP	2.9
1	F	8	PRO	2.7
1	A	366	ALA	2.6
1	F	345	ALA	2.6
1	B	431	SER	2.5
1	E	2	VAL	2.5
1	C	400	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	369	CYS	2.5
1	E	196	LYS	2.4
1	F	224	ASP	2.4
1	E	108	ASP	2.4
1	D	327	LEU	2.4
1	C	194	PRO	2.3
1	C	367	VAL	2.3
1	D	370	VAL	2.3
1	A	431	SER	2.3
1	B	223	LYS	2.3
1	F	223	LYS	2.3
1	D	421	ASP	2.3
1	F	196	LYS	2.3
1	F	108	ASP	2.2
1	F	366	ALA	2.2
1	C	365	VAL	2.2
1	C	33	SER	2.2
1	C	192	ASP	2.2
1	D	369	CYS	2.1
1	F	193	ASP	2.1
1	C	421	ASP	2.1
1	A	195	SER	2.1
1	E	159	ASN	2.1
1	D	365	VAL	2.1
1	F	365	VAL	2.1
1	E	7	SER	2.1
1	C	347	GLU	2.1
1	F	54	ARG	2.1
1	D	367	VAL	2.1
1	F	360	ILE	2.1
1	D	159	ASN	2.0
1	D	296	LEU	2.0
1	D	323	CYS	2.0
1	E	8	PRO	2.0
1	F	367	VAL	2.0
1	D	224	ASP	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, 95th 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 ²)	Q<0.9
3	GOL	E	1433	6/6	0.74	0.30	10.07	46,47,48,48	0
3	GOL	E	1435	6/6	0.40	0.39	7.56	58,59,59,59	0
3	GOL	C	1435	6/6	0.84	0.34	6.07	48,49,50,50	0
3	GOL	D	1432	6/6	0.77	0.35	5.40	52,52,54,55	0
3	GOL	A	1433	6/6	0.43	0.24	5.30	57,57,58,59	0
3	GOL	E	1434	6/6	0.67	0.34	4.93	45,48,49,50	0
3	GOL	B	1434	6/6	0.67	0.28	4.89	45,46,48,48	0
3	GOL	C	1437	6/6	0.59	0.33	4.86	42,44,45,45	0
3	GOL	F	1434	6/6	0.69	0.32	4.65	47,51,53,54	0
3	GOL	D	1435	6/6	0.83	0.18	4.57	45,46,48,49	0
4	SPM	C	1434	14/14	0.65	0.27	3.75	45,46,47,49	0
3	GOL	C	1432	6/6	0.78	0.25	3.28	52,54,54,55	0
3	GOL	D	1437	6/6	0.85	0.22	2.85	43,45,46,47	0
4	SPM	D	1434	14/14	0.86	0.20	2.13	40,52,56,56	0
4	SPM	F	1433	14/14	0.79	0.18	2.04	33,43,48,49	0
5	PE4	F	1435	24/24	0.65	0.20	1.87	49,53,55,57	0
5	PE4	B	1436	24/24	0.69	0.20	1.75	43,47,56,60	0
3	GOL	D	1436	6/6	0.86	0.20	1.18	48,49,49,50	0
4	SPM	B	1433	14/14	0.89	0.15	1.10	34,42,50,51	0
3	GOL	C	1436	6/6	0.88	0.12	0.19	39,41,42,42	0
2	FAD	D	1433	53/53	0.96	0.08	-0.41	16,21,23,26	0
2	FAD	A	1432	53/53	0.96	0.09	-0.45	16,20,22,22	0
2	FAD	C	1433	53/53	0.97	0.10	-0.59	15,19,23,25	0
2	FAD	E	1432	53/53	0.97	0.09	-0.60	15,18,21,22	0
2	FAD	B	1432	53/53	0.97	0.09	-0.67	15,19,22,24	0
2	FAD	F	1432	53/53	0.96	0.08	-0.88	13,17,22,24	0
3	GOL	B	1435	6/6	0.67	0.28	-	53,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.