Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:27 AM GMT

PDB ID	:	3LSK
Title	:	Pyranose 2-oxidase T169S acetate complex
Authors	:	Tan, T.C.; Spadiut, O.; Divne, C.
Deposited on	:	2010-02-12
Resolution	:	1.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

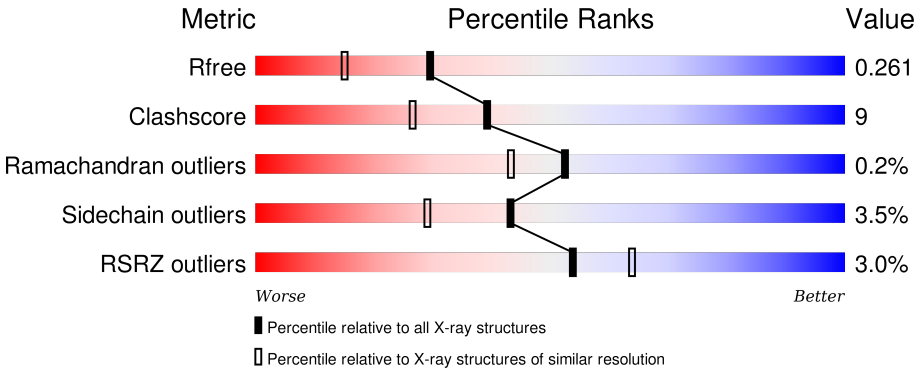
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	623	2% 79% 13% • 8%
1	B	623	2% 75% 15% • 8%
1	C	623	3% 71% 19% • 8%
1	D	623	4% 76% 14% • 8%

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	ACT	A	901	-	-	X	X
3	ACT	B	901	-	-	X	X
3	ACT	C	901	-	-	X	X
3	ACT	D	901	-	-	X	-
4	12P	A	903	-	-	-	X
4	12P	A	904	-	-	-	X
4	12P	B	902	-	-	-	X
4	12P	C	905	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20361 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.

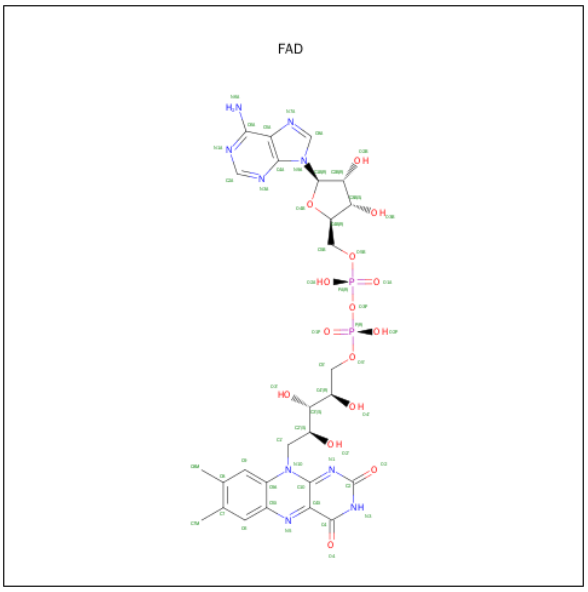
- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4541	2867	777	872	25			
1	B	576	Total	C	N	O	S	0	0	0
			4541	2867	777	872	25			
1	C	575	Total	C	N	O	S	0	0	0
			4532	2862	776	870	24			
1	D	574	Total	C	N	O	S	0	0	0
			4525	2858	775	868	24			

There are 4 discrepancies between the modelled and reference sequences:

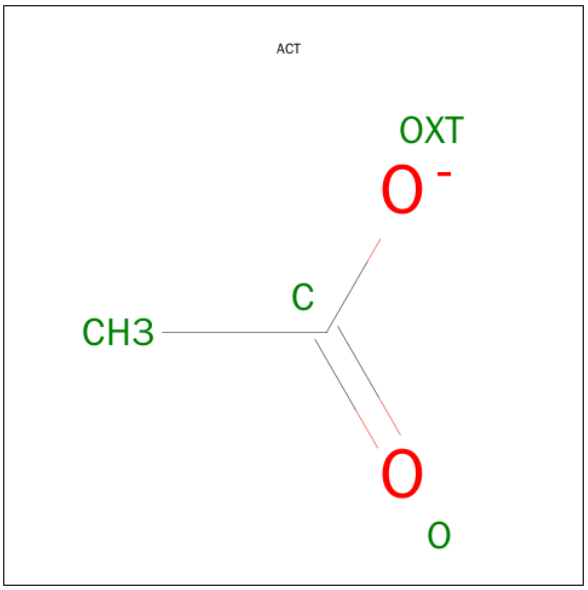
Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	THR	ENGINEERED	UNP Q7ZA32
B	169	SER	THR	ENGINEERED	UNP Q7ZA32
C	169	SER	THR	ENGINEERED	UNP Q7ZA32
D	169	SER	THR	ENGINEERED	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



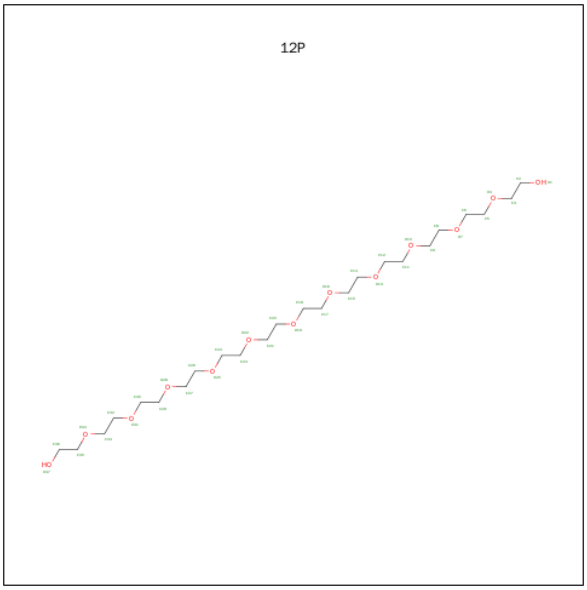
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 11 5	0	0
4	A	1	Total C O 16 11 5	0	0
4	B	1	Total C O 16 10 6	0	0
4	C	1	Total C O 14 10 4	0	0
4	D	1	Total C O 12 8 4	0	0
4	D	1	Total C O 11 7 4	0	0

- Molecule 5 is water.

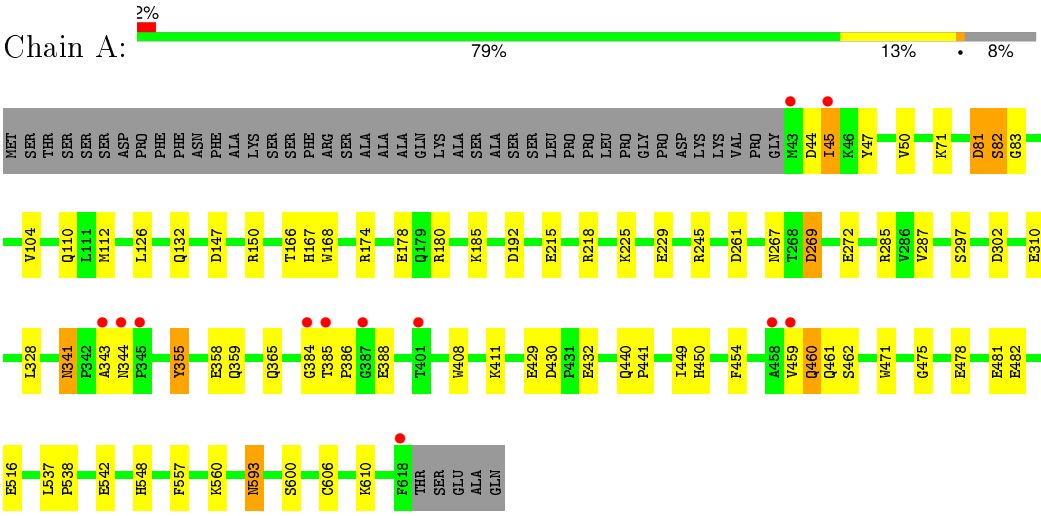
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	518	Total O 518 518	0	0
5	B	534	Total O 534 534	0	0
5	C	457	Total O 457 457	0	0
5	D	400	Total O 400 400	0	0

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.

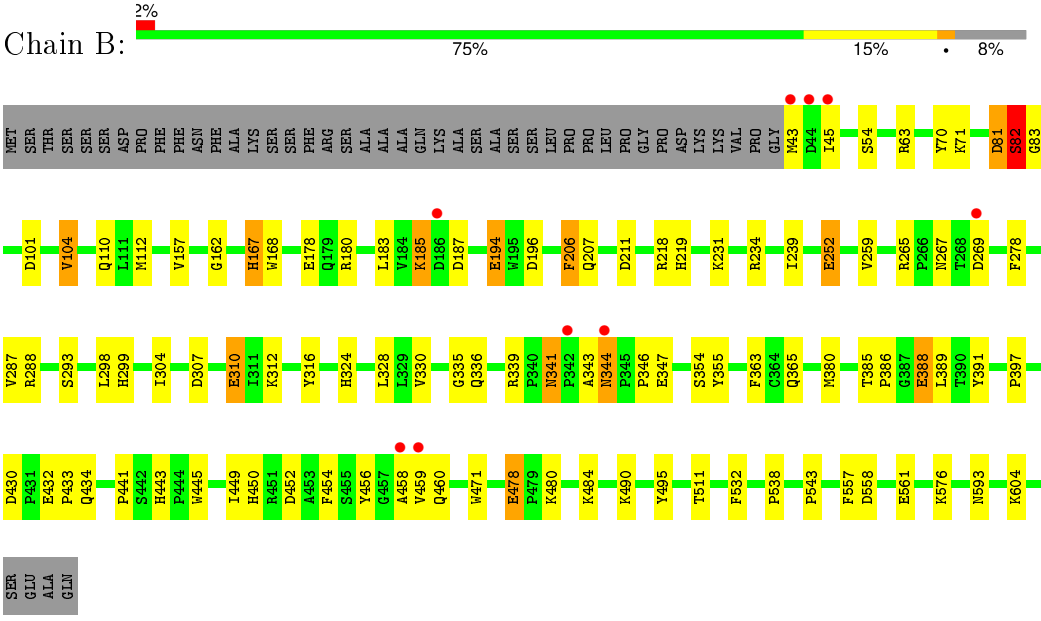
- Molecule 1: Pyranose 2-oxidase

Chain A:

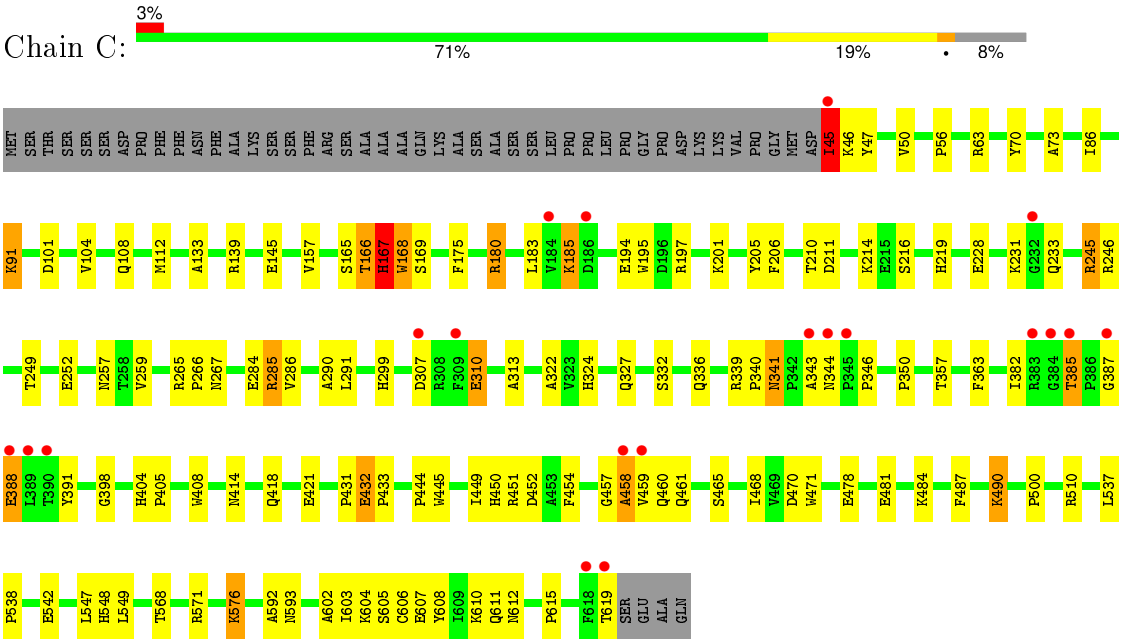


- Molecule 1: Pyranose 2-oxidase

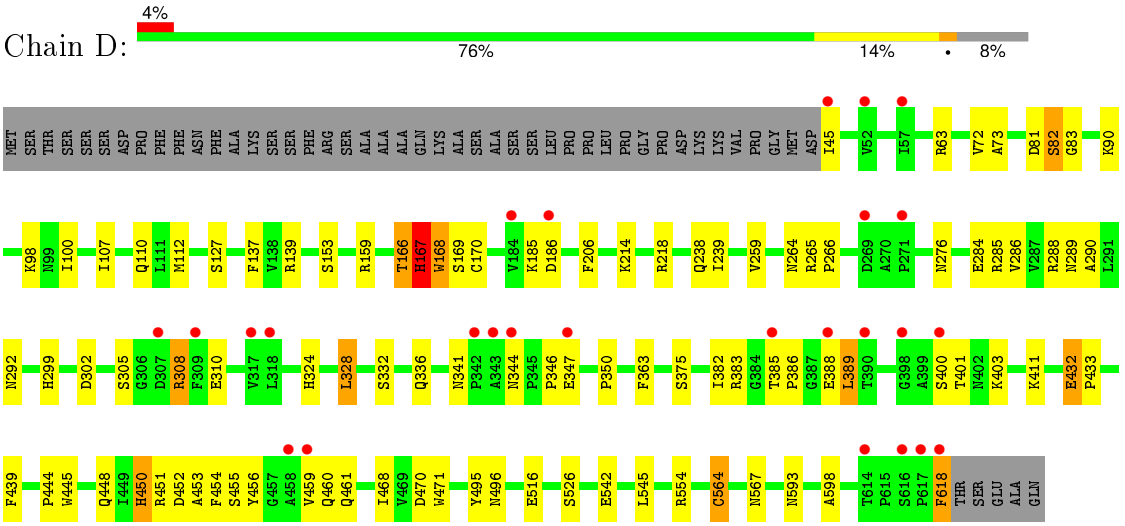
Chain B:



- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.26Å 102.45Å 136.72Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.95) 98.8 (29.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.196 , 0.256 0.207 , 0.261	Depositor DCC
R_{free} test set	2008 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.3	EDS
Estimated twinning fraction	0.059 for -k,-h,-l 0.048 for k,h,-l 0.039 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 198620 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20361	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 12P, FAD, ACT

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	1.19	11/4657 (0.2%)	1.01	11/6331 (0.2%)
1	B	1.18	10/4657 (0.2%)	1.02	13/6331 (0.2%)
1	C	1.02	7/4648 (0.2%)	0.97	10/6320 (0.2%)
1	D	0.99	5/4641 (0.1%)	0.91	3/6310 (0.0%)
All	All	1.10	33/18603 (0.2%)	0.98	37/25292 (0.1%)

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
1	C	0	3
1	D	0	2
All	All	0	6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	THR	C-N	13.15	1.64	1.34
1	B	206	PHE	CE1-CZ	-7.30	1.23	1.37
1	B	316	TYR	CD2-CE2	-7.16	1.28	1.39
1	C	322	ALA	CA-CB	-6.94	1.37	1.52
1	A	429	GLU	CB-CG	6.89	1.65	1.52
1	D	127	SER	CB-OG	-6.75	1.33	1.42
1	B	316	TYR	CD1-CE1	-6.55	1.29	1.39
1	A	478	GLU	CD-OE1	6.36	1.32	1.25
1	D	166	THR	C-N	6.29	1.48	1.34
1	A	482	GLU	CG-CD	6.15	1.61	1.51
1	C	478	GLU	CG-CD	6.03	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	ALA	CA-CB	-5.96	1.40	1.52
1	A	358	GLU	CG-CD	5.93	1.60	1.51
1	A	600	SER	CB-OG	5.82	1.49	1.42
1	B	104	VAL	CB-CG2	-5.80	1.40	1.52
1	B	445	TRP	CB-CG	5.74	1.60	1.50
1	B	495	TYR	CE2-CZ	-5.62	1.31	1.38
1	A	486	TRP	CB-CG	5.60	1.60	1.50
1	D	432	GLU	CB-CG	-5.58	1.41	1.52
1	C	421	GLU	CB-CG	5.47	1.62	1.52
1	A	358	GLU	CB-CG	5.45	1.62	1.52
1	C	310	GLU	CG-CD	5.44	1.60	1.51
1	D	598	ALA	CA-CB	-5.44	1.41	1.52
1	A	355	TYR	CD2-CE2	-5.42	1.31	1.39
1	C	478	GLU	CD-OE2	5.40	1.31	1.25
1	A	317	VAL	CB-CG2	5.39	1.64	1.52
1	B	310	GLU	CG-CD	5.21	1.59	1.51
1	B	330	VAL	CB-CG1	-5.20	1.42	1.52
1	A	542	GLU	CG-CD	5.19	1.59	1.51
1	C	542	GLU	CG-CD	5.15	1.59	1.51
1	B	478	GLU	CG-CD	5.10	1.59	1.51
1	D	564	CYS	CB-SG	-5.09	1.73	1.81
1	B	194	GLU	CG-CD	5.03	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	ASP	CB-CG-OD1	-10.00	109.30	118.30
1	D	167	HIS	O-C-N	-8.50	109.10	122.70
1	A	147	ASP	CB-CG-OD1	7.44	124.99	118.30
1	C	470	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	307	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	339	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	B	288	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	174	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	B	81	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	B	380	MET	CG-SD-CE	-6.59	89.66	100.20
1	C	45	ILE	CB-CA-C	-6.56	98.48	111.60
1	C	139	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	187	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	180	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	82	SER	N-CA-C	6.37	128.21	111.00
1	A	245	ARG	NE-CZ-NH2	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	167	HIS	O-C-N	-6.04	113.04	122.70
1	A	302	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	470	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	265	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	211	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	261	ASP	CB-CG-OD1	5.68	123.42	118.30
1	C	307	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	166	THR	O-C-N	-5.57	113.80	122.70
1	D	389	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	C	510	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	180	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	307	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	166	THR	C-N-CA	-5.38	108.26	121.70
1	C	167	HIS	O-C-N	-5.37	114.11	122.70
1	A	81	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	82	SER	N-CA-C	5.30	125.31	111.00
1	A	82	SER	CB-CA-C	-5.29	100.05	110.10
1	C	167	HIS	C-N-CA	5.21	134.72	121.70
1	B	196	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	285	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	192	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	449	ILE	Peptide
1	C	166	THR	Mainchain
1	C	167	HIS	Mainchain
1	C	457	GLY	Peptide
1	D	166	THR	Mainchain
1	D	167	HIS	Mainchain

5.2 Too-close contacts (i)

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	4541	0	4386	56	0
1	B	4541	0	4386	77	0
1	C	4532	0	4380	96	0
1	D	4525	0	4373	93	0
2	A	53	0	27	1	0
2	B	53	0	26	0	0
2	C	53	0	29	14	0
2	D	53	0	26	1	0
3	A	4	0	3	3	0
3	B	4	0	3	2	0
3	C	4	0	3	2	0
3	D	4	0	3	2	0
4	A	32	0	36	0	0
4	B	16	0	21	0	0
4	C	14	0	16	1	0
4	D	23	0	26	9	0
5	A	518	0	0	9	0
5	B	534	0	0	21	0
5	C	457	0	0	12	0
5	D	400	0	0	19	0
All	All	20361	0	17744	321	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 9.

All (321) 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:C:167:HIS:HE2	2:C:801:FAD:C8M	1.00	1.58
1:C:167:HIS:NE2	2:C:801:FAD:HM82	1.04	1.35
1:B:312:LYS:HG3	5:B:2396:HOH:O	1.41	1.19
1:A:385:THR:O	1:A:388:GLU:HG2	1.38	1.18
1:C:299:HIS:CE1	1:C:310:GLU:HG2	1.78	1.17
1:B:101:ASP:O	1:B:104:VAL:HG12	1.47	1.15
1:D:385:THR:HG23	1:D:388:GLU:HG3	1.29	1.14
1:B:389:LEU:HB2	5:B:2263:HOH:O	1.50	1.09
1:C:458:ALA:HA	5:C:2694:HOH:O	1.56	1.06
1:D:214:LYS:HD2	5:D:2117:HOH:O	1.69	0.93
1:C:167:HIS:CD2	2:C:801:FAD:HM82	2.04	0.91
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.36	0.89
1:A:459:VAL:HA	5:A:2120:HOH:O	1.73	0.87
1:D:382:ILE:HD13	5:D:2710:HOH:O	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASP:OD2	1:B:561:GLU:HG3	1.76	0.86
1:D:382:ILE:CD1	5:D:2710:HOH:O	2.24	0.85
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.20	0.85
1:D:385:THR:HG23	1:D:388:GLU:CG	2.06	0.84
1:C:388:GLU:OE1	1:C:388:GLU:N	2.10	0.83
1:D:385:THR:CG2	1:D:388:GLU:HG3	2.08	0.82
1:B:365:GLN:OE1	1:B:458:ALA:HB2	1.79	0.82
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.25	0.81
1:B:207:GLN:HG3	5:B:2725:HOH:O	1.80	0.81
1:B:478:GLU:HG3	1:B:511:THR:OG1	1.80	0.80
1:D:308:ARG:HG3	1:D:308:ARG:HH11	1.46	0.80
1:A:385:THR:HB	1:A:386:PRO:HD2	1.63	0.80
1:B:459:VAL:HG12	1:B:459:VAL:O	1.81	0.79
1:B:178:GLU:OE2	1:B:441:PRO:HG3	1.81	0.78
1:C:167:HIS:CE1	2:C:801:FAD:HM82	2.12	0.78
1:C:341:ASN:ND2	1:C:343:ALA:H	1.82	0.77
1:D:308:ARG:CG	1:D:308:ARG:HH11	1.98	0.76
1:B:267:ASN:HB2	5:B:2679:HOH:O	1.85	0.75
1:D:288:ARG:NH1	4:D:907:12P:H121	2.01	0.75
1:C:167:HIS:HE2	2:C:801:FAD:C8	1.98	0.74
1:A:385:THR:H	1:A:388:GLU:CD	1.91	0.74
1:A:45:ILE:H	1:A:45:ILE:HD12	1.53	0.73
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.71	0.73
1:A:225:LYS:HE3	1:A:229:GLU:OE2	1.89	0.72
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.35	0.72
1:D:411:LYS:HE2	5:D:2736:HOH:O	1.88	0.71
1:D:545:LEU:HD12	5:D:2399:HOH:O	1.88	0.71
1:A:185:LYS:HD3	5:A:2648:HOH:O	1.91	0.71
1:A:83:GLY:N	1:B:81:ASP:O	2.23	0.70
1:C:216:SER:HB3	1:C:219:HIS:HB3	1.74	0.70
1:C:341:ASN:HD22	1:C:343:ALA:H	1.40	0.69
1:B:101:ASP:O	1:B:104:VAL:CG1	2.35	0.69
1:B:310:GLU:O	1:B:310:GLU:HG3	1.93	0.69
1:D:456:TYR:HB3	5:D:2705:HOH:O	1.93	0.68
1:A:365:GLN:HE22	1:A:459:VAL:HG22	1.59	0.68
1:C:341:ASN:C	1:C:341:ASN:HD22	1.98	0.67
5:C:2195:HOH:O	1:D:461:GLN:HG2	1.96	0.66
1:D:81:ASP:OD2	1:D:90:LYS:NZ	2.28	0.65
1:B:185:LYS:HD3	1:B:557:PHE:CD2	2.30	0.65
1:D:288:ARG:O	4:D:907:12P:H152	1.96	0.65
1:C:432:GLU:HB2	1:C:433:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:GLN:HE22	3:D:901:ACT:CH3	2.09	0.65
1:B:344:ASN:N	1:B:344:ASN:ND2	2.44	0.65
1:A:81:ASP:N	1:A:81:ASP:OD1	2.24	0.64
1:B:397:PRO:HD3	5:B:2573:HOH:O	1.97	0.64
1:C:228:GLU:HA	1:C:231:LYS:HE2	1.80	0.64
1:B:456:TYR:CD1	1:B:456:TYR:N	2.66	0.63
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.80	0.63
1:D:137:PHE:CE2	1:D:139:ARG:HG3	2.34	0.63
1:D:299:HIS:ND1	1:D:310:GLU:OE2	2.29	0.62
1:B:490:LYS:HG3	5:B:1609:HOH:O	1.99	0.62
1:C:465:SER:HA	1:C:468:ILE:HD12	1.80	0.62
1:C:194:GLU:OE2	1:C:604:LYS:NZ	2.33	0.61
1:A:269:ASP:N	1:A:269:ASP:OD1	2.33	0.61
1:D:459:VAL:HG12	1:D:461:GLN:NE2	2.16	0.61
1:D:452:ASP:HB3	1:D:454:PHE:CE1	2.35	0.61
1:D:81:ASP:O	1:D:83:GLY:N	2.33	0.60
1:D:452:ASP:HB3	1:D:454:PHE:HE1	1.65	0.60
1:B:185:LYS:HD3	1:B:557:PHE:CE2	2.36	0.60
1:C:449:ILE:HD13	1:C:471:TRP:CZ3	2.36	0.60
1:B:459:VAL:CG1	1:B:459:VAL:O	2.49	0.60
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.34	0.60
1:D:290:ALA:HB3	5:D:2315:HOH:O	2.00	0.60
1:A:185:LYS:HE3	1:A:557:PHE:CD2	2.37	0.59
1:C:547:LEU:CD1	2:C:801:FAD:HM83	2.32	0.59
1:B:71:LYS:HE3	5:B:2295:HOH:O	2.02	0.59
2:A:801:FAD:O4	3:A:901:ACT:H2	2.03	0.59
1:A:45:ILE:HD12	1:A:45:ILE:N	2.17	0.58
1:B:344:ASN:HD22	1:B:344:ASN:N	2.01	0.58
1:B:82:SER:CB	5:B:1614:HOH:O	2.50	0.58
1:B:81:ASP:N	1:B:81:ASP:OD1	2.32	0.58
1:C:619:THR:CG2	1:C:619:THR:O	2.52	0.58
1:A:44:ASP:OD2	1:A:71:LYS:NZ	2.34	0.57
1:A:343:ALA:C	1:A:344:ASN:HD22	2.07	0.57
1:C:336:GLN:NE2	1:C:344:ASN:O	2.38	0.57
1:C:167:HIS:NE2	2:C:801:FAD:C8	2.64	0.57
1:B:234:ARG:HD3	1:B:443:HIS:CE1	2.40	0.57
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.40	0.57
1:D:459:VAL:HG12	1:D:461:GLN:HE22	1.70	0.56
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.41	0.56
1:D:288:ARG:HH12	4:D:907:12P:C12	2.18	0.56
1:A:81:ASP:O	1:B:81:ASP:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:SER:O	1:B:355:TYR:HB2	2.04	0.56
1:B:269:ASP:HB2	5:B:2322:HOH:O	2.05	0.56
1:C:461:GLN:HA	1:C:461:GLN:HE21	1.71	0.56
1:A:440:GLN:HB3	1:A:441:PRO:HD2	1.87	0.56
1:C:619:THR:O	1:C:619:THR:HG22	2.06	0.56
1:D:288:ARG:HH12	4:D:907:12P:H121	1.71	0.55
1:B:341:ASN:ND2	1:B:343:ALA:H	2.03	0.55
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.88	0.55
1:C:214:LYS:HG3	5:C:1393:HOH:O	2.07	0.55
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.71	0.55
1:D:567:ASN:HB2	5:D:2758:HOH:O	2.05	0.55
1:D:545:LEU:CD1	5:D:2399:HOH:O	2.52	0.54
1:B:343:ALA:C	1:B:344:ASN:HD22	2.11	0.54
1:C:175:PHE:CE1	1:C:592:ALA:HB3	2.42	0.54
1:C:414:ASN:HB3	1:C:418:GLN:HE22	1.72	0.54
1:C:245:ARG:HG2	5:C:2461:HOH:O	2.08	0.54
1:D:265:ARG:HB3	1:D:266:PRO:HA	1.89	0.54
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.08	0.54
1:D:153:SER:OG	1:D:542:GLU:HG3	2.07	0.53
1:B:543:PRO:HG3	5:D:1751:HOH:O	2.08	0.53
1:B:43:MET:HG2	1:B:278:PHE:CE1	2.44	0.53
1:C:265:ARG:HB3	1:C:266:PRO:HA	1.91	0.53
1:B:335:GLY:O	1:B:346:PRO:HB3	2.08	0.53
1:B:82:SER:HB2	5:B:1614:HOH:O	2.06	0.53
1:D:450:HIS:O	1:D:470:ASP:HB2	2.08	0.53
1:C:284:GLU:C	1:C:285:ARG:HG2	2.29	0.53
1:A:440:GLN:HB3	1:A:441:PRO:CD	2.38	0.52
1:A:606:CYS:O	1:A:610:LYS:HG3	2.10	0.52
1:A:516:GLU:HB3	5:A:2035:HOH:O	2.09	0.52
1:D:299:HIS:HD1	1:D:310:GLU:CD	2.13	0.52
1:C:228:GLU:HG3	1:C:231:LYS:NZ	2.24	0.52
1:D:432:GLU:CB	1:D:433:PRO:HD2	2.40	0.52
1:C:216:SER:OG	1:C:431:PRO:O	2.20	0.52
1:D:290:ALA:HB2	5:D:2440:HOH:O	2.09	0.52
1:C:165:SER:HA	1:C:168:TRP:CD1	2.44	0.52
1:C:197:ARG:HG2	1:C:197:ARG:NH1	2.23	0.52
1:D:82:SER:HB2	5:D:2176:HOH:O	2.10	0.52
1:A:341:ASN:HD21	1:A:343:ALA:HB3	1.75	0.51
1:A:344:ASN:N	1:A:344:ASN:HD22	2.09	0.51
1:D:328:LEU:CD1	1:D:328:LEU:C	2.78	0.51
1:D:299:HIS:NE2	1:D:308:ARG:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.93	0.51
1:C:547:LEU:HD12	2:C:801:FAD:HM83	1.93	0.51
1:D:302:ASP:OD2	1:D:305:SER:OG	2.22	0.51
1:D:218:ARG:HD2	5:D:1518:HOH:O	2.11	0.51
1:B:63:ARG:HD2	1:B:259:VAL:O	2.11	0.51
1:D:185:LYS:O	1:D:186:ASP:C	2.48	0.51
1:C:169:SER:OG	2:C:801:FAD:N5	2.44	0.50
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.47	0.50
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.75	0.50
1:D:451:ARG:HD3	1:D:468:ILE:O	2.12	0.50
1:D:292:ASN:OD1	4:D:907:12P:H121	2.11	0.50
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.12	0.50
1:A:215:GLU:O	1:A:411:LYS:NZ	2.45	0.50
1:D:453:ALA:C	1:D:454:PHE:CD1	2.85	0.50
1:A:365:GLN:HE22	1:A:459:VAL:CG2	2.24	0.50
1:C:387:GLY:C	1:C:388:GLU:OE1	2.50	0.50
1:D:336:GLN:NE2	1:D:344:ASN:O	2.45	0.50
1:D:168:TRP:H	1:D:168:TRP:HD1	1.59	0.50
1:D:328:LEU:C	1:D:328:LEU:HD12	2.32	0.49
1:C:145:GLU:OE2	1:C:490:LYS:NZ	2.40	0.49
1:A:218:ARG:HD2	5:A:1538:HOH:O	2.10	0.49
1:A:384:GLY:N	5:A:2691:HOH:O	2.45	0.49
1:B:269:ASP:CB	5:B:2322:HOH:O	2.60	0.49
1:C:324:HIS:HD2	1:C:327:GLN:OE1	1.96	0.49
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.12	0.49
1:D:288:ARG:NH1	4:D:907:12P:C12	2.72	0.49
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.95	0.49
1:B:336:GLN:HG2	5:B:2181:HOH:O	2.12	0.49
1:C:461:GLN:HA	1:C:461:GLN:NE2	2.29	0.48
1:A:548:HIS:NE2	3:A:901:ACT:O	2.46	0.48
1:D:284:GLU:O	1:D:285:ARG:HB3	2.14	0.48
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.49	0.48
1:D:169:SER:O	1:D:170:CYS:HB2	2.13	0.48
1:C:414:ASN:HB3	1:C:418:GLN:NE2	2.28	0.48
1:C:183:LEU:HD12	1:C:195:TRP:CE2	2.47	0.48
1:A:297:SER:OG	1:A:310:GLU:OE1	2.27	0.48
1:D:459:VAL:CG1	1:D:460:GLN:N	2.76	0.48
1:D:185:LYS:HD2	1:D:186:ASP:OD2	2.13	0.48
1:D:81:ASP:OD1	1:D:81:ASP:N	2.47	0.48
1:B:454:PHE:CE2	3:B:901:ACT:H1	2.49	0.48
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:OD1	1:A:267:ASN:C	2.52	0.48
1:B:484:LYS:HB3	5:B:2003:HOH:O	2.14	0.47
1:B:336:GLN:NE2	1:B:344:ASN:O	2.47	0.47
1:D:324:HIS:CE1	5:D:2193:HOH:O	2.67	0.47
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.97	0.47
1:C:56:PRO:HD3	1:C:165:SER:HB3	1.97	0.47
1:A:44:ASP:HB2	1:A:47:TYR:CZ	2.50	0.47
1:B:267:ASN:CB	5:B:2679:HOH:O	2.54	0.46
1:B:269:ASP:HA	5:B:2322:HOH:O	2.15	0.46
1:D:618:PHE:C	1:D:618:PHE:CD2	2.88	0.46
1:C:341:ASN:C	1:C:341:ASN:ND2	2.68	0.46
1:C:104:VAL:HG13	1:C:454:PHE:O	2.15	0.46
1:C:571:ARG:NH2	5:C:2535:HOH:O	2.38	0.46
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.50	0.46
1:D:516:GLU:HB3	5:D:2049:HOH:O	2.15	0.46
1:A:132:GLN:OE1	5:A:1776:HOH:O	2.20	0.46
1:C:246:ARG:NH2	1:C:252:GLU:OE1	2.43	0.46
1:C:185:LYS:HD3	1:C:185:LYS:HA	1.70	0.46
1:C:490:LYS:HG2	5:C:2430:HOH:O	2.15	0.46
1:C:608:TYR:CE2	1:C:612:ASN:ND2	2.84	0.46
1:D:336:GLN:HG3	5:D:2042:HOH:O	2.15	0.46
1:C:357:THR:O	1:C:549:LEU:HD12	2.16	0.46
1:D:100:ILE:O	1:D:100:ILE:HG13	2.15	0.46
1:D:411:LYS:CE	5:D:2736:HOH:O	2.56	0.46
1:D:459:VAL:CG1	1:D:461:GLN:NE2	2.78	0.46
1:B:219:HIS:HB2	1:B:433:PRO:HA	1.97	0.46
1:D:308:ARG:NH1	1:D:308:ARG:CG	2.63	0.45
1:B:408:TRP:C	1:B:408:TRP:CD1	2.89	0.45
1:C:233:GLN:NE2	5:C:2213:HOH:O	2.49	0.45
1:D:375:SER:HA	5:D:2094:HOH:O	2.17	0.45
1:B:304:ILE:HG12	5:B:2217:HOH:O	2.17	0.45
1:C:167:HIS:CE1	2:C:801:FAD:C8M	2.85	0.45
1:A:459:VAL:HG22	5:A:2120:HOH:O	2.17	0.45
1:B:283:CYS:HB3	1:B:298:LEU:HD11	1.98	0.45
1:C:398:GLY:HA3	5:C:2523:HOH:O	2.17	0.45
1:D:385:THR:O	1:D:386:PRO:C	2.54	0.45
1:D:448:GLN:HE22	3:D:901:ACT:H3	1.82	0.45
1:B:432:GLU:HB2	1:B:433:PRO:HD2	1.97	0.45
1:D:98:LYS:HG2	5:D:2364:HOH:O	2.17	0.45
1:A:328:LEU:HD23	1:A:328:LEU:C	2.37	0.45
1:B:532:PHE:CE1	1:B:538:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:SER:OG	1:D:545:LEU:HD11	2.17	0.44
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.82	0.44
1:C:461:GLN:HE21	1:C:461:GLN:CA	2.28	0.44
1:D:618:PHE:C	1:D:618:PHE:HD2	2.20	0.44
1:C:454:PHE:CE2	3:C:901:ACT:H1	2.52	0.44
1:A:81:ASP:O	1:B:83:GLY:N	2.50	0.44
1:B:341:ASN:HD22	1:B:341:ASN:C	2.20	0.44
1:B:70:TYR:HA	1:B:615:PRO:HB3	1.99	0.44
1:B:410:GLU:OE2	5:B:2343:HOH:O	2.21	0.44
1:A:225:LYS:CE	1:A:229:GLU:OE2	2.63	0.44
1:C:290:ALA:HA	4:C:905:12P:H122	1.99	0.44
1:D:289:ASN:O	4:D:907:12P:H141	2.18	0.44
1:A:285:ARG:NH1	1:A:287:VAL:HG22	2.32	0.44
1:D:341:ASN:ND2	1:D:341:ASN:C	2.71	0.44
1:A:150:ARG:NH1	5:A:1483:HOH:O	2.42	0.44
1:C:432:GLU:HB2	1:C:451:ARG:HB2	1.99	0.44
1:C:568:THR:O	1:C:604:LYS:HD3	2.17	0.44
1:A:593:ASN:ND2	3:A:901:ACT:H3	2.32	0.44
1:C:606:CYS:O	1:C:610:LYS:HG3	2.18	0.44
1:C:404:HIS:HB3	1:C:405:PRO:HD2	1.99	0.44
1:A:537:LEU:HB3	1:A:538:PRO:HD2	1.99	0.44
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.90	0.44
1:D:439:PHE:C	1:D:439:PHE:CD1	2.92	0.44
1:B:452:ASP:HB3	1:B:454:PHE:CE1	2.52	0.43
1:C:91:LYS:NZ	1:C:452:ASP:OD1	2.51	0.43
1:C:481:GLU:OE2	1:C:484:LYS:NZ	2.48	0.43
1:A:460:GLN:HG3	1:A:460:GLN:H	1.47	0.43
1:B:478:GLU:HG3	1:B:478:GLU:H	1.64	0.43
1:C:104:VAL:O	1:C:108:GLN:HG3	2.17	0.43
1:B:433:PRO:C	1:B:434:GLN:HG2	2.39	0.43
1:D:346:PRO:HG2	1:D:350:PRO:HA	2.00	0.43
1:D:363:PHE:HA	1:D:471:TRP:O	2.18	0.43
1:D:288:ARG:O	4:D:907:12P:C15	2.65	0.43
1:B:180:ARG:NH1	5:B:2571:HOH:O	2.32	0.43
1:D:185:LYS:HG2	1:D:186:ASP:N	2.33	0.43
1:C:86:ILE:O	1:C:257:ASN:HB2	2.18	0.43
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.17	0.43
1:B:183:LEU:HA	1:B:183:LEU:HD23	1.78	0.43
1:D:167:HIS:C	1:D:167:HIS:CD2	2.92	0.43
1:D:265:ARG:HA	1:D:266:PRO:C	2.39	0.43
1:A:328:LEU:HD23	1:A:328:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:HB	1:B:388:GLU:HG3	2.00	0.43
1:A:90:LYS:NZ	1:A:110:GLN:OE1	2.42	0.43
1:D:459:VAL:CG1	1:D:461:GLN:HE22	2.32	0.43
1:D:328:LEU:CD1	1:D:328:LEU:O	2.66	0.43
1:C:70:TYR:HA	1:C:615:PRO:HB3	2.01	0.43
1:B:252:GLU:OE2	5:B:1817:HOH:O	2.21	0.43
1:B:354:SER:O	1:B:355:TYR:CB	2.66	0.42
1:C:63:ARG:HD2	1:C:259:VAL:O	2.19	0.42
1:A:104:VAL:HG13	1:A:454:PHE:O	2.19	0.42
1:C:167:HIS:NE2	2:C:801:FAD:HM81	2.11	0.42
1:B:239:ILE:HD13	1:B:239:ILE:HG21	1.85	0.42
1:A:460:GLN:O	1:A:461:GLN:NE2	2.52	0.42
1:D:238:GLN:HG2	1:D:239:ILE:N	2.34	0.42
1:C:363:PHE:HA	1:C:471:TRP:O	2.20	0.42
1:D:286:VAL:O	1:D:332:SER:HB3	2.19	0.42
1:C:602:ALA:O	1:C:605:SER:HB3	2.19	0.42
1:C:291:LEU:HG	5:C:2216:HOH:O	2.19	0.42
1:C:341:ASN:HD21	1:C:343:ALA:CB	2.32	0.42
1:B:293:SER:O	1:B:576:LYS:NZ	2.52	0.42
1:B:363:PHE:HA	1:B:471:TRP:O	2.20	0.42
1:D:554:ARG:O	1:D:564:CYS:HB2	2.20	0.42
1:C:45:ILE:N	5:C:2639:HOH:O	2.52	0.42
1:B:386:PRO:HG3	1:B:391:TYR:CE1	2.54	0.42
1:A:341:ASN:C	1:A:341:ASN:HD22	2.23	0.42
1:C:537:LEU:HB3	1:C:538:PRO:HD2	2.02	0.42
1:B:328:LEU:HD23	1:B:328:LEU:C	2.39	0.42
1:D:285:ARG:HA	1:D:328:LEU:HD13	2.02	0.41
2:C:801:FAD:H8A	5:C:1581:HOH:O	2.20	0.41
1:B:267:ASN:CA	5:B:2679:HOH:O	2.67	0.41
1:B:454:PHE:CZ	3:B:901:ACT:H1	2.55	0.41
1:C:548:HIS:NE2	3:C:901:ACT:O	2.53	0.41
1:B:194:GLU:OE2	1:B:604:LYS:NZ	2.48	0.41
1:A:355:TYR:CZ	1:A:481:GLU:HB2	2.54	0.41
1:D:63:ARG:HD2	1:D:259:VAL:O	2.20	0.41
1:D:264:ASN:OD1	1:D:276:ASN:HA	2.20	0.41
1:C:385:THR:O	1:C:391:TYR:HB2	2.20	0.41
1:C:167:HIS:CD2	2:C:801:FAD:C8M	2.85	0.41
1:D:347:GLU:OE1	4:D:907:12P:H82	2.20	0.41
1:A:215:GLU:OE2	5:A:2805:HOH:O	2.21	0.41
1:C:201:LYS:HE2	1:C:205:TYR:OH	2.21	0.41
1:B:82:SER:HB2	5:B:1650:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:SER:HB3	1:C:219:HIS:CB	2.46	0.41
1:C:603:ILE:O	1:C:607:GLU:HG3	2.20	0.41
1:A:385:THR:CB	1:A:386:PRO:HD2	2.39	0.41
1:D:107:ILE:HG12	1:D:167:HIS:HB2	2.03	0.41
1:B:355:TYR:HA	1:B:480:LYS:O	2.21	0.41
1:C:286:VAL:O	1:C:332:SER:HB3	2.21	0.41
1:B:54:SER:O	1:B:162:GLY:HA2	2.21	0.41
1:C:210:THR:HG23	5:C:2860:HOH:O	2.19	0.41
1:D:72:VAL:HG12	1:D:73:ALA:N	2.36	0.41
1:C:487:PHE:CE1	1:C:500:PRO:HB3	2.56	0.41
1:B:341:ASN:HD21	1:B:343:ALA:HB3	1.86	0.41
1:D:471:TRP:CH2	1:D:526:SER:HA	2.56	0.41
1:A:359:GLN:HG2	1:A:475:GLY:O	2.21	0.41
1:C:388:GLU:N	1:C:388:GLU:CD	2.71	0.40
1:B:287:VAL:CG2	1:B:299:HIS:CD2	3.04	0.40
1:C:267:ASN:C	1:C:267:ASN:OD1	2.59	0.40
1:C:180:ARG:HD2	1:C:195:TRP:CD2	2.57	0.40
1:C:576:LYS:HA	1:C:576:LYS:HD2	1.72	0.40
1:D:495:TYR:O	1:D:496:ASN:HB2	2.20	0.40
1:A:459:VAL:CG1	1:A:460:GLN:N	2.84	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	574/623 (92%)	551 (96%)	22 (4%)	1 (0%)	52	43
1	B	574/623 (92%)	553 (96%)	20 (4%)	1 (0%)	52	43
1	C	573/623 (92%)	545 (95%)	26 (4%)	2 (0%)	46	35
1	D	572/623 (92%)	546 (96%)	25 (4%)	1 (0%)	52	43
All	All	2293/2492 (92%)	2195 (96%)	93 (4%)	5 (0%)	52	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	B	82	SER
1	C	458	ALA
1	C	459	VAL
1	D	82	SER

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	504/542 (93%)	489 (97%)	15 (3%)	48	36
1	B	504/542 (93%)	486 (96%)	18 (4%)	42	28
1	C	503/542 (93%)	479 (95%)	24 (5%)	31	15
1	D	502/542 (93%)	489 (97%)	13 (3%)	54	43
All	All	2013/2168 (93%)	1943 (96%)	70 (4%)	43	29

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	112	MET
1	A	168	TRP
1	A	178	GLU
1	A	269	ASP
1	A	272	GLU
1	A	341	ASN
1	A	408	TRP
1	A	432	GLU
1	A	450	HIS
1	A	460	GLN
1	A	462	SER
1	A	490	LYS
1	A	560	LYS
1	A	593	ASN

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Mol	Chain	Res	Type
1	B	45	ILE
1	B	82	SER
1	B	85	LYS
1	B	112	MET
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	231	LYS
1	B	252	GLU
1	B	285	ARG
1	B	341	ASN
1	B	344	ASN
1	B	347	GLU
1	B	388	GLU
1	B	408	TRP
1	B	450	HIS
1	B	460	GLN
1	B	593	ASN
1	C	45	ILE
1	C	46	LYS
1	C	91	LYS
1	C	101	ASP
1	C	112	MET
1	C	168	TRP
1	C	185	LYS
1	C	206	PHE
1	C	211	ASP
1	C	245	ARG
1	C	249	THR
1	C	285	ARG
1	C	341	ASN
1	C	382	ILE
1	C	385	THR
1	C	388	GLU
1	C	408	TRP
1	C	432	GLU
1	C	450	HIS
1	C	460	GLN
1	C	490	LYS
1	C	576	LYS
1	C	593	ASN
1	C	611	GLN

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Mol	Chain	Res	Type
1	D	45	ILE
1	D	112	MET
1	D	168	TRP
1	D	206	PHE
1	D	308	ARG
1	D	328	LEU
1	D	383	ARG
1	D	400	SER
1	D	401	THR
1	D	403	LYS
1	D	450	HIS
1	D	593	ASN
1	D	618	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	263	GLN
1	A	341	ASN
1	A	344	ASN
1	A	365	GLN
1	A	461	GLN
1	B	110	GLN
1	B	263	GLN
1	B	341	ASN
1	B	344	ASN
1	C	132	GLN
1	C	299	HIS
1	C	324	HIS
1	C	341	ASN
1	C	418	GLN
1	C	461	GLN
1	C	612	ASN
1	D	110	GLN
1	D	237	GLN
1	D	341	ASN
1	D	461	GLN
1	D	563	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

14 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	801	1	48,58,58	1.57	9 (18%)	54,89,89	2.92	17 (31%)
3	ACT	A	901	-	1,3,3	2.38	1 (100%)	0,3,3	0.00	-
4	12P	A	903	-	15,15,36	0.70	0	14,14,35	0.53	0
4	12P	A	904	-	15,15,36	0.72	0	14,14,35	0.44	0
2	FAD	B	801	1	48,58,58	1.46	6 (12%)	54,89,89	4.32	14 (25%)
3	ACT	B	901	-	1,3,3	1.85	0	0,3,3	0.00	-
4	12P	B	902	-	15,15,36	0.48	0	14,14,35	0.43	0
2	FAD	C	801	1	48,58,58	1.30	4 (8%)	54,89,89	3.18	21 (38%)
3	ACT	C	901	-	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
4	12P	C	905	-	13,13,36	0.78	0	12,12,35	0.31	0
2	FAD	D	801	1	48,58,58	1.31	5 (10%)	54,89,89	3.02	21 (38%)
3	ACT	D	901	-	1,3,3	1.60	0	0,3,3	0.00	-
4	12P	D	906	-	11,11,36	0.53	0	10,10,35	0.28	0
4	12P	D	907	-	10,10,36	0.63	0	9,9,35	0.26	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	801	1	-	0/30/50/50	0/6/6/6
3	ACT	A	901	-	-	0/0/0/0	0/0/0/0
4	12P	A	903	-	-	0/13/13/34	0/0/0/0
4	12P	A	904	-	-	0/13/13/34	0/0/0/0
2	FAD	B	801	1	-	0/30/50/50	0/6/6/6
3	ACT	B	901	-	-	0/0/0/0	0/0/0/0
4	12P	B	902	-	-	0/13/13/34	0/0/0/0
2	FAD	C	801	1	-	0/30/50/50	0/6/6/6
3	ACT	C	901	-	-	0/0/0/0	0/0/0/0
4	12P	C	905	-	-	0/11/11/34	0/0/0/0
2	FAD	D	801	1	-	0/30/50/50	0/6/6/6
3	ACT	D	901	-	-	0/0/0/0	0/0/0/0
4	12P	D	906	-	-	0/9/9/34	0/0/0/0
4	12P	D	907	-	-	0/8/8/34	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C4A-N3A	-4.14	1.29	1.35
2	A	801	FAD	O4B-C4B	-3.76	1.36	1.45
2	B	801	FAD	PA-O1A	-3.08	1.39	1.51
2	D	801	FAD	O4B-C4B	-2.54	1.39	1.45
2	B	801	FAD	O3B-C3B	-2.36	1.37	1.43
2	A	801	FAD	O2B-C2B	-2.30	1.37	1.43
2	C	801	FAD	O4B-C4B	-2.28	1.39	1.45
2	A	801	FAD	C2B-C3B	-2.23	1.47	1.53
2	B	801	FAD	O4B-C4B	-2.22	1.39	1.45
2	A	801	FAD	O3B-C3B	-2.07	1.38	1.43
2	D	801	FAD	C2A-N1A	2.35	1.38	1.33
3	A	901	ACT	CH3-C	2.38	1.52	1.48
2	C	801	FAD	C4-N3	2.40	1.37	1.33
2	A	801	FAD	C2A-N3A	2.65	1.36	1.32
3	C	901	ACT	CH3-C	2.79	1.52	1.48
2	A	801	FAD	C4-C4X	2.89	1.47	1.41
2	B	801	FAD	C2A-N3A	2.93	1.37	1.32
2	D	801	FAD	C2A-N3A	2.95	1.37	1.32
2	D	801	FAD	C4-N3	3.05	1.38	1.33
2	C	801	FAD	C2A-N3A	3.18	1.37	1.32
2	A	801	FAD	C4-N3	3.32	1.39	1.33
2	B	801	FAD	C4-C4X	3.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C2A-N1A	3.67	1.40	1.33
2	A	801	FAD	C1'-N10	3.89	1.52	1.48
2	D	801	FAD	C4-C4X	4.15	1.49	1.41
2	C	801	FAD	C4-C4X	5.06	1.51	1.41

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FAD	N3A-C2A-N1A	-14.35	117.91	128.89
2	B	801	FAD	C4X-C4-N3	-12.72	106.20	123.59
2	C	801	FAD	C4-C4X-C10	-11.14	112.81	119.94
2	A	801	FAD	N3A-C2A-N1A	-10.86	120.58	128.89
2	D	801	FAD	N3A-C2A-N1A	-9.98	121.26	128.89
2	C	801	FAD	N3A-C2A-N1A	-8.87	122.10	128.89
2	D	801	FAD	C4X-C4-N3	-7.65	113.13	123.59
2	A	801	FAD	C4-C4X-C10	-6.86	115.55	119.94
2	C	801	FAD	C4X-C4-N3	-5.29	116.36	123.59
2	A	801	FAD	C4A-C5A-N7A	-3.91	105.88	109.48
2	D	801	FAD	C4-C4X-C10	-3.69	117.58	119.94
2	A	801	FAD	C4X-C10-N10	-3.31	118.57	120.52
2	D	801	FAD	C4X-C10-N10	-3.29	118.58	120.52
2	C	801	FAD	O5'-P-O1P	-3.16	97.34	109.62
2	C	801	FAD	C4X-C10-N10	-2.89	118.81	120.52
2	D	801	FAD	C9A-C5X-N5	-2.80	118.22	122.36
2	D	801	FAD	C4B-O4B-C1B	-2.61	106.85	109.72
2	B	801	FAD	O5'-P-O1P	-2.54	99.76	109.62
2	B	801	FAD	C8M-C8-C7	-2.44	115.36	120.73
2	A	801	FAD	C4X-C4-N3	-2.34	120.39	123.59
2	D	801	FAD	O4'-C4'-C5'	-2.28	105.23	110.19
2	D	801	FAD	C4A-C5A-N7A	-2.26	107.40	109.48
2	C	801	FAD	C4B-O4B-C1B	-2.23	107.27	109.72
2	A	801	FAD	C9A-C5X-N5	-2.21	119.08	122.36
2	C	801	FAD	C4A-C5A-N7A	-2.17	107.48	109.48
2	A	801	FAD	O3P-PA-O5B	-2.13	97.27	102.94
2	C	801	FAD	N6A-C6A-N1A	-2.00	114.91	119.20
2	C	801	FAD	C5X-C9A-N10	2.06	119.19	117.62
2	B	801	FAD	O2P-P-O5'	2.20	119.55	108.46
2	C	801	FAD	O4B-C4B-C5B	2.33	117.65	109.32
2	D	801	FAD	O2P-P-O5'	2.36	120.36	108.46
2	D	801	FAD	O2A-PA-O3P	2.37	115.86	105.09
2	C	801	FAD	C4X-N5-C5X	2.43	119.55	116.76
2	C	801	FAD	C1'-C2'-C3'	2.45	116.81	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FAD	O2A-PA-O1A	2.45	125.79	112.53
2	D	801	FAD	O3B-C3B-C2B	2.63	120.38	111.83
2	B	801	FAD	C4-C4X-C10	2.68	121.65	119.94
2	C	801	FAD	O4'-C4'-C3'	2.72	115.87	109.02
2	A	801	FAD	C4X-N5-C5X	2.76	119.94	116.76
2	D	801	FAD	C1'-N10-C9A	2.85	122.06	118.86
2	C	801	FAD	C5B-C4B-C3B	2.87	126.59	115.21
2	D	801	FAD	O4B-C4B-C5B	2.92	119.78	109.32
2	B	801	FAD	O4B-C1B-N9A	2.94	114.26	108.10
2	D	801	FAD	C5B-C4B-C3B	2.98	127.05	115.21
2	A	801	FAD	C4-C4X-N5	3.04	122.41	118.72
2	B	801	FAD	C5B-C4B-C3B	3.06	127.35	115.21
2	B	801	FAD	O3B-C3B-C4B	3.09	120.33	111.05
2	D	801	FAD	O2B-C2B-C3B	3.12	121.97	111.83
2	A	801	FAD	C5B-C4B-C3B	3.31	128.33	115.21
2	C	801	FAD	O4B-C1B-N9A	3.49	115.40	108.10
2	A	801	FAD	C4-N3-C2	3.56	118.32	115.25
2	A	801	FAD	O3P-P-O5'	3.67	112.68	102.94
2	D	801	FAD	C4-C4X-N5	3.70	123.21	118.72
2	C	801	FAD	C1'-N10-C9A	3.78	123.10	118.86
2	B	801	FAD	O2B-C2B-C3B	4.09	125.13	111.83
2	A	801	FAD	C1'-N10-C9A	4.41	123.82	118.86
2	D	801	FAD	C4-N3-C2	4.63	119.25	115.25
2	D	801	FAD	O4B-C1B-N9A	4.79	118.12	108.10
2	A	801	FAD	O2B-C2B-C3B	4.86	127.64	111.83
2	C	801	FAD	O2B-C2B-C3B	4.97	127.99	111.83
2	C	801	FAD	C4-C4X-N5	5.05	124.85	118.72
2	C	801	FAD	O3B-C3B-C4B	5.47	127.47	111.05
2	B	801	FAD	C1'-N10-C9A	5.49	125.03	118.86
2	D	801	FAD	C4X-N5-C5X	5.51	123.10	116.76
2	A	801	FAD	O3B-C3B-C4B	5.59	127.82	111.05
2	A	801	FAD	O4B-C1B-N9A	5.64	119.91	108.10
2	D	801	FAD	O3B-C3B-C4B	5.93	128.83	111.05
2	C	801	FAD	C2B-C1B-N9A	6.95	124.92	114.29
2	A	801	FAD	C2B-C1B-N9A	7.41	125.61	114.29
2	C	801	FAD	C4-N3-C2	7.64	121.86	115.25
2	D	801	FAD	C2B-C1B-N9A	9.12	128.22	114.29
2	B	801	FAD	C2B-C1B-N9A	9.72	129.15	114.29
2	B	801	FAD	C4-N3-C2	19.75	132.32	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	1	0
3	A	901	ACT	3	0
3	B	901	ACT	2	0
2	C	801	FAD	14	0
3	C	901	ACT	2	0
4	C	905	12P	1	0
2	D	801	FAD	1	0
3	D	901	ACT	2	0
4	D	907	12P	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	576/623 (92%)	0.02	12 (2%)	67	75	7, 13, 31, 43	0
1	B	576/623 (92%)	-0.01	10 (1%)	73	81	7, 13, 27, 48	0
1	C	575/623 (92%)	0.19	20 (3%)	48	58	9, 18, 36, 55	0
1	D	574/623 (92%)	0.32	26 (4%)	37	48	10, 22, 41, 51	0
All	All	2301/2492 (92%)	0.13	68 (2%)	54	64	7, 17, 35, 55	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	459	VAL	7.8
1	D	459	VAL	6.6
1	D	458	ALA	6.4
1	C	458	ALA	6.0
1	B	459	VAL	6.0
1	C	383	ARG	5.2
1	C	389	LEU	4.5
1	B	44	ASP	4.4
1	C	387	GLY	4.3
1	C	384	GLY	4.2
1	A	385	THR	4.1
1	D	45	ILE	3.9
1	C	619	THR	3.8
1	D	618	PHE	3.5
1	A	458	ALA	3.5
1	B	618	PHE	3.4
1	A	345	PRO	3.4
1	D	309	PHE	3.4
1	A	459	VAL	3.4
1	B	43	MET	3.3
1	C	390	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	385	THR	3.3
1	C	385	THR	3.3
1	D	343	ALA	3.3
1	B	458	ALA	3.2
1	D	342	PRO	3.2
1	B	186	ASP	3.1
1	D	318	LEU	3.0
1	C	388	GLU	3.0
1	A	343	ALA	3.0
1	A	43	MET	2.9
1	D	388	GLU	2.9
1	C	345	PRO	2.8
1	B	342	PRO	2.8
1	D	617	PRO	2.8
1	A	401	THR	2.7
1	A	384	GLY	2.7
1	D	344	ASN	2.7
1	C	186	ASP	2.6
1	D	347	GLU	2.6
1	B	269	ASP	2.6
1	D	317	VAL	2.6
1	C	45	ILE	2.6
1	D	400	SER	2.5
1	C	309	PHE	2.5
1	A	618	PHE	2.4
1	C	343	ALA	2.4
1	C	344	ASN	2.4
1	D	307	ASP	2.4
1	A	344	ASN	2.4
1	D	184	VAL	2.3
1	D	269	ASP	2.3
1	B	344	ASN	2.2
1	D	57	ILE	2.2
1	D	52	VAL	2.2
1	C	618	PHE	2.2
1	D	398	GLY	2.2
1	C	232	GLY	2.2
1	D	616	SER	2.2
1	D	271	PRO	2.2
1	A	45	ILE	2.2
1	D	614	THR	2.2
1	C	307	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	184	VAL	2.1
1	B	45	ILE	2.1
1	D	186	ASP	2.1
1	A	387	GLY	2.0
1	D	390	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	ACT	C	901	4/4	0.88	0.22	5.66	30,31,31,31	0
4	12P	B	902	16/37	0.93	0.13	2.94	22,24,39,42	0
3	ACT	A	901	4/4	0.95	0.15	2.67	29,31,32,33	0
3	ACT	B	901	4/4	0.93	0.17	2.64	27,27,27,29	0
4	12P	C	905	14/37	0.72	0.26	2.38	35,42,44,45	0
4	12P	A	903	16/37	0.91	0.13	2.29	21,26,38,38	0
4	12P	A	904	16/37	0.90	0.12	2.07	23,26,39,40	0
4	12P	D	907	11/37	0.75	0.26	1.52	45,47,48,49	0
3	ACT	D	901	4/4	0.91	0.14	0.98	26,27,28,28	0
4	12P	D	906	12/37	0.89	0.13	0.74	23,27,34,34	0
2	FAD	A	801	53/53	0.97	0.11	0.11	4,10,13,16	0
2	FAD	B	801	53/53	0.97	0.11	-0.50	2,9,14,18	0
2	FAD	D	801	53/53	0.95	0.11	-0.55	12,16,19,21	0
2	FAD	C	801	53/53	0.97	0.10	-0.75	7,14,18,19	0

6.5 Other polymers (i)

There are no such residues in this entry.