



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:49 PM GMT

PDB ID : 1UDY
Title : Medium-Chain Acyl-CoA Dehydrogenase with 3-Thiaoctanoyl-CoA
Authors : Satoh, A.; Nakajima, Y.; Miyahara, I.; Hirotsu, K.; Tanaka, T.; Nishina, Y.;
Shiga, K.; Tamaoki, H.; Setoyama, C.; Miura, R.
Deposited on : 2003-05-07
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

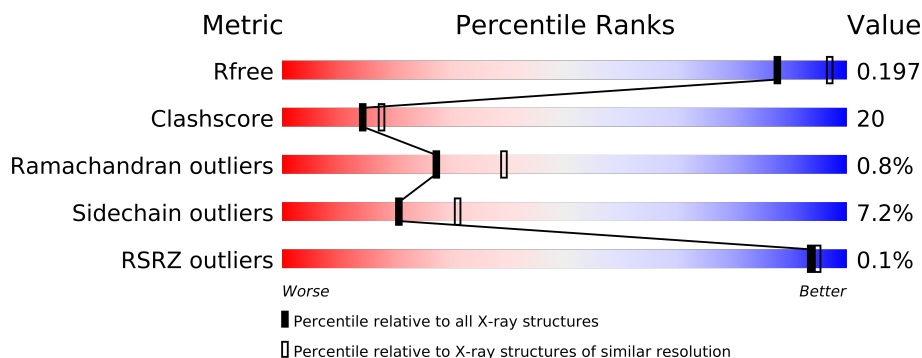
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	<div><div></div><div></div></div>
1	B	396	<div><div></div><div></div></div>
1	C	396	<div><div></div><div></div></div>
1	D	396	<div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CS8	B	1400	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12594 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

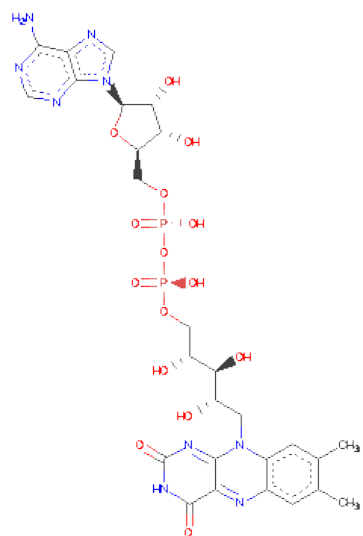
- Molecule 1 is a protein called Acyl-CoA dehydrogenase, medium-chain specific.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2981	1891	514	562	14			
1	B	383	Total	C	N	O	S	0	0	0
			2960	1876	511	559	14			
1	C	385	Total	C	N	O	S	0	0	0
			2981	1891	514	562	14			
1	D	385	Total	C	N	O	S	0	0	0
			2981	1891	514	562	14			

There are 16 discrepancies between the modelled and reference sequences:

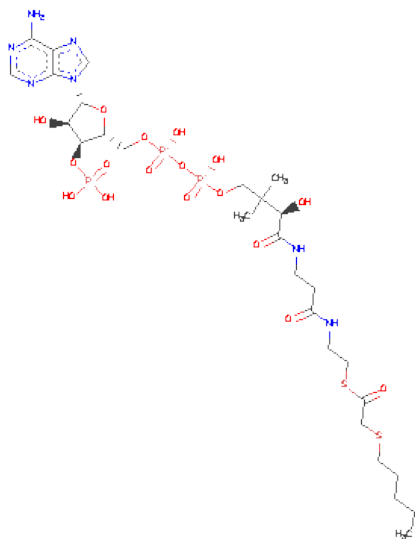
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	SEE REMARK 999	UNP P41367
A	258	PRO	SER	SEE REMARK 999	UNP P41367
A	280	GLU	GLY	SEE REMARK 999	UNP P41367
A	306	GLU	ASP	SEE REMARK 999	UNP P41367
B	15	GLU	LYS	SEE REMARK 999	UNP P41367
B	258	PRO	SER	SEE REMARK 999	UNP P41367
B	280	GLU	GLY	SEE REMARK 999	UNP P41367
B	306	GLU	ASP	SEE REMARK 999	UNP P41367
C	15	GLU	LYS	SEE REMARK 999	UNP P41367
C	258	PRO	SER	SEE REMARK 999	UNP P41367
C	280	GLU	GLY	SEE REMARK 999	UNP P41367
C	306	GLU	ASP	SEE REMARK 999	UNP P41367
D	15	GLU	LYS	SEE REMARK 999	UNP P41367
D	258	PRO	SER	SEE REMARK 999	UNP P41367
D	280	GLU	GLY	SEE REMARK 999	UNP P41367
D	306	GLU	ASP	SEE REMARK 999	UNP P41367

- 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 3-THIAOCTANOYL-COENZYME (three-letter code: CS8) (formula: $C_{28}H_{48}N_7O_{17}P_3S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	B	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	C	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	D	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		

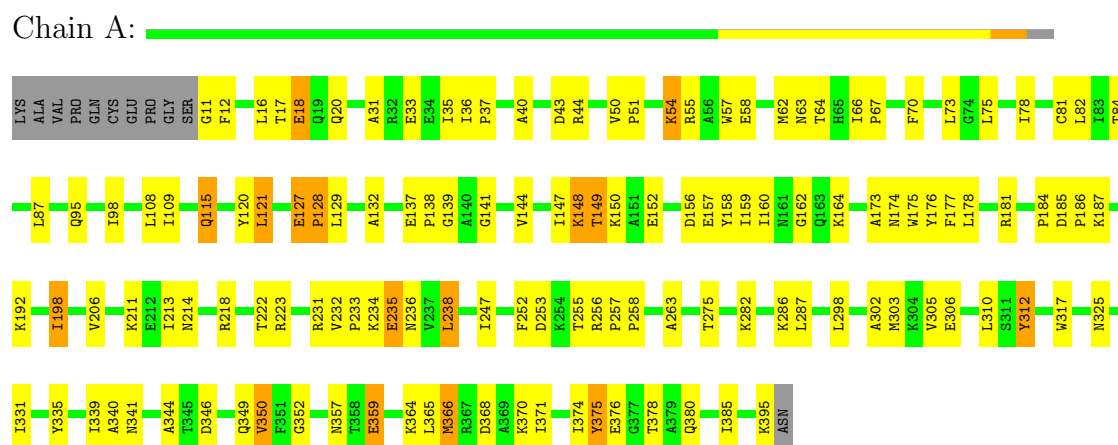
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	63	Total	O	0	0
			63	63		
4	C	52	Total	O	0	0
			52	52		
4	D	76	Total	O	0	0
			76	76		

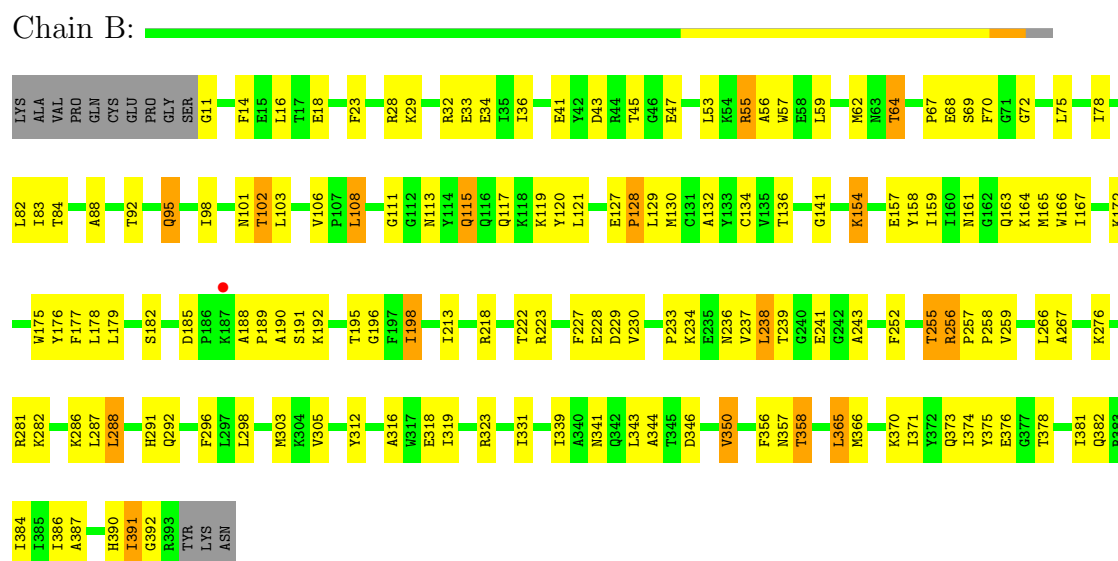
3 Residue-property plots

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

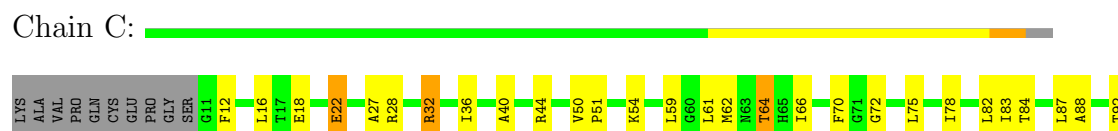
- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific

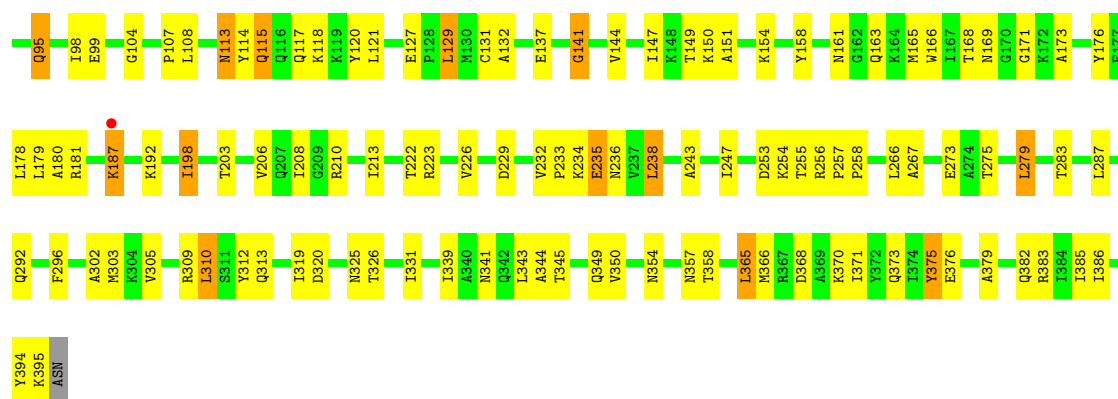


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific



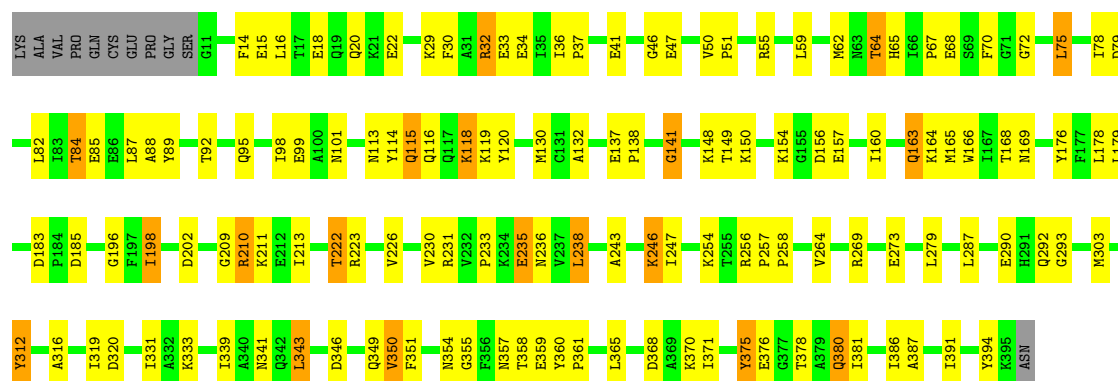
- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific





- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.00Å 110.60Å 147.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 45.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 82.2 (45.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.260 0.192 , 0.197	Depositor DCC
R_{free} test set	2729 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59765 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12594	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 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: CS8, 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	0.37	0/3038	0.62	0/4101
1	B	0.37	0/3016	0.61	1/4072 (0.0%)
1	C	0.37	0/3038	0.61	0/4101
1	D	0.37	0/3038	0.60	0/4101
All	All	0.37	0/12130	0.61	1/16375 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	PHE	N-CA-C	-5.91	95.05	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2981	0	2974	127	0
1	B	2960	0	2952	139	0
1	C	2981	0	2974	120	0
1	D	2981	0	2974	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	6	0
2	B	53	0	31	4	0
2	C	53	0	31	4	0
2	D	53	0	31	5	0
3	A	57	0	44	3	0
3	B	57	0	44	5	0
3	C	57	0	44	1	0
3	D	57	0	44	0	0
4	A	60	0	0	3	0
4	B	63	0	0	3	0
4	C	52	0	0	0	0
4	D	76	0	0	4	0
All	All	12594	0	12174	481	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (481) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:ASN:ND2	1:B:229:ASP:H	1.59	1.01
1:B:341:ASN:HD21	1:B:370:LYS:HA	1.34	0.92
1:D:378:THR:HG22	1:D:381:ILE:HG12	1.52	0.91
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.36	0.90
1:A:186:PRO:HG2	1:A:187:LYS:HD2	1.54	0.89
1:A:137:GLU:OE2	1:A:149:THR:HG22	1.73	0.88
1:C:32:ARG:HA	1:C:36:ILE:HD12	1.55	0.86
1:B:115:GLN:HE21	1:B:115:GLN:H	1.23	0.86
1:B:292:GLN:HE21	1:D:293:GLY:H	1.23	0.85
1:D:32:ARG:HH11	1:D:32:ARG:HG2	1.40	0.85
1:A:115:GLN:NE2	1:A:115:GLN:H	1.72	0.85
1:C:99:GLU:HB3	3:C:2400:CS8:H7'1	1.58	0.85
1:C:108:LEU:HD23	1:C:238:LEU:HD21	1.59	0.84
1:B:23:PHE:HB3	1:B:83:ILE:HD11	1.59	0.84
1:B:127:GLU:HG3	1:B:129:LEU:HD13	1.61	0.82
1:D:341:ASN:HD21	1:D:370:LYS:HA	1.44	0.81
1:A:282:LYS:HE3	1:A:287:LEU:HD22	1.62	0.81
1:D:163:GLN:NE2	1:D:226:VAL:HG22	1.96	0.80
1:A:78:ILE:O	1:A:82:LEU:HD13	1.82	0.80
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.45	0.80
1:C:187:LYS:NZ	1:C:187:LYS:HA	1.97	0.80
1:B:55:ARG:O	1:B:59:LEU:HB2	1.83	0.79
1:B:161:ASN:HD21	1:B:229:ASP:H	1.27	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:THR:O	1:A:258:PRO:HD2	1.83	0.79
1:C:127:GLU:HG3	1:C:129:LEU:HD22	1.64	0.78
1:A:139:GLY:HA2	1:B:281:ARG:HH12	1.48	0.78
1:A:286:LYS:HE3	4:A:1008:HOH:O	1.84	0.77
1:C:78:ILE:HG13	1:C:320:ASP:OD2	1.84	0.76
1:D:246:LYS:H	1:D:246:LYS:HE3	1.51	0.76
1:C:64:THR:HG23	1:C:75:LEU:HB2	1.68	0.75
1:B:163:GLN:HG2	1:B:164:LYS:N	2.00	0.75
1:A:62:MET:HG3	1:A:98:ILE:HG23	1.69	0.74
1:B:252:PHE:HA	1:B:255:THR:HG23	1.69	0.74
1:B:34:GLU:OE1	1:B:55:ARG:HD3	1.89	0.73
1:B:127:GLU:HG3	1:B:129:LEU:CD1	2.18	0.73
1:B:292:GLN:HE21	1:D:293:GLY:N	1.85	0.73
1:B:154:LYS:HD3	1:B:154:LYS:O	1.88	0.73
1:A:108:LEU:HD12	1:A:238:LEU:HD11	1.69	0.73
1:A:43:ASP:OD1	1:A:218:ARG:HD3	1.89	0.73
1:A:149:THR:HG21	1:A:164:LYS:HE2	1.71	0.72
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.52	0.72
1:A:159:ILE:CD1	1:A:231:ARG:HG2	2.19	0.72
1:B:331:ILE:HG23	1:C:303:MET:HG3	1.70	0.72
1:D:118:LYS:NZ	1:D:118:LYS:HB2	2.04	0.71
1:B:255:THR:O	1:B:258:PRO:HD2	1.90	0.71
1:A:303:MET:HG3	1:D:331:ILE:HG23	1.72	0.71
1:B:256:ARG:HG2	1:B:256:ARG:NH1	2.05	0.71
1:D:64:THR:HG23	1:D:75:LEU:HB2	1.71	0.71
1:D:378:THR:HG22	1:D:381:ILE:CG1	2.20	0.71
1:D:32:ARG:NH1	1:D:32:ARG:HG2	2.04	0.70
1:B:292:GLN:NE2	1:D:293:GLY:H	1.89	0.70
1:D:29:LYS:O	1:D:33:GLU:HG2	1.92	0.69
1:D:378:THR:CG2	1:D:381:ILE:HG12	2.22	0.69
1:D:246:LYS:CE	1:D:246:LYS:H	2.04	0.69
1:D:256:ARG:HG3	1:D:333:LYS:HG3	1.74	0.69
1:D:115:GLN:NE2	1:D:115:GLN:H	1.91	0.69
1:A:73:LEU:HB3	1:A:75:LEU:HD13	1.74	0.69
1:B:45:THR:OG1	1:B:47:GLU:HG2	1.94	0.68
1:B:257:PRO:HB2	1:B:258:PRO:HD3	1.76	0.68
1:A:331:ILE:HG23	1:D:303:MET:HG3	1.77	0.67
1:B:115:GLN:NE2	1:B:115:GLN:H	1.91	0.67
1:C:341:ASN:HD21	1:C:370:LYS:HA	1.60	0.67
1:B:161:ASN:HD21	1:B:229:ASP:N	1.91	0.67
1:A:198:ILE:HG23	1:A:236:ASN:HB3	1.75	0.67
1:D:16:LEU:CD2	1:D:82:LEU:HD21	2.23	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:PHE:HA	1:A:255:THR:HG22	1.76	0.67
1:A:156:ASP:HA	1:A:234:LYS:HD3	1.77	0.67
1:A:150:LYS:HD2	1:A:181:ARG:O	1.93	0.67
1:C:141:GLY:HA3	2:C:2399:FAD:H5'1	1.76	0.67
1:A:54:LYS:HB2	1:A:54:LYS:NZ	2.09	0.67
1:B:390:HIS:C	1:B:392:GLY:H	1.99	0.66
1:A:62:MET:CG	1:A:98:ILE:HG23	2.25	0.66
1:C:233:PRO:HB2	1:C:235:GLU:OE2	1.95	0.66
1:B:233:PRO:HG2	1:B:236:ASN:OD1	1.94	0.66
1:C:187:LYS:HA	1:C:187:LYS:HZ3	1.61	0.66
1:C:158:TYR:HB2	1:C:232:VAL:CG1	2.26	0.65
1:C:137:GLU:OE2	1:C:149:THR:HB	1.96	0.65
1:A:302:ALA:O	1:A:305:VAL:HG12	1.96	0.65
1:B:55:ARG:NH2	1:B:59:LEU:HD13	2.11	0.65
1:B:57:TRP:CD2	1:B:128:PRO:HG3	2.31	0.65
1:B:84:THR:HG23	1:B:95:GLN:OE1	1.97	0.65
1:B:291:HIS:HD2	4:B:944:HOH:O	1.81	0.64
1:C:257:PRO:HB2	1:C:258:PRO:HD3	1.79	0.64
1:D:163:GLN:HE22	1:D:226:VAL:HG22	1.62	0.64
1:A:17:THR:H	1:A:20:GLN:HE21	1.44	0.64
1:D:222:THR:HB	4:D:860:HOH:O	1.97	0.64
1:B:346:ASP:O	1:B:350:VAL:HG13	1.98	0.63
1:C:158:TYR:HB2	1:C:232:VAL:HG13	1.80	0.63
1:D:55:ARG:O	1:D:59:LEU:HD13	1.98	0.63
1:C:275:THR:O	1:C:279:LEU:HD22	1.99	0.63
1:B:78:ILE:O	1:B:82:LEU:HD13	1.97	0.63
1:A:137:GLU:HB3	1:A:138:PRO:HD2	1.80	0.63
1:C:150:LYS:HG3	1:C:151:ALA:H	1.63	0.62
1:B:161:ASN:ND2	1:B:229:ASP:N	2.40	0.62
1:A:395:LYS:NZ	1:A:395:LYS:CB	2.62	0.62
1:C:115:GLN:H	1:C:115:GLN:CD	2.03	0.62
1:D:41:GLU:HB2	4:D:1025:HOH:O	1.99	0.61
1:C:150:LYS:HD2	1:C:181:ARG:O	2.00	0.61
1:C:357:ASN:HD22	1:C:358:THR:H	1.46	0.61
1:C:187:LYS:HA	1:C:187:LYS:HZ2	1.65	0.61
1:C:370:LYS:HZ3	1:D:349:GLN:HG2	1.64	0.61
1:C:345:THR:HA	1:C:366:MET:HE2	1.81	0.61
1:A:137:GLU:OE2	1:A:147:ILE:HB	2.01	0.61
1:D:387:ALA:O	1:D:391:ILE:HD13	2.01	0.61
1:D:16:LEU:HD22	1:D:82:LEU:HD21	1.83	0.60
1:B:276:LYS:HE2	4:B:901:HOH:O	2.01	0.60
1:A:115:GLN:HE21	1:A:115:GLN:H	1.50	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:233:PRO:HG2	1:D:236:ASN:ND2	2.16	0.60
1:C:370:LYS:NZ	1:D:349:GLN:HG2	2.17	0.60
1:A:206:VAL:O	1:A:206:VAL:HG23	2.01	0.59
1:B:108:LEU:HD22	1:B:238:LEU:HD11	1.83	0.59
1:B:164:LYS:HB3	1:B:167:ILE:HD11	1.83	0.59
1:D:198:ILE:C	1:D:198:ILE:HD13	2.22	0.59
1:B:16:LEU:HD23	1:B:82:LEU:HD21	1.83	0.59
1:A:198:ILE:HG22	1:A:236:ASN:O	2.03	0.59
1:A:375:TYR:O	1:A:376:GLU:HB2	2.02	0.58
1:D:257:PRO:HB2	1:D:258:PRO:HD3	1.84	0.58
1:C:83:ILE:O	1:C:87:LEU:HD13	2.03	0.58
1:A:395:LYS:HZ2	1:A:395:LYS:HB2	1.69	0.58
1:C:50:VAL:O	1:C:54:LYS:HD3	2.04	0.58
1:A:149:THR:HB	1:A:162:GLY:HA3	1.85	0.58
1:C:213:ILE:O	1:D:358:THR:HG22	2.04	0.57
1:B:11:GLY:N	4:B:864:HOH:O	2.37	0.57
1:D:165:MET:HG3	1:D:166:TRP:CD1	2.39	0.57
1:C:171:GLY:HA2	1:C:208:ILE:HD13	1.86	0.57
1:A:78:ILE:HD11	1:A:317:TRP:HA	1.85	0.57
1:A:395:LYS:NZ	1:A:395:LYS:HB2	2.18	0.57
1:D:65:HIS:HE1	1:D:254:LYS:NZ	2.02	0.57
1:A:282:LYS:HE3	1:A:287:LEU:CD2	2.33	0.57
1:B:381:ILE:HG23	3:B:1400:CS8:H133	1.87	0.57
1:D:55:ARG:NH2	1:D:59:LEU:HD11	2.19	0.57
1:A:173:ALA:HB3	1:A:176:TYR:CE1	2.39	0.57
1:D:339:ILE:O	1:D:343:LEU:HD12	2.05	0.57
1:A:368:ASP:O	1:A:371:ILE:HG22	2.05	0.56
1:D:210:ARG:HG3	1:D:210:ARG:HH11	1.69	0.56
1:B:384:ILE:HD11	1:C:292:GLN:HE21	1.69	0.56
1:D:202:ASP:HB3	4:D:1048:HOH:O	2.04	0.56
1:A:375:TYR:HD1	1:A:375:TYR:O	1.88	0.56
1:A:252:PHE:CE1	3:A:400:CS8:H31	2.40	0.56
1:B:117:GLN:O	1:B:121:LEU:HB2	2.06	0.56
1:C:163:GLN:HG2	1:C:226:VAL:HG22	1.86	0.56
1:B:111:GLY:O	1:B:239:THR:HG22	2.05	0.56
1:B:371:ILE:CD1	2:B:1399:FAD:HM83	2.35	0.56
1:D:380:GLN:H	1:D:380:GLN:NE2	2.03	0.56
1:A:252:PHE:O	1:A:256:ARG:HB2	2.04	0.56
1:D:246:LYS:HD3	1:D:246:LYS:N	2.21	0.56
1:C:150:LYS:HG3	1:C:151:ALA:N	2.19	0.56
1:C:132:ALA:HB3	1:C:176:TYR:HD1	1.70	0.56
1:B:163:GLN:HG2	1:B:164:LYS:H	1.71	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:368:ASP:O	1:C:371:ILE:HG22	2.05	0.55
1:B:56:ALA:HB3	1:B:62:MET:HE3	1.87	0.55
1:A:282:LYS:HG3	1:A:287:LEU:HD13	1.88	0.55
1:C:344:ALA:HB1	1:C:366:MET:HA	1.89	0.55
1:D:292:GLN:NE2	4:D:813:HOH:O	2.39	0.55
1:C:16:LEU:HD22	1:C:82:LEU:HD21	1.87	0.55
1:B:16:LEU:HD23	1:B:82:LEU:CD2	2.36	0.55
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.72	0.55
1:D:378:THR:HG21	2:D:3399:FAD:O2B	2.07	0.55
1:A:152:GLU:O	1:A:158:TYR:HA	2.07	0.55
1:D:114:TYR:HB3	1:D:115:GLN:HE21	1.71	0.55
1:C:32:ARG:NH1	1:C:32:ARG:HG2	2.21	0.54
1:A:43:ASP:HB2	1:A:364:LYS:HE2	1.87	0.54
1:B:103:LEU:HD22	3:B:1400:CS8:H4'1	1.89	0.54
1:C:154:LYS:NZ	1:C:154:LYS:HB3	2.22	0.54
1:A:357:ASN:ND2	1:B:213:ILE:O	2.39	0.54
1:C:357:ASN:HD22	1:C:358:THR:N	2.05	0.54
1:C:255:THR:C	1:C:258:PRO:HD2	2.28	0.54
1:A:16:LEU:HG	1:A:20:GLN:HB2	1.89	0.54
1:A:17:THR:OG1	1:A:20:GLN:HG3	2.07	0.54
2:A:399:FAD:H8A	2:A:399:FAD:O1A	2.08	0.54
1:D:246:LYS:CD	1:D:246:LYS:N	2.71	0.54
1:B:227:PHE:HD2	1:B:230:VAL:HG21	1.72	0.54
1:A:371:ILE:HD12	1:A:374:ILE:HB	1.90	0.54
1:D:115:GLN:CD	1:D:115:GLN:H	2.11	0.54
1:C:166:TRP:HZ2	1:D:354:ASN:HD22	1.56	0.54
1:B:175:TRP:CE3	1:B:198:ILE:HD13	2.42	0.54
1:C:287:LEU:HD22	1:C:287:LEU:H	1.73	0.54
1:A:357:ASN:OD1	1:A:359:GLU:HB2	2.08	0.54
1:C:192:LYS:NZ	1:C:192:LYS:HB2	2.23	0.54
1:C:394:TYR:O	1:C:395:LYS:HB3	2.08	0.54
1:B:292:GLN:HE21	1:D:293:GLY:CA	2.20	0.53
1:A:159:ILE:HD11	1:A:231:ARG:NH1	2.23	0.53
1:C:357:ASN:ND2	1:C:358:THR:N	2.56	0.53
1:C:178:LEU:HD13	1:C:179:LEU:N	2.22	0.53
1:C:394:TYR:O	1:C:395:LYS:CB	2.57	0.53
1:D:16:LEU:HD21	1:D:82:LEU:HD21	1.88	0.53
1:B:43:ASP:CG	1:B:218:ARG:HH21	2.12	0.53
1:B:16:LEU:H	1:B:16:LEU:HD12	1.72	0.53
1:C:345:THR:HA	1:C:366:MET:CE	2.39	0.53
1:C:371:ILE:HD11	2:C:2399:FAD:HM83	1.91	0.53
1:C:255:THR:O	1:C:258:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:PRO:HB2	1:A:235:GLU:HG2	1.90	0.53
1:C:302:ALA:O	1:C:305:VAL:HG12	2.07	0.53
1:B:382:GLN:O	1:B:386:ILE:HG13	2.09	0.53
1:C:161:ASN:ND2	1:C:229:ASP:H	2.07	0.53
1:A:255:THR:C	1:A:258:PRO:HD2	2.29	0.52
1:D:64:THR:HG23	1:D:75:LEU:CB	2.37	0.52
1:C:254:LYS:HD2	1:C:319:ILE:HG12	1.92	0.52
1:A:198:ILE:HG23	1:A:236:ASN:CB	2.39	0.52
1:C:115:GLN:OE1	1:C:115:GLN:N	2.26	0.52
1:B:371:ILE:HD11	2:B:1399:FAD:HM83	1.90	0.52
1:D:55:ARG:CZ	1:D:59:LEU:HD11	2.40	0.52
1:B:292:GLN:HB3	1:D:292:GLN:HB3	1.92	0.52
1:A:177:PHE:HE1	1:A:238:LEU:HD22	1.74	0.52
1:B:370:LYS:HZ2	1:B:373:GLN:NE2	2.08	0.52
1:C:149:THR:HG23	1:C:180:ALA:HA	1.91	0.52
1:A:149:THR:HG21	1:A:164:LYS:CE	2.38	0.52
1:C:357:ASN:ND2	1:D:213:ILE:O	2.42	0.52
1:D:316:ALA:O	1:D:319:ILE:HG22	2.09	0.52
1:A:40:ALA:O	1:A:44:ARG:HG3	2.10	0.52
1:B:282:LYS:HE2	1:B:287:LEU:HD13	1.91	0.52
1:D:118:LYS:HZ2	1:D:118:LYS:HB2	1.74	0.51
1:B:119:LYS:HD3	1:B:120:TYR:CE2	2.45	0.51
1:A:255:THR:HG23	1:A:376:GLU:OE2	2.11	0.51
1:A:129:LEU:HG	1:A:174:ASN:ND2	2.26	0.51
1:C:203:THR:O	1:C:206:VAL:HG13	2.11	0.51
1:B:282:LYS:HG3	1:B:286:LYS:O	2.10	0.51
1:B:102:THR:O	1:B:106:VAL:HG23	2.11	0.51
1:D:371:ILE:HD11	2:D:3399:FAD:HM83	1.91	0.51
1:A:317:TRP:CH2	1:D:15:GLU:HG2	2.46	0.51
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.93	0.51
1:C:117:GLN:O	1:C:121:LEU:HB2	2.10	0.51
1:B:390:HIS:C	1:B:392:GLY:N	2.64	0.51
1:C:62:MET:HG3	1:C:98:ILE:HG23	1.93	0.51
1:D:62:MET:HG3	1:D:98:ILE:HG23	1.92	0.51
1:C:357:ASN:ND2	1:C:358:THR:H	2.10	0.50
1:C:113:ASN:O	1:C:117:GLN:HG3	2.11	0.50
1:B:387:ALA:O	1:B:391:ILE:HG13	2.10	0.50
1:A:213:ILE:HB	1:B:358:THR:HG21	1.94	0.50
1:A:253:ASP:HB3	1:A:325:ASN:OD1	2.11	0.50
1:A:346:ASP:O	1:A:350:VAL:HG13	2.12	0.50
1:D:183:ASP:OD1	1:D:185:ASP:HB3	2.11	0.50
1:B:189:PRO:O	1:B:191:SER:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:371:ILE:CD1	2:D:3399:FAD:HM83	2.41	0.50
1:B:158:TYR:CE1	1:B:237:VAL:HG21	2.46	0.50
1:B:88:ALA:HB1	1:B:92:THR:HG22	1.93	0.50
1:C:120:TYR:CE2	1:C:198:ILE:HG12	2.46	0.50
1:A:158:TYR:HB2	1:A:232:VAL:HG13	1.94	0.50
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.46	0.50
1:B:53:LEU:HD13	1:B:130:MET:CE	2.42	0.50
1:D:246:LYS:H	1:D:246:LYS:CD	2.25	0.50
1:B:198:ILE:HG13	1:B:198:ILE:O	2.11	0.50
1:C:108:LEU:CD2	1:C:238:LEU:HD21	2.37	0.50
2:A:399:FAD:O2'	3:A:400:CS8:H21	2.12	0.50
1:B:108:LEU:HB3	1:B:121:LEU:HD11	1.94	0.50
1:B:384:ILE:HD11	1:C:292:GLN:NE2	2.27	0.50
1:D:88:ALA:HB1	1:D:92:THR:HG22	1.94	0.50
1:A:11:GLY:N	4:A:887:HOH:O	2.45	0.50
1:D:114:TYR:HB3	1:D:115:GLN:NE2	2.26	0.49
1:C:88:ALA:HB1	1:C:92:THR:HG22	1.93	0.49
1:B:370:LYS:NZ	1:B:373:GLN:NE2	2.60	0.49
1:B:281:ARG:HB3	1:B:288:LEU:HD22	1.94	0.49
1:D:132:ALA:HB3	1:D:176:TYR:HD1	1.77	0.49
1:D:141:GLY:HA3	2:D:3399:FAD:H5'1	1.94	0.49
1:C:235:GLU:H	1:C:235:GLU:CD	2.16	0.49
1:B:195:THR:HG23	1:B:241:GLU:HA	1.93	0.49
1:B:163:GLN:HG2	1:B:164:LYS:O	2.12	0.49
1:A:206:VAL:O	1:A:206:VAL:CG2	2.60	0.49
1:B:196:GLY:C	1:B:238:LEU:HD23	2.33	0.49
1:B:141:GLY:HA3	2:B:1399:FAD:H5'1	1.94	0.49
1:B:53:LEU:HD13	1:B:130:MET:HE1	1.95	0.49
1:D:46:GLY:O	1:D:211:LYS:NZ	2.45	0.49
1:B:292:GLN:HG3	1:B:296:PHE:CE1	2.47	0.49
1:D:78:ILE:HG23	1:D:79:ASP:N	2.27	0.49
1:B:136:THR:OG1	3:B:1400:CS8:H32	2.12	0.49
1:B:132:ALA:HB3	1:B:176:TYR:HD1	1.76	0.49
1:A:349:GLN:HE21	1:B:370:LYS:NZ	2.11	0.49
1:D:32:ARG:HH11	1:D:32:ARG:CG	2.18	0.49
1:C:192:LYS:O	1:C:192:LYS:HG2	2.13	0.49
1:A:156:ASP:O	1:A:234:LYS:HG3	2.13	0.48
1:C:382:GLN:O	1:C:386:ILE:HG13	2.12	0.48
1:D:375:TYR:O	1:D:376:GLU:HB2	2.13	0.48
1:B:255:THR:C	1:B:258:PRO:HD2	2.32	0.48
1:D:118:LYS:HZ3	1:D:118:LYS:HB2	1.77	0.48
1:B:64:THR:O	1:B:75:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165:MET:HG3	1:C:166:TRP:CD1	2.49	0.48
1:A:192:LYS:HG2	1:A:192:LYS:O	2.12	0.48
1:A:238:LEU:HD23	1:A:247:ILE:HD13	1.94	0.48
1:D:196:GLY:O	1:D:238:LEU:HD13	2.14	0.48
1:B:182:SER:HB3	1:B:195:THR:OG1	2.13	0.48
1:A:127:GLU:HB3	1:A:129:LEU:HD22	1.96	0.48
1:D:346:ASP:O	1:D:350:VAL:HG13	2.14	0.48
1:B:175:TRP:HB2	1:B:198:ILE:CD1	2.44	0.48
1:D:154:LYS:O	1:D:157:GLU:HG2	2.13	0.48
1:A:109:ILE:HG23	4:A:875:HOH:O	2.13	0.48
1:C:350:VAL:O	2:D:3399:FAD:H51A	2.14	0.47
1:C:131:CYS:HA	1:C:173:ALA:HB1	1.97	0.47
1:C:114:TYR:HB3	1:C:115:GLN:OE1	2.14	0.47
1:A:214:ASN:ND2	1:B:357:ASN:HD22	2.11	0.47
1:B:178:LEU:C	1:B:178:LEU:HD13	2.35	0.47
1:D:119:LYS:HD3	1:D:120:TYR:CE2	2.50	0.47
1:A:371:ILE:HB	1:B:356:PHE:CZ	2.50	0.47
1:B:154:LYS:HE3	1:B:157:GLU:OE2	2.14	0.47
1:B:103:LEU:CD2	3:B:1400:CS8:H2'2	2.44	0.47
1:B:108:LEU:HD12	1:B:117:GLN:HA	1.96	0.47
1:C:178:LEU:HD13	1:C:178:LEU:C	2.35	0.47
1:D:50:VAL:HB	1:D:51:PRO:HD3	1.95	0.47
1:D:85:GLU:HG3	1:D:264:VAL:HG22	1.95	0.47
1:D:67:PRO:HB2	1:D:70:PHE:CD2	2.50	0.47
1:C:349:GLN:HE21	1:D:380:GLN:HE22	1.62	0.47
1:B:303:MET:HG3	1:C:331:ILE:HG23	1.97	0.47
1:D:164:LYS:HE3	1:D:178:LEU:CD2	2.45	0.47
1:B:115:GLN:N	1:B:115:GLN:HE21	2.00	0.47
1:B:134:CYS:SG	1:B:167:ILE:HG21	2.54	0.47
1:D:20:GLN:HB3	1:D:82:LEU:CD2	2.44	0.47
1:A:16:LEU:HD11	1:A:82:LEU:HD21	1.97	0.47
1:A:141:GLY:HA3	2:A:399:FAD:H5'1	1.96	0.47
1:C:371:ILE:CD1	2:C:2399:FAD:HM83	2.45	0.46
1:C:120:TYR:CD2	1:C:198:ILE:HG12	2.50	0.46
1:D:168:THR:O	1:D:169:ASN:HB2	2.14	0.46
1:C:266:LEU:CD1	1:C:365:LEU:HG	2.46	0.46
1:D:233:PRO:HB2	1:D:235:GLU:HG2	1.97	0.46
1:A:63:ASN:HB3	1:A:66:ILE:HD12	1.97	0.46
1:A:275:THR:HG21	1:D:394:TYR:CE1	2.50	0.46
1:A:395:LYS:HZ3	1:A:395:LYS:HB3	1.79	0.46
1:B:316:ALA:O	1:B:319:ILE:HG22	2.15	0.46
1:C:309:ARG:HA	1:C:312:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:27:ALA:HB2	1:C:83:ILE:HG23	1.98	0.46
2:B:1399:FAD:C2	3:B:1400:CS8:H21	2.45	0.46
1:A:33:GLU:O	1:A:37:PRO:HG2	2.15	0.46
1:D:312:TYR:CD1	1:D:312:TYR:C	2.88	0.46
1:D:333:LYS:HD3	1:D:333:LYS:O	2.16	0.46
1:C:256:ARG:HH12	1:C:385:ILE:HD13	1.81	0.46
1:C:40:ALA:O	1:C:44:ARG:HG3	2.16	0.46
1:A:12:PHE:CD1	1:D:14:PHE:HA	2.51	0.46
1:A:374:ILE:HA	1:A:378:THR:HG22	1.97	0.46
1:D:78:ILE:HG22	1:D:320:ASP:OD2	2.15	0.46
1:B:29:LYS:HE3	1:B:33:GLU:OE1	2.16	0.46
1:A:380:GLN:HB2	2:A:399:FAD:O2B	2.16	0.46
1:D:157:GLU:OE1	1:D:231:ARG:CZ	2.63	0.46
1:A:67:PRO:HB2	1:A:70:PHE:CD2	2.51	0.46
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.98	0.45
1:B:163:GLN:CG	1:B:164:LYS:N	2.74	0.45
1:A:159:ILE:HD11	1:A:231:ARG:HH11	1.81	0.45
1:D:154:LYS:HG2	1:D:154:LYS:O	2.17	0.45
1:C:379:ALA:O	1:C:383:ARG:HG2	2.16	0.45
1:A:54:LYS:HB2	1:A:54:LYS:HZ3	1.79	0.45
1:D:55:ARG:NE	1:D:59:LEU:HD11	2.31	0.45
1:D:36:ILE:HB	1:D:37:PRO:HD3	1.98	0.45
1:B:267:ALA:HB1	1:B:343:LEU:HD22	1.97	0.45
1:C:210:ARG:O	1:C:223:ARG:HB2	2.16	0.45
1:C:273:GLU:OE1	1:C:273:GLU:HA	2.16	0.45
1:B:237:VAL:O	1:B:238:LEU:O	2.34	0.45
1:A:36:ILE:HB	1:A:37:PRO:HD3	1.98	0.45
1:A:148:LYS:HD3	1:A:148:LYS:N	2.32	0.45
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.17	0.45
1:A:144:VAL:O	1:A:147:ILE:HG23	2.17	0.45
1:B:292:GLN:HE21	1:D:293:GLY:HA3	1.82	0.45
1:D:210:ARG:HD3	1:D:210:ARG:H	1.82	0.45
1:B:384:ILE:HD13	1:C:296:PHE:HE1	1.82	0.45
1:A:31:ALA:HA	1:A:35:ILE:HD12	1.99	0.45
1:D:163:GLN:HE22	1:D:226:VAL:CG2	2.27	0.45
1:A:108:LEU:CD1	1:A:238:LEU:HD11	2.42	0.45
1:C:132:ALA:HB3	1:C:176:TYR:CD1	2.50	0.45
1:B:111:GLY:O	1:B:239:THR:CG2	2.65	0.45
1:B:344:ALA:HB1	1:B:366:MET:HA	1.98	0.45
1:D:148:LYS:O	1:D:149:THR:C	2.55	0.45
1:C:50:VAL:HB	1:C:51:PRO:HD3	1.99	0.45
1:C:375:TYR:O	1:C:376:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:243:ALA:O	1:C:247:ILE:HG13	2.17	0.44
1:D:113:ASN:OD1	1:D:116:GLN:HG3	2.16	0.44
1:D:341:ASN:HD21	1:D:370:LYS:CA	2.23	0.44
1:A:63:ASN:HB3	1:A:66:ILE:CD1	2.47	0.44
1:A:371:ILE:CD1	2:A:399:FAD:HM83	2.47	0.44
1:C:61:LEU:HD22	1:C:83:ILE:CG2	2.48	0.44
1:A:344:ALA:HB1	1:A:366:MET:HA	1.98	0.44
1:D:55:ARG:HD2	1:D:55:ARG:HA	1.78	0.44
1:D:68:GLU:HA	1:D:72:GLY:O	2.17	0.44
1:B:32:ARG:HA	1:B:36:ILE:HD12	2.00	0.44
1:C:104:GLY:O	1:C:107:PRO:HD2	2.17	0.44
1:D:269:ARG:O	1:D:273:GLU:HG2	2.17	0.44
1:B:127:GLU:HA	1:B:128:PRO:HD3	1.82	0.44
1:A:159:ILE:HD12	1:A:231:ARG:HG2	1.97	0.44
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.83	0.44
1:C:144:VAL:O	1:C:147:ILE:HG23	2.17	0.44
1:B:266:LEU:CD1	1:B:365:LEU:HG	2.48	0.44
1:A:349:GLN:HE21	1:B:370:LYS:HZ1	1.65	0.44
1:B:67:PRO:HG2	1:B:70:PHE:CD2	2.53	0.44
1:A:132:ALA:HB3	1:A:176:TYR:CD1	2.53	0.44
1:D:178:LEU:HD13	1:D:179:LEU:N	2.33	0.44
1:A:55:ARG:HD2	1:A:58:GLU:OE1	2.18	0.44
1:B:98:ILE:O	1:B:101:ASN:HB2	2.18	0.44
1:B:161:ASN:HD22	1:B:228:GLU:HA	1.83	0.44
2:C:2399:FAD:H8A	2:C:2399:FAD:O1A	2.18	0.44
1:B:64:THR:OG1	1:B:75:LEU:HD22	2.17	0.44
1:D:156:ASP:O	1:D:157:GLU:HB3	2.18	0.44
1:A:57:TRP:CD2	1:A:128:PRO:HG3	2.52	0.44
1:A:160:ILE:HD13	1:A:178:LEU:HD23	2.01	0.43
1:D:357:ASN:OD1	1:D:359:GLU:HB2	2.18	0.43
1:A:256:ARG:HD2	1:A:376:GLU:O	2.18	0.43
1:B:371:ILE:HD12	1:B:374:ILE:HB	1.99	0.43
1:A:211:LYS:HB2	1:A:223:ARG:NH2	2.32	0.43
1:C:95:GLN:HE21	1:C:95:GLN:HB3	1.66	0.43
1:D:59:LEU:N	1:D:59:LEU:HD12	2.33	0.43
1:B:154:LYS:HD2	1:B:159:ILE:HD11	2.01	0.43
1:B:189:PRO:O	1:B:192:LYS:N	2.51	0.43
1:C:395:LYS:O	1:C:395:LYS:HG3	2.18	0.43
1:C:234:LYS:C	1:C:236:ASN:H	2.20	0.43
1:D:160:ILE:HB	1:D:230:VAL:HB	1.99	0.43
1:C:168:THR:O	1:C:169:ASN:HB2	2.18	0.43
1:C:198:ILE:HG13	1:C:198:ILE:O	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:351:PHE:HB3	1:D:355:GLY:N	2.32	0.43
1:B:256:ARG:CG	1:B:256:ARG:HH11	2.18	0.43
1:C:253:ASP:OD1	1:C:326:THR:HA	2.19	0.43
1:A:175:TRP:CE3	1:A:198:ILE:HD13	2.54	0.43
1:B:239:THR:OG1	1:B:243:ALA:HB3	2.19	0.43
1:D:178:LEU:C	1:D:178:LEU:HD13	2.39	0.43
1:D:360:TYR:HB3	1:D:361:PRO:HD2	2.00	0.43
1:D:89:TYR:CE1	1:D:269:ARG:HD3	2.53	0.43
1:C:166:TRP:HZ2	1:D:354:ASN:ND2	2.15	0.43
1:A:109:ILE:CG1	1:A:121:LEU:HD21	2.49	0.43
1:B:28:ARG:O	1:B:32:ARG:HG2	2.19	0.43
1:C:339:ILE:O	1:C:343:LEU:HD13	2.19	0.43
1:A:335:TYR:CE2	1:A:339:ILE:HG21	2.54	0.43
1:D:185:ASP:OD2	1:D:185:ASP:C	2.57	0.42
1:A:214:ASN:HD22	1:B:357:ASN:HD22	1.66	0.42
1:C:309:ARG:HA	1:C:312:TYR:CE2	2.54	0.42
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.54	0.42
1:B:41:GLU:O	1:B:45:THR:HG23	2.19	0.42
1:A:156:ASP:C	1:A:234:LYS:HG3	2.39	0.42
1:B:282:LYS:HE2	1:B:287:LEU:CD1	2.49	0.42
1:C:253:ASP:HB3	1:C:325:ASN:OD1	2.19	0.42
1:C:267:ALA:HB1	1:C:343:LEU:HD22	2.01	0.42
1:A:395:LYS:HZ3	1:A:395:LYS:CB	2.31	0.42
1:A:303:MET:HE2	1:D:386:ILE:HD13	2.00	0.42
1:C:370:LYS:NZ	1:C:373:GLN:NE2	2.67	0.42
1:B:113:ASN:O	1:B:117:GLN:HG3	2.19	0.42
1:D:287:LEU:O	1:D:290:GLU:HB2	2.19	0.42
1:A:385:ILE:HD11	3:A:400:CS8:H142	2.02	0.42
1:D:150:LYS:HZ1	1:D:183:ASP:C	2.23	0.42
1:D:164:LYS:HE3	1:D:178:LEU:HD22	2.00	0.42
1:B:14:PHE:HA	1:C:12:PHE:CD1	2.54	0.42
1:A:18:GLU:CA	1:A:18:GLU:OE2	2.66	0.42
1:C:66:ILE:O	1:C:72:GLY:HA3	2.20	0.42
1:C:32:ARG:N	1:C:32:ARG:HD2	2.35	0.42
1:C:354:ASN:HD22	1:D:166:TRP:HZ2	1.66	0.42
1:D:98:ILE:O	1:D:101:ASN:HB2	2.19	0.42
1:B:339:ILE:HD12	1:B:339:ILE:C	2.40	0.42
1:A:352:GLY:O	1:B:374:ILE:HD13	2.20	0.42
1:C:266:LEU:HD11	1:C:365:LEU:HG	2.02	0.42
1:C:257:PRO:CB	1:C:258:PRO:HD3	2.49	0.42
1:D:209:GLY:O	1:D:223:ARG:HD3	2.20	0.42
1:A:160:ILE:HD13	1:A:178:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:243:ALA:O	1:D:247:ILE:HG13	2.20	0.41
1:D:30:PHE:O	1:D:34:GLU:HB2	2.20	0.41
1:D:65:HIS:HE1	1:D:254:LYS:HZ1	1.66	0.41
1:C:256:ARG:N	1:C:257:PRO:CD	2.83	0.41
1:C:61:LEU:HD22	1:C:83:ILE:HG23	2.03	0.41
1:B:378:THR:O	1:B:382:GLN:HG2	2.20	0.41
1:A:371:ILE:HD13	2:A:399:FAD:HM83	2.01	0.41
1:B:257:PRO:CB	1:B:258:PRO:HD3	2.48	0.41
1:D:115:GLN:N	1:D:115:GLN:NE2	2.63	0.41
1:B:192:LYS:HA	1:B:192:LYS:HD2	1.91	0.41
1:B:130:MET:HB2	1:B:172:LYS:O	2.20	0.41
1:A:305:VAL:HG13	1:A:306:GLU:N	2.36	0.41
1:D:202:ASP:OD2	1:D:202:ASP:C	2.59	0.41
1:B:62:MET:C	1:B:64:THR:N	2.72	0.41
1:B:305:VAL:HG23	1:B:343:LEU:HD21	2.01	0.41
1:D:84:THR:OG1	1:D:99:GLU:OE2	2.39	0.41
1:A:184:PRO:O	1:A:185:ASP:C	2.58	0.41
1:B:185:ASP:HB3	1:B:188:ALA:HB2	2.03	0.41
1:B:68:GLU:HA	1:B:72:GLY:O	2.21	0.41
1:C:28:ARG:HG3	1:C:32:ARG:HD3	2.03	0.41
1:B:16:LEU:HD12	1:B:16:LEU:N	2.36	0.41
1:D:257:PRO:N	1:D:258:PRO:CD	2.84	0.41
1:C:87:LEU:N	1:C:87:LEU:HD12	2.35	0.41
1:A:36:ILE:N	1:A:37:PRO:CD	2.84	0.41
1:D:368:ASP:O	1:D:371:ILE:HG22	2.21	0.40
1:A:16:LEU:HG	1:A:20:GLN:CB	2.50	0.40
1:B:195:THR:CG2	1:B:241:GLU:HA	2.51	0.40
1:C:59:LEU:HA	1:C:59:LEU:HD12	1.89	0.40
1:A:17:THR:HG1	1:A:20:GLN:HG3	1.85	0.40
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.86	0.40
1:B:259:VAL:HG21	1:B:376:GLU:HG2	2.03	0.40
1:B:318:GLU:OE2	1:B:323:ARG:HD2	2.20	0.40
1:D:137:GLU:HB3	1:D:138:PRO:HD2	2.04	0.40
1:C:70:PHE:HD1	1:C:118:LYS:HD2	1.86	0.40
1:C:310:LEU:HD12	1:C:313:GLN:HE22	1.85	0.40
1:A:120:TYR:CE2	1:A:198:ILE:HG12	2.56	0.40
1:B:391:ILE:HG22	1:B:391:ILE:O	2.22	0.40
1:A:263:ALA:HB1	1:A:340:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	383/396 (97%)	366 (96%)	15 (4%)	2 (0%)	38	53
1	B	381/396 (96%)	350 (92%)	24 (6%)	7 (2%)	13	15
1	C	383/396 (97%)	371 (97%)	10 (3%)	2 (0%)	38	53
1	D	383/396 (97%)	367 (96%)	14 (4%)	2 (0%)	38	53
All	All	1530/1584 (97%)	1454 (95%)	63 (4%)	13 (1%)	27	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	ALA
1	B	238	LEU
1	C	238	LEU
1	A	238	LEU
1	B	64	THR
1	B	69	SER
1	D	238	LEU
1	B	128	PRO
1	B	234	LYS
1	B	391	ILE
1	A	128	PRO
1	C	141	GLY
1	D	141	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/310 (97%)	278 (92%)	23 (8%)	19	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	299/310 (96%)	279 (93%)	20 (7%)	23	35
1	C	301/310 (97%)	283 (94%)	18 (6%)	27	41
1	D	301/310 (97%)	276 (92%)	25 (8%)	16	24
All	All	1202/1240 (97%)	1116 (93%)	86 (7%)	21	31

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	54	LYS
1	A	64	THR
1	A	84	THR
1	A	87	LEU
1	A	95	GLN
1	A	115	GLN
1	A	121	LEU
1	A	127	GLU
1	A	148	LYS
1	A	149	THR
1	A	157	GLU
1	A	198	ILE
1	A	222	THR
1	A	235	GLU
1	A	298	LEU
1	A	310	LEU
1	A	312	TYR
1	A	350	VAL
1	A	359	GLU
1	A	365	LEU
1	A	366	MET
1	A	375	TYR
1	B	18	GLU
1	B	55	ARG
1	B	95	GLN
1	B	102	THR
1	B	108	LEU
1	B	115	GLN
1	B	154	LYS
1	B	179	LEU
1	B	198	ILE
1	B	222	THR

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Mol	Chain	Res	Type
1	B	223	ARG
1	B	255	THR
1	B	256	ARG
1	B	288	LEU
1	B	298	LEU
1	B	312	TYR
1	B	350	VAL
1	B	358	THR
1	B	365	LEU
1	B	375	TYR
1	C	18	GLU
1	C	22	GLU
1	C	32	ARG
1	C	64	THR
1	C	84	THR
1	C	95	GLN
1	C	113	ASN
1	C	115	GLN
1	C	129	LEU
1	C	187	LYS
1	C	198	ILE
1	C	222	THR
1	C	235	GLU
1	C	279	LEU
1	C	283	THR
1	C	310	LEU
1	C	365	LEU
1	C	375	TYR
1	D	18	GLU
1	D	22	GLU
1	D	32	ARG
1	D	47	GLU
1	D	64	THR
1	D	75	LEU
1	D	84	THR
1	D	87	LEU
1	D	95	GLN
1	D	115	GLN
1	D	118	LYS
1	D	130	MET
1	D	163	GLN
1	D	198	ILE

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Mol	Chain	Res	Type
1	D	210	ARG
1	D	222	THR
1	D	235	GLU
1	D	246	LYS
1	D	279	LEU
1	D	312	TYR
1	D	343	LEU
1	D	350	VAL
1	D	365	LEU
1	D	375	TYR
1	D	380	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	95	GLN
1	A	105	GLN
1	A	115	GLN
1	A	163	GLN
1	A	169	ASN
1	A	174	ASN
1	A	214	ASN
1	A	217	GLN
1	A	236	ASN
1	A	313	GLN
1	A	341	ASN
1	A	349	GLN
1	B	19	GLN
1	B	105	GLN
1	B	115	GLN
1	B	117	GLN
1	B	161	ASN
1	B	169	ASN
1	B	217	GLN
1	B	291	HIS
1	B	292	GLN
1	B	313	GLN
1	B	341	ASN
1	B	373	GLN
1	C	19	GLN
1	C	20	GLN

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Mol	Chain	Res	Type
1	C	65	HIS
1	C	95	GLN
1	C	105	GLN
1	C	161	ASN
1	C	169	ASN
1	C	217	GLN
1	C	313	GLN
1	C	341	ASN
1	C	354	ASN
1	C	357	ASN
1	C	373	GLN
1	C	380	GLN
1	D	19	GLN
1	D	65	HIS
1	D	95	GLN
1	D	105	GLN
1	D	115	GLN
1	D	161	ASN
1	D	163	GLN
1	D	169	ASN
1	D	207	GLN
1	D	217	GLN
1	D	236	ASN
1	D	313	GLN
1	D	341	ASN
1	D	354	ASN
1	D	380	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	399	-	58,58,58	2.66	18 (31%)	85,89,89	2.03	21 (24%)
3	CS8	A	400	-	59,59,59	0.89	2 (3%)	85,85,85	2.39	16 (18%)
2	FAD	B	1399	-	58,58,58	2.53	20 (34%)	85,89,89	2.10	19 (22%)
3	CS8	B	1400	-	59,59,59	1.19	5 (8%)	85,85,85	2.51	19 (22%)
2	FAD	C	2399	-	58,58,58	2.52	17 (29%)	85,89,89	1.96	18 (21%)
3	CS8	C	2400	-	59,59,59	0.85	2 (3%)	85,85,85	2.35	18 (21%)
2	FAD	D	3399	-	58,58,58	2.51	20 (34%)	85,89,89	2.06	18 (21%)
3	CS8	D	3400	-	59,59,59	0.86	2 (3%)	85,85,85	2.42	15 (17%)

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	399	-	-	0/34/50/50	0/1/6/6
3	CS8	A	400	-	-	0/58/74/74	0/1/3/3
2	FAD	B	1399	-	-	0/34/50/50	0/1/6/6
3	CS8	B	1400	-	-	0/58/74/74	0/1/3/3
2	FAD	C	2399	-	-	0/34/50/50	0/1/6/6
3	CS8	C	2400	-	-	0/58/74/74	0/1/3/3
2	FAD	D	3399	-	-	0/34/50/50	0/1/6/6
3	CS8	D	3400	-	-	0/58/74/74	0/1/3/3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	399	FAD	P-O3P	-9.83	1.42	1.59
2	C	2399	FAD	P-O3P	-9.73	1.42	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1399	FAD	P-O3P	-9.02	1.43	1.59
2	D	3399	FAD	P-O3P	-8.61	1.44	1.59
2	C	2399	FAD	C1'-C2'	8.01	1.59	1.51
2	B	1399	FAD	C1'-C2'	7.01	1.58	1.51
2	A	399	FAD	C1'-C2'	6.97	1.58	1.51
2	D	3399	FAD	C1'-C2'	6.72	1.58	1.51
2	A	399	FAD	O4B-C1B	5.20	1.49	1.41
2	B	1399	FAD	O4B-C1B	5.03	1.49	1.41
2	D	3399	FAD	C2'-C3'	-4.97	1.43	1.53
2	B	1399	FAD	C2'-C3'	-4.67	1.43	1.53
2	C	2399	FAD	O4B-C1B	4.67	1.48	1.41
2	B	1399	FAD	PA-O2A	-4.60	1.34	1.55
2	D	3399	FAD	PA-O2A	-4.54	1.34	1.55
2	A	399	FAD	C2'-C3'	-4.50	1.44	1.53
2	D	3399	FAD	O4B-C1B	4.50	1.48	1.41
2	C	2399	FAD	PA-O2A	-4.47	1.35	1.55
2	A	399	FAD	PA-O2A	-4.29	1.35	1.55
2	A	399	FAD	C9A-N10	4.12	1.44	1.38
2	B	1399	FAD	PA-O3P	-4.06	1.52	1.59
2	A	399	FAD	C4-C4X	4.03	1.47	1.41
2	A	399	FAD	C4X-C10	3.99	1.47	1.40
2	C	2399	FAD	C2'-C3'	-3.96	1.45	1.53
2	D	3399	FAD	C9A-N10	3.94	1.44	1.38
2	D	3399	FAD	C1'-N10	-3.89	1.43	1.48
2	A	399	FAD	PA-O3P	-3.88	1.52	1.59
2	B	1399	FAD	C5'-C4'	-3.78	1.45	1.51
2	D	3399	FAD	C4X-C10	3.75	1.47	1.40
3	B	1400	CS8	C5P-N4P	3.73	1.42	1.33
2	A	399	FAD	C5X-N5	3.71	1.41	1.35
2	C	2399	FAD	P-O2P	-3.69	1.38	1.55
2	C	2399	FAD	C4X-C10	3.67	1.47	1.40
2	A	399	FAD	P-O2P	-3.65	1.38	1.55
2	D	3399	FAD	C2-N3	3.59	1.44	1.37
2	A	399	FAD	C2-N3	3.58	1.44	1.37
2	B	1399	FAD	C1'-N10	-3.53	1.44	1.48
2	B	1399	FAD	C9A-N10	3.51	1.44	1.38
3	A	400	CS8	C5P-N4P	3.36	1.41	1.33
2	C	2399	FAD	C9A-N10	3.32	1.43	1.38
2	D	3399	FAD	P-O2P	-3.30	1.40	1.55
2	C	2399	FAD	PA-O3P	-3.28	1.53	1.59
2	B	1399	FAD	P-O2P	-3.23	1.40	1.55
3	C	2400	CS8	C5P-N4P	3.22	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2399	FAD	C2-N3	3.21	1.43	1.37
2	D	3399	FAD	C5'-C4'	-3.16	1.46	1.51
3	D	3400	CS8	C5P-N4P	3.15	1.40	1.33
3	B	1400	CS8	C9P-N8P	3.14	1.40	1.33
2	A	399	FAD	C1'-N10	-3.09	1.44	1.48
2	D	3399	FAD	PA-O3P	-3.06	1.54	1.59
2	D	3399	FAD	C4-C4X	3.05	1.46	1.41
2	B	1399	FAD	C4X-C10	2.94	1.46	1.40
2	B	1399	FAD	C4-C4X	2.91	1.46	1.41
2	A	399	FAD	C5'-C4'	-2.77	1.47	1.51
3	B	1400	CS8	P2A-O3A	2.75	1.64	1.59
2	C	2399	FAD	C2B-C1B	-2.74	1.49	1.53
2	C	2399	FAD	C4-C4X	2.74	1.45	1.41
2	B	1399	FAD	C2-N3	2.73	1.42	1.37
2	A	399	FAD	C2B-C1B	-2.64	1.49	1.53
3	A	400	CS8	C9P-N8P	2.59	1.39	1.33
3	B	1400	CS8	P1A-O3A	2.51	1.64	1.59
2	C	2399	FAD	C1'-N10	-2.51	1.45	1.48
2	A	399	FAD	C6-C5X	2.48	1.44	1.41
2	B	1399	FAD	C8-C7	2.45	1.47	1.40
2	B	1399	FAD	C5X-N5	2.42	1.39	1.35
2	D	3399	FAD	P-O5'	-2.38	1.48	1.59
2	A	399	FAD	P-O5'	-2.36	1.48	1.59
2	D	3399	FAD	C5X-N5	2.30	1.38	1.35
2	B	1399	FAD	O2-C2	-2.30	1.18	1.23
2	D	3399	FAD	C8-C7	2.26	1.47	1.40
3	C	2400	CS8	C9P-N8P	2.24	1.38	1.33
3	D	3400	CS8	C9P-N8P	2.24	1.38	1.33
2	D	3399	FAD	C5B-C4B	2.22	1.58	1.51
2	B	1399	FAD	P-O5'	-2.21	1.49	1.59
2	A	399	FAD	C8-C7	2.18	1.47	1.40
2	C	2399	FAD	C4A-N3A	2.17	1.38	1.35
3	B	1400	CS8	C1'-S1P	2.17	1.80	1.76
2	D	3399	FAD	C2B-C1B	-2.16	1.50	1.53
2	C	2399	FAD	C5X-N5	2.15	1.38	1.35
2	C	2399	FAD	C8-C7	2.15	1.47	1.40
2	D	3399	FAD	C10-N10	-2.15	1.34	1.38
2	B	1399	FAD	C2B-C1B	-2.14	1.50	1.53
2	B	1399	FAD	O3B-C3B	-2.06	1.38	1.43
2	D	3399	FAD	C4A-N3A	2.03	1.38	1.35
2	C	2399	FAD	O4-C4	-2.01	1.20	1.24
2	B	1399	FAD	C2A-N1A	2.01	1.37	1.33

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1400	CS8	O1'-C1'-S1P	-11.00	111.27	122.85
2	B	1399	FAD	C5'-C4'-C3'	-10.60	92.05	112.06
2	D	3399	FAD	C5'-C4'-C3'	-10.13	92.95	112.06
3	B	1400	CS8	P3B-O3B-C3B	10.09	143.20	121.96
3	D	3400	CS8	O1'-C1'-S1P	-9.78	112.55	122.85
2	A	399	FAD	C5'-C4'-C3'	-9.68	93.79	112.06
3	A	400	CS8	O1'-C1'-S1P	-9.47	112.88	122.85
3	A	400	CS8	P3B-O3B-C3B	9.40	141.76	121.96
2	C	2399	FAD	C5'-C4'-C3'	-9.37	94.38	112.06
3	B	1400	CS8	C2'-C1'-S1P	9.29	123.95	113.31
3	C	2400	CS8	P3B-O3B-C3B	9.28	141.50	121.96
3	C	2400	CS8	O1'-C1'-S1P	-9.28	113.08	122.85
3	A	400	CS8	C2'-C1'-S1P	9.17	123.81	113.31
3	D	3400	CS8	P3B-O3B-C3B	9.14	141.20	121.96
3	D	3400	CS8	C2'-C1'-S1P	9.11	123.74	113.31
3	C	2400	CS8	C2'-C1'-S1P	8.20	122.70	113.31
3	C	2400	CS8	O6A-CCP-CBP	6.72	121.81	110.57
3	D	3400	CS8	O6A-CCP-CBP	6.40	121.28	110.57
3	A	400	CS8	O4B-C1B-N9A	6.38	114.38	108.44
3	D	3400	CS8	O4B-C1B-N9A	6.29	114.29	108.44
3	A	400	CS8	O6A-CCP-CBP	6.05	120.69	110.57
2	B	1399	FAD	O4B-C1B-N9A	-5.87	102.98	108.44
3	D	3400	CS8	C3P-N4P-C5P	-5.73	111.16	122.84
2	B	1399	FAD	C2-N1-C10	5.52	120.54	114.98
3	B	1400	CS8	O6A-CCP-CBP	5.49	119.75	110.57
2	A	399	FAD	C2-N1-C10	5.37	120.39	114.98
3	A	400	CS8	C3P-N4P-C5P	-5.20	112.24	122.84
3	B	1400	CS8	C3P-N4P-C5P	-5.12	112.41	122.84
3	C	2400	CS8	O4B-C1B-N9A	5.11	113.19	108.44
2	D	3399	FAD	O4B-C1B-N9A	-5.09	103.71	108.44
2	C	2399	FAD	C2-N1-C10	5.09	120.10	114.98
2	C	2399	FAD	O4B-C1B-N9A	-5.05	103.75	108.44
2	D	3399	FAD	C2-N1-C10	5.04	120.06	114.98
3	C	2400	CS8	C3P-N4P-C5P	-4.94	112.78	122.84
2	A	399	FAD	C4B-O4B-C1B	-4.93	104.40	109.75
3	B	1400	CS8	O4B-C1B-N9A	4.80	112.91	108.44
2	D	3399	FAD	C4X-C10-N10	-4.78	118.12	120.51
2	C	2399	FAD	C4B-O4B-C1B	-4.57	104.78	109.75
2	D	3399	FAD	C4B-O4B-C1B	-4.52	104.84	109.75
2	B	1399	FAD	C4B-O4B-C1B	-4.43	104.94	109.75
2	B	1399	FAD	C4X-C10-N10	-4.42	118.30	120.51
2	A	399	FAD	C2'-C1'-N10	4.21	118.03	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3399	FAD	C1'-C2'-C3'	-4.17	97.88	109.82
2	A	399	FAD	O4B-C1B-C2B	-4.15	100.41	106.77
2	A	399	FAD	C1'-C2'-C3'	-4.08	98.14	109.82
2	C	2399	FAD	C1'-C2'-C3'	-3.88	98.73	109.82
2	B	1399	FAD	C1'-C2'-C3'	-3.83	98.87	109.82
2	C	2399	FAD	C4X-C10-N10	-3.81	118.61	120.51
3	D	3400	CS8	CBP-CAP-C9P	3.68	116.30	112.73
2	A	399	FAD	O4B-C1B-N9A	-3.62	105.07	108.44
3	B	1400	CS8	O3A-P2A-O6A	3.61	119.56	103.41
3	C	2400	CS8	CBP-CAP-C9P	3.59	116.21	112.73
2	B	1399	FAD	O4B-C1B-C2B	-3.56	101.31	106.77
2	A	399	FAD	C4X-C10-N10	-3.55	118.74	120.51
3	C	2400	CS8	O3A-P2A-O6A	3.53	119.19	103.41
2	C	2399	FAD	O4B-C1B-C2B	-3.52	101.37	106.77
3	C	2400	CS8	P1A-O3A-P2A	-3.48	121.47	131.68
2	D	3399	FAD	C1'-N10-C9A	-3.45	115.52	118.87
3	B	1400	CS8	CAP-C9P-N8P	3.35	123.75	116.57
2	D	3399	FAD	O4B-C1B-C2B	-3.22	101.83	106.77
3	D	3400	CS8	C8A-N9A-C1B	3.21	132.71	126.38
2	D	3399	FAD	N3A-C2A-N1A	-3.18	126.05	128.71
2	A	399	FAD	N3A-C2A-N1A	-3.17	126.06	128.71
3	A	400	CS8	C8A-N9A-C1B	3.14	132.58	126.38
2	B	1399	FAD	N3A-C2A-N1A	-3.13	126.09	128.71
2	D	3399	FAD	O5B-PA-O1A	-3.09	97.26	109.37
3	A	400	CS8	CBP-CAP-C9P	3.09	115.73	112.73
2	C	2399	FAD	N3A-C2A-N1A	-3.08	126.13	128.71
3	D	3400	CS8	O3A-P2A-O6A	3.08	117.17	103.41
3	B	1400	CS8	C8A-N9A-C1B	3.06	132.42	126.38
2	A	399	FAD	P-O3P-PA	3.06	140.66	131.68
3	C	2400	CS8	C8A-N9A-C1B	3.03	132.36	126.38
2	C	2399	FAD	C2'-C1'-N10	3.03	116.48	112.45
2	C	2399	FAD	O5B-PA-O1A	-3.02	97.56	109.37
3	C	2400	CS8	CAP-C9P-N8P	3.01	123.01	116.57
3	B	1400	CS8	C1'-C2'-S3'	3.00	118.30	113.05
3	A	400	CS8	CAP-C9P-N8P	2.97	122.94	116.57
3	B	1400	CS8	CBP-CAP-C9P	2.94	115.58	112.73
3	A	400	CS8	O3A-P2A-O6A	2.90	116.39	103.41
3	A	400	CS8	P1A-O3A-P2A	-2.88	123.23	131.68
2	B	1399	FAD	C4'-C3'-C2'	2.78	119.54	113.25
2	B	1399	FAD	O5B-PA-O1A	-2.78	98.48	109.37
3	D	3400	CS8	P1A-O3A-P2A	-2.77	123.56	131.68
3	D	3400	CS8	C1B-N9A-C4A	-2.77	121.85	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3400	CS8	CAP-C9P-N8P	2.75	122.45	116.57
2	A	399	FAD	O5B-PA-O1A	-2.71	98.78	109.37
2	D	3399	FAD	C4'-C3'-C2'	2.70	119.35	113.25
3	B	1400	CS8	P1A-O3A-P2A	-2.68	123.84	131.68
2	C	2399	FAD	C4'-C3'-C2'	2.66	119.25	113.25
2	A	399	FAD	O2A-PA-O3P	2.63	117.62	105.14
3	D	3400	CS8	C7P-N8P-C9P	-2.61	117.21	122.57
3	A	400	CS8	C1B-N9A-C4A	-2.60	122.15	126.64
2	B	1399	FAD	C1'-N10-C9A	-2.58	116.36	118.87
2	A	399	FAD	C4'-C3'-C2'	2.57	119.06	113.25
3	B	1400	CS8	C8A-N9A-C4A	-2.50	104.99	106.90
3	C	2400	CS8	C1B-N9A-C4A	-2.49	122.33	126.64
2	B	1399	FAD	N3A-C4A-N9A	2.48	129.91	125.43
3	C	2400	CS8	O5P-C5P-N4P	2.44	127.77	122.94
2	A	399	FAD	C1'-N10-C9A	-2.43	116.51	118.87
2	A	399	FAD	N3A-C4A-N9A	2.42	129.81	125.43
2	B	1399	FAD	O2A-PA-O3P	2.41	116.59	105.14
2	D	3399	FAD	C2'-C1'-N10	2.38	115.61	112.45
3	A	400	CS8	C7P-N8P-C9P	-2.38	117.69	122.57
2	C	2399	FAD	C4A-C5A-N7A	2.35	111.54	109.52
2	C	2399	FAD	N3A-C4A-N9A	2.34	129.66	125.43
3	B	1400	CS8	C1B-N9A-C4A	-2.34	122.59	126.64
3	B	1400	CS8	C3B-C2B-C1B	2.33	105.52	99.98
3	A	400	CS8	O5P-C5P-N4P	2.33	127.56	122.94
3	C	2400	CS8	C6P-C7P-N8P	-2.32	106.87	111.87
3	C	2400	CS8	O5P-C5P-C6P	-2.32	117.32	121.92
3	B	1400	CS8	O5P-C5P-N4P	2.31	127.52	122.94
3	A	400	CS8	O5P-C5P-C6P	-2.31	117.33	121.92
3	D	3400	CS8	O5P-C5P-N4P	2.31	127.51	122.94
2	C	2399	FAD	O3'-C3'-C4'	-2.30	102.91	108.74
2	D	3399	FAD	O4'-C4'-C5'	2.29	114.83	110.12
2	D	3399	FAD	N3A-C4A-N9A	2.29	129.57	125.43
2	C	2399	FAD	C5A-C4A-N9A	-2.28	103.87	107.16
2	D	3399	FAD	C2A-N1A-C6A	2.26	122.86	118.77
3	D	3400	CS8	O5P-C5P-C6P	-2.26	117.42	121.92
2	B	1399	FAD	P-O3P-PA	2.25	138.29	131.68
2	B	1399	FAD	C5A-C4A-N9A	-2.24	103.92	107.16
2	B	1399	FAD	O4'-C4'-C5'	2.24	114.71	110.12
2	B	1399	FAD	O3'-C3'-C4'	-2.23	103.09	108.74
2	D	3399	FAD	O3'-C3'-C4'	-2.23	103.10	108.74
2	B	1399	FAD	C2A-N1A-C6A	2.23	122.79	118.77
2	A	399	FAD	O3'-C3'-C4'	-2.22	103.13	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	399	FAD	O3B-C3B-C2B	2.22	119.04	111.83
2	C	2399	FAD	O4'-C4'-C5'	2.21	114.67	110.12
2	A	399	FAD	C2A-N1A-C6A	2.20	122.74	118.77
2	A	399	FAD	C5A-C4A-N9A	-2.18	104.01	107.16
2	B	1399	FAD	C4A-C5A-N7A	2.18	111.39	109.52
3	B	1400	CS8	C7P-N8P-C9P	-2.18	118.10	122.57
3	C	2400	CS8	C7P-N8P-C9P	-2.17	118.11	122.57
2	C	2399	FAD	C2A-N1A-C6A	2.16	122.67	118.77
3	C	2400	CS8	O9P-C9P-CAP	-2.15	116.56	120.48
2	A	399	FAD	C4A-C5A-N7A	2.15	111.36	109.52
2	A	399	FAD	O4'-C4'-C5'	2.13	114.50	110.12
3	A	400	CS8	C8A-N9A-C4A	-2.13	105.27	106.90
2	C	2399	FAD	O2A-PA-O3P	2.12	115.18	105.14
2	D	3399	FAD	C5A-C4A-N9A	-2.09	104.15	107.16
3	C	2400	CS8	C8A-N9A-C4A	-2.08	105.31	106.90
3	B	1400	CS8	C7P-C6P-C5P	2.07	115.78	112.25
2	D	3399	FAD	O2A-PA-O3P	2.06	114.90	105.14
3	B	1400	CS8	O9P-C9P-CAP	-2.05	116.74	120.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	385/396 (97%)	-0.68	0 100 100	14, 26, 38, 50	0
1	B	383/396 (96%)	-0.57	1 (0%) 91 92	17, 30, 44, 58	0
1	C	385/396 (97%)	-0.73	1 (0%) 91 92	14, 25, 38, 46	0
1	D	385/396 (97%)	-0.67	0 100 100	14, 25, 40, 49	0
All	All	1538/1584 (97%)	-0.66	2 (0%) 93 95	14, 27, 41, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	LYS	2.5
1	B	187	LYS	2.1

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CS8	B	1400	57/57	0.36	9.49	25,43,49,49	57
2	FAD	C	2399	53/53	0.13	1.74	20,24,32,38	0
2	FAD	D	3399	53/53	0.14	1.57	21,25,30,32	0
2	FAD	B	1399	53/53	0.13	1.44	20,27,33,35	0
2	FAD	A	399	53/53	0.13	1.15	16,23,27,32	0
3	CS8	D	3400	57/57	0.12	0.57	20,29,41,43	57
3	CS8	A	400	57/57	0.12	0.32	15,30,38,40	57
3	CS8	C	2400	57/57	0.10	0.21	15,29,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.