Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:49 PM GMT

PDB ID	:	3V3O
Title	:	Crystal structure of TetX2 T280A: an adaptive mutant in complex with tigecycline
Authors	:	Walkiewicz, K.; Shamoo, Y.
Deposited on	:	2011-12-13
Resolution	:	2.90 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:

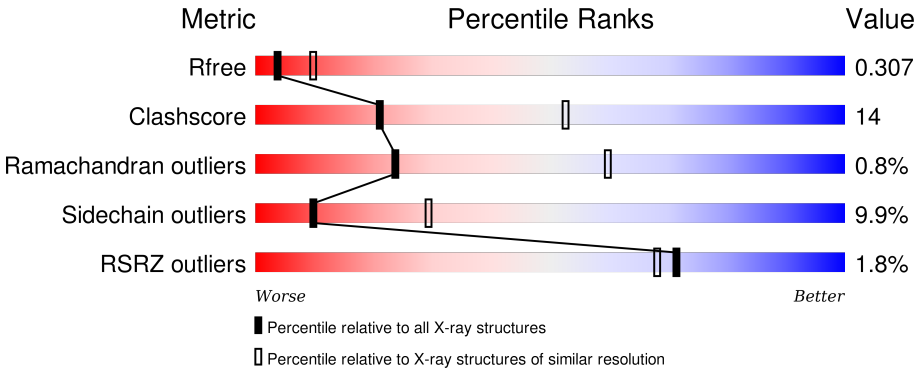
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	378	64% 28% 5%
1	B	378	63% 30%
1	C	378	59% 33%
1	D	378	4% 63% 28% 5%

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
4	T1C	B	405	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11946 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.

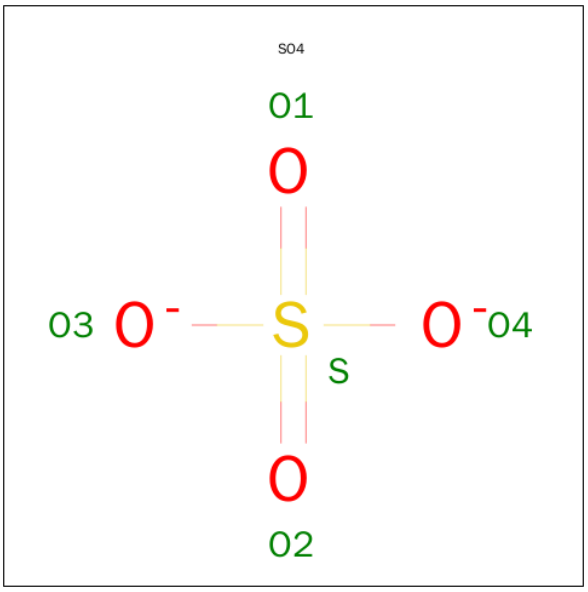
- Molecule 1 is a protein called TetX2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2895	1837	497	549	12			
1	B	365	Total	C	N	O	S	0	0	0
			2878	1826	492	548	12			
1	C	364	Total	C	N	O	S	0	0	0
			2866	1817	490	547	12			
1	D	364	Total	C	N	O	S	0	0	0
			2874	1823	492	547	12			

There are 12 discrepancies between the modelled and reference sequences:

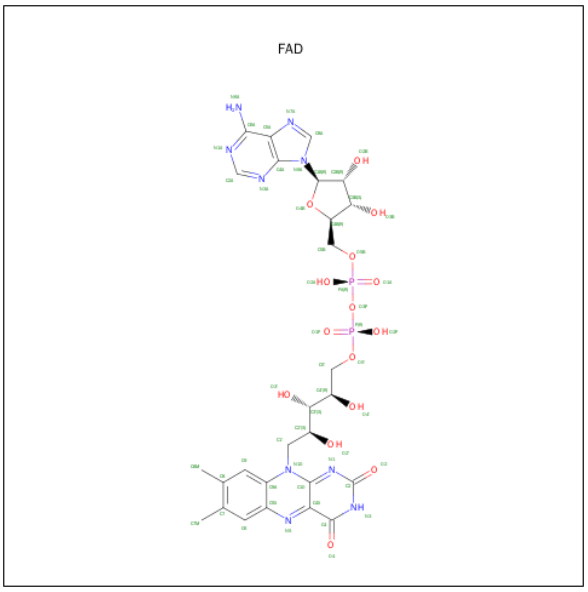
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
A	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
A	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
B	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
B	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
C	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
C	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51
D	94	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	266	LYS	GLU	ENGINEERED MUTATION	UNP Q93L51
D	280	ALA	THR	ENGINEERED MUTATION	UNP Q93L51

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



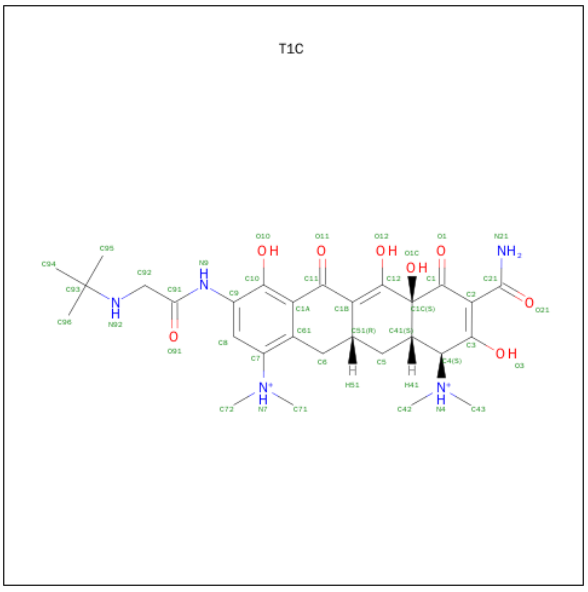
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			42	29	5	8		
4	B	1	Total	C	N	O	0	0
			42	29	5	8		
4	C	1	Total	C	N	O	0	0
			42	29	5	8		
4	D	1	Total	C	N	O	0	0
			42	29	5	8		

- Molecule 5 is water.

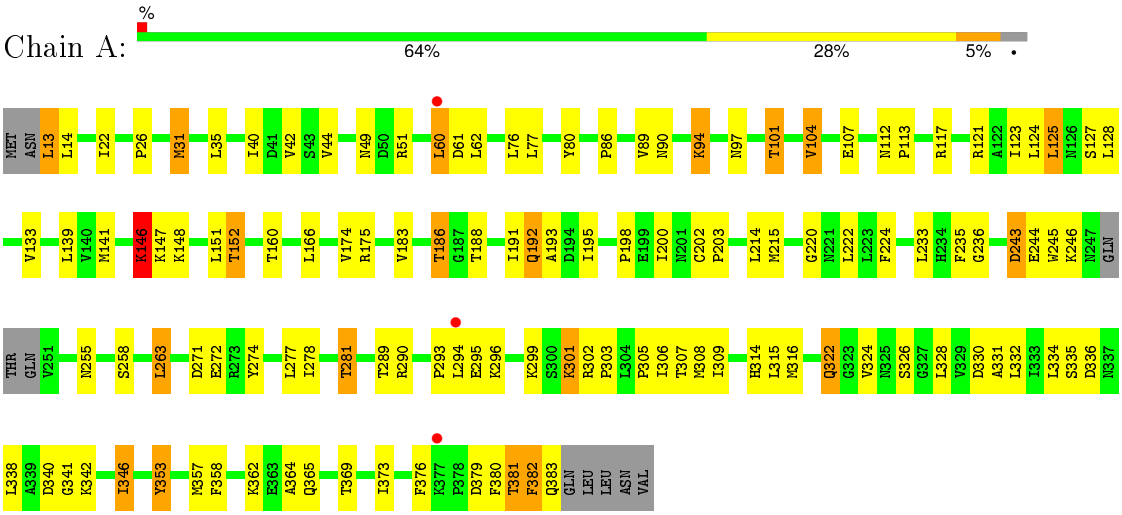
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	9	Total	O	0	0
			9	9		
5	C	2	Total	O	0	0
			2	2		
5	D	5	Total	O	0	0
			5	5		

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.

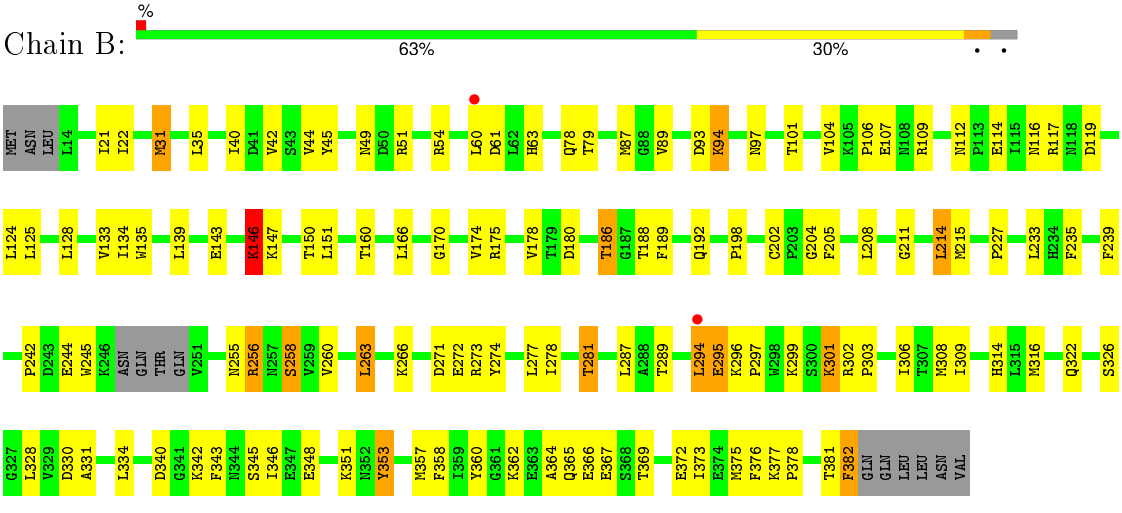
- Molecule 1: TetX2 protein

Chain A:



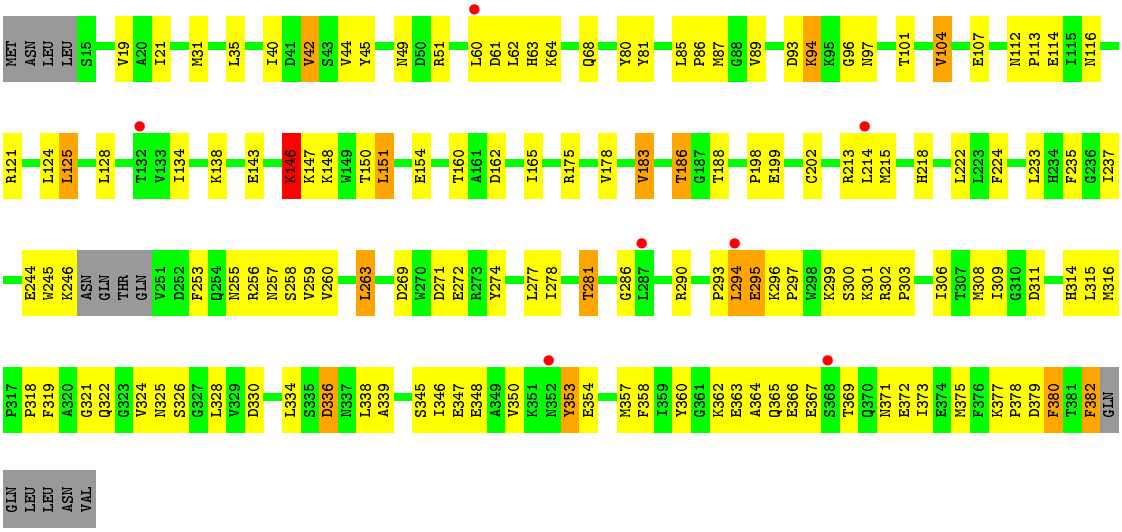
- Molecule 1: TetX2 protein

Chain B:



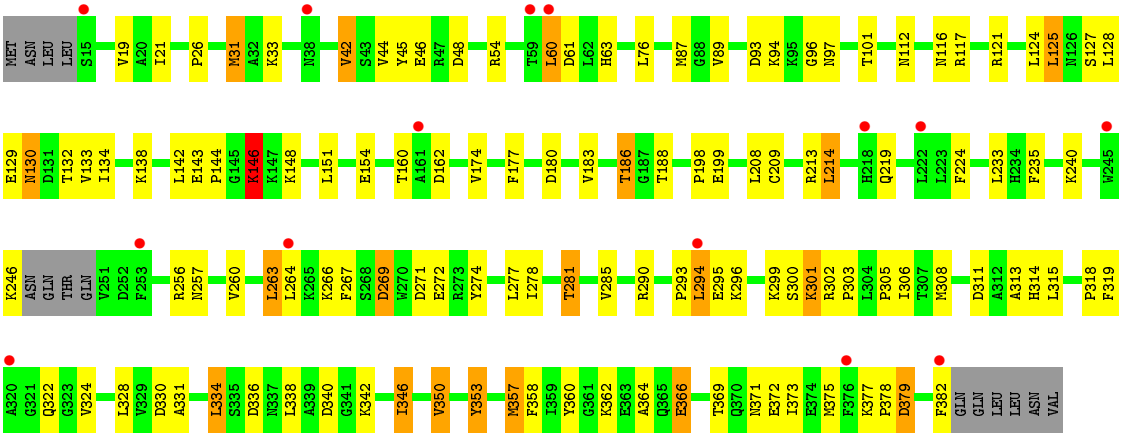
- Molecule 1: TetX2 protein

Chain C:



• Molecule 1: TetX2 protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.13Å 80.08Å 87.24Å 111.02° 89.97° 92.97°	Depositor
Resolution (Å)	48.95 – 2.90 48.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.95-2.90) 82.7 (48.95-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.297 0.239 , 0.307	Depositor DCC
R_{free} test set	1824 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 36868 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11946	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: SO4, FAD, T1C

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	0.54	0/2953	0.70	0/3991
1	B	0.53	0/2936	0.69	0/3967
1	C	0.46	0/2924	0.66	0/3952
1	D	0.46	0/2932	0.64	0/3960
All	All	0.50	0/11745	0.67	0/15870

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2895	0	2859	83	0
1	B	2878	0	2842	80	0
1	C	2866	0	2820	88	0
1	D	2874	0	2842	83	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
3	C	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	53	0	31	2	0
4	A	42	0	41	7	0
4	B	42	0	40	2	0
4	C	42	0	41	1	0
4	D	42	0	41	4	0
5	A	7	0	0	0	0
5	B	9	0	0	2	0
5	C	2	0	0	0	0
5	D	5	0	0	1	0
All	All	11946	0	11650	338	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 14.

All (338) 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:B:61:ASP:HB2	1:B:112:ASN:HB2	1.52	0.92
1:B:330:ASP:HB2	1:B:353:TYR:HE1	1.41	0.85
1:B:78:GLN:HG2	1:C:64:LYS:HB3	1.61	0.83
1:B:186:THR:HG22	1:B:188:THR:H	1.45	0.80
1:D:293:PRO:HB2	1:D:295:GLU:HG2	1.62	0.80
1:C:263:LEU:HB3	1:C:278:ILE:HD13	1.64	0.79
1:C:322:GLN:HG2	1:C:364:ALA:HB1	1.65	0.77
1:A:294:LEU:HD21	1:A:314:HIS:HB3	1.65	0.77
1:A:35:LEU:HD22	1:A:40:ILE:HD12	1.65	0.76
1:A:146:LYS:HE3	1:A:147:LYS:H	1.51	0.75
1:D:330:ASP:HB2	1:D:353:TYR:HE1	1.53	0.72
1:D:322:GLN:HG2	1:D:364:ALA:HB1	1.72	0.72
1:C:293:PRO:HB2	1:C:295:GLU:HG2	1.71	0.72
1:C:330:ASP:HB2	1:C:353:TYR:HE1	1.54	0.71
1:C:186:THR:HG22	1:C:188:THR:H	1.56	0.71
1:A:307:THR:HG21	1:A:334:LEU:HD11	1.73	0.70
1:A:166:LEU:HD21	1:A:174:VAL:HG23	1.74	0.70
1:D:186:THR:HG22	1:D:188:THR:H	1.55	0.70
1:C:148:LYS:HD3	1:C:160:THR:HB	1.74	0.70
1:B:93:ASP:OD1	1:B:97:ASN:N	2.22	0.69
1:A:235:PHE:HZ	1:A:281:THR:HG21	1.57	0.69
1:B:117:ARG:NH2	3:B:403:FAD:O2'	2.20	0.69
1:A:44:VAL:HB	1:A:133:VAL:HG22	1.73	0.69
1:C:61:ASP:HB2	1:C:112:ASN:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:HB2	1:A:112:ASN:HB2	1.74	0.68
1:D:330:ASP:HB2	1:D:353:TYR:CE1	2.29	0.67
1:B:146:LYS:HE3	1:B:147:LYS:H	1.58	0.67
1:D:235:PHE:HZ	1:D:281:THR:HG21	1.60	0.66
1:C:21:ILE:HB	1:C:44:VAL:HG22	1.78	0.66
1:A:330:ASP:HB2	1:A:353:TYR:HE1	1.61	0.66
1:B:295:GLU:HG3	1:B:296:LYS:H	1.60	0.65
1:B:21:ILE:HB	1:B:44:VAL:HG22	1.77	0.65
1:B:35:LEU:HD22	1:B:40:ILE:HD12	1.78	0.65
1:A:305:PRO:HB3	1:A:346:ILE:HD12	1.78	0.64
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.78	0.64
1:A:222:LEU:HD23	1:A:224:PHE:CZ	2.33	0.63
1:A:186:THR:HG22	1:A:188:THR:H	1.62	0.63
1:D:44:VAL:HB	1:D:133:VAL:HG22	1.80	0.63
1:A:293:PRO:HB2	1:A:295:GLU:HG2	1.81	0.62
1:D:290:ARG:HB2	1:D:315:LEU:HD21	1.81	0.62
1:D:302:ARG:NH2	1:D:306:ILE:O	2.25	0.62
1:D:121:ARG:HG2	1:D:125:LEU:HD22	1.81	0.61
1:B:94:LYS:O	1:B:271:ASP:N	2.32	0.61
1:A:299:LYS:O	1:A:302:ARG:HD2	2.00	0.61
1:A:31:MET:HG3	1:A:309:ILE:CD1	2.30	0.61
1:C:373:ILE:HG22	1:C:377:LYS:HE2	1.81	0.61
1:A:148:LYS:HD3	1:A:160:THR:HB	1.82	0.60
1:B:208:LEU:HD23	1:B:214:LEU:HD21	1.82	0.60
1:C:31:MET:HG3	1:C:309:ILE:HD13	1.83	0.60
1:B:348:GLU:HA	1:B:351:LYS:HE3	1.83	0.60
1:B:330:ASP:HB2	1:B:353:TYR:CE1	2.31	0.60
1:B:211:GLY:O	5:B:505:HOH:O	2.17	0.59
1:D:21:ILE:HB	1:D:44:VAL:HG22	1.84	0.59
1:C:345:SER:O	1:C:348:GLU:HG2	2.02	0.59
1:D:369:THR:O	1:D:373:ILE:HG12	2.03	0.59
1:D:33:LYS:HE2	1:D:127:SER:HB2	1.86	0.58
1:D:19:VAL:HB	1:D:42:VAL:HG13	1.85	0.58
1:D:219:GLN:NE2	1:D:269:ASP:OD2	2.36	0.58
1:D:271:ASP:OD1	1:D:272:GLU:N	2.36	0.58
1:B:175:ARG:HG2	1:B:308:MET:SD	2.43	0.58
1:A:107:GLU:N	1:A:107:GLU:OE1	2.35	0.57
1:C:68:GLN:OE1	1:C:81:TYR:OH	2.18	0.57
1:D:314:HIS:NE2	1:D:330:ASP:OD2	2.32	0.57
1:A:316:MET:HE3	1:A:365:GLN:HA	1.87	0.57
1:C:244:GLU:HG3	1:C:245:TRP:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLU:HG3	1:D:296:LYS:H	1.70	0.56
1:D:294:LEU:HD21	1:D:314:HIS:HB3	1.87	0.56
1:A:330:ASP:HB2	1:A:353:TYR:CE1	2.40	0.56
1:C:377:LYS:O	1:C:379:ASP:N	2.38	0.56
1:C:334:LEU:O	1:C:338:LEU:HG	2.05	0.56
1:D:130:ASN:OD1	1:D:130:ASN:N	2.37	0.56
1:A:307:THR:OG1	1:A:308:MET:N	2.39	0.56
3:B:403:FAD:N1	3:B:403:FAD:H2'	2.21	0.56
1:A:271:ASP:OD1	1:A:272:GLU:N	2.38	0.56
1:D:334:LEU:O	1:D:338:LEU:HG	2.05	0.55
1:D:377:LYS:O	1:D:379:ASP:N	2.39	0.55
1:A:290:ARG:HB2	1:A:315:LEU:HD21	1.89	0.55
1:C:271:ASP:OD1	1:C:272:GLU:N	2.38	0.55
1:D:117:ARG:NH2	3:D:402:FAD:O2'	2.26	0.55
1:A:97:ASN:ND2	1:B:366:GLU:HG2	2.21	0.55
1:D:366:GLU:HA	1:D:369:THR:HG22	1.88	0.55
1:C:31:MET:HG3	1:C:309:ILE:CD1	2.37	0.55
1:D:357:MET:HA	1:D:360:TYR:CZ	2.42	0.54
1:B:316:MET:HE3	1:B:365:GLN:HA	1.88	0.54
1:C:198:PRO:HB3	1:C:233:LEU:HB2	1.89	0.54
1:C:45:TYR:HE1	1:C:134:ILE:HD12	1.72	0.54
1:B:235:PHE:HZ	1:B:281:THR:HG21	1.73	0.54
1:D:300:SER:H	1:D:301:LYS:HE3	1.72	0.54
1:B:44:VAL:HB	1:B:133:VAL:HG22	1.89	0.54
1:D:209:CYS:HA	1:D:214:LEU:HD23	1.90	0.54
1:D:277:LEU:O	1:D:281:THR:HG22	2.08	0.53
1:D:93:ASP:OD1	1:D:97:ASN:N	2.40	0.53
1:A:222:LEU:HD23	1:A:224:PHE:HZ	1.71	0.53
1:A:60:LEU:HD22	1:A:117:ARG:HG2	1.91	0.53
1:A:94:LYS:O	1:A:271:ASP:N	2.40	0.53
1:A:86:PRO:HB2	1:A:104:VAL:HG11	1.90	0.53
1:D:60:LEU:HG	1:D:324:VAL:HG11	1.89	0.53
1:A:381:THR:O	1:A:382:PHE:HB2	2.08	0.53
1:C:358:PHE:O	1:C:362:LYS:HB2	2.08	0.53
1:D:129:GLU:O	1:D:132:THR:OG1	2.16	0.52
1:B:271:ASP:OD1	1:B:272:GLU:N	2.42	0.52
1:D:324:VAL:HG12	3:D:402:FAD:O2	2.09	0.52
4:D:401:T1C:O12	4:D:401:T1C:O11	2.27	0.52
1:C:87:MET:HE2	1:C:213:ARG:HG2	1.91	0.52
1:D:87:MET:HE2	1:D:213:ARG:HG2	1.91	0.52
4:A:404:T1C:O11	4:A:404:T1C:O12	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:HG3	1:B:245:TRP:CD1	2.45	0.52
1:B:87:MET:HE1	1:B:227:PRO:HD2	1.92	0.52
1:C:375:MET:HG2	1:C:380:PHE:CZ	2.45	0.52
1:C:369:THR:HA	1:C:372:GLU:HG2	1.91	0.52
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.91	0.52
1:B:180:ASP:OD1	1:B:296:LYS:NZ	2.24	0.51
1:B:348:GLU:HA	1:B:351:LYS:HB3	1.92	0.51
1:C:357:MET:HA	1:C:360:TYR:CZ	2.46	0.51
1:B:294:LEU:HD21	1:B:314:HIS:HB3	1.92	0.51
1:D:142:LEU:HD12	1:D:174:VAL:HB	1.93	0.51
1:D:358:PHE:O	1:D:362:LYS:HB2	2.11	0.51
1:A:26:PRO:HD2	3:A:403:FAD:O1P	2.11	0.51
1:C:124:LEU:O	1:C:128:LEU:HG	2.11	0.51
1:A:383:GLN:HB3	4:A:404:T1C:H963	1.93	0.51
1:C:321:GLY:O	1:C:325:ASN:ND2	2.44	0.51
1:A:324:VAL:O	1:A:328:LEU:N	2.37	0.51
1:D:61:ASP:HB2	1:D:112:ASN:HB2	1.93	0.50
1:C:324:VAL:HG12	3:C:402:FAD:O2	2.11	0.50
1:B:314:HIS:NE2	1:B:330:ASP:OD2	2.37	0.50
1:C:255:ASN:O	1:C:258:SER:HB3	2.12	0.50
1:A:31:MET:HG3	1:A:309:ILE:HD13	1.92	0.50
1:D:318:PRO:HD2	1:D:319:PHE:CE2	2.45	0.50
1:A:198:PRO:HB3	1:A:233:LEU:HB2	1.93	0.50
1:A:175:ARG:HG2	1:A:308:MET:CE	2.42	0.50
1:A:202:CYS:SG	1:A:233:LEU:HD13	2.52	0.50
1:B:263:LEU:HD23	1:B:278:ILE:HG23	1.94	0.50
1:B:358:PHE:O	1:B:362:LYS:HB2	2.12	0.50
1:A:324:VAL:HG12	3:A:403:FAD:O2	2.12	0.50
1:A:77:LEU:HD12	1:A:80:TYR:HD2	1.77	0.49
1:D:124:LEU:O	1:D:128:LEU:HG	2.12	0.49
1:B:31:MET:HG3	1:B:309:ILE:HD12	1.93	0.49
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.43	0.49
1:C:143:GLU:O	1:C:150:THR:N	2.35	0.49
1:B:214:LEU:HD12	1:B:215:MET:N	2.27	0.49
1:A:328:LEU:O	1:A:331:ALA:HB3	2.13	0.49
1:C:253:PHE:CE2	1:C:286:GLY:HA3	2.48	0.49
1:C:302:ARG:NH2	1:C:306:ILE:O	2.37	0.49
1:A:62:LEU:HB2	1:A:80:TYR:CZ	2.48	0.49
1:A:255:ASN:O	1:A:258:SER:HB3	2.11	0.49
1:C:222:LEU:O	1:C:237:ILE:HA	2.13	0.48
1:A:358:PHE:O	1:A:362:LYS:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HA	1:A:113:PRO:HA	1.95	0.48
1:A:236:GLY:HA3	4:A:404:T1C:H421	1.96	0.48
1:A:308:MET:O	1:A:353:TYR:OH	2.20	0.48
1:C:371:ASN:O	1:C:375:MET:HG3	2.13	0.48
1:B:166:LEU:HD21	1:B:174:VAL:HG23	1.96	0.48
1:A:243:ASP:N	1:A:243:ASP:OD1	2.47	0.48
1:D:302:ARG:HA	1:D:303:PRO:HD3	1.71	0.48
1:D:146:LYS:HB2	1:D:146:LYS:NZ	2.28	0.48
1:D:324:VAL:O	1:D:328:LEU:N	2.35	0.48
1:C:45:TYR:CE1	1:C:134:ILE:HD12	2.49	0.48
1:D:371:ASN:O	1:D:375:MET:HG3	2.13	0.48
1:D:146:LYS:HG3	1:D:146:LYS:H	1.44	0.48
1:C:277:LEU:O	1:C:281:THR:HG22	2.14	0.48
1:C:86:PRO:HA	1:C:113:PRO:HA	1.95	0.48
4:B:405:T1C:O12	4:B:405:T1C:O11	2.21	0.47
1:A:166:LEU:HD13	1:A:306:ILE:HD11	1.96	0.47
1:C:330:ASP:HB2	1:C:353:TYR:CE1	2.44	0.47
1:C:363:GLU:O	1:C:367:GLU:HG3	2.14	0.47
1:C:324:VAL:O	1:C:328:LEU:N	2.36	0.47
1:A:302:ARG:NH2	1:A:306:ILE:O	2.34	0.47
1:B:45:TYR:CE1	1:B:134:ILE:HD12	2.50	0.47
1:A:244:GLU:HG3	1:A:245:TRP:CD1	2.49	0.47
1:B:215:MET:HB3	1:B:382:PHE:CZ	2.49	0.47
1:B:107:GLU:N	1:B:107:GLU:OE1	2.41	0.47
1:D:199:GLU:CD	1:D:199:GLU:H	2.18	0.47
1:B:116:ASN:HB3	1:B:119:ASP:OD2	2.14	0.47
1:C:86:PRO:HB2	1:C:104:VAL:HG11	1.95	0.47
1:B:345:SER:O	1:B:348:GLU:HG2	2.15	0.47
1:A:76:LEU:HD13	1:A:123:ILE:HG22	1.97	0.47
1:B:296:LYS:HG2	1:B:297:PRO:O	2.15	0.47
1:C:87:MET:HG3	1:C:114:GLU:HG3	1.97	0.47
1:B:255:ASN:O	1:B:258:SER:HB3	2.15	0.47
1:B:322:GLN:HG2	1:B:364:ALA:HB1	1.97	0.47
1:D:45:TYR:HE1	1:D:134:ILE:HD12	1.79	0.46
4:A:404:T1C:H433	4:A:404:T1C:H41	1.62	0.46
1:C:299:LYS:O	1:C:302:ARG:HD2	2.15	0.46
1:C:318:PRO:O	4:C:401:T1C:H433	2.15	0.46
1:A:277:LEU:O	1:A:281:THR:HG22	2.16	0.46
1:A:235:PHE:CZ	1:A:281:THR:HG21	2.45	0.46
1:A:340:ASP:HB3	1:A:342:LYS:HB2	1.96	0.46
1:D:198:PRO:HB3	1:D:233:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LYS:HG3	1:C:146:LYS:H	1.37	0.46
1:D:31:MET:HE3	1:D:31:MET:O	2.14	0.46
1:B:277:LEU:O	1:B:281:THR:HG22	2.15	0.46
1:B:328:LEU:O	1:B:331:ALA:HB3	2.16	0.46
1:D:308:MET:O	1:D:313:ALA:HB2	2.16	0.46
1:C:257:ASN:HA	1:C:260:VAL:HB	1.97	0.46
1:A:90:ASN:OD1	1:A:101:THR:HB	2.16	0.46
1:C:316:MET:HE3	1:C:365:GLN:HA	1.98	0.46
1:A:215:MET:HG2	1:A:224:PHE:HD2	1.80	0.46
1:D:198:PRO:HD2	1:D:199:GLU:OE1	2.16	0.46
1:D:144:PRO:HD3	1:D:177:PHE:CE2	2.51	0.46
1:D:148:LYS:HD3	1:D:160:THR:HB	1.98	0.46
1:D:46:GLU:HG3	1:D:48:ASP:H	1.81	0.46
1:D:144:PRO:HD3	1:D:177:PHE:HE2	1.81	0.46
1:B:189:PHE:HB3	1:B:239:PHE:CE1	2.51	0.46
1:C:138:LYS:HD3	1:C:154:GLU:OE1	2.15	0.46
1:A:295:GLU:HG3	1:A:296:LYS:H	1.81	0.46
1:B:198:PRO:HG3	1:B:233:LEU:H	1.80	0.46
1:B:106:PRO:HA	1:B:109:ARG:HE	1.81	0.45
1:A:224:PHE:HB2	4:A:404:T1C:H423	1.98	0.45
1:C:198:PRO:HD2	1:C:199:GLU:OE1	2.16	0.45
1:C:202:CYS:SG	1:C:233:LEU:HD13	2.57	0.45
1:D:63:HIS:CD2	4:D:401:T1C:H961	2.51	0.45
1:C:357:MET:HA	1:C:360:TYR:CE2	2.52	0.45
1:C:183:VAL:HG21	1:C:290:ARG:HD3	1.98	0.45
1:D:299:LYS:O	1:D:302:ARG:HD2	2.17	0.45
1:D:369:THR:HA	1:D:372:GLU:HG2	1.99	0.45
1:C:215:MET:HB3	1:C:382:PHE:CZ	2.52	0.45
1:A:31:MET:HE3	1:A:334:LEU:HD13	1.99	0.45
1:C:35:LEU:HD22	1:C:40:ILE:HD12	1.98	0.45
1:B:124:LEU:O	1:B:128:LEU:HG	2.16	0.45
1:B:343:PHE:CE1	1:B:348:GLU:HG3	2.51	0.45
1:C:198:PRO:HG3	1:C:233:LEU:H	1.81	0.45
1:B:301:LYS:HD2	1:B:301:LYS:H	1.81	0.45
1:B:150:THR:HA	1:B:160:THR:HG22	1.99	0.45
1:B:256:ARG:O	1:B:260:VAL:HG23	2.16	0.45
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.85	0.45
1:B:22:ILE:HG21	1:B:139:LEU:HD22	1.98	0.45
1:D:96:GLY:O	1:D:208:LEU:HD11	2.17	0.44
1:C:222:LEU:HB3	1:C:224:PHE:HE1	1.82	0.44
1:A:220:GLY:HA2	1:A:376:PHE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LYS:HD3	1:D:154:GLU:OE1	2.17	0.44
1:B:186:THR:HB	1:B:289:THR:O	2.17	0.44
1:D:300:SER:N	1:D:301:LYS:HE3	2.32	0.44
4:B:405:T1C:H41	4:B:405:T1C:H423	1.66	0.44
1:C:369:THR:O	1:C:373:ILE:HG12	2.16	0.44
1:C:222:LEU:HB3	1:C:224:PHE:CE1	2.52	0.44
1:D:274:TYR:O	1:D:277:LEU:HB2	2.17	0.44
1:C:360:TYR:O	1:C:363:GLU:HB3	2.17	0.44
1:D:375:MET:HG3	1:D:375:MET:H	1.58	0.44
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.80	0.44
1:C:178:VAL:HG22	1:C:306:ILE:HG23	2.00	0.44
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.98	0.44
1:C:274:TYR:O	1:C:277:LEU:HB2	2.17	0.44
1:D:340:ASP:HB3	1:D:342:LYS:H	1.81	0.44
1:C:21:ILE:HG12	1:C:165:ILE:HB	1.99	0.43
1:A:236:GLY:HA3	4:A:404:T1C:C42	2.48	0.43
1:C:373:ILE:O	1:C:377:LYS:HG3	2.17	0.43
1:D:305:PRO:HB3	1:D:346:ILE:HD12	2.00	0.43
1:D:180:ASP:OD1	1:D:296:LYS:NZ	2.38	0.43
1:C:61:ASP:OD2	1:C:63:HIS:NE2	2.51	0.43
1:B:22:ILE:HD11	1:B:151:LEU:HD23	2.01	0.43
1:A:121:ARG:HG2	1:A:125:LEU:HD22	2.01	0.43
1:D:183:VAL:HG21	1:D:290:ARG:HD3	2.00	0.43
1:A:76:LEU:HD21	1:A:127:SER:HB3	1.99	0.43
1:A:186:THR:HB	1:A:289:THR:O	2.19	0.43
1:C:296:LYS:HG2	1:C:297:PRO:O	2.18	0.43
1:A:274:TYR:O	1:A:277:LEU:HB2	2.19	0.43
4:A:404:T1C:H951	4:A:404:T1C:H922	1.78	0.43
1:D:301:LYS:CD	1:D:301:LYS:H	2.32	0.43
1:B:375:MET:C	1:B:377:LYS:H	2.22	0.43
1:B:170:GLY:O	1:B:175:ARG:NH2	2.42	0.43
1:D:257:ASN:HA	1:D:260:VAL:HB	2.01	0.43
1:C:93:ASP:OD1	1:C:96:GLY:N	2.52	0.43
1:D:328:LEU:O	1:D:331:ALA:HB3	2.18	0.43
1:D:26:PRO:HD3	5:D:503:HOH:O	2.19	0.43
1:D:208:LEU:HD23	1:D:214:LEU:HD21	2.01	0.42
1:B:87:MET:HG3	1:B:114:GLU:HG3	2.01	0.42
1:B:372:GLU:O	1:B:376:PHE:HD2	2.02	0.42
1:A:141:MET:HB3	1:A:152:THR:HG23	2.01	0.42
1:B:362:LYS:O	1:B:366:GLU:HB2	2.19	0.42
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:HH21	1:D:54:ARG:NE	2.17	0.42
1:C:256:ARG:O	1:C:260:VAL:HG23	2.19	0.42
1:A:322:GLN:HG2	1:A:364:ALA:HB1	2.01	0.42
1:A:146:LYS:HE3	1:A:146:LYS:HB2	1.80	0.42
1:A:22:ILE:HG21	1:A:139:LEU:HD22	2.00	0.42
1:A:369:THR:O	1:A:373:ILE:HG12	2.19	0.42
1:B:299:LYS:O	1:B:302:ARG:HD2	2.19	0.42
1:A:299:LYS:HB3	1:A:301:LYS:HD2	2.01	0.42
1:D:308:MET:O	1:D:353:TYR:OH	2.35	0.42
1:C:235:PHE:HZ	1:C:281:THR:HG21	1.84	0.42
1:B:369:THR:O	1:B:373:ILE:HG12	2.20	0.42
1:A:302:ARG:HA	1:A:303:PRO:HD3	1.73	0.42
1:B:343:PHE:CD1	1:B:348:GLU:HG3	2.53	0.42
1:C:302:ARG:HA	1:C:303:PRO:HD3	1.72	0.42
1:B:204:GLY:HA3	1:B:273:ARG:HG2	2.02	0.42
1:A:332:LEU:O	1:A:335:SER:OG	2.38	0.42
1:B:61:ASP:OD2	1:B:63:HIS:NE2	2.53	0.42
1:C:318:PRO:HD2	1:C:319:PHE:CE2	2.54	0.42
1:A:200:ILE:O	1:A:203:PRO:HD3	2.19	0.42
1:B:180:ASP:H	1:B:296:LYS:NZ	2.18	0.42
1:C:296:LYS:NZ	1:C:299:LYS:HG3	2.34	0.42
1:C:146:LYS:HB2	1:C:147:LYS:H	1.72	0.42
1:B:202:CYS:SG	1:B:233:LEU:HD13	2.60	0.42
1:B:274:TYR:O	1:B:277:LEU:HB2	2.20	0.42
1:D:224:PHE:HB2	4:D:401:T1C:O3	2.20	0.42
1:A:198:PRO:HG3	1:A:233:LEU:H	1.84	0.42
1:B:205:PHE:HD2	1:B:233:LEU:HD11	1.85	0.42
1:C:151:LEU:HD23	1:C:151:LEU:N	2.35	0.42
1:A:193:ALA:HB3	1:A:235:PHE:CE1	2.55	0.41
1:B:125:LEU:HD21	1:B:135:TRP:CZ2	2.55	0.41
1:B:125:LEU:HD21	1:B:135:TRP:HZ2	1.84	0.41
1:D:188:THR:HA	1:D:240:LYS:HA	2.01	0.41
3:C:402:FAD:N1	3:C:402:FAD:H2'	2.35	0.41
1:D:45:TYR:CE1	1:D:134:ILE:HD12	2.55	0.41
1:D:346:ILE:O	1:D:350:VAL:HG13	2.20	0.41
1:A:124:LEU:O	1:A:128:LEU:HG	2.20	0.41
1:C:121:ARG:HG2	1:C:125:LEU:HD22	2.02	0.41
1:C:354:GLU:HA	1:C:357:MET:HG2	2.02	0.41
1:B:340:ASP:HB3	1:B:342:LYS:H	1.86	0.41
1:C:294:LEU:HD12	1:C:294:LEU:HA	1.92	0.41
1:B:178:VAL:HG22	1:B:306:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:HG2	1:C:308:MET:CE	2.50	0.41
1:C:259:VAL:O	1:C:263:LEU:HB2	2.20	0.41
4:D:401:T1C:H433	4:D:401:T1C:H41	1.72	0.41
1:C:107:GLU:N	1:C:107:GLU:OE1	2.48	0.41
1:A:121:ARG:O	1:A:125:LEU:HB2	2.20	0.41
1:B:302:ARG:HA	1:B:303:PRO:HD3	1.75	0.41
1:C:290:ARG:HB2	1:C:315:LEU:HD21	2.02	0.41
1:B:266:LYS:NZ	5:B:506:HOH:O	2.31	0.41
1:C:62:LEU:HB2	1:C:80:TYR:CZ	2.56	0.41
1:A:35:LEU:HD21	1:A:338:LEU:HD12	2.03	0.41
1:C:336:ASP:O	1:C:339:ALA:N	2.54	0.41
1:C:300:SER:H	1:C:301:LYS:NZ	2.19	0.41
1:C:94:LYS:HD2	1:C:218:HIS:CE1	2.56	0.41
1:C:85:LEU:O	1:C:87:MET:HG2	2.21	0.41
1:A:13:LEU:HB2	1:A:341:GLY:HA2	2.03	0.41
1:B:330:ASP:HB3	1:B:360:TYR:OH	2.21	0.40
1:D:269:ASP:N	1:D:269:ASP:OD1	2.48	0.40
1:C:93:ASP:OD1	1:C:97:ASN:N	2.46	0.40
1:A:191:ILE:C	1:A:192:GLN:HG2	2.41	0.40
1:D:266:LYS:HB3	1:D:267:PHE:HD1	1.86	0.40
1:B:54:ARG:HE	1:D:54:ARG:HE	1.69	0.40
1:A:94:LYS:NZ	1:B:367:GLU:OE2	2.55	0.40
1:D:334:LEU:HD22	1:D:338:LEU:HD11	2.02	0.40
1:B:143:GLU:O	1:B:150:THR:N	2.33	0.40
1:D:76:LEU:HD21	1:D:127:SER:HB3	2.03	0.40
1:B:242:PRO:HG2	1:B:245:TRP:CZ2	2.56	0.40
1:C:19:VAL:HB	1:C:42:VAL:HG13	2.04	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	364/378 (96%)	337 (93%)	24 (7%)	3 (1%)	24 60
1	B	361/378 (96%)	333 (92%)	24 (7%)	4 (1%)	17 51
1	C	360/378 (95%)	329 (91%)	28 (8%)	3 (1%)	24 60
1	D	360/378 (95%)	334 (93%)	24 (7%)	2 (1%)	30 67
All	All	1445/1512 (96%)	1333 (92%)	100 (7%)	12 (1%)	24 60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	LYS
1	A	379	ASP
1	B	146	LYS
1	C	146	LYS
1	C	378	PRO
1	C	380	PHE
1	D	146	LYS
1	D	378	PRO
1	A	382	PHE
1	B	295	GLU
1	B	258	SER
1	B	378	PRO

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	314/327 (96%)	281 (90%)	33 (10%)	8 25
1	B	313/327 (96%)	286 (91%)	27 (9%)	13 36
1	C	311/327 (95%)	280 (90%)	31 (10%)	9 28
1	D	313/327 (96%)	280 (90%)	33 (10%)	8 25
All	All	1251/1308 (96%)	1127 (90%)	124 (10%)	10 29

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	LEU
1	A	31	MET
1	A	42	VAL
1	A	49	ASN
1	A	51	ARG
1	A	60	LEU
1	A	89	VAL
1	A	94	LYS
1	A	101	THR
1	A	104	VAL
1	A	125	LEU
1	A	146	LYS
1	A	151	LEU
1	A	152	THR
1	A	183	VAL
1	A	186	THR
1	A	192	GLN
1	A	195	ILE
1	A	214	LEU
1	A	243	ASP
1	A	246	LYS
1	A	263	LEU
1	A	281	THR
1	A	301	LYS
1	A	322	GLN
1	A	326	SER
1	A	336	ASP
1	A	346	ILE
1	A	353	TYR
1	A	357	MET
1	A	380	PHE
1	A	381	THR
1	B	31	MET
1	B	42	VAL
1	B	49	ASN
1	B	51	ARG
1	B	60	LEU
1	B	79	THR
1	B	89	VAL
1	B	94	LYS
1	B	101	THR
1	B	104	VAL

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Mol	Chain	Res	Type
1	B	146	LYS
1	B	186	THR
1	B	192	GLN
1	B	214	LEU
1	B	256	ARG
1	B	263	LEU
1	B	281	THR
1	B	287	LEU
1	B	294	LEU
1	B	301	LYS
1	B	326	SER
1	B	334	LEU
1	B	346	ILE
1	B	353	TYR
1	B	357	MET
1	B	381	THR
1	B	382	PHE
1	C	42	VAL
1	C	49	ASN
1	C	51	ARG
1	C	60	LEU
1	C	89	VAL
1	C	94	LYS
1	C	101	THR
1	C	104	VAL
1	C	116	ASN
1	C	125	LEU
1	C	146	LYS
1	C	151	LEU
1	C	162	ASP
1	C	183	VAL
1	C	186	THR
1	C	214	LEU
1	C	246	LYS
1	C	263	LEU
1	C	269	ASP
1	C	281	THR
1	C	294	LEU
1	C	295	GLU
1	C	311	ASP
1	C	326	SER
1	C	336	ASP

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Mol	Chain	Res	Type
1	C	346	ILE
1	C	347	GLU
1	C	350	VAL
1	C	353	TYR
1	C	366	GLU
1	C	382	PHE
1	D	31	MET
1	D	42	VAL
1	D	60	LEU
1	D	89	VAL
1	D	94	LYS
1	D	101	THR
1	D	116	ASN
1	D	125	LEU
1	D	130	ASN
1	D	143	GLU
1	D	146	LYS
1	D	151	LEU
1	D	162	ASP
1	D	186	THR
1	D	214	LEU
1	D	246	LYS
1	D	256	ARG
1	D	263	LEU
1	D	269	ASP
1	D	281	THR
1	D	285	VAL
1	D	294	LEU
1	D	301	LYS
1	D	311	ASP
1	D	334	LEU
1	D	336	ASP
1	D	346	ILE
1	D	350	VAL
1	D	353	TYR
1	D	357	MET
1	D	366	GLU
1	D	379	ASP
1	D	382	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	218	HIS
1	C	325	ASN
1	D	219	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	SO4	A	401	-	4,4,4	0.10	0	6,6,6	0.19	0
2	SO4	A	402	-	4,4,4	0.08	0	6,6,6	0.16	0
3	FAD	A	403	-	48,58,58	1.75	9 (18%)	54,89,89	2.82	20 (37%)
4	T1C	A	404	-	44,45,45	3.46	22 (50%)	48,72,72	2.51	15 (31%)
2	SO4	B	401	-	4,4,4	0.07	0	6,6,6	0.19	0
2	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.46	0
3	FAD	B	403	-	48,58,58	1.67	8 (16%)	54,89,89	2.35	14 (25%)
2	SO4	B	404	-	4,4,4	0.07	0	6,6,6	0.17	0
4	T1C	B	405	-	44,45,45	3.41	22 (50%)	48,72,72	2.26	16 (33%)
2	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.12	0
4	T1C	C	401	-	44,45,45	3.29	19 (43%)	48,72,72	1.85	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FAD	C	402	-	48,58,58	1.75	7 (14%)	54,89,89	2.84	14 (25%)
4	T1C	D	401	-	44,45,45	3.33	20 (45%)	48,72,72	1.89	15 (31%)
3	FAD	D	402	-	48,58,58	1.74	7 (14%)	54,89,89	2.97	17 (31%)

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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	FAD	A	403	-	-	0/30/50/50	0/6/6/6
4	T1C	A	404	-	-	0/22/80/80	0/4/4/4
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
3	FAD	B	403	-	-	0/30/50/50	0/6/6/6
2	SO4	B	404	-	-	0/0/0/0	0/0/0/0
4	T1C	B	405	-	-	0/22/80/80	0/4/4/4
2	SO4	B	406	-	-	0/0/0/0	0/0/0/0
4	T1C	C	401	-	-	0/22/80/80	0/4/4/4
3	FAD	C	402	-	-	0/30/50/50	0/6/6/6
4	T1C	D	401	-	-	0/22/80/80	0/4/4/4
3	FAD	D	402	-	-	0/30/50/50	0/6/6/6

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	FAD	C2B-C3B	-3.95	1.42	1.53
3	C	402	FAD	C2B-C3B	-3.93	1.42	1.53
3	D	402	FAD	C2B-C3B	-3.61	1.43	1.53
4	B	405	T1C	O1C-C1C	-3.58	1.36	1.42
3	A	403	FAD	C2B-C3B	-3.48	1.43	1.53
4	A	404	T1C	C51-C1B	-3.42	1.47	1.51
4	A	404	T1C	O1C-C1C	-3.38	1.37	1.42
4	D	401	T1C	O1C-C1C	-3.36	1.37	1.42
4	C	401	T1C	O1C-C1C	-3.33	1.37	1.42
4	D	401	T1C	C51-C1B	-3.12	1.48	1.51
4	A	404	T1C	C1B-C12	-2.90	1.32	1.36
3	C	402	FAD	O4'-C4'	-2.73	1.37	1.43
4	B	405	T1C	C1C-C1	-2.73	1.50	1.55
4	C	401	T1C	C51-C1B	-2.64	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	T1C	C1C-C1	-2.58	1.51	1.55
4	D	401	T1C	C1A-C61	-2.58	1.36	1.40
4	B	405	T1C	C51-C1B	-2.56	1.48	1.51
4	D	401	T1C	C1C-C1	-2.47	1.51	1.55
4	A	404	T1C	C1A-C61	-2.45	1.36	1.40
4	C	401	T1C	C1A-C61	-2.44	1.36	1.40
4	B	405	T1C	C1A-C61	-2.33	1.37	1.40
3	D	402	FAD	O4'-C4'	-2.29	1.38	1.43
3	D	402	FAD	C9A-C5X	-2.19	1.38	1.42
3	B	403	FAD	O4'-C4'	-2.11	1.38	1.43
3	A	403	FAD	O4'-C4'	-2.06	1.38	1.43
4	D	401	T1C	O3-C3	2.02	1.39	1.33
3	A	403	FAD	C2'-C3'	2.02	1.57	1.53
3	C	402	FAD	C2'-C3'	2.02	1.57	1.53
3	A	403	FAD	C2A-N3A	2.05	1.35	1.32
3	B	403	FAD	C4-C4X	2.05	1.45	1.41
4	D	401	T1C	C1C-C41	2.06	1.55	1.53
4	C	401	T1C	C4-C3	2.06	1.56	1.51
4	C	401	T1C	C2-C21	2.10	1.51	1.47
3	B	403	FAD	C2'-C3'	2.13	1.57	1.53
4	C	401	T1C	C7-N7	2.13	1.48	1.42
4	B	405	T1C	C6-C51	2.14	1.58	1.52
3	A	403	FAD	C5'-C4'	2.14	1.54	1.51
4	D	401	T1C	C7-N7	2.15	1.48	1.42
4	B	405	T1C	O3-C3	2.23	1.40	1.33
4	B	405	T1C	C8-C9	2.24	1.43	1.39
4	B	405	T1C	C8-C7	2.28	1.43	1.39
4	A	404	T1C	C2-C21	2.28	1.51	1.47
4	C	401	T1C	O3-C3	2.30	1.40	1.33
3	B	403	FAD	C6A-N6A	2.32	1.42	1.34
3	C	402	FAD	C6A-N6A	2.32	1.42	1.34
4	B	405	T1C	C7-N7	2.37	1.48	1.42
3	A	403	FAD	C6A-N6A	2.37	1.42	1.34
4	D	401	T1C	C8-C7	2.37	1.43	1.39
3	B	403	FAD	C2A-N3A	2.41	1.36	1.32
4	A	404	T1C	C4-C3	2.45	1.56	1.51
4	A	404	T1C	O3-C3	2.45	1.40	1.33
3	D	402	FAD	C6A-N6A	2.46	1.42	1.34
3	A	403	FAD	C4-C4X	2.48	1.46	1.41
4	C	401	T1C	C1C-C41	2.53	1.55	1.53
4	A	404	T1C	C8-C9	2.56	1.43	1.39
4	D	401	T1C	C2-C21	2.59	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	T1C	C4-C3	2.62	1.57	1.51
4	C	401	T1C	C8-C9	2.62	1.43	1.39
4	A	404	T1C	C7-N7	2.68	1.49	1.42
4	A	404	T1C	C8-C7	2.69	1.44	1.39
4	B	405	T1C	C1C-C41	2.88	1.55	1.53
4	D	401	T1C	C8-C9	2.94	1.44	1.39
3	D	402	FAD	C4-C4X	3.11	1.47	1.41
4	B	405	T1C	C9-C10	3.17	1.45	1.40
4	A	404	T1C	C9-C10	3.41	1.46	1.40
4	C	401	T1C	C6-C61	3.46	1.57	1.51
3	C	402	FAD	C4-C4X	3.47	1.48	1.41
4	D	401	T1C	C41-C4	3.59	1.58	1.54
4	C	401	T1C	C9-C10	3.61	1.46	1.40
4	B	405	T1C	C41-C4	3.63	1.58	1.54
4	A	404	T1C	C1C-C41	3.64	1.56	1.53
4	D	401	T1C	C9-C10	3.66	1.46	1.40
4	A	404	T1C	C21-N21	3.67	1.44	1.33
4	D	401	T1C	C6-C61	3.77	1.58	1.51
4	B	405	T1C	C2-C21	3.79	1.54	1.47
4	C	401	T1C	C21-N21	3.84	1.44	1.33
4	A	404	T1C	C41-C4	3.85	1.58	1.54
4	B	405	T1C	C9-N9	3.94	1.49	1.41
4	C	401	T1C	C41-C4	3.96	1.59	1.54
4	C	401	T1C	C9-N9	4.07	1.49	1.41
3	B	403	FAD	C4-N3	4.08	1.40	1.33
4	D	401	T1C	C21-N21	4.08	1.45	1.33
4	B	405	T1C	C6-C61	4.09	1.58	1.51
4	A	404	T1C	C6-C61	4.12	1.58	1.51
4	A	404	T1C	C9-N9	4.16	1.49	1.41
4	D	401	T1C	C9-N9	4.33	1.50	1.41
3	A	403	FAD	C4-N3	4.56	1.41	1.33
4	B	405	T1C	C21-N21	4.58	1.46	1.33
3	D	402	FAD	C4-N3	4.61	1.41	1.33
3	C	402	FAD	C4-N3	4.62	1.41	1.33
4	A	404	T1C	C91-N9	5.51	1.48	1.35
4	B	405	T1C	C91-N9	5.68	1.49	1.35
4	C	401	T1C	C91-N9	5.75	1.49	1.35
4	D	401	T1C	C91-N9	5.76	1.49	1.35
4	A	404	T1C	C1A-C10	5.86	1.53	1.41
3	C	402	FAD	C10-N1	6.08	1.45	1.35
4	B	405	T1C	C1A-C10	6.19	1.54	1.41
3	B	403	FAD	C10-N1	6.23	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	FAD	C10-N1	6.27	1.46	1.35
4	C	401	T1C	C1A-C10	6.31	1.54	1.41
4	D	401	T1C	C1A-C10	6.49	1.55	1.41
3	A	403	FAD	C10-N1	6.82	1.46	1.35
4	D	401	T1C	O11-C11	7.59	1.39	1.23
4	C	401	T1C	O11-C11	7.62	1.39	1.23
4	B	405	T1C	O11-C11	7.74	1.39	1.23
4	A	404	T1C	O11-C11	7.85	1.40	1.23
4	D	401	T1C	C7-C61	9.48	1.54	1.40
4	C	401	T1C	C7-C61	9.57	1.54	1.40
4	B	405	T1C	O1-C1	9.60	1.40	1.22
4	D	401	T1C	O1-C1	9.65	1.40	1.22
4	A	404	T1C	O1-C1	9.78	1.40	1.22
4	C	401	T1C	O1-C1	9.83	1.40	1.22
4	B	405	T1C	C7-C61	10.38	1.55	1.40
4	A	404	T1C	C7-C61	10.70	1.55	1.40

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	FAD	N3A-C2A-N1A	-10.50	120.85	128.89
3	C	402	FAD	N3A-C2A-N1A	-9.24	121.82	128.89
3	C	402	FAD	O3P-P-O5'	-8.87	79.40	102.94
3	A	403	FAD	O3P-P-O5'	-8.69	79.87	102.94
3	A	403	FAD	N3A-C2A-N1A	-8.51	122.38	128.89
3	B	403	FAD	N3A-C2A-N1A	-8.34	122.51	128.89
3	D	402	FAD	O3P-P-O5'	-7.51	83.02	102.94
4	A	404	T1C	O1C-C1C-C41	-6.94	101.42	110.17
4	D	401	T1C	O12-C12-C1B	-6.19	117.91	123.84
4	B	405	T1C	O12-C12-C1B	-6.11	117.99	123.84
3	D	402	FAD	O2P-P-O5'	-5.86	78.92	108.46
3	A	403	FAD	O2P-P-O5'	-5.82	79.14	108.46
4	A	404	T1C	O12-C12-C1B	-5.75	118.34	123.84
3	C	402	FAD	O2P-P-O5'	-5.28	81.84	108.46
4	C	401	T1C	O12-C12-C1B	-5.14	118.92	123.84
3	A	403	FAD	P-O3P-PA	-4.75	119.39	132.73
4	B	405	T1C	O1C-C1C-C41	-4.73	104.21	110.17
3	C	402	FAD	C4X-C4-N3	-4.40	117.57	123.59
3	D	402	FAD	O5'-P-O1P	-4.40	92.54	109.62
3	C	402	FAD	O5'-P-O1P	-4.36	92.71	109.62
4	A	404	T1C	C11-C1B-C12	-4.25	115.31	118.93
4	D	401	T1C	O1C-C1C-C41	-4.17	104.92	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	FAD	O5'-P-O1P	-4.12	93.61	109.62
3	D	402	FAD	C4A-C5A-N7A	-3.89	105.90	109.48
3	D	402	FAD	C4X-C4-N3	-3.86	118.31	123.59
4	C	401	T1C	O1C-C1C-C41	-3.76	105.44	110.17
4	A	404	T1C	C21-C2-C1	-3.64	116.59	120.87
3	B	403	FAD	C4X-C4-N3	-3.59	118.68	123.59
4	B	405	T1C	C21-C2-C1	-3.34	116.94	120.87
3	C	402	FAD	C4A-C5A-N7A	-3.27	106.47	109.48
4	C	401	T1C	C51-C5-C41	-3.22	104.50	110.71
3	D	402	FAD	C4B-O4B-C1B	-3.13	106.28	109.72
3	B	403	FAD	C4A-C5A-N7A	-3.11	106.61	109.48
3	B	403	FAD	P-O3P-PA	-2.96	124.42	132.73
4	A	404	T1C	O1-C1-C2	-2.95	117.54	123.59
3	D	402	FAD	C2B-C1B-N9A	-2.90	109.87	114.29
3	A	403	FAD	C4A-C5A-N7A	-2.90	106.81	109.48
3	A	403	FAD	C4X-C4-N3	-2.88	119.65	123.59
4	D	401	T1C	O1-C1-C2	-2.88	117.69	123.59
4	B	405	T1C	O21-C21-N21	-2.79	115.82	122.76
3	B	403	FAD	C6-C5X-N5	-2.71	115.47	118.96
3	D	402	FAD	C1B-N9A-C4A	-2.64	122.96	126.94
4	B	405	T1C	C11-C1B-C12	-2.63	116.69	118.93
3	C	402	FAD	C6-C5X-N5	-2.59	115.64	118.96
4	A	404	T1C	C72-N7-C71	-2.57	107.49	115.96
4	B	405	T1C	O11-C11-C1B	-2.44	117.10	120.73
4	B	405	T1C	O1-C1-C2	-2.39	118.68	123.59
3	A	403	FAD	C4X-C10-N10	-2.37	119.12	120.52
3	D	402	FAD	C4X-C10-N10	-2.34	119.14	120.52
4	A	404	T1C	C8-C7-C61	-2.33	118.23	122.57
3	A	403	FAD	C6-C5X-N5	-2.31	115.99	118.96
4	B	405	T1C	C72-N7-C71	-2.28	108.42	115.96
4	D	401	T1C	C21-C2-C1	-2.19	118.29	120.87
4	D	401	T1C	O11-C11-C1B	-2.18	117.48	120.73
4	B	405	T1C	C8-C7-N7	-2.17	117.27	120.54
4	A	404	T1C	C8-C7-N7	-2.16	117.29	120.54
3	B	403	FAD	O2P-P-O1P	-2.16	100.83	112.53
3	A	403	FAD	C4B-O4B-C1B	-2.13	107.38	109.72
3	B	403	FAD	C4B-O4B-C1B	-2.09	107.42	109.72
4	C	401	T1C	O1-C1-C2	-2.09	119.30	123.59
4	D	401	T1C	O21-C21-N21	-2.05	117.66	122.76
4	D	401	T1C	C11-C1B-C12	-2.02	117.21	118.93
4	A	404	T1C	O11-C11-C1B	-2.01	117.73	120.73
4	C	401	T1C	C1A-C11-C1B	2.02	121.87	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	T1C	C61-C7-N7	2.05	120.68	118.94
3	B	403	FAD	C6-C5X-C9A	2.06	121.69	118.98
4	A	404	T1C	C1C-C41-C4	2.07	114.50	111.73
4	C	401	T1C	O12-C12-C1C	2.10	116.84	113.50
3	D	402	FAD	C4-C4X-N5	2.12	121.29	118.72
3	A	403	FAD	O3'-C3'-C4'	2.18	114.25	108.75
3	D	402	FAD	O2'-C2'-C1'	2.20	115.36	109.94
4	D	401	T1C	C1C-C41-C4	2.22	114.70	111.73
3	B	403	FAD	O2'-C2'-C1'	2.22	115.40	109.94
4	D	401	T1C	C1A-C11-C1B	2.22	122.19	118.68
4	C	401	T1C	C61-C7-N7	2.29	120.89	118.94
3	A	403	FAD	C4-C4X-C10	2.29	121.41	119.94
4	C	401	T1C	C6-C61-C1A	2.29	122.28	117.77
4	D	401	T1C	C6-C61-C1A	2.31	122.31	117.77
3	A	403	FAD	C6-C5X-C9A	2.32	122.03	118.98
3	C	402	FAD	C1'-C2'-C3'	2.35	116.53	109.82
3	C	402	FAD	O3P-PA-O5B	2.42	109.37	102.94
4	B	405	T1C	O12-C12-C1C	2.43	117.38	113.50
4	C	401	T1C	C1C-C1-C2	2.47	120.09	116.13
4	D	401	T1C	O12-C12-C1C	2.50	117.48	113.50
3	B	403	FAD	O2A-PA-O3P	2.51	116.46	105.09
4	B	405	T1C	C1A-C11-C1B	2.55	122.71	118.68
4	C	401	T1C	C1-C1C-C12	2.58	112.97	109.73
3	B	403	FAD	C1'-C2'-C3'	2.67	117.46	109.82
3	A	403	FAD	O2'-C2'-C1'	2.73	116.65	109.94
3	C	402	FAD	C4X-N5-C5X	2.76	119.94	116.76
3	A	403	FAD	O2A-PA-O3P	2.85	118.03	105.09
3	C	402	FAD	O4B-C1B-N9A	2.87	114.10	108.10
3	D	402	FAD	O2P-P-O3P	2.93	118.38	105.09
3	A	403	FAD	C1'-C2'-C3'	2.96	118.27	109.82
4	A	404	T1C	O12-C12-C1C	3.03	118.33	113.50
4	D	401	T1C	C41-C1C-C1	3.10	114.70	111.17
4	B	405	T1C	C2-C21-N21	3.23	125.49	119.27
3	C	402	FAD	O2P-P-O3P	3.25	119.83	105.09
4	D	401	T1C	C92-C91-N9	3.28	119.27	114.56
4	D	401	T1C	C1C-C1-C2	3.30	121.41	116.13
4	B	405	T1C	C92-C91-N9	3.38	119.40	114.56
3	D	402	FAD	C4X-N5-C5X	3.40	120.68	116.76
3	B	403	FAD	C4X-N5-C5X	3.43	120.70	116.76
4	C	401	T1C	C1C-C41-C4	3.46	116.38	111.73
4	A	404	T1C	C92-C91-N9	3.47	119.53	114.56
3	A	403	FAD	C1'-N10-C9A	3.58	122.88	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	405	T1C	C1C-C1-C2	3.59	121.88	116.13
3	A	403	FAD	C4X-N5-C5X	3.85	121.19	116.76
3	D	402	FAD	C1'-N10-C9A	3.87	123.21	118.86
3	A	403	FAD	O2P-P-O3P	3.98	123.17	105.09
4	A	404	T1C	C1C-C1-C2	4.09	122.68	116.13
4	C	401	T1C	C92-C91-N9	4.30	120.72	114.56
3	C	402	FAD	C1'-N10-C9A	4.54	123.96	118.86
3	D	402	FAD	O4B-C1B-N9A	4.57	117.67	108.10
3	B	403	FAD	C1'-N10-C9A	4.83	124.28	118.86
4	B	405	T1C	C61-C7-N7	5.50	123.62	118.94
4	B	405	T1C	C41-C1C-C1	5.91	117.90	111.17
4	A	404	T1C	C61-C7-N7	6.52	124.48	118.94
4	A	404	T1C	C41-C1C-C1	7.15	119.31	111.17
3	A	403	FAD	C4-N3-C2	8.25	122.38	115.25
3	D	402	FAD	C4-N3-C2	9.61	123.56	115.25
3	C	402	FAD	C4-N3-C2	9.63	123.57	115.25
3	B	403	FAD	C4-N3-C2	9.78	123.70	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	FAD	2	0
4	A	404	T1C	7	0
3	B	403	FAD	2	0
4	B	405	T1C	2	0
4	C	401	T1C	1	0
3	C	402	FAD	2	0
4	D	401	T1C	4	0
3	D	402	FAD	2	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	368/378 (97%)	0.07	3 (0%)	87 86	37, 58, 86, 113	0
1	B	365/378 (96%)	0.13	2 (0%)	91 90	37, 59, 88, 103	0
1	C	364/378 (96%)	0.27	7 (1%)	70 66	45, 73, 100, 112	0
1	D	364/378 (96%)	0.29	14 (3%)	44 37	46, 74, 101, 114	0
All	All	1461/1512 (96%)	0.19	26 (1%)	71 68	37, 66, 97, 114	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	LEU	4.5
1	D	60	LEU	4.2
1	D	245	TRP	3.3
1	C	60	LEU	3.3
1	D	264	LEU	3.0
1	B	60	LEU	2.9
1	C	214	LEU	2.8
1	D	222	LEU	2.8
1	C	368	SER	2.7
1	D	38	ASN	2.6
1	D	15	SER	2.5
1	B	294	LEU	2.5
1	D	320	ALA	2.4
1	A	294	LEU	2.4
1	D	161	ALA	2.4
1	D	294	LEU	2.3
1	C	287	LEU	2.3
1	D	59	THR	2.3
1	D	382	PHE	2.3
1	A	377	LYS	2.3
1	C	352	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	218	HIS	2.2
1	C	132	THR	2.2
1	D	376	PHE	2.2
1	D	253	PHE	2.1
1	A	60	LEU	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
4	T1C	B	405	42/42	0.81	0.32	2.26	41,77,98,109	0
4	T1C	D	401	42/42	0.76	0.34	1.48	62,90,114,120	0
4	T1C	C	401	42/42	0.84	0.29	1.29	62,86,114,117	0
4	T1C	A	404	42/42	0.84	0.23	0.73	44,65,81,87	0
3	FAD	D	402	53/53	0.94	0.20	-0.39	42,56,77,83	0
3	FAD	B	403	53/53	0.96	0.19	-0.51	30,46,61,75	0
3	FAD	C	402	53/53	0.95	0.19	-0.54	41,58,72,77	0
2	SO4	B	402	5/5	0.92	0.17	-0.70	63,66,72,85	0
3	FAD	A	403	53/53	0.97	0.18	-0.73	32,47,62,68	0
2	SO4	A	402	5/5	0.93	0.11	-1.70	68,70,85,88	0
2	SO4	B	404	5/5	0.92	0.11	-	79,79,87,95	0
2	SO4	A	401	5/5	0.97	0.08	-	61,71,78,93	0
2	SO4	B	401	5/5	0.96	0.10	-	74,85,87,93	0
2	SO4	B	406	5/5	0.98	0.09	-	58,64,81,86	0

6.5 Other polymers (i)

There are no such residues in this entry.