



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:56 AM GMT

PDB ID : 1TB3
Title : Crystal Structure Analysis of Recombinant Rat Kidney Long-chain Hydroxy
Acid Oxidase
Authors : Cunane, L.M.; Barton, J.D.; Chen, Z.W.; Le, K.H.D.; Amar, D.; Lederer, F.;
Mathews, F.S.
Deposited on : 2004-05-19
Resolution : 2.30 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>

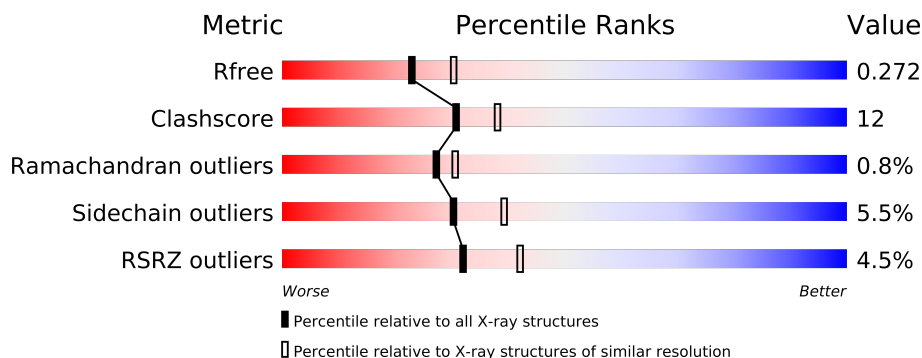
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	352	
1	B	352	
1	C	352	
1	D	352	
1	E	352	
1	F	352	
1	G	352	
1	H	352	

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	ACY	A	1402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACY	B	2402	-	X
3	ACY	C	3402	-	X
3	ACY	F	6402	-	X
3	ACY	H	8402	-	X

2 Entry composition

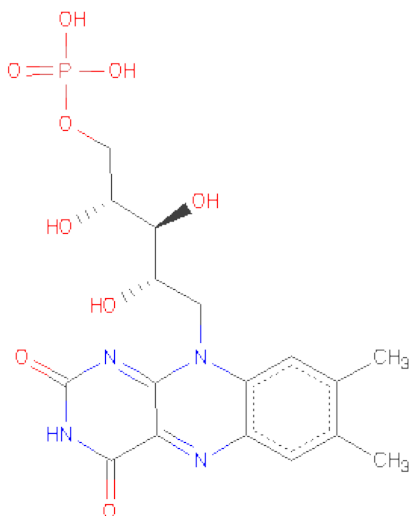
There are 4 unique types of molecules in this entry. The entry contains 21605 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hydroxyacid oxidase 3.

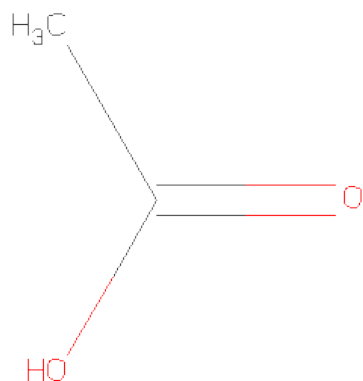
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	B	327	Total	C	N	O	S	0	0	0
			2537	1605	444	474	14			
1	C	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	D	329	Total	C	N	O	S	0	0	0
			2550	1614	446	476	14			
1	E	324	Total	C	N	O	S	0	0	0
			2519	1593	441	471	14			
1	F	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			
1	G	329	Total	C	N	O	S	0	0	0
			2547	1611	446	476	14			
1	H	332	Total	C	N	O	S	0	0	0
			2568	1624	449	481	14			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	130	Total O 130 130	0	0
4	B	75	Total O 75 75	0	0
4	C	106	Total O 106 106	0	0
4	D	115	Total O 115 115	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	71	Total 71	O 71	0	0
4	F	166	Total 166	O 166	0	0
4	G	109	Total 109	O 109	0	0
4	H	128	Total 128	O 128	0	0

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.

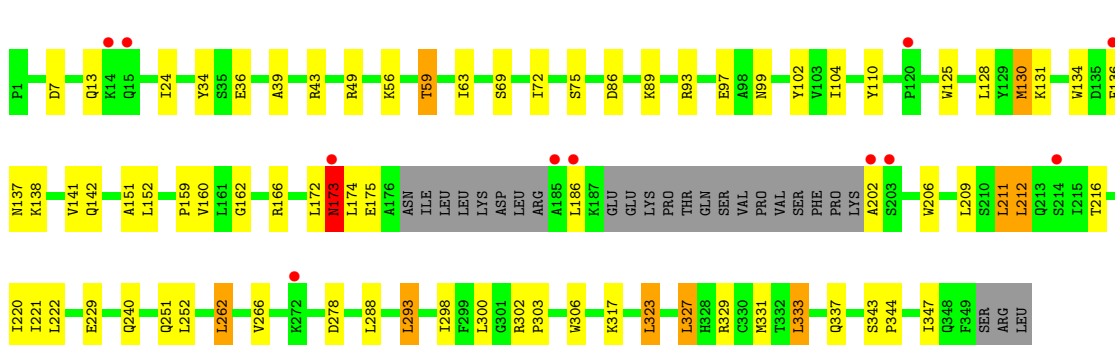
• Molecule 1: Hydroxyacid oxidase 3

Chain A:



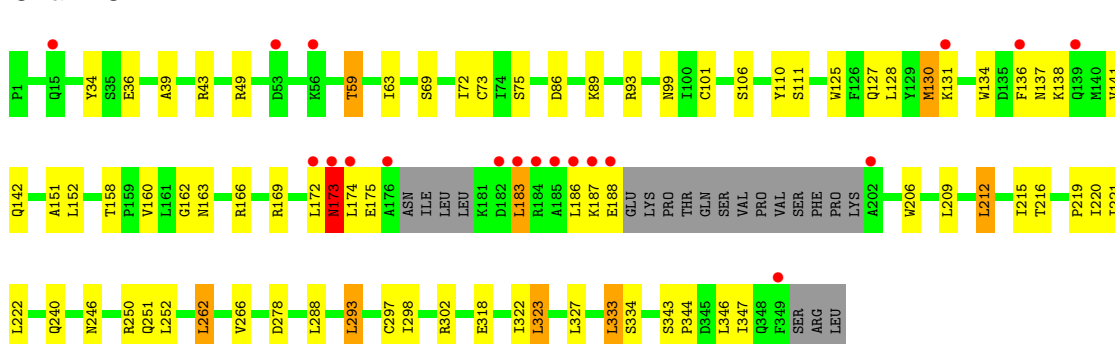
• Molecule 1: Hydroxyacid oxidase 3

Chain B:



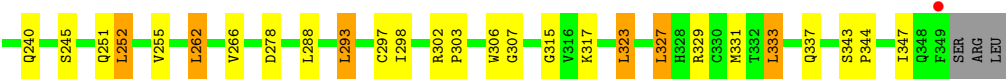
• Molecule 1: Hydroxyacid oxidase 3

Chain C:



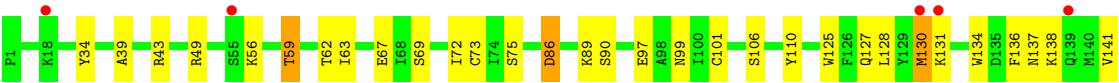
Chain D:





● Molecule 1: Hydroxyacid oxidase 3

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.84Å 151.10Å 222.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 39.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.1 (40.00-2.30) 83.2 (39.99-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.269 0.241 , 0.272	Depositor DCC
R_{free} test set	7147 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 159563 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21605	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 90.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6809e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ACY

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	0.35	0/2610	0.62	0/3528
1	B	0.34	0/2579	0.60	0/3485
1	C	0.34	0/2610	0.60	0/3528
1	D	0.35	0/2592	0.60	0/3503
1	E	0.34	0/2562	0.59	0/3463
1	F	0.36	0/2610	0.62	0/3528
1	G	0.36	0/2589	0.60	0/3499
1	H	0.35	0/2610	0.61	0/3528
All	All	0.35	0/20762	0.60	0/28062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2568	0	2584	58	0
1	B	2537	0	2563	64	0
1	C	2568	0	2584	63	0
1	D	2550	0	2576	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2519	0	2546	61	0
1	F	2568	0	2584	64	0
1	G	2547	0	2567	70	0
1	H	2568	0	2584	69	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	0	0
3	H	4	0	3	0	0
4	A	130	0	0	4	0
4	B	75	0	0	2	0
4	C	106	0	0	2	0
4	D	115	0	0	2	0
4	E	71	0	0	3	0
4	F	166	0	0	6	0
4	G	109	0	0	2	0
4	H	128	0	0	4	0
All	All	21605	0	20764	489	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 12.

All (489) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:220:ILE:H	1:B:240:GLN:HE21	1.13	0.96
1:F:220:ILE:H	1:F:240:GLN:HE21	1.12	0.94
1:G:220:ILE:H	1:G:240:GLN:HE21	1.16	0.94
1:D:220:ILE:H	1:D:240:GLN:HE21	1.16	0.93
1:E:220:ILE:H	1:E:240:GLN:HE21	1.18	0.91
1:A:220:ILE:H	1:A:240:GLN:HE21	1.14	0.90
1:C:220:ILE:H	1:C:240:GLN:HE21	1.19	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:220:ILE:H	1:H:240:GLN:HE21	1.19	0.85
1:F:130:MET:HA	1:F:130:MET:HE2	1.61	0.83
1:A:130:MET:HA	1:A:130:MET:HE3	1.64	0.79
1:E:130:MET:HE2	1:E:130:MET:HA	1.65	0.79
1:B:130:MET:HE3	1:B:130:MET:HA	1.66	0.77
1:H:130:MET:HA	1:H:130:MET:HE3	1.68	0.76
1:C:130:MET:HA	1:C:130:MET:HE3	1.70	0.74
1:C:141:VAL:HG11	1:C:216:THR:HB	1.70	0.73
1:F:213:GLN:HG2	1:F:220:ILE:HD12	1.70	0.73
1:A:220:ILE:H	1:A:240:GLN:NE2	1.87	0.73
1:H:220:ILE:H	1:H:240:GLN:NE2	1.87	0.72
1:C:220:ILE:H	1:C:240:GLN:NE2	1.87	0.72
1:H:141:VAL:HG11	1:H:216:THR:HB	1.72	0.71
1:F:220:ILE:H	1:F:240:GLN:NE2	1.86	0.71
1:B:220:ILE:H	1:B:240:GLN:NE2	1.86	0.70
1:E:220:ILE:H	1:E:240:GLN:NE2	1.89	0.70
1:H:138:LYS:HA	1:H:215:ILE:HD12	1.72	0.70
1:G:130:MET:HA	1:G:130:MET:HE3	1.74	0.70
1:G:220:ILE:H	1:G:240:GLN:NE2	1.89	0.68
1:D:220:ILE:H	1:D:240:GLN:NE2	1.90	0.67
1:B:141:VAL:HG11	1:B:216:THR:HB	1.76	0.67
1:F:169:ARG:NH2	4:F:6537:HOH:O	2.27	0.66
1:F:164:ARG:HD3	4:F:6507:HOH:O	1.96	0.66
1:E:162:GLY:H	1:E:251:GLN:HE22	1.43	0.65
1:F:173:ASN:O	1:F:175:GLU:HG2	1.96	0.65
1:F:131:LYS:H	1:F:137:ASN:HD21	1.43	0.65
1:F:172:LEU:HD13	4:F:6514:HOH:O	1.95	0.64
1:A:213:GLN:HG2	1:A:220:ILE:HD12	1.79	0.63
1:B:211:LEU:HD12	1:B:211:LEU:C	2.18	0.63
1:D:130:MET:HA	1:D:130:MET:HE2	1.80	0.63
1:H:128:LEU:HG	1:H:130:MET:HE1	1.80	0.63
1:A:131:LYS:H	1:A:137:ASN:HD21	1.47	0.63
1:C:128:LEU:HG	1:C:130:MET:HE1	1.81	0.63
1:B:131:LYS:H	1:B:137:ASN:HD21	1.45	0.62
1:A:212:LEU:O	1:A:215:ILE:HG12	2.00	0.62
1:B:220:ILE:N	1:B:240:GLN:HE21	1.93	0.62
1:B:298:ILE:C	1:B:298:ILE:HD12	2.19	0.61
1:G:212:LEU:O	1:G:216:THR:HG22	2.01	0.61
1:F:128:LEU:HG	1:F:130:MET:HE3	1.83	0.61
1:H:220:ILE:N	1:H:240:GLN:HE21	1.97	0.60
1:D:125:TRP:CD1	1:D:151:ALA:HB3	2.36	0.60
1:H:131:LYS:HE2	1:H:136:PHE:CE1	2.37	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:131:LYS:H	1:E:137:ASN:HD21	1.46	0.60
1:E:141:VAL:HG11	1:E:216:THR:HB	1.84	0.60
1:A:220:ILE:N	1:A:240:GLN:HE21	1.94	0.60
1:G:162:GLY:H	1:G:251:GLN:HE22	1.48	0.59
1:D:173:ASN:O	1:D:175:GLU:HG2	2.02	0.59
1:C:220:ILE:N	1:C:240:GLN:HE21	1.96	0.59
1:A:128:LEU:HG	1:A:130:MET:HE1	1.84	0.59
1:G:262:LEU:HD22	1:G:266:VAL:HG23	1.85	0.59
1:F:212:LEU:O	1:F:215:ILE:HG12	2.02	0.59
1:G:298:ILE:HD12	1:G:298:ILE:C	2.23	0.59
1:A:160:VAL:HG12	1:D:333:LEU:HD13	1.84	0.59
1:E:298:ILE:C	1:E:298:ILE:HD12	2.24	0.59
1:H:298:ILE:HD12	1:H:298:ILE:C	2.23	0.59
1:G:131:LYS:HE2	1:G:136:PHE:CE1	2.38	0.59
1:A:173:ASN:HA	4:A:1507:HOH:O	2.02	0.59
1:F:141:VAL:HG11	1:F:216:THR:HB	1.84	0.59
1:A:262:LEU:HD22	1:A:266:VAL:HG23	1.85	0.58
1:H:162:GLY:H	1:H:251:GLN:HE22	1.52	0.58
1:G:128:LEU:HG	1:G:130:MET:HE1	1.86	0.58
1:C:298:ILE:C	1:C:298:ILE:HD12	2.24	0.58
1:G:162:GLY:H	1:G:251:GLN:NE2	2.02	0.57
1:D:298:ILE:C	1:D:298:ILE:HD12	2.24	0.57
1:F:131:LYS:HE2	1:F:136:PHE:CE1	2.39	0.57
1:B:162:GLY:H	1:B:251:GLN:HE22	1.50	0.57
1:A:343:SER:HB2	1:A:344:PRO:HD2	1.86	0.57
1:B:343:SER:HB2	1:B:344:PRO:HD2	1.87	0.57
1:D:131:LYS:HE2	1:D:136:PHE:CE1	2.40	0.56
1:D:343:SER:HB2	1:D:344:PRO:HD2	1.86	0.56
1:H:128:LEU:CD2	1:H:130:MET:HE1	2.36	0.56
1:D:128:LEU:HG	1:D:130:MET:HE3	1.87	0.56
1:D:166:ARG:HG2	1:D:166:ARG:HH11	1.71	0.56
1:D:262:LEU:HD22	1:D:266:VAL:HG23	1.86	0.56
1:E:162:GLY:H	1:E:251:GLN:NE2	2.04	0.56
1:H:169:ARG:NH2	4:H:8440:HOH:O	2.38	0.56
1:A:169:ARG:NH1	1:D:7:ASP:OD1	2.38	0.56
1:C:173:ASN:O	1:C:175:GLU:HG2	2.05	0.56
1:F:124:ARG:NH1	4:F:6516:HOH:O	2.38	0.56
1:F:188:GLU:HA	4:F:6553:HOH:O	2.06	0.56
1:E:72:ILE:HD13	1:E:323:LEU:HB3	1.88	0.56
1:E:202:ALA:HA	4:E:5470:HOH:O	2.04	0.55
1:F:343:SER:HB2	1:F:344:PRO:HD2	1.87	0.55
1:A:173:ASN:O	1:A:175:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:162:GLY:H	1:D:251:GLN:HE22	1.55	0.55
1:A:162:GLY:H	1:A:251:GLN:HE22	1.54	0.55
1:C:343:SER:HB2	1:C:344:PRO:HD2	1.88	0.55
1:A:141:VAL:HG11	1:A:216:THR:HB	1.88	0.55
1:E:220:ILE:N	1:E:240:GLN:HE21	1.97	0.55
1:C:162:GLY:H	1:C:251:GLN:HE22	1.55	0.55
1:F:220:ILE:N	1:F:240:GLN:HE21	1.92	0.55
1:F:59:THR:HG23	1:F:69:SER:O	2.06	0.55
1:F:298:ILE:HD12	1:F:298:ILE:C	2.27	0.54
1:B:128:LEU:HG	1:B:130:MET:HE1	1.89	0.54
1:A:298:ILE:C	1:A:298:ILE:HD12	2.27	0.54
1:G:343:SER:HB2	1:G:344:PRO:HD2	1.89	0.54
1:H:343:SER:HB2	1:H:344:PRO:HD2	1.88	0.54
1:E:343:SER:HB2	1:E:344:PRO:HD2	1.90	0.54
1:D:293:LEU:HD13	1:D:347:ILE:HG13	1.90	0.54
1:E:128:LEU:HG	1:E:130:MET:HE3	1.90	0.54
1:G:128:LEU:CD2	1:G:130:MET:HE1	2.37	0.54
1:B:293:LEU:HD13	1:B:347:ILE:HG13	1.90	0.54
1:B:160:VAL:HG12	1:C:333:LEU:HD13	1.90	0.54
1:E:293:LEU:HD13	1:E:347:ILE:HG13	1.88	0.54
1:F:162:GLY:H	1:F:251:GLN:HE22	1.55	0.54
1:C:293:LEU:HD13	1:C:347:ILE:HG13	1.90	0.54
1:A:293:LEU:HD13	1:A:347:ILE:HG13	1.89	0.54
1:G:89:LYS:HE2	1:G:110:TYR:CE2	2.42	0.54
1:A:131:LYS:HE2	1:A:136:PHE:CE1	2.43	0.54
1:G:166:ARG:HH11	1:G:166:ARG:HG2	1.71	0.54
1:G:220:ILE:N	1:G:240:GLN:HE21	1.97	0.53
1:F:160:VAL:HG12	1:G:333:LEU:HD13	1.89	0.53
1:B:138:LYS:O	1:B:142:GLN:HG3	2.08	0.53
1:F:145:GLU:HG3	1:F:218:LEU:HD11	1.90	0.53
1:H:39:ALA:O	1:H:43:ARG:HG3	2.08	0.53
1:C:59:THR:HG23	1:C:69:SER:O	2.09	0.53
1:H:293:LEU:HD13	1:H:347:ILE:HG13	1.90	0.53
1:B:262:LEU:HD22	1:B:266:VAL:HG23	1.90	0.53
1:G:293:LEU:HD13	1:G:347:ILE:HG13	1.90	0.53
1:B:7:ASP:OD1	1:D:169:ARG:NH1	2.42	0.53
1:D:327:LEU:HD22	1:D:331:MET:HG3	1.91	0.53
1:E:130:MET:HG3	1:E:137:ASN:OD1	2.08	0.53
1:F:293:LEU:HD13	1:F:347:ILE:HG13	1.91	0.53
1:F:262:LEU:HD22	1:F:266:VAL:HG23	1.90	0.53
1:G:173:ASN:O	1:G:175:GLU:HG2	2.09	0.53
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:136:PHE:HD1	1:G:137:ASN:HD22	1.55	0.52
1:H:131:LYS:HE2	1:H:136:PHE:CD1	2.45	0.52
1:B:134:TRP:CD2	1:B:211:LEU:HD21	2.44	0.52
1:C:130:MET:HA	1:C:130:MET:CE	2.40	0.52
1:D:26:GLY:HA2	4:D:4437:HOH:O	2.09	0.52
1:F:221:ILE:N	1:F:221:ILE:HD12	2.24	0.52
1:H:72:ILE:HD13	1:H:323:LEU:HB3	1.91	0.52
1:C:246:ASN:HA	4:C:3410:HOH:O	2.09	0.52
1:H:130:MET:CE	1:H:130:MET:HA	2.38	0.52
1:B:72:ILE:HD13	1:B:323:LEU:HB3	1.91	0.52
1:D:162:GLY:H	1:D:251:GLN:NE2	2.07	0.52
1:G:186:LEU:C	1:G:188:GLU:H	2.13	0.52
1:E:138:LYS:O	1:E:142:GLN:HG3	2.10	0.52
1:H:221:ILE:N	1:H:221:ILE:HD12	2.25	0.51
1:D:89:LYS:HE2	1:D:110:TYR:CE2	2.45	0.51
1:A:221:ILE:HD12	1:A:221:ILE:N	2.26	0.51
1:A:111:SER:HA	1:A:183:LEU:HD11	1.92	0.51
1:G:59:THR:HG23	1:G:69:SER:O	2.11	0.51
1:G:131:LYS:H	1:G:137:ASN:HD21	1.57	0.51
1:B:162:GLY:H	1:B:251:GLN:NE2	2.08	0.51
1:E:125:TRP:CD1	1:E:151:ALA:HB3	2.45	0.51
1:E:160:VAL:HG12	1:H:333:LEU:HD13	1.92	0.51
1:C:138:LYS:O	1:C:142:GLN:HG3	2.11	0.51
1:A:172:LEU:O	1:A:173:ASN:HB3	2.11	0.51
1:H:166:ARG:HB2	4:H:8470:HOH:O	2.10	0.51
1:F:130:MET:HA	1:F:130:MET:CE	2.39	0.51
1:D:136:PHE:HD1	1:D:137:ASN:ND2	2.09	0.51
1:H:166:ARG:HH11	1:H:166:ARG:HG2	1.75	0.51
1:C:131:LYS:HE2	1:C:136:PHE:CE1	2.46	0.51
1:C:72:ILE:HD13	1:C:323:LEU:HB3	1.92	0.51
1:F:131:LYS:HE2	1:F:136:PHE:CZ	2.45	0.51
1:H:34:TYR:HE1	1:H:302:ARG:CZ	2.24	0.51
1:C:186:LEU:C	1:C:188:GLU:H	2.12	0.51
1:C:128:LEU:CD2	1:C:130:MET:HE1	2.40	0.50
1:H:138:LYS:O	1:H:142:GLN:HG3	2.12	0.50
1:H:138:LYS:CA	1:H:215:ILE:HD12	2.41	0.50
1:C:106:SER:HB2	1:C:127:GLN:O	2.11	0.50
1:B:125:TRP:CD1	1:B:151:ALA:HB3	2.47	0.50
1:C:221:ILE:N	1:C:221:ILE:HD12	2.27	0.50
1:C:34:TYR:HE1	1:C:302:ARG:CZ	2.25	0.50
1:B:173:ASN:O	1:B:175:GLU:HG2	2.11	0.50
1:G:141:VAL:HG11	1:G:216:THR:HB	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:125:TRP:CG	1:D:151:ALA:HB3	2.47	0.50
1:H:173:ASN:O	1:H:175:GLU:HG2	2.12	0.50
1:C:39:ALA:O	1:C:43:ARG:HG3	2.12	0.50
1:G:125:TRP:CD1	1:G:151:ALA:HB3	2.47	0.50
1:A:166:ARG:HH11	1:A:166:ARG:HG2	1.77	0.50
1:B:59:THR:HG23	1:B:69:SER:O	2.11	0.50
1:C:172:LEU:O	1:C:173:ASN:HB3	2.10	0.50
1:A:59:THR:HG23	1:A:69:SER:O	2.12	0.50
1:B:221:ILE:N	1:B:221:ILE:HD12	2.27	0.50
1:B:211:LEU:O	1:B:211:LEU:HD12	2.11	0.50
1:C:187:LYS:O	1:C:188:GLU:CB	2.59	0.50
1:E:69:SER:OG	1:E:99:ASN:HB3	2.12	0.50
1:F:172:LEU:O	1:F:173:ASN:HB3	2.12	0.49
1:H:187:LYS:O	1:H:188:GLU:CB	2.59	0.49
1:F:163:ASN:HB2	1:G:329:ARG:NE	2.27	0.49
1:F:169:ARG:NH1	1:G:7:ASP:OD1	2.45	0.49
1:B:130:MET:HG3	1:B:137:ASN:OD1	2.12	0.49
1:H:128:LEU:CG	1:H:130:MET:HE1	2.43	0.49
1:H:186:LEU:C	1:H:188:GLU:H	2.14	0.49
1:A:130:MET:HA	1:A:130:MET:CE	2.40	0.49
1:A:7:ASP:OD1	1:C:169:ARG:NH1	2.46	0.49
1:F:34:TYR:HE1	1:F:302:ARG:CZ	2.24	0.49
1:F:97:GLU:HG2	1:F:317:LYS:HE3	1.94	0.49
1:D:220:ILE:N	1:D:240:GLN:HE21	1.97	0.49
1:G:136:PHE:HD1	1:G:137:ASN:ND2	2.10	0.49
1:E:135:ASP:O	1:E:138:LYS:HG2	2.12	0.49
1:F:333:LEU:HD13	1:H:160:VAL:HG12	1.95	0.49
4:A:1468:HOH:O	1:D:329:ARG:HD3	2.12	0.49
1:E:327:LEU:HD22	1:E:331:MET:SD	2.52	0.49
1:A:128:LEU:CD2	1:A:130:MET:HE1	2.43	0.49
1:B:125:TRP:CG	1:B:151:ALA:HB3	2.47	0.49
1:C:262:LEU:HD22	1:C:266:VAL:HG23	1.95	0.49
1:E:262:LEU:HD22	1:E:266:VAL:HG23	1.95	0.49
1:A:162:GLY:H	1:A:251:GLN:NE2	2.10	0.49
1:F:329:ARG:HD3	4:H:8476:HOH:O	2.12	0.49
1:G:138:LYS:O	1:G:142:GLN:HG3	2.13	0.49
1:G:39:ALA:O	1:G:43:ARG:HG3	2.13	0.49
1:C:212:LEU:O	1:C:215:ILE:HG12	2.13	0.49
1:F:162:GLY:H	1:F:251:GLN:NE2	2.11	0.48
1:E:59:THR:HG23	1:E:69:SER:O	2.13	0.48
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.78	0.48
1:F:59:THR:CG2	1:F:69:SER:O	2.60	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:59:THR:CG2	1:A:69:SER:O	2.62	0.48
1:B:97:GLU:HG2	1:B:317:LYS:HE3	1.96	0.48
1:G:221:ILE:N	1:G:221:ILE:HD12	2.28	0.48
1:B:202:ALA:HA	4:B:2453:HOH:O	2.13	0.48
1:E:130:MET:HA	1:E:130:MET:CE	2.42	0.48
1:F:327:LEU:HD22	1:F:331:MET:HG3	1.95	0.48
1:D:39:ALA:O	1:D:43:ARG:HG3	2.13	0.48
1:B:333:LEU:HD13	1:D:160:VAL:HG12	1.95	0.48
1:A:163:ASN:HB2	1:D:329:ARG:NE	2.29	0.48
1:C:89:LYS:HE2	1:C:110:TYR:CE2	2.49	0.48
1:E:145:GLU:HG2	1:E:218:LEU:HG	1.96	0.48
1:E:173:ASN:O	1:E:175:GLU:HG2	2.14	0.48
1:C:131:LYS:H	1:C:137:ASN:HD21	1.60	0.48
1:E:7:ASP:OD1	1:G:169:ARG:NH1	2.47	0.48
1:D:72:ILE:HD13	1:D:323:LEU:HB3	1.96	0.48
1:B:13:GLN:HG3	4:B:2477:HOH:O	2.13	0.48
1:H:262:LEU:HD22	1:H:266:VAL:HG23	1.95	0.48
1:A:131:LYS:HE2	1:A:136:PHE:CZ	2.49	0.47
1:D:136:PHE:HD1	1:D:137:ASN:HD22	1.61	0.47
1:D:131:LYS:H	1:D:137:ASN:HD21	1.61	0.47
1:F:206:TRP:O	1:F:209:LEU:HB2	2.14	0.47
1:F:166:ARG:HG2	1:F:166:ARG:HH11	1.78	0.47
1:G:327:LEU:HD22	1:G:331:MET:HG3	1.96	0.47
1:E:89:LYS:O	1:E:93:ARG:HG3	2.15	0.47
1:A:206:TRP:O	1:A:209:LEU:HB2	2.14	0.47
1:C:173:ASN:HA	4:C:3468:HOH:O	2.13	0.47
1:H:89:LYS:HE2	1:H:110:TYR:CE2	2.50	0.47
1:A:333:LEU:HD13	1:C:160:VAL:HG12	1.94	0.47
1:A:97:GLU:HG2	1:A:317:LYS:HE3	1.95	0.47
1:A:211:LEU:O	1:A:215:ILE:HG23	2.14	0.47
1:C:172:LEU:O	1:C:173:ASN:CB	2.62	0.47
1:E:327:LEU:HD22	1:E:331:MET:HG3	1.97	0.47
1:C:166:ARG:HH11	1:C:166:ARG:HG2	1.79	0.47
1:G:125:TRP:CG	1:G:151:ALA:HB3	2.50	0.47
1:H:125:TRP:CD1	1:H:151:ALA:HB3	2.50	0.47
1:D:131:LYS:HE2	1:D:136:PHE:CD1	2.49	0.47
1:H:162:GLY:H	1:H:251:GLN:NE2	2.12	0.47
1:E:97:GLU:HG2	1:E:317:LYS:HE3	1.96	0.47
1:F:138:LYS:O	1:F:142:GLN:HG3	2.14	0.47
1:B:39:ALA:O	1:B:43:ARG:HG3	2.14	0.47
1:F:213:GLN:CG	1:F:220:ILE:HD12	2.44	0.47
1:C:59:THR:CG2	1:C:69:SER:O	2.63	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:333:LEU:HD13	1:G:160:VAL:HG12	1.96	0.47
1:A:69:SER:OG	1:A:99:ASN:HB3	2.16	0.46
1:A:138:LYS:O	1:A:142:GLN:HG3	2.14	0.46
1:B:327:LEU:HD22	1:B:331:MET:SD	2.55	0.46
1:F:211:LEU:O	1:F:215:ILE:HG23	2.14	0.46
1:C:125:TRP:CD1	1:C:151:ALA:HB3	2.50	0.46
1:A:34:TYR:HE1	1:A:302:ARG:CZ	2.28	0.46
1:F:102:TYR:CZ	1:F:104:ILE:HG12	2.50	0.46
1:F:158:THR:HG22	1:F:158:THR:O	2.15	0.46
1:B:206:TRP:O	1:B:209:LEU:HB2	2.16	0.46
1:E:39:ALA:O	1:E:43:ARG:HG3	2.15	0.46
1:B:128:LEU:CD2	1:B:130:MET:HE1	2.46	0.46
1:B:212:LEU:O	1:B:216:THR:HG22	2.14	0.46
1:D:166:ARG:HG2	1:D:166:ARG:NH1	2.30	0.46
1:B:300:LEU:HD11	1:B:323:LEU:HD12	1.97	0.46
1:C:125:TRP:CG	1:C:151:ALA:HB3	2.51	0.46
1:D:59:THR:HG23	1:D:69:SER:O	2.15	0.46
1:E:128:LEU:CD2	1:E:130:MET:HE3	2.46	0.46
1:H:136:PHE:HD1	1:H:137:ASN:HD22	1.64	0.46
1:A:172:LEU:O	1:A:173:ASN:CB	2.63	0.46
1:F:39:ALA:O	1:F:43:ARG:HG3	2.16	0.46
1:H:59:THR:CG2	1:H:69:SER:O	2.64	0.46
1:C:69:SER:OG	1:C:99:ASN:HB3	2.16	0.46
1:H:59:THR:HG23	1:H:69:SER:O	2.15	0.46
1:D:133:ASP:OD2	1:D:135:ASP:HB2	2.16	0.46
1:D:245:SER:HB2	1:D:278:ASP:OD2	2.15	0.46
1:C:111:SER:HA	1:C:183:LEU:HD11	1.98	0.46
1:B:278:ASP:OD2	1:B:278:ASP:C	2.54	0.46
1:E:206:TRP:O	1:E:209:LEU:HB2	2.16	0.46
1:E:278:ASP:C	1:E:278:ASP:OD2	2.53	0.46
1:E:172:LEU:O	1:E:173:ASN:OD1	2.33	0.46
1:F:172:LEU:O	1:F:173:ASN:CB	2.64	0.45
1:G:166:ARG:HG2	1:G:166:ARG:NH1	2.31	0.45
1:A:327:LEU:HD22	1:A:331:MET:HG3	1.97	0.45
1:D:128:LEU:CD2	1:D:130:MET:HE3	2.47	0.45
1:G:327:LEU:HD22	1:G:331:MET:SD	2.56	0.45
1:F:26:GLY:HA2	4:F:6458:HOH:O	2.16	0.45
1:B:89:LYS:HE2	1:B:110:TYR:CE2	2.51	0.45
1:F:128:LEU:CD2	1:F:130:MET:HE3	2.46	0.45
1:G:172:LEU:O	1:G:173:ASN:HB3	2.16	0.45
1:D:278:ASP:OD2	1:D:278:ASP:C	2.54	0.45
1:B:329:ARG:NE	1:D:163:ASN:HB2	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:323:LEU:HD23	1:G:323:LEU:HA	1.86	0.45
1:H:209:LEU:O	1:H:213:GLN:HG3	2.17	0.45
1:A:72:ILE:HD13	1:A:323:LEU:HB3	1.98	0.45
1:D:172:LEU:O	1:D:173:ASN:HB3	2.16	0.45
1:G:26:GLY:HA2	4:G:7444:HOH:O	2.16	0.45
1:D:138:LYS:O	1:D:142:GLN:HG3	2.17	0.45
1:G:240:GLN:N	1:G:240:GLN:CD	2.70	0.45
1:F:7:ASP:OD1	1:H:169:ARG:NH1	2.50	0.45
1:H:327:LEU:HD22	1:H:331:MET:HG3	1.98	0.45
1:C:186:LEU:C	1:C:188:GLU:N	2.70	0.45
1:A:102:TYR:CZ	1:A:104:ILE:HG12	2.51	0.45
1:B:49:ARG:NH2	1:D:229:GLU:HB3	2.31	0.45
1:A:26:GLY:HA2	4:A:1445:HOH:O	2.17	0.45
1:G:206:TRP:O	1:G:209:LEU:HB2	2.17	0.45
1:H:106:SER:HB2	1:H:127:GLN:O	2.17	0.45
1:B:56:LYS:O	1:B:337:GLN:HG2	2.17	0.45
1:C:162:GLY:H	1:C:251:GLN:NE2	2.14	0.45
1:G:172:LEU:O	1:G:173:ASN:CB	2.65	0.45
1:D:221:ILE:HD12	1:D:221:ILE:N	2.32	0.45
1:E:221:ILE:HD12	1:E:221:ILE:N	2.31	0.45
1:B:102:TYR:CZ	1:B:104:ILE:HG12	2.52	0.45
1:B:240:GLN:N	1:B:240:GLN:CD	2.69	0.44
1:E:212:LEU:O	1:E:216:THR:HG22	2.17	0.44
1:E:329:ARG:NE	1:G:163:ASN:HB2	2.31	0.44
1:E:125:TRP:CG	1:E:151:ALA:HB3	2.52	0.44
1:H:334:SER:HB2	1:H:346:LEU:HD11	1.99	0.44
1:H:73:CYS:HB3	1:H:101:CYS:O	2.17	0.44
1:E:303:PRO:HA	1:E:306:TRP:CE3	2.53	0.44
1:E:137:ASN:O	1:E:141:VAL:HG23	2.17	0.44
1:B:160:VAL:HG12	1:C:333:LEU:CD1	2.47	0.44
1:D:172:LEU:O	1:D:173:ASN:CB	2.65	0.44
1:B:69:SER:OG	1:B:99:ASN:HB3	2.18	0.44
1:F:111:SER:HA	1:F:183:LEU:HD11	1.98	0.44
1:F:72:ILE:HD13	1:F:323:LEU:HB3	1.98	0.44
1:G:102:TYR:CZ	1:G:104:ILE:HG12	2.53	0.44
1:A:125:TRP:CD1	1:A:151:ALA:HB3	2.52	0.44
1:A:136:PHE:HD1	1:A:137:ASN:HD22	1.66	0.44
1:G:89:LYS:O	1:G:93:ARG:HG3	2.17	0.44
1:H:172:LEU:O	1:H:173:ASN:CB	2.64	0.44
1:G:59:THR:O	1:G:70:ALA:HA	2.18	0.44
1:H:56:LYS:O	1:H:337:GLN:HG2	2.18	0.44
1:E:63:ILE:O	1:E:63:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:125:TRP:CG	1:H:151:ALA:HB3	2.53	0.44
1:G:27:GLU:H	1:G:27:GLU:CD	2.21	0.44
1:E:169:ARG:NH2	4:E:5462:HOH:O	2.51	0.44
1:G:130:MET:CE	1:G:130:MET:HA	2.47	0.43
1:G:128:LEU:CG	1:G:130:MET:HE1	2.47	0.43
1:D:130:MET:HG3	1:D:137:ASN:OD1	2.17	0.43
1:G:137:ASN:O	1:G:141:VAL:HG23	2.18	0.43
1:C:63:ILE:O	1:C:63:ILE:HG13	2.18	0.43
1:A:99:ASN:ND2	4:A:1517:HOH:O	2.51	0.43
1:C:206:TRP:O	1:C:209:LEU:HB2	2.17	0.43
1:G:34:TYR:HE1	1:G:302:ARG:CZ	2.31	0.43
1:E:163:ASN:HB2	1:H:329:ARG:NE	2.33	0.43
1:H:172:LEU:O	1:H:173:ASN:HB3	2.18	0.43
1:F:74:ILE:HG23	1:F:304:ILE:HG13	2.00	0.43
1:C:128:LEU:CG	1:C:130:MET:HE1	2.46	0.43
1:C:131:LYS:HE2	1:C:136:PHE:CD1	2.53	0.43
1:B:172:LEU:O	1:B:173:ASN:CB	2.66	0.43
1:E:329:ARG:HD3	4:E:5461:HOH:O	2.18	0.43
1:B:63:ILE:HG13	1:B:63:ILE:O	2.18	0.43
1:G:245:SER:HB2	1:G:278:ASP:OD2	2.19	0.43
1:H:131:LYS:H	1:H:137:ASN:HD21	1.66	0.43
1:A:130:MET:HG3	1:A:137:ASN:OD1	2.19	0.43
1:B:172:LEU:O	1:B:173:ASN:HB3	2.18	0.43
1:B:89:LYS:O	1:B:93:ARG:HG3	2.19	0.43
1:F:56:LYS:O	1:F:337:GLN:HG2	2.19	0.43
1:E:212:LEU:O	1:E:212:LEU:HD23	2.18	0.43
1:G:131:LYS:HE2	1:G:136:PHE:CD1	2.53	0.43
1:G:131:LYS:HE2	1:G:136:PHE:CZ	2.53	0.43
1:A:167:ASP:HB3	1:A:172:LEU:HD23	2.01	0.43
1:B:323:LEU:HA	1:B:323:LEU:HD23	1.88	0.43
1:C:318:GLU:O	1:C:322:ILE:HG13	2.18	0.43
1:C:134:TRP:HA	1:C:137:ASN:HB2	2.00	0.43
1:H:206:TRP:O	1:H:209:LEU:HB2	2.19	0.43
1:D:252:LEU:HD13	1:D:255:VAL:CG1	2.48	0.43
1:A:56:LYS:O	1:A:337:GLN:HG2	2.18	0.43
1:D:206:TRP:O	1:D:209:LEU:HB2	2.18	0.43
1:D:76:PRO:HD3	1:D:103:VAL:HG11	2.01	0.43
1:D:141:VAL:HG11	1:D:216:THR:HB	2.00	0.43
1:A:126:PHE:HB2	1:A:149:PHE:CD2	2.53	0.43
1:E:56:LYS:O	1:E:337:GLN:HG2	2.19	0.43
1:A:141:VAL:HG22	1:A:152:LEU:HD21	2.01	0.42
1:G:106:SER:HB2	1:G:127:GLN:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:318:GLU:O	1:F:322:ILE:HG13	2.19	0.42
1:H:138:LYS:CB	1:H:215:ILE:HD12	2.49	0.42
1:H:323:LEU:HA	1:H:323:LEU:HD23	1.90	0.42
1:D:36:GLU:CD	1:D:43:ARG:HH22	2.22	0.42
1:E:172:LEU:O	1:E:173:ASN:CB	2.67	0.42
1:D:73:CYS:HB3	1:D:101:CYS:O	2.19	0.42
1:H:63:ILE:O	1:H:63:ILE:HG13	2.20	0.42
1:B:141:VAL:HG22	1:B:152:LEU:HD21	2.01	0.42
1:H:131:LYS:HE2	1:H:136:PHE:CZ	2.54	0.42
1:G:262:LEU:HD22	1:G:266:VAL:CG2	2.49	0.42
1:E:229:GLU:HB3	1:H:49:ARG:NH2	2.34	0.42
1:B:131:LYS:HE2	1:B:136:PHE:CE1	2.54	0.42
1:G:187:LYS:O	1:G:188:GLU:CB	2.67	0.42
1:E:138:LYS:HB3	1:E:215:ILE:HD12	2.00	0.42
1:D:59:THR:CG2	1:D:69:SER:O	2.68	0.42
1:B:24:ILE:HA	2:B:2401:FMN:HM71	2.01	0.42
1:C:334:SER:HB2	1:C:346:LEU:HD11	2.00	0.42
1:H:97:GLU:HG2	1:H:317:LYS:HE3	2.01	0.42
1:F:130:MET:HG3	1:F:137:ASN:OD1	2.18	0.42
1:F:186:LEU:C	1:F:188:GLU:H	2.22	0.42
1:E:300:LEU:HD11	1:E:323:LEU:HD12	2.01	0.42
1:D:59:THR:O	1:D:70:ALA:HA	2.20	0.42
1:G:278:ASP:OD2	1:G:278:ASP:C	2.58	0.42
1:F:159:PRO:HA	1:F:202:ALA:HB3	2.02	0.42
1:G:252:LEU:HD13	1:G:255:VAL:CG1	2.50	0.42
1:E:240:GLN:N	1:E:240:GLN:CD	2.73	0.42
1:A:300:LEU:HD11	1:A:323:LEU:HD12	2.01	0.42
1:D:104:ILE:HD13	1:D:115:ILE:HG21	2.01	0.42
1:F:89:LYS:HE2	1:F:110:TYR:CE2	2.54	0.42
1:G:56:LYS:O	1:G:337:GLN:HG2	2.19	0.42
1:C:141:VAL:HG22	1:C:152:LEU:HD21	2.01	0.42
1:E:160:VAL:HG12	1:H:333:LEU:CD1	2.50	0.42
1:G:36:GLU:CD	1:G:43:ARG:HH22	2.23	0.42
1:D:97:GLU:HG2	1:D:317:LYS:HE3	2.01	0.42
1:G:97:GLU:HG2	1:G:317:LYS:HE3	2.02	0.42
1:H:322:ILE:O	1:H:326:GLU:HG3	2.20	0.42
1:D:130:MET:HA	1:D:130:MET:CE	2.47	0.42
1:E:323:LEU:HA	1:E:323:LEU:HD23	1.90	0.42
1:F:69:SER:OG	1:F:99:ASN:HB3	2.20	0.42
1:H:166:ARG:NH1	1:H:166:ARG:HG2	2.35	0.42
1:F:329:ARG:NE	1:H:163:ASN:HB2	2.35	0.42
1:G:302:ARG:HG3	2:G:7401:FMN:O2P	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:303:PRO:HA	1:D:306:TRP:CE3	2.55	0.42
1:D:100:ILE:C	1:D:100:ILE:HD12	2.40	0.42
1:G:303:PRO:HA	1:G:306:TRP:CE3	2.53	0.42
1:H:134:TRP:HA	1:H:137:ASN:HB2	2.01	0.42
1:E:158:THR:O	1:E:158:THR:HG22	2.19	0.42
1:C:219:PRO:HA	1:C:240:GLN:HE21	1.84	0.41
1:F:128:LEU:CG	1:F:130:MET:HE3	2.49	0.41
1:H:69:SER:OG	1:H:99:ASN:HB3	2.20	0.41
1:D:85:PRO:HB2	4:D:4491:HOH:O	2.18	0.41
1:B:229:GLU:HB3	1:C:49:ARG:NH2	2.35	0.41
1:G:307:GLY:O	1:G:315:GLY:HA3	2.20	0.41
1:D:262:LEU:HD22	1:D:266:VAL:CG2	2.51	0.41
1:E:73:CYS:HB3	1:E:101:CYS:O	2.20	0.41
1:A:36:GLU:CD	1:A:43:ARG:HH22	2.22	0.41
1:B:34:TYR:HE1	1:B:302:ARG:CZ	2.33	0.41
1:D:56:LYS:O	1:D:337:GLN:HG2	2.20	0.41
1:C:158:THR:HG22	1:C:158:THR:O	2.20	0.41
1:B:212:LEU:HD23	1:B:212:LEU:O	2.21	0.41
1:C:36:GLU:CD	1:C:43:ARG:HH22	2.23	0.41
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.90	0.41
1:A:329:ARG:NE	1:C:163:ASN:HB2	2.34	0.41
1:E:34:TYR:HE1	1:E:302:ARG:CZ	2.33	0.41
1:F:73:CYS:HB3	1:F:101:CYS:O	2.20	0.41
1:C:278:ASP:C	1:C:278:ASP:OD2	2.59	0.41
1:C:73:CYS:HB3	1:C:101:CYS:O	2.21	0.41
1:A:128:LEU:CG	1:A:130:MET:HE1	2.48	0.41
1:F:126:PHE:HB2	1:F:149:PHE:CD2	2.56	0.41
1:B:303:PRO:HA	1:B:306:TRP:CE3	2.55	0.41
1:H:212:LEU:O	1:H:216:THR:HG22	2.21	0.41
1:F:141:VAL:HG22	1:F:152:LEU:HD21	2.02	0.41
1:C:136:PHE:HD1	1:C:137:ASN:HD22	1.67	0.41
1:A:318:GLU:O	1:A:322:ILE:HG13	2.21	0.41
1:A:166:ARG:NH1	1:A:166:ARG:HG2	2.36	0.41
1:C:89:LYS:O	1:C:93:ARG:HG3	2.20	0.41
1:D:213:GLN:HG2	1:D:220:ILE:HD12	2.03	0.41
1:B:211:LEU:C	1:B:211:LEU:CD1	2.87	0.41
1:G:211:LEU:HG	1:G:212:LEU:N	2.36	0.41
1:C:136:PHE:C	1:C:136:PHE:CD1	2.93	0.41
1:B:36:GLU:CD	1:B:43:ARG:HH22	2.21	0.41
1:D:141:VAL:HG22	1:D:152:LEU:HD21	2.02	0.41
1:H:62:THR:HG22	1:H:67:GLU:HA	2.02	0.41
1:B:130:MET:CE	1:B:130:MET:HA	2.42	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:186:LEU:HB2	4:H:8521:HOH:O	2.21	0.41
1:H:86:ASP:HB3	1:H:90:SER:OG	2.21	0.41
1:H:34:TYR:CE1	1:H:302:ARG:CZ	3.04	0.40
1:C:250:ARG:NH1	2:C:3401:FMN:HM82	2.36	0.40
1:D:240:GLN:CD	1:D:240:GLN:N	2.75	0.40
1:H:141:VAL:HG22	1:H:152:LEU:HD21	2.02	0.40
1:B:134:TRP:CZ3	1:B:211:LEU:HG	2.55	0.40
1:E:59:THR:O	1:E:70:ALA:HA	2.21	0.40
1:G:329:ARG:NH2	4:G:7440:HOH:O	2.40	0.40
1:G:72:ILE:HD13	1:G:323:LEU:HB3	2.03	0.40
1:H:219:PRO:HA	1:H:240:GLN:HE21	1.86	0.40
1:D:327:LEU:HD22	1:D:331:MET:SD	2.62	0.40
1:G:186:LEU:C	1:G:188:GLU:N	2.75	0.40
1:C:138:LYS:HA	1:C:215:ILE:HD12	2.03	0.40
1:B:159:PRO:HA	1:B:202:ALA:HB3	2.02	0.40
1:D:34:TYR:HE1	1:D:302:ARG:CZ	2.34	0.40
1:G:213:GLN:HG2	1:G:220:ILE:HD12	2.04	0.40
1:E:343:SER:O	1:E:346:LEU:HB2	2.22	0.40
1:B:327:LEU:HD22	1:B:331:MET:HG3	2.03	0.40
1:D:134:TRP:HA	1:D:137:ASN: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	326/352 (93%)	310 (95%)	13 (4%)	3 (1%)	25	26
1	B	321/352 (91%)	308 (96%)	11 (3%)	2 (1%)	33	39
1	C	326/352 (93%)	309 (95%)	14 (4%)	3 (1%)	25	26
1	D	323/352 (92%)	310 (96%)	11 (3%)	2 (1%)	33	39
1	E	320/352 (91%)	306 (96%)	12 (4%)	2 (1%)	33	39
1	F	326/352 (93%)	311 (95%)	12 (4%)	3 (1%)	25	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	323/352 (92%)	309 (96%)	12 (4%)	2 (1%)	33	39
1	H	326/352 (93%)	311 (95%)	12 (4%)	3 (1%)	25	26
All	All	2591/2816 (92%)	2474 (96%)	97 (4%)	20 (1%)	27	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	B	173	ASN
1	C	173	ASN
1	D	173	ASN
1	E	173	ASN
1	F	173	ASN
1	G	173	ASN
1	H	173	ASN
1	A	174	LEU
1	A	183	LEU
1	B	174	LEU
1	D	174	LEU
1	F	174	LEU
1	F	183	LEU
1	G	174	LEU
1	H	174	LEU
1	C	174	LEU
1	C	183	LEU
1	E	174	LEU
1	H	183	LEU

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	272/296 (92%)	256 (94%)	16 (6%)	28	35
1	B	270/296 (91%)	254 (94%)	16 (6%)	28	35
1	C	272/296 (92%)	257 (94%)	15 (6%)	30	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	271/296 (92%)	256 (94%)	15 (6%)	30	39
1	E	269/296 (91%)	256 (95%)	13 (5%)	35	46
1	F	272/296 (92%)	257 (94%)	15 (6%)	30	39
1	G	270/296 (91%)	255 (94%)	15 (6%)	30	38
1	H	272/296 (92%)	257 (94%)	15 (6%)	30	39
All	All	2168/2368 (92%)	2048 (94%)	120 (6%)	30	39

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	A	75	SER
1	A	86	ASP
1	A	130	MET
1	A	173	ASN
1	A	186	LEU
1	A	212	LEU
1	A	222	LEU
1	A	252	LEU
1	A	262	LEU
1	A	288	LEU
1	A	293	LEU
1	A	297	CYS
1	A	323	LEU
1	A	327	LEU
1	A	333	LEU
1	B	59	THR
1	B	75	SER
1	B	86	ASP
1	B	130	MET
1	B	173	ASN
1	B	186	LEU
1	B	211	LEU
1	B	212	LEU
1	B	222	LEU
1	B	252	LEU
1	B	262	LEU
1	B	288	LEU
1	B	293	LEU
1	B	323	LEU

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Mol	Chain	Res	Type
1	B	327	LEU
1	B	333	LEU
1	C	59	THR
1	C	75	SER
1	C	86	ASP
1	C	130	MET
1	C	173	ASN
1	C	212	LEU
1	C	222	LEU
1	C	252	LEU
1	C	262	LEU
1	C	288	LEU
1	C	293	LEU
1	C	297	CYS
1	C	323	LEU
1	C	327	LEU
1	C	333	LEU
1	D	59	THR
1	D	75	SER
1	D	86	ASP
1	D	130	MET
1	D	173	ASN
1	D	212	LEU
1	D	222	LEU
1	D	252	LEU
1	D	262	LEU
1	D	288	LEU
1	D	293	LEU
1	D	297	CYS
1	D	323	LEU
1	D	327	LEU
1	D	333	LEU
1	E	59	THR
1	E	75	SER
1	E	86	ASP
1	E	130	MET
1	E	173	ASN
1	E	222	LEU
1	E	252	LEU
1	E	262	LEU
1	E	288	LEU
1	E	293	LEU

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Mol	Chain	Res	Type
1	E	323	LEU
1	E	327	LEU
1	E	333	LEU
1	F	59	THR
1	F	75	SER
1	F	86	ASP
1	F	130	MET
1	F	173	ASN
1	F	212	LEU
1	F	222	LEU
1	F	252	LEU
1	F	262	LEU
1	F	288	LEU
1	F	293	LEU
1	F	297	CYS
1	F	323	LEU
1	F	327	LEU
1	F	333	LEU
1	G	59	THR
1	G	75	SER
1	G	86	ASP
1	G	130	MET
1	G	173	ASN
1	G	186	LEU
1	G	222	LEU
1	G	252	LEU
1	G	262	LEU
1	G	288	LEU
1	G	293	LEU
1	G	297	CYS
1	G	323	LEU
1	G	327	LEU
1	G	333	LEU
1	H	59	THR
1	H	75	SER
1	H	86	ASP
1	H	130	MET
1	H	173	ASN
1	H	212	LEU
1	H	222	LEU
1	H	252	LEU
1	H	262	LEU

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Mol	Chain	Res	Type
1	H	288	LEU
1	H	293	LEU
1	H	297	CYS
1	H	323	LEU
1	H	327	LEU
1	H	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	99	ASN
1	A	137	ASN
1	A	163	ASN
1	A	171	GLN
1	A	237	HIS
1	A	240	GLN
1	A	251	GLN
1	B	64	GLN
1	B	99	ASN
1	B	137	ASN
1	B	163	ASN
1	B	171	GLN
1	B	173	ASN
1	B	237	HIS
1	B	240	GLN
1	B	251	GLN
1	C	64	GLN
1	C	99	ASN
1	C	137	ASN
1	C	163	ASN
1	C	171	GLN
1	C	237	HIS
1	C	240	GLN
1	C	251	GLN
1	D	64	GLN
1	D	99	ASN
1	D	137	ASN
1	D	163	ASN
1	D	171	GLN
1	D	173	ASN
1	D	237	HIS

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Mol	Chain	Res	Type
1	D	240	GLN
1	D	251	GLN
1	E	64	GLN
1	E	99	ASN
1	E	137	ASN
1	E	163	ASN
1	E	171	GLN
1	E	173	ASN
1	E	237	HIS
1	E	240	GLN
1	E	251	GLN
1	F	64	GLN
1	F	99	ASN
1	F	137	ASN
1	F	163	ASN
1	F	171	GLN
1	F	237	HIS
1	F	240	GLN
1	F	251	GLN
1	G	64	GLN
1	G	99	ASN
1	G	137	ASN
1	G	163	ASN
1	G	171	GLN
1	G	173	ASN
1	G	240	GLN
1	G	251	GLN
1	H	64	GLN
1	H	99	ASN
1	H	137	ASN
1	H	163	ASN
1	H	171	GLN
1	H	237	HIS
1	H	240	GLN
1	H	251	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 ⓘ

16 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	FMN	A	1401	-	33,33,33	2.51	12 (36%)	46,50,50	3.04	12 (26%)
3	ACY	A	1402	-	3,3,3	1.18	0	3,3,3	1.42	0
2	FMN	B	2401	-	33,33,33	2.53	11 (33%)	46,50,50	2.99	12 (26%)
3	ACY	B	2402	-	3,3,3	1.18	0	3,3,3	1.41	0
2	FMN	C	3401	-	33,33,33	2.46	10 (30%)	46,50,50	3.01	12 (26%)
3	ACY	C	3402	-	3,3,3	1.13	0	3,3,3	1.40	0
2	FMN	D	4401	-	33,33,33	2.53	11 (33%)	46,50,50	2.94	12 (26%)
3	ACY	D	4402	-	3,3,3	1.14	0	3,3,3	1.38	0
2	FMN	E	5401	-	33,33,33	2.51	13 (39%)	46,50,50	2.99	12 (26%)
3	ACY	E	5402	-	3,3,3	1.16	0	3,3,3	1.39	0
2	FMN	F	6401	-	33,33,33	2.58	13 (39%)	46,50,50	3.02	12 (26%)
3	ACY	F	6402	-	3,3,3	1.19	0	3,3,3	1.41	0
2	FMN	G	7401	-	33,33,33	2.60	12 (36%)	46,50,50	2.96	12 (26%)
3	ACY	G	7402	-	3,3,3	1.10	0	3,3,3	1.38	0
2	FMN	H	8401	-	33,33,33	2.54	11 (33%)	46,50,50	2.95	12 (26%)
3	ACY	H	8402	-	3,3,3	1.15	0	3,3,3	1.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	1401	-	-	0/18/18/18	0/0/3/3
3	ACY	A	1402	-	-	0/0/0/0	0/0/0/0
2	FMN	B	2401	-	-	0/18/18/18	0/0/3/3
3	ACY	B	2402	-	-	0/0/0/0	0/0/0/0
2	FMN	C	3401	-	-	0/18/18/18	0/0/3/3
3	ACY	C	3402	-	-	0/0/0/0	0/0/0/0
2	FMN	D	4401	-	-	0/18/18/18	0/0/3/3
3	ACY	D	4402	-	-	0/0/0/0	0/0/0/0
2	FMN	E	5401	-	-	0/18/18/18	0/0/3/3
3	ACY	E	5402	-	-	0/0/0/0	0/0/0/0
2	FMN	F	6401	-	-	0/18/18/18	0/0/3/3
3	ACY	F	6402	-	-	0/0/0/0	0/0/0/0
2	FMN	G	7401	-	-	0/18/18/18	0/0/3/3
3	ACY	G	7402	-	-	0/0/0/0	0/0/0/0
2	FMN	H	8401	-	-	0/18/18/18	0/0/3/3
3	ACY	H	8402	-	-	0/0/0/0	0/0/0/0

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7401	FMN	C1'-N10	-10.08	1.36	1.48
2	H	8401	FMN	C1'-N10	-9.77	1.37	1.48
2	E	5401	FMN	C1'-N10	-9.74	1.37	1.48
2	D	4401	FMN	C1'-N10	-9.71	1.37	1.48
2	B	2401	FMN	C1'-N10	-9.55	1.37	1.48
2	C	3401	FMN	C1'-N10	-9.42	1.37	1.48
2	A	1401	FMN	C1'-N10	-8.92	1.38	1.48
2	F	6401	FMN	C1'-N10	-8.72	1.38	1.48
2	F	6401	FMN	C1'-C2'	7.01	1.58	1.51
2	A	1401	FMN	C1'-C2'	5.74	1.57	1.51
2	H	8401	FMN	C1'-C2'	5.31	1.56	1.51
2	G	7401	FMN	C1'-C2'	5.30	1.56	1.51
2	D	4401	FMN	C1'-C2'	5.07	1.56	1.51
2	B	2401	FMN	C1'-C2'	4.83	1.56	1.51
2	C	3401	FMN	C1'-C2'	4.69	1.56	1.51
2	E	5401	FMN	C1'-C2'	4.62	1.56	1.51
2	D	4401	FMN	C5A-N5	4.00	1.41	1.35
2	B	2401	FMN	C5A-N5	3.89	1.41	1.35
2	G	7401	FMN	C5A-N5	3.83	1.41	1.35
2	E	5401	FMN	C5A-N5	3.80	1.41	1.35
2	H	8401	FMN	C5A-N5	3.70	1.41	1.35
2	C	3401	FMN	C5A-N5	3.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6401	FMN	C9A-N10	3.68	1.44	1.38
2	A	1401	FMN	C4-C4A	3.60	1.47	1.41
2	A	1401	FMN	C9A-N10	3.54	1.44	1.38
2	F	6401	FMN	C5A-N5	3.54	1.40	1.35
2	H	8401	FMN	C9A-N10	3.49	1.44	1.38
2	B	2401	FMN	C4-C4A	3.45	1.46	1.41
2	E	5401	FMN	C4-C4A	3.42	1.46	1.41
2	G	7401	FMN	C4-C4A	3.41	1.46	1.41
2	F	6401	FMN	C4-C4A	3.37	1.46	1.41
2	A	1401	FMN	C5A-N5	3.35	1.40	1.35
2	D	4401	FMN	C4-C4A	3.28	1.46	1.41
2	G	7401	FMN	C9A-N10	3.23	1.43	1.38
2	C	3401	FMN	C4-C4A	3.19	1.46	1.41
2	C	3401	FMN	C9A-N10	3.19	1.43	1.38
2	B	2401	FMN	C9A-N10	3.13	1.43	1.38
2	D	4401	FMN	C9A-N10	3.10	1.43	1.38
2	E	5401	FMN	C9A-N10	2.97	1.43	1.38
2	H	8401	FMN	C4-C4A	2.96	1.46	1.41
2	A	1401	FMN	C4A-N5	2.94	1.42	1.36
2	C	3401	FMN	C4A-N5	2.90	1.42	1.36
2	B	2401	FMN	C4A-N5	2.88	1.42	1.36
2	E	5401	FMN	C4A-N5	2.86	1.42	1.36
2	H	8401	FMN	C4A-N5	2.86	1.42	1.36
2	G	7401	FMN	C4A-N5	2.85	1.42	1.36
2	D	4401	FMN	C4A-N5	2.83	1.42	1.36
2	B	2401	FMN	P-O2P	-2.83	1.44	1.54
2	F	6401	FMN	C4A-N5	2.81	1.42	1.36
2	G	7401	FMN	P-O3P	-2.79	1.44	1.54
2	F	6401	FMN	P-O3P	-2.66	1.45	1.54
2	E	5401	FMN	P-O2P	-2.65	1.45	1.54
2	D	4401	FMN	P-O3P	-2.60	1.45	1.54
2	C	3401	FMN	P-O2P	-2.59	1.45	1.54
2	G	7401	FMN	P-O2P	-2.57	1.45	1.54
2	H	8401	FMN	P-O2P	-2.57	1.45	1.54
2	F	6401	FMN	P-O5'	-2.55	1.51	1.60
2	A	1401	FMN	P-O5'	-2.53	1.51	1.60
2	A	1401	FMN	P-O3P	-2.53	1.45	1.54
2	A	1401	FMN	P-O2P	-2.51	1.45	1.54
2	B	2401	FMN	P-O3P	-2.49	1.45	1.54
2	D	4401	FMN	P-O2P	-2.46	1.45	1.54
2	E	5401	FMN	C6-C5A	-2.43	1.38	1.41
2	B	2401	FMN	P-O5'	-2.42	1.51	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6401	FMN	C6-C5A	-2.35	1.38	1.41
2	H	8401	FMN	C4-N3	2.32	1.41	1.37
2	A	1401	FMN	C6-C5A	-2.30	1.39	1.41
2	H	8401	FMN	C10-N1	2.30	1.39	1.35
2	G	7401	FMN	P-O5'	-2.28	1.52	1.60
2	E	5401	FMN	P-O5'	-2.26	1.52	1.60
2	C	3401	FMN	P-O3P	-2.24	1.46	1.54
2	F	6401	FMN	P-O2P	-2.24	1.46	1.54
2	B	2401	FMN	C4-N3	2.24	1.41	1.37
2	A	1401	FMN	C4-N3	2.22	1.41	1.37
2	H	8401	FMN	P-O5'	-2.19	1.52	1.60
2	D	4401	FMN	C4-N3	2.19	1.40	1.37
2	E	5401	FMN	P-O3P	-2.19	1.46	1.54
2	C	3401	FMN	P-O5'	-2.15	1.52	1.60
2	E	5401	FMN	C10-N1	2.15	1.39	1.35
2	C	3401	FMN	C4-N3	2.13	1.40	1.37
2	B	2401	FMN	C6-C5A	-2.12	1.39	1.41
2	E	5401	FMN	C10-N10	2.11	1.43	1.38
2	H	8401	FMN	P-O3P	-2.11	1.47	1.54
2	D	4401	FMN	C6-C5A	-2.11	1.39	1.41
2	F	6401	FMN	C4-N3	2.08	1.40	1.37
2	G	7401	FMN	C10-N1	2.07	1.39	1.35
2	E	5401	FMN	C4-N3	2.07	1.40	1.37
2	A	1401	FMN	C10-N1	2.07	1.39	1.35
2	D	4401	FMN	P-O5'	-2.05	1.53	1.60
2	F	6401	FMN	C2-N3	2.05	1.41	1.37
2	G	7401	FMN	C6-C5A	-2.04	1.39	1.41
2	G	7401	FMN	C4-N3	2.04	1.40	1.37
2	F	6401	FMN	C10-N1	2.02	1.39	1.35

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	FMN	C2-N1-C10	14.70	129.80	114.98
2	C	3401	FMN	C2-N1-C10	14.63	129.73	114.98
2	B	2401	FMN	C2-N1-C10	14.55	129.65	114.98
2	F	6401	FMN	C2-N1-C10	14.48	129.57	114.98
2	D	4401	FMN	C2-N1-C10	14.45	129.55	114.98
2	E	5401	FMN	C2-N1-C10	14.44	129.53	114.98
2	G	7401	FMN	C2-N1-C10	14.39	129.49	114.98
2	H	8401	FMN	C2-N1-C10	14.14	129.23	114.98
2	E	5401	FMN	C4A-C10-N1	-8.62	114.12	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7401	FMN	C4A-C10-N1	-8.56	114.18	122.73
2	A	1401	FMN	C4A-C10-N1	-8.55	114.19	122.73
2	F	6401	FMN	C4A-C10-N1	-8.50	114.24	122.73
2	C	3401	FMN	C4A-C10-N1	-8.42	114.31	122.73
2	B	2401	FMN	C4A-C10-N1	-8.42	114.32	122.73
2	H	8401	FMN	C4A-C10-N1	-8.33	114.41	122.73
2	D	4401	FMN	C4A-C10-N1	-8.27	114.47	122.73
2	F	6401	FMN	C5'-C4'-C3'	-4.69	103.20	112.06
2	A	1401	FMN	C5'-C4'-C3'	-4.47	103.62	112.06
2	E	5401	FMN	N3-C2-N1	-4.35	111.94	121.19
2	A	1401	FMN	N3-C2-N1	-4.35	111.94	121.19
2	F	6401	FMN	N3-C2-N1	-4.35	111.94	121.19
2	B	2401	FMN	N3-C2-N1	-4.33	111.99	121.19
2	C	3401	FMN	N3-C2-N1	-4.32	112.00	121.19
2	D	4401	FMN	N3-C2-N1	-4.28	112.08	121.19
2	G	7401	FMN	N3-C2-N1	-4.27	112.11	121.19
2	G	7401	FMN	C5'-C4'-C3'	-4.23	104.07	112.06
2	B	2401	FMN	C5'-C4'-C3'	-4.23	104.08	112.06
2	C	3401	FMN	C5'-C4'-C3'	-4.22	104.09	112.06
2	H	8401	FMN	N3-C2-N1	-4.21	112.24	121.19
2	H	8401	FMN	C5'-C4'-C3'	-4.20	104.12	112.06
2	E	5401	FMN	C5'-C4'-C3'	-4.19	104.15	112.06
2	A	1401	FMN	P-O5'-C5'	4.02	129.82	118.19
2	D	4401	FMN	C5'-C4'-C3'	-3.89	104.72	112.06
2	H	8401	FMN	P-O5'-C5'	3.89	129.43	118.19
2	C	3401	FMN	P-O5'-C5'	3.87	129.38	118.19
2	F	6401	FMN	P-O5'-C5'	3.83	129.26	118.19
2	E	5401	FMN	C4-C4A-C10	3.75	123.01	116.95
2	F	6401	FMN	C4-C4A-C10	3.74	122.98	116.95
2	G	7401	FMN	C4-C4A-C10	3.73	122.97	116.95
2	H	8401	FMN	C4-C4A-C10	3.69	122.91	116.95
2	A	1401	FMN	C4-C4A-C10	3.69	122.90	116.95
2	B	2401	FMN	C4-C4A-C10	3.65	122.84	116.95
2	D	4401	FMN	C4-C4A-C10	3.60	122.77	116.95
2	C	3401	FMN	C4-C4A-C10	3.59	122.75	116.95
2	D	4401	FMN	P-O5'-C5'	3.58	128.54	118.19
2	G	7401	FMN	P-O5'-C5'	3.58	128.53	118.19
2	E	5401	FMN	P-O5'-C5'	3.57	128.51	118.19
2	E	5401	FMN	N1-C10-N10	3.53	125.25	115.97
2	C	3401	FMN	N1-C10-N10	3.47	125.10	115.97
2	A	1401	FMN	N1-C10-N10	3.46	125.07	115.97
2	G	7401	FMN	N1-C10-N10	3.46	125.06	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2401	FMN	P-O5'-C5'	3.46	128.19	118.19
2	H	8401	FMN	N1-C10-N10	3.45	125.05	115.97
2	F	6401	FMN	N1-C10-N10	3.45	125.03	115.97
2	B	2401	FMN	N1-C10-N10	3.39	124.88	115.97
2	F	6401	FMN	C1'-N10-C9A	3.32	122.10	118.87
2	D	4401	FMN	N1-C10-N10	3.30	124.64	115.97
2	A	1401	FMN	C1'-N10-C9A	3.16	121.95	118.87
2	D	4401	FMN	C1'-N10-C9A	3.12	121.90	118.87
2	B	2401	FMN	O4'-C4'-C3'	3.05	116.64	109.05
2	C	3401	FMN	O4'-C4'-C3'	3.04	116.61	109.05
2	H	8401	FMN	C1'-N10-C9A	2.98	121.78	118.87
2	H	8401	FMN	O4'-C4'-C3'	2.97	116.45	109.05
2	E	5401	FMN	O4'-C4'-C3'	2.93	116.33	109.05
2	G	7401	FMN	O4'-C4'-C3'	2.91	116.30	109.05
2	D	4401	FMN	O4'-C4'-C3'	2.80	116.02	109.05
2	B	2401	FMN	C1'-N10-C9A	2.74	121.54	118.87
2	G	7401	FMN	C1'-N10-C9A	2.74	121.54	118.87
2	C	3401	FMN	C1'-N10-C9A	2.70	121.50	118.87
2	A	1401	FMN	O4'-C4'-C3'	2.69	115.74	109.05
2	F	6401	FMN	O4'-C4'-C3'	2.64	115.63	109.05
2	E	5401	FMN	C1'-N10-C9A	2.57	121.37	118.87
2	A	1401	FMN	C4A-N5-C5A	2.50	119.50	116.69
2	C	3401	FMN	C4A-N5-C5A	2.46	119.45	116.69
2	F	6401	FMN	C4A-N5-C5A	2.45	119.45	116.69
2	G	7401	FMN	C4A-N5-C5A	2.45	119.44	116.69
2	F	6401	FMN	C9A-N10-C10	-2.40	119.41	121.77
2	E	5401	FMN	C4A-N5-C5A	2.40	119.39	116.69
2	H	8401	FMN	O2P-P-O1P	2.40	118.27	110.44
2	B	2401	FMN	C4A-N5-C5A	2.38	119.36	116.69
2	C	3401	FMN	O2P-P-O1P	2.36	118.16	110.44
2	A	1401	FMN	C9A-N10-C10	-2.31	119.50	121.77
2	F	6401	FMN	O2P-P-O1P	2.27	117.86	110.44
2	H	8401	FMN	C4A-N5-C5A	2.25	119.22	116.69
2	D	4401	FMN	O2P-P-O1P	2.25	117.79	110.44
2	A	1401	FMN	O2P-P-O1P	2.22	117.69	110.44
2	E	5401	FMN	O2P-P-O1P	2.22	117.69	110.44
2	E	5401	FMN	C9A-N10-C10	-2.20	119.61	121.77
2	B	2401	FMN	C9A-N10-C10	-2.20	119.61	121.77
2	D	4401	FMN	C4A-N5-C5A	2.20	119.16	116.69
2	H	8401	FMN	C9A-N10-C10	-2.18	119.62	121.77
2	B	2401	FMN	O2P-P-O1P	2.18	117.57	110.44
2	D	4401	FMN	C9A-N10-C10	-2.17	119.64	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3401	FMN	C9A-N10-C10	-2.13	119.67	121.77
2	G	7401	FMN	C9A-N10-C10	-2.11	119.69	121.77
2	G	7401	FMN	O2P-P-O1P	2.10	117.32	110.44

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	332/352 (94%)	-0.18	10 (3%)	48	58	16, 31, 73, 98	0
1	B	327/352 (92%)	0.03	11 (3%)	43	53	22, 39, 73, 96	0
1	C	332/352 (94%)	-0.04	19 (5%)	23	32	21, 35, 78, 99	0
1	D	329/352 (93%)	-0.11	14 (4%)	34	44	20, 36, 76, 96	0
1	E	324/352 (92%)	0.22	19 (5%)	22	30	22, 40, 73, 95	0
1	F	332/352 (94%)	-0.18	12 (3%)	41	51	13, 28, 72, 97	0
1	G	329/352 (93%)	0.02	19 (5%)	22	31	18, 35, 77, 99	0
1	H	332/352 (94%)	-0.06	16 (4%)	29	39	19, 34, 76, 99	0
All	All	2637/2816 (93%)	-0.04	120 (4%)	32	41	13, 35, 76, 99	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ASP	6.5
1	B	185	ALA	6.1
1	E	202	ALA	6.1
1	C	185	ALA	5.9
1	F	182	ASP	5.8
1	C	183	LEU	5.7
1	C	182	ASP	5.5
1	B	202	ALA	5.3
1	C	202	ALA	5.1
1	D	202	ALA	4.9
1	G	203	SER	4.9
1	D	183	LEU	4.9
1	G	188	GLU	4.9
1	G	185	ALA	4.8
1	C	173	ASN	4.7
1	H	173	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	173	ASN	4.6
1	H	185	ALA	4.5
1	H	183	LEU	4.5
1	C	139	GLN	4.4
1	D	203	SER	4.3
1	D	185	ALA	4.2
1	B	173	ASN	4.2
1	E	173	ASN	4.1
1	C	186	LEU	4.1
1	F	183	LEU	4.1
1	H	172	LEU	4.1
1	D	349	PHE	4.1
1	F	172	LEU	4.0
1	H	182	ASP	4.0
1	H	139	GLN	3.9
1	A	202	ALA	3.9
1	G	186	LEU	3.7
1	E	132	SER	3.7
1	E	56	LYS	3.6
1	A	172	LEU	3.6
1	H	186	LEU	3.5
1	A	173	ASN	3.5
1	G	202	ALA	3.5
1	E	136	PHE	3.4
1	G	173	ASN	3.4
1	D	173	ASN	3.3
1	F	202	ALA	3.3
1	G	349	PHE	3.3
1	B	15	GLN	3.2
1	F	185	ALA	3.2
1	A	183	LEU	3.2
1	C	188	GLU	3.2
1	C	131	LYS	3.2
1	G	207	ASN	3.1
1	A	136	PHE	3.0
1	H	188	GLU	3.0
1	G	132	SER	3.0
1	E	172	LEU	2.9
1	E	203	SER	2.9
1	D	172	LEU	2.9
1	F	184	ARG	2.8
1	A	186	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	186	LEU	2.8
1	E	85	PRO	2.8
1	E	272	LYS	2.8
1	E	131	LYS	2.7
1	B	136	PHE	2.7
1	D	184	ARG	2.7
1	C	172	LEU	2.7
1	G	133	ASP	2.7
1	H	202	ALA	2.7
1	D	176	ALA	2.7
1	C	184	ARG	2.7
1	D	186	LEU	2.7
1	F	136	PHE	2.6
1	B	203	SER	2.6
1	D	132	SER	2.6
1	D	139	GLN	2.6
1	C	53	ASP	2.5
1	G	172	LEU	2.5
1	E	129	TYR	2.5
1	A	185	ALA	2.5
1	E	120	PRO	2.5
1	G	215	ILE	2.5
1	F	176	ALA	2.4
1	B	272	LYS	2.4
1	G	136	PHE	2.4
1	E	210	SER	2.3
1	H	55	SER	2.3
1	E	161	LEU	2.3
1	C	349	PHE	2.3
1	G	135	ASP	2.3
1	H	349	PHE	2.3
1	H	171	GLN	2.3
1	H	18	LYS	2.3
1	C	187	LYS	2.3
1	F	131	LYS	2.3
1	A	130	MET	2.2
1	D	207	ASN	2.2
1	G	139	GLN	2.2
1	H	131	LYS	2.2
1	C	56	LYS	2.2
1	F	18	LYS	2.2
1	C	176	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	211	LEU	2.2
1	G	131	LYS	2.2
1	C	174	LEU	2.2
1	A	131	LYS	2.1
1	B	120	PRO	2.1
1	E	340	ALA	2.1
1	H	203	SER	2.1
1	B	14	LYS	2.1
1	E	135	ASP	2.1
1	F	130	MET	2.1
1	H	130	MET	2.1
1	C	15	GLN	2.0
1	E	137	ASN	2.0
1	G	129	TYR	2.0
1	D	135	ASP	2.0
1	G	184	ARG	2.0
1	E	15	GLN	2.0
1	C	136	PHE	2.0
1	B	214	SER	2.0
1	E	84	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACY	C	3402	4/4	0.26	6.49	46,48,49,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ACY	H	8402	4/4	0.23	4.64	45,47,48,51	0
3	ACY	B	2402	4/4	0.34	3.88	57,58,63,64	0
3	ACY	A	1402	4/4	0.22	3.81	36,39,41,45	0
3	ACY	F	6402	4/4	0.25	3.58	35,36,38,42	0
2	FMN	F	6401	31/31	0.15	1.45	11,21,28,30	0
2	FMN	A	1401	31/31	0.13	1.17	15,25,36,37	0
2	FMN	B	2401	31/31	0.15	1.13	21,36,43,45	0
2	FMN	C	3401	31/31	0.14	0.90	18,33,37,40	0
2	FMN	D	4401	31/31	0.13	0.77	22,33,37,41	0
2	FMN	E	5401	31/31	0.15	0.71	19,37,43,45	0
2	FMN	H	8401	31/31	0.15	0.70	11,29,34,36	0
3	ACY	E	5402	4/4	0.19	0.57	59,62,64,64	0
3	ACY	D	4402	4/4	0.15	0.51	41,51,51,52	0
3	ACY	G	7402	4/4	0.15	0.18	57,60,63,64	0
2	FMN	G	7401	31/31	0.12	0.02	17,37,43,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.