



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:37 PM GMT

PDB ID : 2W3S
Title : CRYSTAL STRUCTURE OF XANTHINE DEHYDROGENASE (DESULFO
FORM) FROM RHODOBACTER CAPSULATUS IN COMPLEX WITH
XANTHINE
Authors : Dietzel, U.; Kuper, J.; Leimkuhler, S.; Kisker, C.
Deposited on : 2008-11-14
Resolution : 2.60 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>

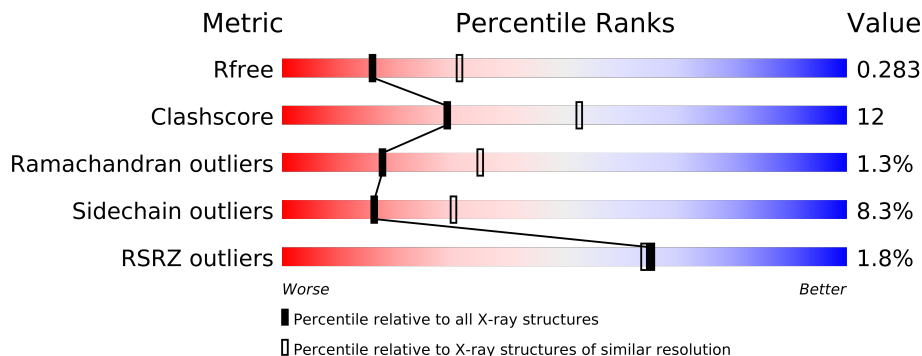
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	462	
1	C	462	
1	E	462	
1	G	462	
2	B	777	
2	D	777	
2	F	777	
2	H	777	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	MPN	B	1778	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	MPN	D	1778	-	X
5	MPN	F	1778	-	X
5	MPN	H	1778	-	X
7	XAN	B	1780[A]	-	X
7	XAN	B	1780[B]	-	X
7	XAN	D	1780[A]	-	X
7	XAN	D	1780[B]	-	X
7	XAN	F	1780[A]	-	X
7	XAN	F	1780[B]	-	X
7	XAN	H	1780[A]	-	X
7	XAN	H	1780[B]	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 36858 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 XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TRP	LEU	CONFLICT	UNP O54050
C	26	TRP	LEU	CONFLICT	UNP O54050
E	26	TRP	LEU	CONFLICT	UNP O54050
G	26	TRP	LEU	CONFLICT	UNP O54050

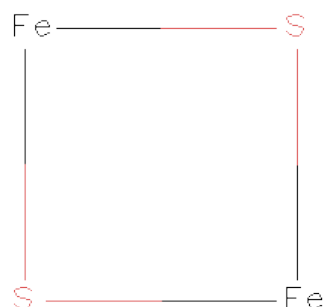
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

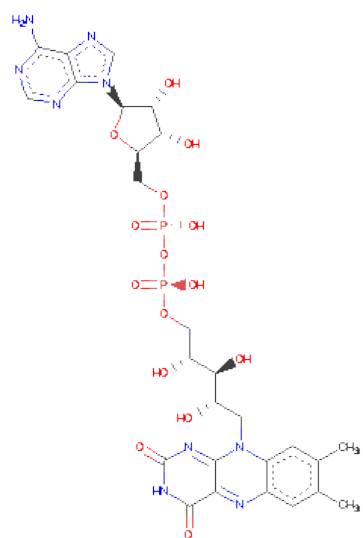
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	CONFLICT	UNP O54051
D	772	ARG	GLY	CONFLICT	UNP O54051
F	772	ARG	GLY	CONFLICT	UNP O54051
H	772	ARG	GLY	CONFLICT	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



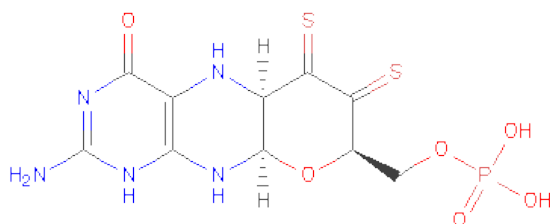
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is PHOSPHORIC ACID MONO-(2-AMINO-4-OXO-5,6-DITHIOXO-1,5,6,7,8A,9,10,10A-OCTAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL)ESTER (three-letter code: MPN) (formula: $C_{10}H_{12}N_5O_6PS_2$).

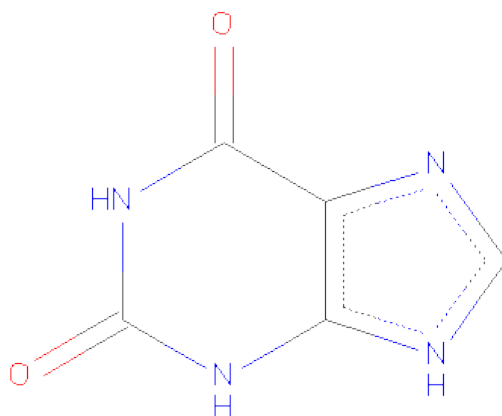


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 7 is XANTHINE (three-letter code: XAN) (formula: C₅H₄N₄O₂).



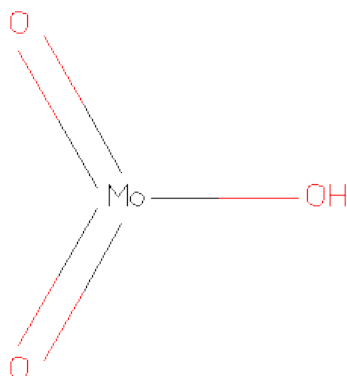
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	1
			22	10	8	4		
7	D	1	Total	C	N	O	0	1
			22	10	8	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	1
			22	10	8	4		
7	H	1	Total	C	N	O	0	1
			22	10	8	4		

- Molecule 8 is HYDROXY(DIOXO)MOLYBDENUM (three-letter code: MOM) (formula: HMoO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Mo	O	0	0
			4	1	3		
8	D	1	Total	Mo	O	0	0
			4	1	3		
8	F	1	Total	Mo	O	0	0
			4	1	3		
8	H	1	Total	Mo	O	0	0
			4	1	3		

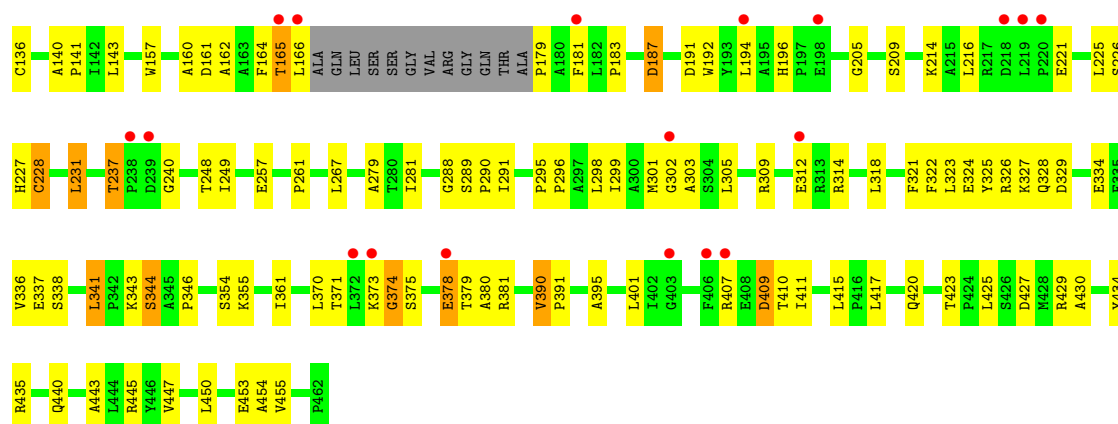
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	9	Total	O	0	0
			9	9		
9	C	4	Total	O	0	0
			4	4		

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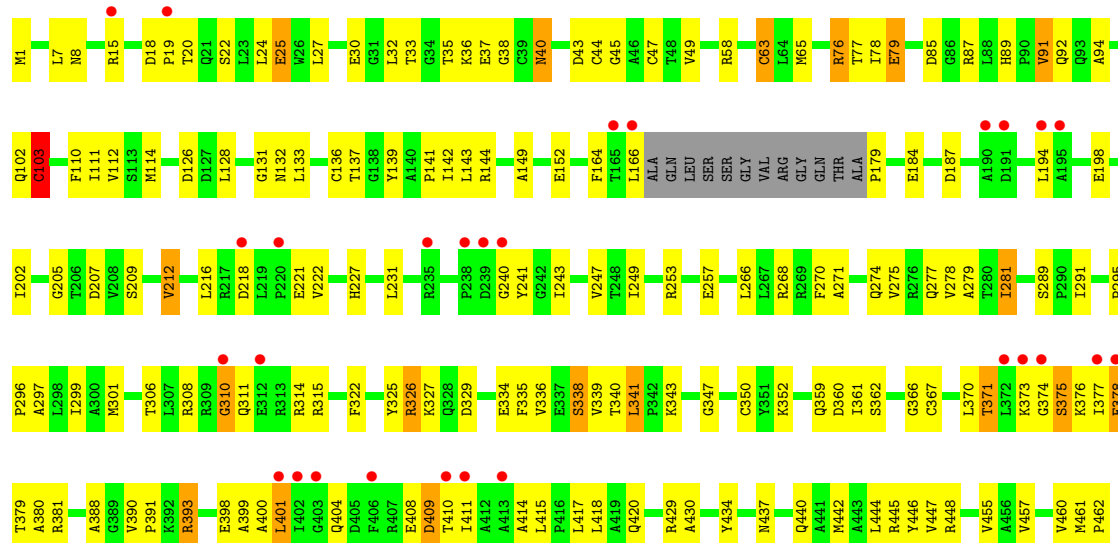
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	7	Total 7	O 7	0	0
9	E	2	Total 2	O 2	0	0
9	F	6	Total 6	O 6	0	0
9	H	7	Total 7	O 7	0	0



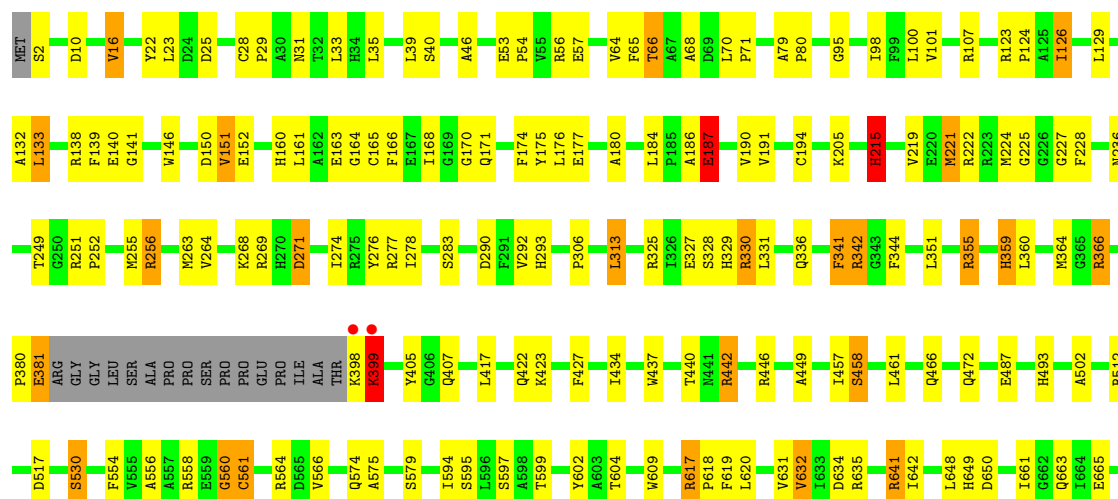
• Molecule 1: XANTHINE DEHYDROGENASE

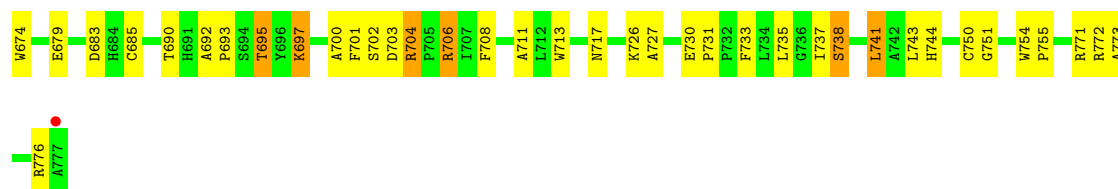
Chain G: 



• Molecule 2: XANTHINE DEHYDROGENASE

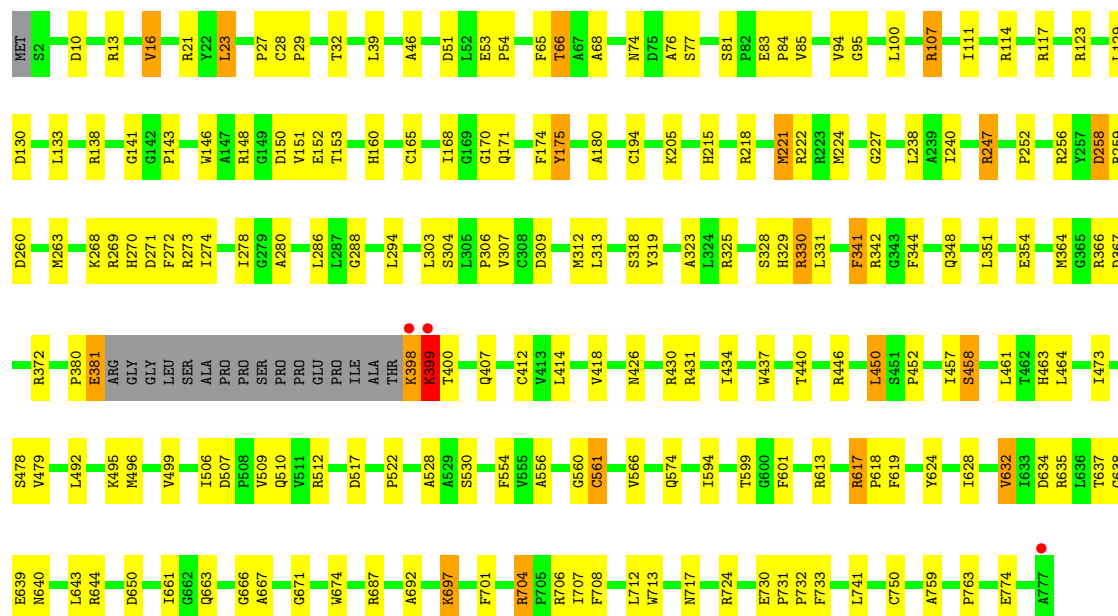
Chain B: 





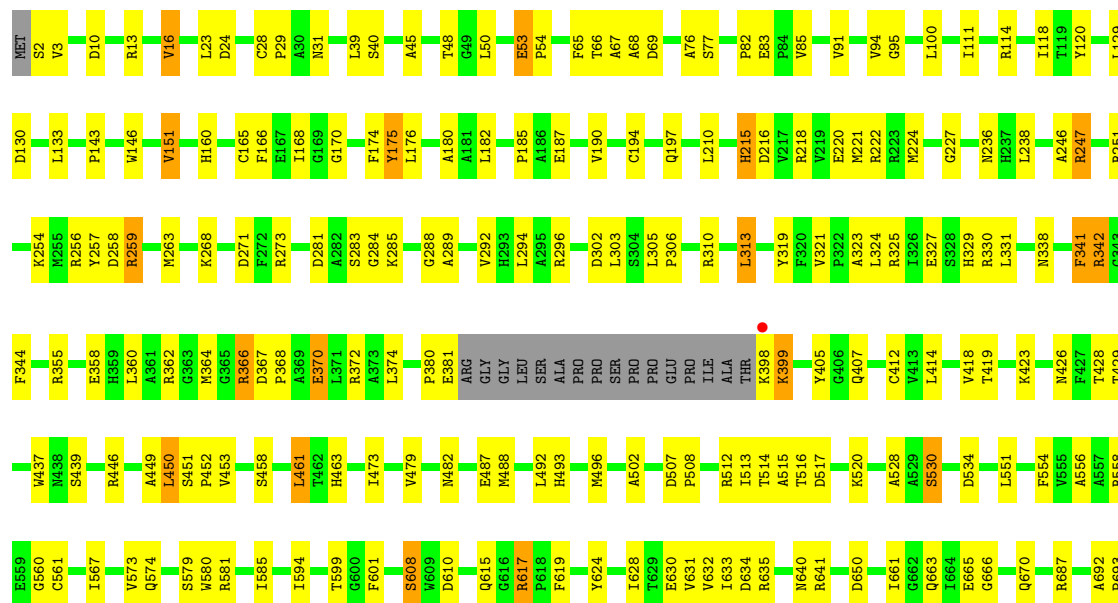
• Molecule 2: XANTHINE DEHYDROGENASE

Chain D: 



• Molecule 2: XANTHINE DEHYDROGENASE

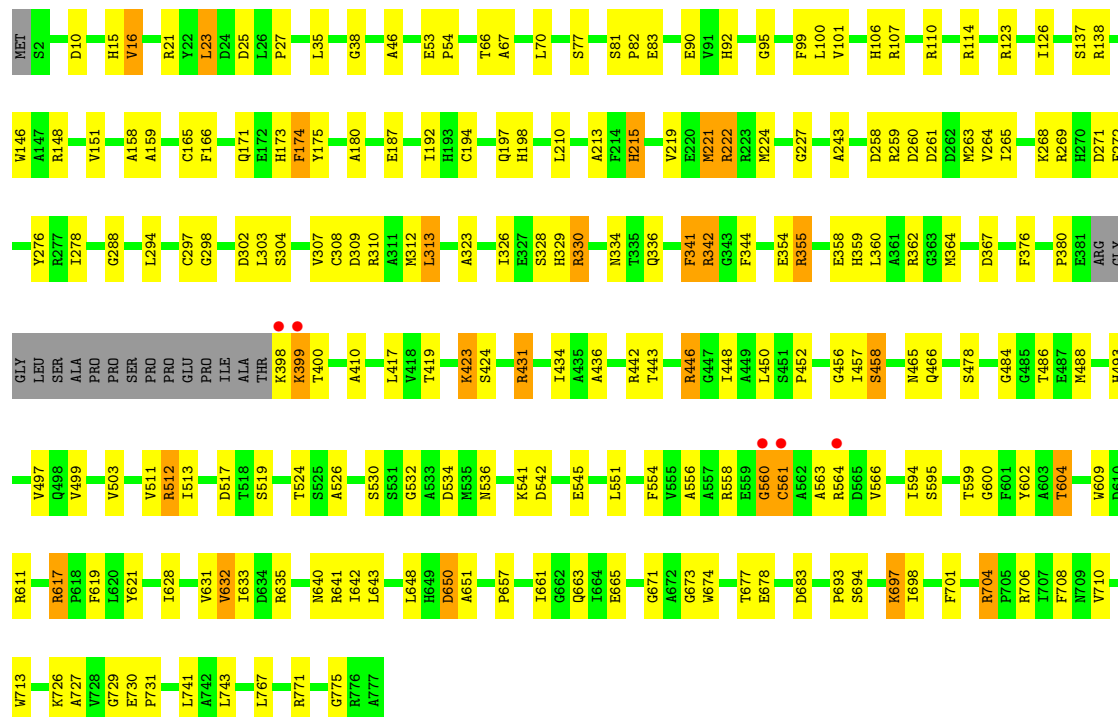
Chain F: 





• Molecule 2: XANTHINE DEHYDROGENASE

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 140.56Å 158.17Å 109.60° 105.89° 101.18°	Depositor
Resolution (Å)	50.12 – 2.60 50.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.12-2.60) 97.7 (50.01-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.232 , 0.284 0.234 , 0.283	Depositor DCC
R_{free} test set	10343 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 206555 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36858	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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: XAN, MPN, CA, FES, MOM, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3439	0.67	0/4659
1	C	0.50	0/3439	0.64	0/4659
1	E	0.51	0/3439	0.66	0/4659
1	G	0.54	1/3439 (0.0%)	0.69	0/4659
2	B	0.56	0/5845	0.70	0/7942
2	D	0.57	1/5845 (0.0%)	0.70	0/7942
2	F	0.58	0/5845	0.71	0/7942
2	H	0.57	0/5845	0.69	0/7942
All	All	0.55	2/37136 (0.0%)	0.69	0/50404

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	103	CYS	CB-SG	-5.70	1.72	1.81
2	D	750	CYS	CB-SG	-5.15	1.73	1.81

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	3376	0	3367	127	0
1	C	3376	0	3367	52	0
1	E	3376	0	3367	94	0
1	G	3376	0	3367	123	0
2	B	5717	0	5631	155	0
2	D	5717	0	5631	126	0
2	F	5717	0	5631	144	0
2	H	5717	0	5630	142	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
3	G	8	0	0	1	0
4	A	53	0	31	6	0
4	C	53	0	31	3	0
4	E	53	0	31	3	0
4	G	53	0	31	4	0
5	B	24	0	8	1	0
5	D	24	0	9	2	0
5	F	24	0	8	3	0
5	H	24	0	8	4	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	22	0	8	0	0
7	D	22	0	8	3	0
7	F	22	0	8	0	0
7	H	22	0	8	0	0
8	B	4	0	0	2	0
8	D	4	0	0	5	0
8	F	4	0	0	2	0
8	H	4	0	0	2	0
9	A	3	0	0	0	0
9	B	9	0	0	0	0
9	C	4	0	0	0	0
9	D	7	0	0	0	0
9	E	2	0	0	0	0
9	F	6	0	0	0	0
9	H	7	0	0	0	0
All	All	36858	0	36180	900	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 (900) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:247:ARG:HH11	2:F:247:ARG:HG2	1.11	1.07
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.34	1.04
2:F:221:MET:HE1	2:F:224:MET:HG3	1.40	1.03
1:A:240:GLY:HA2	1:A:343:LYS:HG2	1.41	1.03
1:G:361:ILE:HD11	1:G:429:ARG:NH2	1.75	1.01
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.27	1.00
2:D:446:ARG:HD3	2:D:632:VAL:HG13	1.44	0.99
1:G:24:LEU:HD21	1:G:37:GLU:HG3	1.42	0.97
1:C:291:ILE:HD13	1:C:361:ILE:HD12	1.45	0.97
1:A:426:SER:H	2:F:574:GLN:HE22	1.15	0.94
1:G:18:ASP:OD2	1:G:20:THR:HG22	1.67	0.94
2:H:701:PHE:O	2:H:704:ARG:HG2	1.73	0.89
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.72	0.88
1:C:240:GLY:HA2	1:C:343:LYS:HG2	1.55	0.88
2:F:247:ARG:NH1	2:F:247:ARG:HG2	1.89	0.87
1:C:216:LEU:HD12	2:D:114:ARG:NH1	1.90	0.86
2:B:690:THR:HA	2:B:695:THR:OG1	1.76	0.86
2:B:126:ILE:HD12	2:B:126:ILE:N	1.89	0.86
1:A:345:ALA:HB3	1:A:346:PRO:HA	1.57	0.86
1:A:361:ILE:HG12	1:A:429:ARG:CZ	2.06	0.85
2:H:360:LEU:HG	2:H:364:MET:HE2	1.59	0.83
2:H:259:ARG:HG3	2:H:263:MET:HE2	1.61	0.82
7:D:1780[A]:XAN:H8	8:D:1781:MOM:OM2	1.79	0.82
2:D:247:ARG:NH1	2:D:247:ARG:HG2	1.83	0.82
2:F:174:PHE:HZ	2:F:693:PRO:HG3	1.44	0.82
1:E:370:LEU:HD22	1:E:380:ALA:HA	1.63	0.81
1:G:444:LEU:O	1:G:448:ARG:HG3	1.80	0.80
1:E:12:ARG:HH11	1:E:12:ARG:HG2	1.46	0.79
2:F:66:THR:HG22	2:F:68:ALA:H	1.48	0.79
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.65	0.78
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.66	0.78
2:D:380:PRO:O	2:D:381:GLU:HB2	1.83	0.78
1:A:190:ALA:HB1	1:A:310:GLY:HA2	1.66	0.78
1:G:361:ILE:HD11	1:G:429:ARG:HH21	1.47	0.78
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.65	0.78
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	1.67	0.77
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.67	0.77
2:F:341:PHE:HD2	2:F:342:ARG:N	1.82	0.76
1:E:7:LEU:HD12	1:E:75:LEU:HD23	1.66	0.76
2:D:247:ARG:HH11	2:D:247:ARG:CG	1.99	0.75
2:D:66:THR:HG22	2:D:68:ALA:H	1.49	0.75
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:32:LEU:HD22	1:C:79:GLU:HG3	1.69	0.74
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.32	0.74
1:A:347:GLY:O	1:A:446:TYR:OH	2.05	0.74
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.70	0.74
2:H:450:LEU:HD12	2:H:628:ILE:HD11	1.69	0.74
1:C:216:LEU:HD12	2:D:114:ARG:HH11	1.53	0.74
1:E:7:LEU:CD1	1:E:75:LEU:HD23	2.18	0.73
1:G:110:PHE:O	1:G:114:MET:HG3	1.88	0.73
2:B:560:GLY:O	2:B:561:CYS:HB3	1.86	0.73
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.71	0.73
2:F:701:PHE:O	2:F:704:ARG:HG2	1.88	0.73
1:A:371:THR:OG1	1:A:379:THR:HB	1.89	0.72
1:C:462:PRO:HA	2:D:643:LEU:HD22	1.72	0.72
1:A:330:ARG:HH21	4:A:1465:FAD:H2A	1.54	0.72
2:F:473:ILE:HG12	2:F:479:VAL:HG22	1.71	0.72
1:G:352:LYS:HG3	1:G:362:SER:HB3	1.72	0.72
1:E:323:LEU:HD21	1:E:329:ASP:HB2	1.71	0.71
2:F:599:THR:HG23	2:H:599:THR:HG23	1.71	0.71
2:B:35:LEU:HB2	2:B:255:MET:HB2	1.71	0.71
1:C:41:GLU:HG3	1:C:214:LYS:HE3	1.72	0.71
1:A:202:ILE:HD13	1:A:222:VAL:HG13	1.72	0.71
2:F:341:PHE:HD2	2:F:342:ARG:H	1.37	0.71
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.71	0.71
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.06	0.70
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.74	0.70
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.72	0.70
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.26	0.70
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.74	0.70
2:H:174:PHE:HZ	2:H:693:PRO:HG3	1.56	0.70
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.21	0.69
1:G:1:MET:HB2	1:G:179:PRO:HG3	1.71	0.69
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.25	0.69
1:G:216:LEU:HD12	2:H:114:ARG:NH1	2.08	0.68
2:H:354:GLU:OE1	2:H:354:GLU:HA	1.93	0.68
1:G:322:PHE:HB3	1:G:390:VAL:HG23	1.76	0.68
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.76	0.68
2:B:126:ILE:CD1	2:B:126:ILE:N	2.57	0.68
2:B:292:VAL:HG22	2:B:327:GLU:HB3	1.75	0.68
1:G:347:GLY:O	1:G:446:TYR:OH	2.10	0.68
2:H:23:LEU:HD22	2:H:180:ALA:HB1	1.76	0.68
2:D:168:ILE:HD13	2:D:351:LEU:HD23	1.75	0.68
1:A:345:ALA:CB	1:A:346:PRO:HA	2.24	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:66:THR:HG22	2:B:68:ALA:H	1.59	0.67
2:D:701:PHE:O	2:D:704:ARG:HG2	1.94	0.67
1:G:253:ARG:NH2	1:G:268:ARG:HG3	2.10	0.67
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.41	0.67
2:H:541:LYS:O	2:H:545:GLU:HG3	1.95	0.67
2:H:259:ARG:HG3	2:H:263:MET:CE	2.23	0.67
1:A:202:ILE:CD1	1:A:222:VAL:HG13	2.25	0.67
1:G:322:PHE:HB3	1:G:390:VAL:CG2	2.25	0.66
1:G:143:LEU:C	1:G:143:LEU:HD23	2.15	0.66
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.76	0.66
2:B:751:GLY:HA3	2:B:773:ALA:O	1.95	0.66
2:B:39:LEU:HD22	2:B:95:GLY:O	1.96	0.66
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.96	0.66
1:C:445:ARG:NH2	2:D:634:ASP:OD2	2.28	0.66
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.29	0.66
2:D:288:GLY:HA2	2:D:323:ALA:O	1.96	0.66
2:H:665:GLU:HG2	2:H:710:VAL:HG21	1.78	0.65
1:C:291:ILE:CD1	1:C:361:ILE:HD12	2.25	0.65
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.44	0.65
2:F:160:HIS:HB3	2:F:364:MET:HE2	1.78	0.65
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.78	0.65
1:G:390:VAL:HG22	1:G:391:PRO:HD2	1.78	0.65
1:A:181:PHE:CZ	1:A:183:PRO:HB3	2.32	0.65
2:D:556:ALA:HB1	2:D:561:CYS:O	1.96	0.65
1:A:231:LEU:HD23	1:A:231:LEU:O	1.96	0.65
2:D:635:ARG:NH1	2:D:774:GLU:OE2	2.26	0.65
2:B:599:THR:HG23	2:D:599:THR:HG23	1.79	0.65
1:G:360:ASP:OD1	2:H:697:LYS:HE3	1.96	0.65
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.77	0.65
2:F:281:ASP:HB2	2:F:285:LYS:H	1.61	0.65
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.79	0.65
2:F:617:ARG:HD3	2:F:619:PHE:O	1.96	0.65
2:H:450:LEU:HD12	2:H:628:ILE:CD1	2.27	0.64
1:G:89:HIS:ND1	1:G:91:VAL:HB	2.12	0.64
1:G:65:MET:HE1	1:G:278:VAL:HG11	1.79	0.64
2:D:76:ALA:HB2	2:D:85:VAL:HG22	1.79	0.64
2:D:205:LYS:HB3	2:D:240:ILE:HD11	1.80	0.64
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.80	0.64
2:H:560:GLY:O	2:H:561:CYS:HB3	1.96	0.64
1:C:407:ARG:HD2	1:C:409:ASP:OD2	1.98	0.64
1:A:2:GLU:OE1	1:A:13:ARG:HG2	1.98	0.64
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:129:LEU:HD12	2:B:129:LEU:H	1.63	0.63
2:D:146:TRP:O	2:D:325:ARG:HG3	1.99	0.63
2:D:270:HIS:NE2	2:D:304:SER:OG	2.31	0.63
1:E:111:ILE:HD11	2:F:16:VAL:CG2	2.29	0.63
2:H:556:ALA:HB2	2:H:563:ALA:HA	1.81	0.63
2:H:360:LEU:HG	2:H:364:MET:CE	2.27	0.63
1:G:297:ALA:HA	1:G:367:CYS:SG	2.38	0.63
1:E:228:CYS:SG	1:E:231:LEU:HB2	2.39	0.63
2:F:360:LEU:HG	2:F:364:MET:HE3	1.81	0.63
1:A:252:LEU:HD22	1:A:281:ILE:HG21	1.81	0.63
8:F:1781:MOM:MO1	8:F:1781:MOM:OM1	1.70	0.63
2:D:617:ARG:HD3	2:D:619:PHE:O	1.99	0.62
2:B:556:ALA:HB1	2:B:561:CYS:O	2.00	0.62
1:E:361:ILE:HD11	1:E:429:ARG:NH1	2.14	0.62
1:G:299:ILE:O	1:G:381:ARG:NH1	2.33	0.62
2:D:554:PHE:HB2	2:D:594:ILE:HD13	1.80	0.62
1:A:426:SER:H	2:F:574:GLN:NE2	1.92	0.62
2:B:126:ILE:HD12	2:B:126:ILE:H	1.65	0.62
7:D:1780[A]:XAN:C8	8:D:1781:MOM:OM2	2.46	0.62
1:G:326:ARG:HH11	1:G:326:ARG:HG2	1.63	0.62
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.15	0.62
1:A:136:CYS:HB2	3:A:1463:FES:S2	2.40	0.61
8:D:1781:MOM:OM1	8:D:1781:MOM:MO1	1.70	0.61
2:H:77:SER:HB2	2:H:83:GLU:HB3	1.82	0.61
2:F:633:ILE:HG22	2:F:640:ASN:HB3	1.82	0.61
1:A:352:LYS:HG3	1:A:362:SER:OG	2.00	0.61
8:F:1781:MOM:MO1	8:F:1781:MOM:OM3	1.71	0.61
1:C:373:LYS:HB2	1:C:378:GLU:CG	2.31	0.61
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.35	0.61
2:B:755:PRO:O	2:B:772:ARG:HD2	2.01	0.61
8:B:1781:MOM:OM3	8:B:1781:MOM:MO1	1.71	0.61
1:E:88:LEU:HD21	2:F:13:ARG:NH1	2.16	0.60
1:A:8:ASN:HA	1:A:76:ARG:HD2	1.81	0.60
2:D:663:GLN:HE22	5:D:1778:MPN:H1	1.50	0.60
1:A:445:ARG:NH2	2:B:634:ASP:OD1	2.34	0.60
1:A:111:ILE:HA	1:A:114:MET:HE2	1.83	0.60
2:B:380:PRO:O	2:B:381:GLU:HB2	2.01	0.60
8:D:1781:MOM:OM3	8:D:1781:MOM:MO1	1.72	0.60
2:B:160:HIS:HB3	2:B:364:MET:CE	2.30	0.60
2:H:192:ILE:HB	2:H:219:VAL:HG22	1.84	0.60
2:B:46:ALA:HB2	2:B:123:ARG:NH2	2.17	0.60
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:24:LEU:CD2	1:G:37:GLU:HG3	2.23	0.60
1:A:32:LEU:HD22	1:A:79:GLU:HG3	1.84	0.60
1:E:370:LEU:HD22	1:E:380:ALA:CA	2.31	0.60
8:H:1781:MOM:OM3	8:H:1781:MOM:MO1	1.71	0.60
1:G:43:ASP:HB3	2:H:693:PRO:HB2	1.84	0.59
2:B:560:GLY:O	2:B:561:CYS:CB	2.50	0.59
8:H:1781:MOM:OM1	8:H:1781:MOM:MO1	1.72	0.59
2:H:198:HIS:ND1	2:H:526:ALA:HB2	2.17	0.59
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.82	0.59
2:H:657:PRO:O	2:H:661:ILE:HG12	2.00	0.59
2:B:635:ARG:HD3	2:B:750:CYS:SG	2.42	0.59
2:B:53:GLU:HG3	2:B:57:GLU:OE2	2.02	0.59
1:E:355:LYS:NZ	1:E:429:ARG:HA	2.18	0.59
2:D:446:ARG:HD3	2:D:632:VAL:CG1	2.24	0.59
2:D:507:ASP:OD1	2:D:509:VAL:HG23	2.02	0.59
1:A:11:THR:HG22	1:A:164:PHE:HE1	1.67	0.59
8:B:1781:MOM:OM1	8:B:1781:MOM:MO1	1.73	0.59
2:B:617:ARG:HD3	2:B:619:PHE:O	2.03	0.59
1:A:347:GLY:O	1:A:369:ASN:HA	2.03	0.59
1:E:1:MET:HB3	1:E:179:PRO:HG2	1.83	0.59
2:F:170:GLY:N	2:F:271:ASP:HB3	2.18	0.58
1:A:330:ARG:NH2	4:A:1465:FAD:H2A	2.18	0.58
1:G:359:GLN:HE22	4:G:1465:FAD:H6	1.67	0.58
1:G:111:ILE:HA	1:G:114:MET:HE2	1.86	0.58
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.86	0.58
1:E:291:ILE:HD13	1:E:361:ILE:HD12	1.85	0.58
1:G:326:ARG:HG2	1:G:326:ARG:NH1	2.16	0.58
2:H:530:SER:HA	5:H:1778:MPN:C4'	2.33	0.58
2:D:171:GLN:NE2	2:D:674:TRP:HB2	2.18	0.58
1:A:18:ASP:OD2	1:A:20:THR:HG22	2.04	0.58
1:C:216:LEU:HD13	2:D:111:ILE:HG13	1.85	0.58
2:D:528:ALA:HA	5:D:1778:MPN:S2'	2.43	0.58
2:B:160:HIS:HB3	2:B:364:MET:HE2	1.85	0.58
2:D:66:THR:HG22	2:D:68:ALA:N	2.17	0.58
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.04	0.58
2:H:767:LEU:O	2:H:771:ARG:HG3	2.02	0.58
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.36	0.58
2:B:274:ILE:HG12	2:B:293:HIS:CD2	2.39	0.58
1:A:401:LEU:HD11	1:A:411:ILE:HD13	1.86	0.58
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.38	0.58
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.36	0.58
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:ARG:NH1	1:A:331:ARG:HG2	2.19	0.57
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.85	0.57
2:D:74:ASN:O	2:D:84:PRO:HA	2.04	0.57
2:F:288:GLY:HA2	2:F:323:ALA:O	2.03	0.57
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.84	0.57
1:A:405:ASP:O	1:A:410:THR:HG21	2.05	0.57
2:B:434:ILE:HG23	2:B:446:ARG:HB2	1.86	0.57
1:G:314:ARG:NH1	1:G:334:GLU:OE2	2.38	0.57
1:A:89:HIS:ND1	1:A:91:VAL:HB	2.20	0.57
2:D:280:ALA:HB3	2:D:364:MET:HE1	1.85	0.57
2:H:92:HIS:O	2:H:334:ASN:HB3	2.04	0.57
2:B:163:GLU:HG2	2:B:277:ARG:HG2	1.87	0.57
2:F:487:GLU:HB2	2:F:493:HIS:CD2	2.40	0.57
2:H:643:LEU:O	2:H:706:ARG:HB2	2.05	0.57
2:H:560:GLY:O	2:H:561:CYS:CB	2.52	0.57
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.68	0.57
1:C:110:PHE:HB3	1:C:114:MET:HE1	1.85	0.57
2:F:28:CYS:HB2	2:F:29:PRO:CD	2.34	0.56
1:A:231:LEU:HD21	1:A:245:ALA:HB3	1.87	0.56
2:F:281:ASP:HB3	2:F:283:SER:H	1.69	0.56
2:F:492:LEU:O	2:F:496:MET:HG2	2.05	0.56
1:G:401:LEU:HD11	1:G:411:ILE:HD13	1.87	0.56
2:B:126:ILE:CD1	2:B:126:ILE:H	2.17	0.56
2:F:530:SER:HA	5:F:1778:MPN:H4'1	1.87	0.56
1:E:374:GLY:O	1:E:375:SER:HB3	2.04	0.56
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.87	0.56
2:H:650:ASP:HA	2:H:713:TRP:HB3	1.87	0.56
2:D:273:ARG:HD2	2:D:294:LEU:HD12	1.87	0.56
1:A:309:ARG:HB3	1:A:312:GLU:HG3	1.88	0.56
2:F:407:GLN:OE1	2:F:617:ARG:HG2	2.05	0.56
2:B:174:PHE:HZ	2:B:693:PRO:HG3	1.70	0.56
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.87	0.56
2:B:163:GLU:CG	2:B:277:ARG:HG2	2.36	0.56
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.86	0.56
2:F:693:PRO:O	2:F:697:LYS:HE2	2.07	0.56
2:H:530:SER:O	2:H:727:ALA:HB1	2.06	0.56
1:A:325:TYR:O	1:A:326:ARG:HB2	2.06	0.55
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.87	0.55
2:B:648:LEU:HD12	2:B:711:ALA:O	2.06	0.55
1:G:361:ILE:CD1	1:G:429:ARG:NH2	2.60	0.55
1:C:141:PRO:HA	1:C:144:ARG:HH11	1.71	0.55
1:A:351:TYR:CE2	1:A:445:ARG:HD3	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.42	0.55
2:B:263:MET:HE3	2:B:692:ALA:HA	1.89	0.55
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.89	0.55
1:G:247:VAL:HB	1:G:281:ILE:HD11	1.88	0.55
1:A:322:PHE:CB	1:A:390:VAL:HG22	2.37	0.55
1:G:216:LEU:HD23	2:H:107:ARG:NH1	2.22	0.55
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.41	0.55
2:B:641:ARG:NH2	2:B:706:ARG:HH12	2.05	0.55
2:H:457:ILE:O	2:H:458:SER:CB	2.54	0.55
1:E:434:TYR:CD1	2:F:764:GLU:HG3	2.41	0.55
1:A:368:LEU:HB2	1:A:446:TYR:CD1	2.41	0.55
1:A:409:ASP:HA	1:A:412:ALA:HB3	1.88	0.55
1:A:418:LEU:HA	1:A:421:ASP:HB2	1.87	0.55
2:B:150:ASP:OD2	2:F:423:LYS:HE2	2.06	0.55
1:A:356:ARG:NH2	1:A:359:GLN:O	2.35	0.55
2:F:581:ARG:NH1	2:F:581:ARG:HB2	2.22	0.55
2:F:247:ARG:NH1	2:F:247:ARG:CG	2.64	0.55
2:D:434:ILE:HG23	2:D:446:ARG:HB2	1.89	0.55
1:E:12:ARG:CG	1:E:12:ARG:HH11	2.19	0.55
2:D:205:LYS:HE2	2:D:205:LYS:HA	1.88	0.55
1:G:85:ASP:OD2	1:G:87:ARG:NH1	2.40	0.55
2:H:303:LEU:O	2:H:307:VAL:HG23	2.07	0.55
1:A:314:ARG:HH12	1:A:331:ARG:HG2	1.71	0.55
2:B:79:ALA:HB1	2:B:80:PRO:HD2	1.88	0.55
2:F:160:HIS:HB3	2:F:364:MET:CE	2.36	0.54
2:F:453:VAL:CG2	2:F:735:LEU:HD23	2.36	0.54
1:A:22:SER:OG	1:A:25:GLU:OE1	2.20	0.54
2:D:74:ASN:OD1	2:D:85:VAL:N	2.35	0.54
2:H:457:ILE:O	2:H:458:SER:HB2	2.07	0.54
2:H:633:ILE:HG22	2:H:640:ASN:HB3	1.89	0.54
1:A:52:ARG:HA	1:A:56:GLY:O	2.07	0.54
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.88	0.54
2:F:66:THR:H	2:F:69:ASP:HB2	1.72	0.54
1:A:400:ALA:CB	1:A:417:LEU:HD13	2.37	0.54
2:B:701:PHE:O	2:B:704:ARG:HG2	2.07	0.54
2:F:185:PRO:HD3	2:F:246:ALA:HB1	1.89	0.54
1:G:411:ILE:O	1:G:415:LEU:HG	2.08	0.54
1:G:44:CYS:O	1:G:132:ASN:HA	2.07	0.54
1:G:408:GLU:OE1	2:H:442:ARG:NH2	2.41	0.54
2:B:66:THR:HG22	2:B:68:ALA:N	2.22	0.54
1:A:428:MET:H	1:A:428:MET:HE3	1.72	0.54
1:C:1:MET:HB3	1:C:179:PRO:HG2	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:111:ILE:HD11	2:D:16:VAL:CG2	2.38	0.54
2:H:530:SER:HA	5:H:1778:MPN:H4'1	1.90	0.54
2:H:221:MET:HE1	2:H:224:MET:HG3	1.90	0.54
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.43	0.54
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.07	0.53
2:D:644:ARG:HG3	2:D:707:ILE:HB	1.88	0.53
4:E:1465:FAD:H2'	4:E:1465:FAD:N1	2.23	0.53
2:B:23:LEU:CD1	2:B:194:CYS:HA	2.38	0.53
1:A:373:LYS:HB2	1:A:378:GLU:HG3	1.90	0.53
1:G:445:ARG:HG3	1:G:455:VAL:CG1	2.38	0.53
1:G:388:ALA:C	1:G:390:VAL:H	2.12	0.53
2:H:609:TRP:CZ3	2:H:611:ARG:HA	2.43	0.53
2:F:40:SER:HB2	2:F:91:VAL:HG11	1.90	0.53
2:B:56:ARG:HG2	2:B:64:VAL:HG21	1.91	0.53
1:A:426:SER:N	2:F:574:GLN:HE22	1.96	0.53
2:B:466:GLN:HA	2:B:602:TYR:O	2.09	0.53
2:F:306:PRO:HB2	2:F:344:PHE:CZ	2.44	0.53
1:E:111:ILE:HA	1:E:114:MET:HE3	1.91	0.53
1:G:32:LEU:HD22	1:G:79:GLU:HG3	1.91	0.53
2:H:380:PRO:HB3	2:H:410:ALA:O	2.08	0.53
1:E:305:LEU:HD11	1:E:336:VAL:HG13	1.90	0.53
1:G:45:GLY:HA3	1:G:131:GLY:O	2.08	0.53
2:B:123:ARG:HB3	2:B:124:PRO:HD2	1.91	0.53
1:G:411:ILE:HG13	1:G:447:VAL:CG2	2.39	0.53
1:E:290:PRO:HA	1:E:391:PRO:HD3	1.91	0.53
2:H:77:SER:HB2	2:H:83:GLU:CB	2.38	0.53
2:D:150:ASP:OD2	2:D:153:THR:OG1	2.27	0.53
1:E:344:SER:OG	1:E:346:PRO:HD3	2.10	0.52
2:D:426:ASN:O	2:D:430:ARG:HG3	2.10	0.52
1:A:354:SER:OG	1:A:356:ARG:O	2.27	0.52
2:H:213:ALA:HB3	2:H:215:HIS:CD2	2.44	0.52
1:A:345:ALA:CB	1:A:346:PRO:CA	2.87	0.52
2:H:174:PHE:HA	2:H:259:ARG:HH21	1.75	0.52
2:H:651:ALA:C	2:H:726:LYS:HB2	2.30	0.52
1:E:77:THR:OG1	1:E:79:GLU:HG2	2.10	0.52
2:B:329:HIS:HB3	2:B:331:LEU:HD21	1.91	0.52
2:B:457:ILE:O	2:B:458:SER:CB	2.58	0.52
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.50	0.52
1:A:425:LEU:HD12	2:F:579:SER:HB2	1.92	0.52
2:D:39:LEU:HD22	2:D:95:GLY:O	2.08	0.52
2:F:23:LEU:CD1	2:F:194:CYS:HA	2.37	0.52
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:33:LEU:HD12	2:B:249:THR:HG21	1.90	0.52
2:B:730:GLU:H	2:B:731:PRO:HD2	1.74	0.52
1:G:409:ASP:OD2	1:G:409:ASP:N	2.43	0.52
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.90	0.52
2:F:426:ASN:HD21	2:F:429:THR:HB	1.75	0.52
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.92	0.52
1:E:430:ALA:HB1	1:E:434:TYR:HD2	1.74	0.52
2:H:632:VAL:O	2:H:640:ASN:HA	2.10	0.52
2:B:631:VAL:HG12	2:B:642:ILE:HA	1.91	0.52
2:D:418:VAL:HG13	2:D:450:LEU:HD11	1.90	0.52
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.92	0.52
1:G:102:GLN:O	2:H:15:HIS:HE1	1.93	0.52
2:H:297:CYS:HB3	2:H:304:SER:OG	2.10	0.52
2:B:95:GLY:HA3	2:B:264:VAL:HG12	1.92	0.52
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.10	0.52
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.40	0.52
1:G:393:ARG:NH1	1:G:398:GLU:OE1	2.43	0.52
1:G:209:SER:HA	1:G:212:VAL:HG13	1.92	0.52
1:E:22:SER:OG	1:E:25:GLU:HG2	2.10	0.52
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.25	0.51
2:D:21:ARG:HH21	2:D:27:PRO:CD	2.23	0.51
2:D:457:ILE:O	2:D:458:SER:CB	2.59	0.51
2:H:673:GLY:O	2:H:678:GLU:HB2	2.10	0.51
2:B:617:ARG:NH1	2:B:620:LEU:HA	2.26	0.51
1:E:192:TRP:O	1:E:196:HIS:HD2	1.93	0.51
1:G:38:GLY:O	2:H:259:ARG:HD3	2.10	0.51
1:E:370:LEU:HD22	1:E:380:ALA:CB	2.39	0.51
1:E:453:GLU:HG2	1:E:454:ALA:N	2.25	0.51
1:E:298:LEU:HB3	1:E:303:ALA:HB3	1.92	0.51
2:F:151:VAL:HG21	2:F:325:ARG:HB3	1.93	0.51
2:H:298:GLY:HA3	2:H:336:GLN:O	2.10	0.51
2:B:278:ILE:HG12	2:B:360:LEU:HD22	1.93	0.51
2:F:601:PHE:CG	2:H:595:SER:HB2	2.45	0.51
1:G:94:ALA:HB2	1:G:149:ALA:HB2	1.93	0.51
2:H:67:ALA:HA	2:H:70:LEU:HD12	1.93	0.51
1:A:51:ILE:HD11	1:A:58:ARG:NH1	2.25	0.51
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.93	0.51
1:A:322:PHE:CB	1:A:390:VAL:CG2	2.86	0.51
1:C:215:ALA:CB	1:C:217:ARG:HH21	2.23	0.51
1:A:430:ALA:HB1	1:A:434:TYR:HD2	1.76	0.51
1:A:110:PHE:O	1:A:114:MET:HG3	2.10	0.51
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:283:SER:O	2:B:366:ARG:NH1	2.42	0.51
1:A:252:LEU:HD22	1:A:281:ILE:CG2	2.41	0.51
1:G:418:LEU:HD12	1:G:440:GLN:HG2	1.92	0.51
1:G:27:LEU:O	1:G:30:GLU:HB2	2.11	0.51
1:G:371:THR:HB	1:G:378:GLU:HB2	1.93	0.51
2:H:694:SER:O	2:H:697:LYS:HE2	2.10	0.51
2:D:129:LEU:HD22	2:D:331:LEU:HD12	1.93	0.51
2:B:228:PHE:O	2:B:341:PHE:HA	2.11	0.51
1:G:187:ASP:HA	1:G:308:ARG:NH2	2.25	0.50
2:F:380:PRO:HD3	2:F:412:CYS:O	2.10	0.50
1:G:377:ILE:N	1:G:404:GLN:O	2.43	0.50
2:F:263:MET:HE3	2:F:692:ALA:HA	1.92	0.50
1:A:409:ASP:N	1:A:409:ASP:OD2	2.44	0.50
2:F:168:ILE:HA	2:F:759:ALA:HB3	1.92	0.50
2:D:730:GLU:N	2:D:731:PRO:CD	2.74	0.50
2:D:730:GLU:H	2:D:731:PRO:CD	2.24	0.50
2:B:663:GLN:HE22	5:B:1778:MPN:H1	1.58	0.50
2:D:28:CYS:HB2	2:D:29:PRO:CD	2.41	0.50
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.46	0.50
1:A:314:ARG:HD3	1:A:334:GLU:OE1	2.12	0.50
2:F:358:GLU:O	2:F:362:ARG:HG2	2.11	0.50
2:F:220:GLU:HG2	2:F:517:ASP:OD1	2.11	0.50
2:H:35:LEU:HB3	2:H:100:LEU:HD11	1.94	0.50
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.40	0.50
2:B:735:LEU:O	2:B:738:SER:HB3	2.12	0.50
2:B:190:VAL:HG22	2:B:191:VAL:N	2.26	0.50
1:C:361:ILE:HG12	1:C:429:ARG:CZ	2.41	0.50
1:E:78:ILE:HG23	1:E:79:GLU:N	2.26	0.50
1:E:111:ILE:HD11	2:F:16:VAL:HG23	1.92	0.50
2:H:146:TRP:HZ3	2:H:313:LEU:HD13	1.76	0.50
2:H:166:PHE:CE2	2:H:355:ARG:HG3	2.46	0.50
2:F:482:ASN:ND2	2:F:514:THR:OG1	2.43	0.50
1:C:212:VAL:O	1:C:216:LEU:HA	2.12	0.50
1:A:361:ILE:HG12	1:A:429:ARG:NE	2.27	0.50
1:G:111:ILE:HD11	2:H:16:VAL:HG22	1.94	0.50
2:B:168:ILE:HD13	2:B:351:LEU:HD23	1.92	0.50
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.93	0.50
1:A:200:THR:HG21	1:A:219:LEU:HD13	1.93	0.50
2:H:53:GLU:HB3	2:H:54:PRO:HD3	1.92	0.50
2:F:77:SER:HB2	2:F:83:GLU:CB	2.38	0.50
1:C:214:LYS:NZ	2:D:258:ASP:OD1	2.43	0.50
1:G:430:ALA:HB1	1:G:434:TYR:HD2	1.77	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:462:PRO:HB3	2:D:706:ARG:HB2	1.94	0.49
2:F:216:ASP:OD1	2:H:512:ARG:HD2	2.11	0.49
1:A:392:LYS:HG3	1:A:422:PHE:HE2	1.77	0.49
2:F:146:TRP:CZ3	2:F:313:LEU:HD13	2.47	0.49
2:D:32:THR:HG23	2:D:252:PRO:HB2	1.93	0.49
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.93	0.49
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.94	0.49
2:B:641:ARG:HH21	2:B:706:ARG:HH12	1.60	0.49
2:H:38:GLY:HA3	2:H:99:PHE:CE2	2.48	0.49
1:E:411:ILE:CG2	1:E:443:ALA:HB1	2.43	0.49
2:D:238:LEU:H	2:D:238:LEU:HD12	1.77	0.49
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.93	0.49
2:B:702:SER:O	2:B:706:ARG:NH2	2.44	0.49
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.93	0.49
2:F:556:ALA:HB1	2:F:561:CYS:O	2.13	0.49
2:D:221:MET:HE1	2:D:224:MET:HG3	1.92	0.49
1:E:136:CYS:O	2:F:666:GLY:HA3	2.11	0.49
1:G:194:LEU:HD22	1:G:310:GLY:HA3	1.95	0.49
2:F:31:ASN:O	2:F:251:ARG:HD3	2.12	0.49
2:F:284:GLY:O	2:F:374:LEU:HD23	2.13	0.49
2:D:638:GLY:HA3	2:D:763:PRO:O	2.13	0.49
2:H:443:THR:O	2:H:635:ARG:HB2	2.12	0.49
1:A:111:ILE:HD11	2:B:16:VAL:HG22	1.94	0.49
2:F:663:GLN:HE22	5:F:1778:MPN:H1	1.59	0.49
1:C:140:ALA:N	1:C:141:PRO:HD2	2.27	0.49
1:A:190:ALA:HB1	1:A:310:GLY:CA	2.40	0.49
1:G:1:MET:HB2	1:G:179:PRO:CG	2.40	0.49
2:B:146:TRP:CZ3	2:B:313:LEU:HD13	2.48	0.49
2:D:309:ASP:OD1	2:D:330:ARG:NH2	2.44	0.49
2:B:554:PHE:HB2	2:B:594:ILE:CD1	2.42	0.49
4:C:1465:FAD:N1	4:C:1465:FAD:H2'	2.28	0.49
2:H:354:GLU:OE2	2:H:452:PRO:HD2	2.13	0.49
2:B:595:SER:HB2	2:D:601:PHE:CG	2.47	0.49
1:E:66:MET:O	1:E:69:GLN:HB2	2.13	0.49
2:H:261:ASP:HB3	2:H:265:ILE:HD12	1.95	0.49
1:A:361:ILE:HG12	1:A:429:ARG:NH2	2.28	0.48
1:C:457:VAL:HG23	2:D:634:ASP:HB2	1.94	0.48
1:C:216:LEU:HD22	2:D:107:ARG:HD3	1.94	0.48
1:G:411:ILE:HG13	1:G:447:VAL:HG21	1.95	0.48
2:D:495:LYS:O	2:D:499:VAL:HG23	2.13	0.48
1:A:444:LEU:O	1:A:448:ARG:HG3	2.12	0.48
2:F:39:LEU:HD22	2:F:95:GLY:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:661:ILE:O	2:F:665:GLU:HG3	2.13	0.48
2:D:319:TYR:OH	2:D:372:ARG:HD3	2.13	0.48
1:E:407:ARG:NH1	1:E:407:ARG:HB2	2.28	0.48
1:E:111:ILE:HD11	2:F:16:VAL:HG22	1.95	0.48
2:D:473:ILE:HG12	2:D:479:VAL:HG22	1.96	0.48
1:G:240:GLY:O	1:G:343:LYS:HE3	2.14	0.48
1:G:22:SER:OG	1:G:25:GLU:HG2	2.12	0.48
2:D:637:THR:OG1	2:D:639:GLU:HG3	2.13	0.48
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.93	0.48
2:B:328:SER:OG	2:B:330:ARG:NH1	2.46	0.48
1:G:164:PHE:O	1:G:166:LEU:HG	2.14	0.48
1:E:415:LEU:HD22	1:E:440:GLN:HB3	1.95	0.48
1:G:126:ASP:OD1	2:H:704:ARG:NH1	2.38	0.48
1:A:414:ALA:O	1:A:417:LEU:HD12	2.14	0.48
1:A:355:LYS:HE2	2:B:679:GLU:OE1	2.14	0.48
2:H:278:ILE:HG23	2:H:360:LEU:HD13	1.96	0.48
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.59	0.48
1:E:21:GLN:HG2	1:E:22:SER:N	2.29	0.48
2:B:398:LYS:HB3	2:B:399:LYS:NZ	2.29	0.48
2:B:446:ARG:HD3	2:B:632:VAL:HG13	1.95	0.48
2:H:341:PHE:O	2:H:342:ARG:C	2.51	0.48
1:G:241:TYR:O	1:G:341:LEU:N	2.43	0.48
1:E:371:THR:O	1:E:378:GLU:HB2	2.14	0.48
1:E:237:THR:HG23	1:E:240:GLY:O	2.14	0.48
1:E:43:ASP:CB	2:F:693:PRO:HB2	2.44	0.48
2:F:697:LYS:HD3	2:F:697:LYS:HA	1.56	0.48
1:G:408:GLU:OE2	1:G:444:LEU:HD22	2.14	0.48
1:A:37:GLU:OE1	2:B:256:ARG:NH2	2.47	0.48
1:A:243:ILE:HG21	1:A:252:LEU:HD13	1.96	0.47
2:B:641:ARG:NH2	2:B:706:ARG:NH1	2.62	0.47
1:A:64:LEU:HD13	1:A:206:THR:HG22	1.97	0.47
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.48	0.47
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.50	0.47
2:H:21:ARG:HH21	2:H:27:PRO:HD3	1.80	0.47
2:H:641:ARG:HH12	2:H:706:ARG:NH1	2.13	0.47
1:A:126:ASP:OD1	2:B:704:ARG:NH1	2.39	0.47
2:D:506:ILE:HD12	2:D:510:GLN:HB2	1.96	0.47
1:E:160:ALA:O	1:E:162:ALA:N	2.47	0.47
1:G:216:LEU:HD12	2:H:114:ARG:HH11	1.79	0.47
2:D:51:ASP:HB3	2:D:117:ARG:HB2	1.96	0.47
2:H:617:ARG:HD3	2:H:619:PHE:O	2.15	0.47
1:G:271:ALA:HB1	1:G:275:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:LEU:HD23	1:A:382:ILE:HG12	1.97	0.47
1:C:445:ARG:HG3	1:C:455:VAL:HG13	1.95	0.47
1:G:136:CYS:HB2	3:G:1463:FES:S2	2.54	0.47
1:E:18:ASP:OD2	1:E:20:THR:HG22	2.15	0.47
1:G:240:GLY:CA	1:G:343:LYS:HG2	2.25	0.47
1:E:289:SER:OG	1:E:291:ILE:HG13	2.15	0.47
1:A:309:ARG:HB3	1:A:312:GLU:CG	2.44	0.47
1:G:376:LYS:HA	1:G:404:GLN:O	2.15	0.47
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.96	0.47
1:E:164:PHE:C	1:E:166:LEU:H	2.18	0.47
2:B:215:HIS:ND1	2:D:478:SER:HB2	2.30	0.47
1:C:243:ILE:HD12	1:C:341:LEU:HG	1.97	0.47
1:C:299:ILE:O	1:C:381:ARG:NH1	2.46	0.47
1:G:359:GLN:O	1:G:359:GLN:HG3	2.15	0.47
2:D:697:LYS:N	2:D:697:LYS:HD2	2.30	0.47
1:G:141:PRO:HA	1:G:144:ARG:HH11	1.80	0.47
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.49	0.47
2:B:174:PHE:CZ	2:B:693:PRO:HG3	2.50	0.47
1:G:187:ASP:HA	1:G:308:ARG:HH22	1.80	0.47
2:F:449:ALA:O	2:F:628:ILE:HA	2.15	0.47
2:F:66:THR:CG2	2:F:67:ALA:N	2.78	0.46
2:F:453:VAL:HG21	2:F:735:LEU:HD23	1.96	0.46
2:H:456:GLY:HA3	2:H:619:PHE:CD1	2.50	0.46
2:B:22:TYR:N	2:B:22:TYR:CD1	2.84	0.46
2:F:341:PHE:CD2	2:F:342:ARG:N	2.73	0.46
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.63	0.46
1:E:111:ILE:CD1	2:F:16:VAL:HG22	2.46	0.46
2:H:35:LEU:HA	2:H:101:VAL:O	2.15	0.46
1:G:306:THR:HB	1:G:338:SER:HB2	1.98	0.46
2:H:517:ASP:OD2	2:H:519:SER:N	2.48	0.46
2:H:466:GLN:HA	2:H:602:TYR:O	2.15	0.46
1:G:390:VAL:CG2	1:G:391:PRO:HD2	2.44	0.46
2:D:168:ILE:HA	2:D:759:ALA:HB3	1.97	0.46
1:C:373:LYS:HB2	1:C:378:GLU:HG3	1.97	0.46
1:A:190:ALA:O	1:A:194:LEU:HB2	2.15	0.46
1:G:77:THR:OG1	1:G:79:GLU:HG2	2.15	0.46
1:E:298:LEU:HB2	1:E:318:LEU:CD2	2.45	0.46
1:G:371:THR:OG1	1:G:379:THR:HB	2.16	0.46
1:G:373:LYS:HB2	1:G:378:GLU:CG	2.45	0.46
2:B:160:HIS:HB3	2:B:364:MET:HE1	1.97	0.46
1:A:43:ASP:CB	2:B:693:PRO:HB2	2.45	0.46
2:F:238:LEU:HD11	2:F:257:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:661:ILE:O	2:B:665:GLU:HG3	2.15	0.46
2:F:197:GLN:HG2	2:F:488:MET:CE	2.45	0.46
2:F:143:PRO:HG3	2:F:329:HIS:CE1	2.50	0.46
2:D:717:ASN:O	2:D:724:ARG:HD2	2.16	0.46
2:D:461:LEU:HG	2:D:463:HIS:CE1	2.51	0.46
1:A:90:PRO:HB3	1:A:152:GLU:HG3	1.96	0.46
2:H:174:PHE:CZ	2:H:693:PRO:HG3	2.42	0.46
2:B:129:LEU:O	2:B:133:LEU:HD22	2.15	0.46
1:G:325:TYR:CE2	1:G:326:ARG:HG3	2.49	0.46
1:C:100:GLY:HA2	1:C:141:PRO:HB2	1.96	0.46
2:F:319:TYR:OH	2:F:372:ARG:HG2	2.15	0.46
2:F:50:LEU:CD1	2:F:118:ILE:HG12	2.45	0.46
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.50	0.46
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.48	0.46
1:G:133:LEU:HD13	2:H:698:ILE:HD11	1.97	0.46
2:H:310:ARG:HD2	2:H:344:PHE:O	2.16	0.46
2:H:771:ARG:O	2:H:775:GLY:N	2.43	0.46
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.40	0.46
2:H:53:GLU:HA	2:H:53:GLU:OE1	2.16	0.46
2:H:532:GLY:O	2:H:536:ASN:HB2	2.16	0.46
2:F:292:VAL:HG22	2:F:327:GLU:HB3	1.97	0.46
2:H:210:LEU:HD11	2:H:243:ALA:HB1	1.98	0.46
2:D:437:TRP:CE3	2:D:446:ARG:HG2	2.52	0.46
2:B:2:SER:N	2:B:502:ALA:HB2	2.31	0.46
1:G:366:GLY:HA3	1:G:442:MET:SD	2.56	0.46
1:E:302:GLY:HA2	1:E:381:ARG:CZ	2.45	0.46
1:A:48:THR:HG21	1:A:113:SER:OG	2.15	0.46
1:E:409:ASP:OD2	1:E:409:ASP:N	2.49	0.46
7:D:1780[B]:XAN:O2	8:D:1781:MOM:OM2	2.33	0.45
2:F:426:ASN:ND2	2:F:429:THR:HB	2.30	0.45
2:F:294:LEU:HD23	2:F:329:HIS:CD2	2.51	0.45
1:E:140:ALA:N	1:E:141:PRO:HD2	2.31	0.45
2:F:414:LEU:O	2:F:418:VAL:HG23	2.15	0.45
2:B:717:ASN:HD22	2:B:726:LYS:HG2	1.81	0.45
2:H:730:GLU:N	2:H:731:PRO:CD	2.80	0.45
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.97	0.45
2:H:465:ASN:HB3	2:H:604:THR:OG1	2.16	0.45
2:B:151:VAL:HG21	2:B:325:ARG:HB3	1.99	0.45
1:A:40:ASN:HA	1:A:40:ASN:HD22	1.61	0.45
2:F:129:LEU:HD21	2:F:296:ARG:HB2	1.99	0.45
1:C:111:ILE:CD1	2:D:16:VAL:HG22	2.46	0.45
1:E:288:GLY:HA2	1:E:322:PHE:HE2	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:276:TYR:OH	2:B:359:HIS:CD2	2.70	0.45
1:C:368:LEU:N	1:C:368:LEU:HD12	2.31	0.45
2:H:450:LEU:C	2:H:450:LEU:HD23	2.36	0.45
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.51	0.45
2:B:457:ILE:O	2:B:458:SER:HB2	2.17	0.45
2:B:151:VAL:HG11	2:B:290:ASP:HB2	1.97	0.45
2:B:139:PHE:O	2:B:140:GLU:HB2	2.17	0.45
2:F:554:PHE:HB2	2:F:594:ILE:CD1	2.46	0.45
2:D:146:TRP:CZ3	2:D:312:MET:HB3	2.51	0.45
1:A:8:ASN:OD1	1:A:80:GLY:HA3	2.15	0.45
2:F:573:VAL:CG2	2:F:585:ILE:HG13	2.46	0.45
2:F:554:PHE:HB2	2:F:594:ILE:HD13	1.98	0.45
1:E:225:LEU:O	1:E:227:HIS:N	2.50	0.45
2:F:215:HIS:ND1	2:H:478:SER:HB2	2.31	0.45
2:B:407:GLN:HG3	2:B:617:ARG:HG2	1.98	0.45
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.31	0.45
2:B:263:MET:CE	2:B:692:ALA:HA	2.47	0.45
1:A:140:ALA:N	1:A:141:PRO:HD2	2.32	0.45
2:D:566:VAL:HA	2:D:574:GLN:O	2.17	0.45
2:B:530:SER:HB2	2:B:727:ALA:HB1	1.99	0.45
1:G:89:HIS:HB3	1:G:92:GLN:HG3	1.99	0.45
2:B:341:PHE:O	2:B:342:ARG:C	2.55	0.45
1:G:370:LEU:HD22	1:G:380:ALA:HA	1.97	0.45
1:E:337:GLU:O	1:E:338:SER:HB3	2.17	0.45
2:D:263:MET:HE3	2:D:692:ALA:HA	1.98	0.45
1:G:325:TYR:O	1:G:326:ARG:HB2	2.17	0.45
1:A:77:THR:OG1	1:A:79:GLU:HG2	2.17	0.45
2:F:296:ARG:O	2:F:338:ASN:ND2	2.44	0.45
2:B:150:ASP:OD2	2:F:423:LYS:CE	2.65	0.45
2:H:302:ASP:OD1	2:H:303:LEU:N	2.50	0.45
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.45
2:B:187:GLU:HG2	2:D:21:ARG:HD2	1.99	0.45
1:E:373:LYS:HB2	1:E:378:GLU:HG3	1.99	0.45
2:B:184:LEU:HD23	2:B:252:PRO:HB3	1.99	0.45
1:E:205:GLY:O	1:E:209:SER:OG	2.24	0.45
1:A:299:ILE:O	1:A:381:ARG:NH1	2.50	0.45
1:C:273:GLU:HA	1:C:276:ARG:NH1	2.31	0.45
1:G:253:ARG:HH21	1:G:268:ARG:HG3	1.77	0.45
2:H:663:GLN:HE22	5:H:1778:MPN:H1	1.65	0.45
2:H:542:ASP:OD2	2:H:600:GLY:HA2	2.17	0.45
2:B:566:VAL:HG13	2:B:575:ALA:HB2	1.98	0.45
1:C:216:LEU:CD2	2:D:107:ARG:HD3	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:283:SER:O	2:F:366:ARG:NH1	2.45	0.44
2:F:321:VAL:HG12	2:F:323:ALA:O	2.17	0.44
1:A:428:MET:H	1:A:428:MET:CE	2.30	0.44
2:F:273:ARG:HD2	2:F:294:LEU:HD12	1.98	0.44
2:H:197:GLN:HG2	2:H:488:MET:HE1	1.99	0.44
2:B:276:TYR:OH	2:B:359:HIS:HD2	2.00	0.44
2:D:175:TYR:O	2:D:259:ARG:NH2	2.37	0.44
2:H:484:GLY:HA3	2:H:524:THR:HG21	2.00	0.44
1:C:216:LEU:HD22	2:D:107:ARG:CD	2.47	0.44
1:G:92:GLN:HB3	2:H:16:VAL:HG13	1.98	0.44
2:B:129:LEU:O	2:B:132:ALA:HB3	2.16	0.44
2:F:580:TRP:HB2	2:F:585:ILE:HD11	1.98	0.44
1:E:240:GLY:HA3	1:E:341:LEU:O	2.18	0.44
1:G:139:TYR:HA	1:G:142:ILE:HD12	1.98	0.44
2:D:398:LYS:HB3	2:D:399:LYS:HD2	1.99	0.44
2:F:222:ARG:HD2	2:F:515:ALA:HB2	1.99	0.44
1:E:228:CYS:SG	1:E:228:CYS:O	2.75	0.44
2:D:450:LEU:HB2	2:D:628:ILE:HG12	1.99	0.44
2:B:236:ASN:N	2:B:236:ASN:HD22	2.15	0.44
2:B:269:ARG:NH2	2:B:733:PHE:CZ	2.85	0.44
1:C:216:LEU:CD1	2:D:114:ARG:NH1	2.71	0.44
1:E:322:PHE:CB	1:E:390:VAL:HG23	2.48	0.44
2:H:434:ILE:HD13	2:H:448:ILE:HB	1.99	0.44
2:H:446:ARG:HD3	2:H:632:VAL:HG13	1.99	0.44
1:A:400:ALA:HB3	1:A:417:LEU:HD13	1.99	0.44
1:G:131:GLY:HA3	1:G:274:GLN:OE1	2.18	0.44
1:E:89:HIS:O	1:E:90:PRO:C	2.56	0.44
2:D:133:LEU:HD12	2:D:133:LEU:HA	1.87	0.44
2:H:171:GLN:NE2	2:H:674:TRP:HB2	2.33	0.44
2:H:499:VAL:O	2:H:503:VAL:HG23	2.18	0.44
1:G:24:LEU:HD13	1:G:47:CYS:HB2	1.99	0.44
2:B:35:LEU:HA	2:B:101:VAL:O	2.17	0.44
1:A:92:GLN:HB3	2:B:16:VAL:HG13	1.99	0.44
2:H:729:GLY:HA3	5:H:1778:MPN:H4'1	1.99	0.44
1:G:460:VAL:HG21	2:H:632:VAL:HG11	1.99	0.44
1:C:393:ARG:HD2	1:C:398:GLU:OE1	2.17	0.44
2:F:767:LEU:O	2:F:771:ARG:HG3	2.18	0.44
2:H:272:PHE:HA	2:H:294:LEU:O	2.17	0.44
1:G:322:PHE:CB	1:G:390:VAL:CG2	2.95	0.44
2:B:360:LEU:O	2:B:364:MET:HE3	2.18	0.44
2:D:46:ALA:HB2	2:D:123:ARG:NH2	2.33	0.44
2:D:306:PRO:HB2	2:D:344:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:7:LEU:HD13	1:E:75:LEU:HD23	1.99	0.44
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.99	0.44
2:H:423:LYS:HE2	2:H:423:LYS:HB3	1.65	0.44
2:F:631:VAL:HG21	2:F:743:LEU:HA	2.00	0.44
1:A:365:CYS:O	1:A:384:PHE:HA	2.17	0.44
2:F:160:HIS:CB	2:F:364:MET:HE2	2.48	0.43
1:E:181:PHE:CZ	1:E:183:PRO:HB3	2.53	0.43
2:D:650:ASP:HA	2:D:713:TRP:HB3	2.00	0.43
2:F:133:LEU:HD12	2:F:133:LEU:HA	1.76	0.43
1:E:12:ARG:NH1	1:E:12:ARG:HG2	2.22	0.43
1:G:205:GLY:O	1:G:209:SER:OG	2.28	0.43
2:B:186:ALA:O	2:B:187:GLU:C	2.57	0.43
2:F:418:VAL:HG13	2:F:450:LEU:HD11	2.00	0.43
2:H:419:THR:O	2:H:423:LYS:HD2	2.19	0.43
1:A:397:PHE:HE1	1:A:415:LEU:HA	1.84	0.43
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.86	0.43
2:D:76:ALA:HB2	2:D:85:VAL:CG2	2.47	0.43
2:H:310:ARG:HA	2:H:313:LEU:HB2	1.99	0.43
2:D:280:ALA:HB3	2:D:364:MET:CE	2.47	0.43
2:F:528:ALA:HA	5:F:1778:MPN:S2'	2.59	0.43
1:C:211:TRP:O	1:C:215:ALA:HB3	2.18	0.43
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.51	0.43
1:E:295:PRO:HB2	1:E:296:PRO:HD3	2.00	0.43
2:F:670:GLN:HG2	2:F:733:PHE:HE1	1.83	0.43
2:H:106:HIS:CE1	2:H:110:ARG:HD3	2.53	0.43
1:G:202:ILE:HD12	1:G:222:VAL:HG11	2.00	0.43
2:F:236:ASN:HD22	2:F:236:ASN:HA	1.69	0.43
1:A:366:GLY:HA3	1:A:442:MET:SD	2.57	0.43
2:H:671:GLY:O	2:H:674:TRP:HB3	2.19	0.43
2:H:376:PHE:HE2	2:H:452:PRO:HG3	1.84	0.43
2:D:354:GLU:OE1	2:D:372:ARG:NE	2.50	0.43
2:H:328:SER:OG	2:H:330:ARG:NH1	2.47	0.43
2:B:700:ALA:O	2:B:703:ASP:HB2	2.18	0.43
1:G:7:LEU:O	1:G:8:ASN:C	2.56	0.43
1:E:325:TYR:O	1:E:326:ARG:HB2	2.18	0.43
1:A:291:ILE:HG12	1:A:291:ILE:H	1.74	0.43
1:G:414:ALA:O	1:G:417:LEU:HD12	2.18	0.43
1:A:207:ASP:OD2	4:A:1465:FAD:O2'	2.27	0.43
2:H:221:MET:HE2	2:H:486:THR:HB	2.01	0.43
2:B:597:SER:HB2	2:D:522:PRO:HG3	1.99	0.43
1:E:6:LEU:HD12	1:E:10:GLU:C	2.38	0.43
1:G:15:ARG:HG2	1:G:15:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:214:LYS:HA	1:E:214:LYS:HD3	1.85	0.43
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.33	0.43
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.99	0.43
2:H:81:SER:HA	2:H:82:PRO:HD3	1.92	0.43
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.53	0.43
1:A:212:VAL:O	2:B:107:ARG:NH1	2.51	0.43
1:A:370:LEU:HD22	1:A:380:ALA:HA	1.99	0.43
2:D:278:ILE:HD11	2:D:286:LEU:HD22	2.00	0.43
2:D:437:TRP:CZ3	2:D:446:ARG:HG2	2.53	0.43
1:E:355:LYS:HZ2	1:E:429:ARG:HA	1.84	0.43
1:A:351:TYR:CZ	1:A:445:ARG:HD3	2.53	0.43
2:D:318:SER:HB3	2:D:414:LEU:HD13	2.00	0.43
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.99	0.43
1:C:357:PHE:HE1	2:D:640:ASN:O	2.01	0.43
2:F:306:PRO:HB2	2:F:344:PHE:HZ	1.84	0.43
1:G:143:LEU:O	1:G:143:LEU:HD23	2.18	0.43
1:E:114:MET:HE3	1:E:114:MET:HB2	1.88	0.43
2:B:683:ASP:OD1	2:B:685:CYS:N	2.49	0.43
1:A:308:ARG:O	1:A:334:GLU:HA	2.19	0.43
2:F:451:SER:HA	2:F:452:PRO:HD3	1.83	0.43
1:A:36:LYS:NZ	2:B:25:ASP:OD2	2.51	0.43
1:G:40:ASN:HA	1:G:40:ASN:HD22	1.54	0.43
1:E:248:THR:HA	1:E:279:ALA:O	2.19	0.42
2:B:313:LEU:HD12	2:B:405:TYR:CD2	2.54	0.42
1:G:8:ASN:HA	1:G:76:ARG:HD3	2.00	0.42
2:B:306:PRO:HB2	2:B:344:PHE:HE2	1.84	0.42
1:C:245:ALA:O	1:C:280:THR:HB	2.18	0.42
2:F:289:ALA:O	2:F:324:LEU:HA	2.19	0.42
2:H:554:PHE:HB2	2:H:594:ILE:CD1	2.48	0.42
2:B:449:ALA:CB	2:B:741:LEU:HB3	2.49	0.42
2:H:683:ASP:OD1	2:H:683:ASP:C	2.58	0.42
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.54	0.42
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.79	0.42
1:C:292:GLY:HA2	4:C:1465:FAD:O2	2.19	0.42
2:F:482:ASN:ND2	2:F:520:LYS:HD3	2.34	0.42
2:H:308:CYS:O	2:H:312:MET:HG3	2.19	0.42
2:H:288:GLY:HA2	2:H:323:ALA:O	2.19	0.42
2:H:497:VAL:HG13	2:H:511:VAL:HB	2.01	0.42
2:F:461:LEU:HD11	2:F:463:HIS:CE1	2.54	0.42
2:B:558:ARG:HB3	2:B:558:ARG:HE	1.70	0.42
2:D:440:THR:O	2:D:440:THR:HG22	2.18	0.42
1:G:102:GLN:HG3	1:G:137:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:335:PHE:HD1	1:G:336:VAL:O	2.01	0.42
2:F:2:SER:N	2:F:502:ALA:HB2	2.34	0.42
2:H:417:LEU:HG	2:H:648:LEU:HD23	1.99	0.42
1:E:324:GLU:HB2	1:E:327:LYS:HD3	2.01	0.42
1:E:321:PHE:CE1	1:E:328:GLN:HB3	2.55	0.42
2:B:487:GLU:HB2	2:B:493:HIS:CD2	2.53	0.42
2:B:70:LEU:HA	2:B:71:PRO:HD3	1.95	0.42
2:H:146:TRP:CH2	2:H:313:LEU:HD13	2.54	0.42
1:E:415:LEU:HD22	1:E:440:GLN:CB	2.49	0.42
1:E:39:CYS:O	1:E:41:GLU:HB2	2.19	0.42
1:G:295:PRO:O	1:G:296:PRO:C	2.58	0.42
1:A:442:MET:O	1:A:445:ARG:HB3	2.19	0.42
1:A:462:PRO:HG3	2:B:706:ARG:HB3	2.02	0.42
1:A:356:ARG:CZ	2:B:697:LYS:HZ3	2.32	0.42
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.55	0.42
2:B:31:ASN:O	2:B:251:ARG:HD3	2.20	0.42
2:D:53:GLU:HB3	2:D:54:PRO:CD	2.48	0.42
2:D:143:PRO:HB3	2:D:329:HIS:CE1	2.55	0.42
1:C:111:ILE:HD11	2:D:16:VAL:HG22	2.02	0.42
1:A:392:LYS:CG	1:A:422:PHE:HE2	2.32	0.42
2:F:437:TRP:CE3	2:F:446:ARG:HG3	2.54	0.42
1:C:96:ILE:HD11	2:D:13:ARG:HA	2.01	0.42
2:H:269:ARG:HH11	2:H:269:ARG:HG3	1.85	0.42
1:G:126:ASP:OD2	2:H:706:ARG:NH2	2.53	0.42
1:E:355:LYS:HZ1	1:E:429:ARG:HA	1.84	0.42
2:H:21:ARG:HB3	2:H:25:ASP:HB2	2.00	0.42
2:F:238:LEU:HD11	2:F:257:TYR:CE1	2.55	0.42
2:F:461:LEU:CD1	2:F:463:HIS:CE1	3.02	0.42
2:B:771:ARG:HD2	2:B:776:ARG:HD2	2.01	0.42
2:D:303:LEU:O	2:D:307:VAL:HG23	2.19	0.42
1:A:192:TRP:O	1:A:196:HIS:HD2	2.01	0.42
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.95	0.42
2:B:160:HIS:CB	2:B:364:MET:CE	2.97	0.42
2:B:407:GLN:HE22	2:B:619:PHE:HB2	1.85	0.42
2:F:419:THR:O	2:F:423:LYS:HG2	2.18	0.42
2:B:186:ALA:O	2:B:187:GLU:O	2.38	0.42
1:G:373:LYS:O	1:G:375:SER:N	2.45	0.42
1:G:103:CYS:HB3	1:G:136:CYS:SG	2.60	0.42
2:H:158:ALA:O	2:H:159:ALA:C	2.57	0.42
2:F:302:ASP:OD1	2:F:303:LEU:N	2.48	0.42
1:A:108:PRO:O	1:A:112:VAL:HG23	2.20	0.42
1:G:43:ASP:CB	2:H:693:PRO:HB2	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:78:ILE:CD1	1:G:111:ILE:HG21	2.50	0.42
2:H:23:LEU:CD1	2:H:194:CYS:HA	2.47	0.42
1:A:234:ILE:HG12	1:A:243:ILE:HG23	2.02	0.42
2:H:530:SER:O	2:H:727:ALA:CB	2.68	0.42
2:F:732:PRO:HA	2:F:735:LEU:HG	2.02	0.42
2:B:730:GLU:N	2:B:731:PRO:HD2	2.34	0.42
1:E:100:GLY:HA2	1:E:141:PRO:HB2	2.02	0.42
1:E:322:PHE:HB3	1:E:390:VAL:HG23	2.02	0.42
2:H:95:GLY:HA3	2:H:264:VAL:HG12	2.02	0.42
1:E:312:GLU:HG3	1:E:312:GLU:H	1.54	0.42
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.73	0.42
2:B:381:GLU:OE2	2:B:381:GLU:HA	2.20	0.42
1:A:345:ALA:HB3	1:A:346:PRO:CA	2.38	0.41
2:F:175:TYR:O	2:F:259:ARG:NH2	2.51	0.41
1:A:301:MET:HB3	1:A:348:LEU:HD22	2.01	0.41
1:G:184:GLU:HA	1:G:227:HIS:O	2.20	0.41
2:F:53:GLU:N	2:F:54:PRO:CD	2.83	0.41
2:F:129:LEU:HD22	2:F:331:LEU:HD12	2.02	0.41
2:B:417:LEU:HG	2:B:648:LEU:HD23	2.02	0.41
1:A:356:ARG:NH2	2:B:697:LYS:NZ	2.68	0.41
2:F:358:GLU:HB2	2:F:372:ARG:HH22	1.85	0.41
1:A:249:ILE:HG23	1:A:267:LEU:HD22	2.03	0.41
1:E:417:LEU:O	1:E:420:GLN:HB2	2.19	0.41
2:F:551:LEU:HD23	2:F:551:LEU:HA	1.92	0.41
1:G:47:CYS:SG	1:G:63:CYS:HB3	2.59	0.41
2:B:53:GLU:HB3	2:B:54:PRO:HD3	2.01	0.41
2:F:271:ASP:OD1	2:F:296:ARG:HD2	2.20	0.41
1:A:314:ARG:NH1	1:A:334:GLU:OE2	2.53	0.41
1:G:149:ALA:O	1:G:152:GLU:HB2	2.20	0.41
1:A:370:LEU:CD2	1:A:380:ALA:HA	2.50	0.41
1:A:192:TRP:O	1:A:196:HIS:CD2	2.74	0.41
1:E:216:LEU:HD13	2:F:111:ILE:HG13	2.02	0.41
2:B:177:GLU:OE1	2:B:225:GLY:N	2.50	0.41
2:B:597:SER:HB2	2:D:522:PRO:CG	2.51	0.41
1:C:136:CYS:O	2:D:666:GLY:HA3	2.20	0.41
2:B:170:GLY:N	2:B:271:ASP:HB3	2.35	0.41
2:B:649:HIS:O	2:B:713:TRP:N	2.52	0.41
1:A:316:MET:HG3	1:A:317:PRO:O	2.21	0.41
2:B:215:HIS:CG	2:D:478:SER:HB2	2.55	0.41
2:H:309:ASP:OD1	2:H:330:ARG:NH2	2.44	0.41
2:F:367:ASP:HA	2:F:368:PRO:HD3	1.85	0.41
1:G:461:MET:HA	1:G:462:PRO:HD2	1.78	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:ASN:HA	1:A:76:ARG:CD	2.50	0.41
1:A:6:LEU:HD13	1:A:164:PHE:CD1	2.56	0.41
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.24	0.41
2:F:493:HIS:CG	2:F:513:ILE:HG12	2.55	0.41
2:H:222:ARG:NH2	2:H:493:HIS:HD2	2.19	0.41
2:B:221:MET:HE1	2:B:224:MET:HG3	2.02	0.41
2:F:650:ASP:HA	2:F:713:TRP:HB3	2.03	0.41
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.52	0.41
2:B:40:SER:HB2	2:B:98:ILE:HD11	2.03	0.41
2:H:126:ILE:HD12	2:H:137:SER:CB	2.50	0.41
2:B:706:ARG:HD3	2:B:706:ARG:HA	1.36	0.41
2:D:328:SER:OG	2:D:330:ARG:NH1	2.48	0.41
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.56	0.41
2:D:492:LEU:O	2:D:496:MET:HG2	2.20	0.41
2:F:45:ALA:HB1	2:F:120:TYR:HB3	2.03	0.41
1:E:78:ILE:HD13	1:E:108:PRO:HA	2.02	0.41
1:A:404:GLN:HB3	1:A:410:THR:CG2	2.50	0.41
1:G:8:ASN:HA	1:G:76:ARG:CD	2.51	0.41
1:E:191:ASP:O	1:E:194:LEU:HB3	2.20	0.41
2:B:574:GLN:HG2	2:B:579:SER:HB3	2.02	0.41
2:H:358:GLU:O	2:H:362:ARG:HG2	2.20	0.41
1:G:36:LYS:HA	1:G:36:LYS:HD3	1.82	0.41
1:C:361:ILE:HG12	1:C:429:ARG:NE	2.35	0.41
4:E:1465:FAD:N1	4:E:1465:FAD:C2'	2.84	0.41
1:A:231:LEU:CD2	1:A:245:ALA:HB3	2.51	0.41
2:H:563:ALA:O	2:H:566:VAL:HG23	2.21	0.41
2:B:437:TRP:CE3	2:B:446:ARG:HG3	2.55	0.41
1:G:399:ALA:C	1:G:401:LEU:H	2.23	0.41
2:D:461:LEU:HD23	2:D:464:LEU:HD11	2.03	0.41
1:G:249:ILE:HG21	1:G:270:PHE:CD2	2.56	0.41
2:D:671:GLY:HA2	2:D:733:PHE:CZ	2.56	0.41
1:E:314:ARG:NH1	1:E:334:GLU:OE2	2.54	0.41
2:D:170:GLY:N	2:D:271:ASP:HB3	2.36	0.41
2:D:632:VAL:HG22	2:D:643:LEU:HD11	2.03	0.41
1:G:207:ASP:OD2	4:G:1465:FAD:O2'	2.35	0.41
1:C:445:ARG:HG3	1:C:455:VAL:CG1	2.51	0.41
2:B:446:ARG:HG2	2:B:632:VAL:HG12	2.02	0.41
2:D:160:HIS:HB2	2:D:364:MET:HE1	2.03	0.41
2:D:21:ARG:HH21	2:D:27:PRO:HD2	1.85	0.41
2:B:325:ARG:HH11	2:B:325:ARG:HG2	1.85	0.41
2:B:205:LYS:HG3	2:B:236:ASN:OD1	2.21	0.41
1:A:295:PRO:O	1:A:296:PRO:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:754:TRP:HA	2:B:755:PRO:HD3	1.94	0.40
2:H:730:GLU:H	2:H:731:PRO:CD	2.35	0.40
2:F:76:ALA:HB2	2:F:85:VAL:HG22	2.03	0.40
2:B:35:LEU:HB3	2:B:100:LEU:HD11	2.02	0.40
2:B:66:THR:CG2	2:B:68:ALA:H	2.29	0.40
2:B:152:GLU:HG2	2:F:423:LYS:HB2	2.02	0.40
1:C:22:SER:OG	1:C:25:GLU:HG2	2.20	0.40
2:F:366:ARG:NE	2:F:370:GLU:OE1	2.47	0.40
2:F:610:ASP:N	2:F:615:GLN:O	2.45	0.40
2:D:165:CYS:HA	2:D:274:ILE:O	2.21	0.40
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.56	0.40
2:B:219:VAL:O	2:B:517:ASP:HA	2.21	0.40
1:G:49:VAL:HA	1:G:112:VAL:HG11	2.03	0.40
2:D:667:ALA:HB3	2:D:732:PRO:HB2	2.04	0.40
1:G:18:ASP:HA	1:G:19:PRO:HD3	1.94	0.40
1:A:203:ALA:HB3	4:A:1465:FAD:O1P	2.21	0.40
2:B:697:LYS:HG3	2:B:697:LYS:HZ2	1.70	0.40
1:E:216:LEU:HD12	2:F:114:ARG:NH1	2.36	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	446/462 (96%)	402 (90%)	38 (8%)	6 (1%)	18	35
1	C	446/462 (96%)	422 (95%)	20 (4%)	4 (1%)	25	49
1	E	446/462 (96%)	389 (87%)	46 (10%)	11 (2%)	9	14
1	G	446/462 (96%)	383 (86%)	56 (13%)	7 (2%)	14	28
2	B	756/777 (97%)	706 (93%)	39 (5%)	11 (2%)	15	30
2	D	756/777 (97%)	713 (94%)	36 (5%)	7 (1%)	25	49
2	F	756/777 (97%)	707 (94%)	41 (5%)	8 (1%)	21	42
2	H	756/777 (97%)	689 (91%)	58 (8%)	9 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4808/4956 (97%)	4411 (92%)	334 (7%)	63 (1%)	18	35

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	A	345	ALA
2	B	187	GLU
2	B	458	SER
2	D	458	SER
1	E	374	GLY
2	F	458	SER
1	G	375	SER
2	H	187	GLU
2	H	458	SER
2	H	561	CYS
1	A	359	GLN
2	B	560	GLY
2	B	561	CYS
1	C	165	THR
1	C	374	GLY
2	D	141	GLY
2	D	560	GLY
1	E	161	ASP
1	E	226	SER
2	F	187	GLU
2	F	399	LYS
2	F	560	GLY
2	F	608	SER
1	G	221	GLU
1	G	378	GLU
2	H	227	GLY
2	H	342	ARG
2	H	399	LYS
2	H	560	GLY
1	A	395	ALA
2	B	141	GLY
2	B	227	GLY
2	B	342	ARG
2	B	738	SER
2	D	342	ARG
2	D	399	LYS

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Mol	Chain	Res	Type
1	E	39	CYS
1	E	221	GLU
1	E	395	ALA
1	E	410	THR
2	F	82	PRO
2	F	342	ARG
1	G	400	ALA
2	H	436	ALA
2	H	558	ARG
1	A	39	CYS
1	C	39	CYS
1	C	359	GLN
1	E	165	THR
1	E	187	ASP
1	E	378	GLU
1	G	310	GLY
1	G	437	ASN
2	B	215	HIS
2	B	336	GLN
2	B	399	LYS
1	G	374	GLY
2	D	227	GLY
2	F	227	GLY
1	A	220	PRO
2	D	452	PRO
1	E	261	PRO

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	339/347 (98%)	311 (92%)	28 (8%)	16	30
1	C	339/347 (98%)	311 (92%)	28 (8%)	16	30
1	E	339/347 (98%)	306 (90%)	33 (10%)	12	22
1	G	339/347 (98%)	304 (90%)	35 (10%)	10	19
2	B	571/584 (98%)	524 (92%)	47 (8%)	17	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	571/584 (98%)	530 (93%)	41 (7%)	21	39
2	F	571/584 (98%)	523 (92%)	48 (8%)	16	29
2	H	571/584 (98%)	529 (93%)	42 (7%)	20	38
All	All	3640/3724 (98%)	3338 (92%)	302 (8%)	16	30

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	20	THR
1	A	33	THR
1	A	40	ASN
1	A	43	ASP
1	A	58	ARG
1	A	76	ARG
1	A	79	GLU
1	A	128	LEU
1	A	143	LEU
1	A	191	ASP
1	A	212	VAL
1	A	239	ASP
1	A	291	ILE
1	A	320	ASP
1	A	338	SER
1	A	361	ILE
1	A	371	THR
1	A	378	GLU
1	A	390	VAL
1	A	393	ARG
1	A	408	GLU
1	A	409	ASP
1	A	410	THR
1	A	411	ILE
1	A	428	MET
1	A	450	LEU
1	A	457	VAL
2	B	10	ASP
2	B	16	VAL
2	B	66	THR
2	B	126	ILE
2	B	133	LEU

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Mol	Chain	Res	Type
2	B	151	VAL
2	B	161	LEU
2	B	165	CYS
2	B	175	TYR
2	B	176	LEU
2	B	187	GLU
2	B	215	HIS
2	B	221	MET
2	B	222	ARG
2	B	256	ARG
2	B	268	LYS
2	B	271	ASP
2	B	313	LEU
2	B	330	ARG
2	B	341	PHE
2	B	355	ARG
2	B	359	HIS
2	B	366	ARG
2	B	381	GLU
2	B	399	LYS
2	B	423	LYS
2	B	440	THR
2	B	442	ARG
2	B	461	LEU
2	B	472	GLN
2	B	512	ARG
2	B	530	SER
2	B	564	ARG
2	B	604	THR
2	B	609	TRP
2	B	617	ARG
2	B	632	VAL
2	B	641	ARG
2	B	650	ASP
2	B	695	THR
2	B	697	LYS
2	B	704	ARG
2	B	706	ARG
2	B	708	PHE
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS

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Mol	Chain	Res	Type
1	C	1	MET
1	C	11	THR
1	C	12	ARG
1	C	33	THR
1	C	40	ASN
1	C	76	ARG
1	C	128	LEU
1	C	143	LEU
1	C	165	THR
1	C	212	VAL
1	C	219	LEU
1	C	231	LEU
1	C	237	THR
1	C	270	PHE
1	C	281	ILE
1	C	309	ARG
1	C	355	LYS
1	C	361	ILE
1	C	376	LYS
1	C	379	THR
1	C	405	ASP
1	C	409	ASP
1	C	420	GLN
1	C	425	LEU
1	C	435	ARG
1	C	447	VAL
1	C	451	SER
1	C	455	VAL
2	D	10	ASP
2	D	16	VAL
2	D	23	LEU
2	D	66	THR
2	D	81	SER
2	D	107	ARG
2	D	130	ASP
2	D	148	ARG
2	D	151	VAL
2	D	152	GLU
2	D	174	PHE
2	D	175	TYR
2	D	215	HIS
2	D	221	MET

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Mol	Chain	Res	Type
2	D	222	ARG
2	D	247	ARG
2	D	256	ARG
2	D	258	ASP
2	D	260	ASP
2	D	268	LYS
2	D	313	LEU
2	D	330	ARG
2	D	341	PHE
2	D	366	ARG
2	D	367	ASP
2	D	381	GLU
2	D	398	LYS
2	D	399	LYS
2	D	400	THR
2	D	431	ARG
2	D	450	LEU
2	D	512	ARG
2	D	530	SER
2	D	561	CYS
2	D	613	ARG
2	D	617	ARG
2	D	632	VAL
2	D	697	LYS
2	D	704	ARG
2	D	708	PHE
2	D	741	LEU
1	E	1	MET
1	E	11	THR
1	E	12	ARG
1	E	33	THR
1	E	40	ASN
1	E	43	ASP
1	E	44	CYS
1	E	69	GLN
1	E	76	ARG
1	E	79	GLU
1	E	101	SER
1	E	128	LEU
1	E	143	LEU
1	E	165	THR
1	E	187	ASP

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Mol	Chain	Res	Type
1	E	228	CYS
1	E	231	LEU
1	E	237	THR
1	E	257	GLU
1	E	281	ILE
1	E	301	MET
1	E	309	ARG
1	E	341	LEU
1	E	344	SER
1	E	354	SER
1	E	379	THR
1	E	390	VAL
1	E	401	LEU
1	E	409	ASP
1	E	423	THR
1	E	425	LEU
1	E	447	VAL
1	E	450	LEU
2	F	10	ASP
2	F	16	VAL
2	F	48	THR
2	F	53	GLU
2	F	130	ASP
2	F	151	VAL
2	F	165	CYS
2	F	166	PHE
2	F	175	TYR
2	F	176	LEU
2	F	182	LEU
2	F	190	VAL
2	F	215	HIS
2	F	218	ARG
2	F	247	ARG
2	F	256	ARG
2	F	258	ASP
2	F	259	ARG
2	F	268	LYS
2	F	310	ARG
2	F	313	LEU
2	F	330	ARG
2	F	341	PHE
2	F	355	ARG

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Mol	Chain	Res	Type
2	F	366	ARG
2	F	370	GLU
2	F	381	GLU
2	F	398	LYS
2	F	399	LYS
2	F	405	TYR
2	F	428	THR
2	F	439	SER
2	F	450	LEU
2	F	461	LEU
2	F	512	ARG
2	F	516	THR
2	F	530	SER
2	F	534	ASP
2	F	558	ARG
2	F	567	ILE
2	F	608	SER
2	F	617	ARG
2	F	630	GLU
2	F	632	VAL
2	F	641	ARG
2	F	704	ARG
2	F	708	PHE
2	F	741	LEU
1	G	25	GLU
1	G	33	THR
1	G	35	THR
1	G	40	ASN
1	G	63	CYS
1	G	76	ARG
1	G	79	GLU
1	G	91	VAL
1	G	103	CYS
1	G	128	LEU
1	G	198	GLU
1	G	212	VAL
1	G	218	ASP
1	G	231	LEU
1	G	243	ILE
1	G	257	GLU
1	G	281	ILE
1	G	289	SER

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Mol	Chain	Res	Type
1	G	291	ILE
1	G	301	MET
1	G	311	GLN
1	G	315	ARG
1	G	326	ARG
1	G	327	LYS
1	G	338	SER
1	G	339	VAL
1	G	340	THR
1	G	341	LEU
1	G	371	THR
1	G	393	ARG
1	G	401	LEU
1	G	409	ASP
1	G	410	THR
1	G	420	GLN
1	G	457	VAL
2	H	10	ASP
2	H	16	VAL
2	H	23	LEU
2	H	66	THR
2	H	90	GLU
2	H	148	ARG
2	H	151	VAL
2	H	165	CYS
2	H	174	PHE
2	H	175	TYR
2	H	215	HIS
2	H	221	MET
2	H	222	ARG
2	H	258	ASP
2	H	260	ASP
2	H	268	LYS
2	H	271	ASP
2	H	313	LEU
2	H	326	ILE
2	H	330	ARG
2	H	341	PHE
2	H	355	ARG
2	H	398	LYS
2	H	399	LYS
2	H	400	THR

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Mol	Chain	Res	Type
2	H	423	LYS
2	H	424	SER
2	H	431	ARG
2	H	446	ARG
2	H	512	ARG
2	H	534	ASP
2	H	564	ARG
2	H	604	THR
2	H	617	ARG
2	H	632	VAL
2	H	650	ASP
2	H	677	THR
2	H	697	LYS
2	H	704	ARG
2	H	708	PHE
2	H	741	LEU
2	H	743	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	196	HIS
1	A	359	GLN
2	B	204	HIS
2	B	208	HIS
2	B	236	ASN
2	B	293	HIS
2	B	359	HIS
2	B	426	ASN
2	B	463	HIS
2	B	574	GLN
1	C	40	ASN
1	C	233	GLN
1	C	359	GLN
1	C	420	GLN
2	D	198	HIS
2	D	208	HIS
2	D	236	ASN
2	D	293	HIS
2	D	359	HIS
2	D	426	ASN

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Mol	Chain	Res	Type
2	D	463	HIS
2	D	744	HIS
1	E	40	ASN
1	E	61	ASN
1	E	196	HIS
1	E	359	GLN
2	F	19	GLN
2	F	204	HIS
2	F	236	ASN
2	F	359	HIS
2	F	426	ASN
2	F	463	HIS
2	F	482	ASN
2	F	574	GLN
2	F	744	HIS
1	G	40	ASN
1	G	196	HIS
1	G	328	GLN
1	G	359	GLN
2	H	106	HIS
2	H	208	HIS
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	441	ASN
2	H	572	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

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

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$
3	FES	A	1463	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	A	1464	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	A	1465	-	58,58,58	1.59	9 (15%)	85,89,89	2.00	16 (18%)
5	MPN	B	1778	8	26,26,26	7.92	7 (26%)	33,40,40	3.09	13 (39%)
7	XAN	B	1780[A]	-	12,12,12	2.02	3 (25%)	11,17,17	8.13	3 (27%)
7	XAN	B	1780[B]	-	12,12,12	2.11	3 (25%)	11,17,17	8.61	3 (27%)
8	MOM	B	1781	5	0,3,3	0.00	-	0,3,3	0.00	-
3	FES	C	1463	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	C	1464	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	C	1465	-	58,58,58	1.59	11 (18%)	85,89,89	2.29	21 (24%)
5	MPN	D	1778	8	26,26,26	8.88	7 (26%)	33,40,40	3.02	15 (45%)
7	XAN	D	1780[A]	-	12,12,12	1.92	3 (25%)	11,17,17	8.03	3 (27%)
7	XAN	D	1780[B]	-	12,12,12	2.08	3 (25%)	11,17,17	9.23	3 (27%)
8	MOM	D	1781	5	0,3,3	0.00	-	0,3,3	0.00	-
3	FES	E	1463	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	E	1464	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	E	1465	-	58,58,58	1.46	8 (13%)	85,89,89	2.02	18 (21%)
5	MPN	F	1778	8	26,26,26	9.32	9 (34%)	33,40,40	2.89	14 (42%)
7	XAN	F	1780[A]	-	12,12,12	2.03	3 (25%)	11,17,17	8.65	3 (27%)
7	XAN	F	1780[B]	-	12,12,12	2.05	3 (25%)	11,17,17	9.13	3 (27%)
8	MOM	F	1781	5	0,3,3	0.00	-	0,3,3	0.00	-
3	FES	G	1463	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	G	1464	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FAD	G	1465	-	58,58,58	1.47	7 (12%)	85,89,89	2.22	17 (20%)
5	MPN	H	1778	8	26,26,26	8.04	8 (30%)	33,40,40	3.05	11 (33%)
7	XAN	H	1780[A]	-	12,12,12	1.98	3 (25%)	11,17,17	8.28	3 (27%)
7	XAN	H	1780[B]	-	12,12,12	2.11	3 (25%)	11,17,17	8.93	3 (27%)
8	MOM	H	1781	5	0,3,3	0.00	-	0,3,3	0.00	-

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
3	FES	A	1463	1	-	0/0/4/4	0/0/1/1
3	FES	A	1464	1	-	0/0/4/4	0/0/1/1
4	FAD	A	1465	-	-	0/34/50/50	0/1/6/6
5	MPN	B	1778	8	1/1/6/8	0/6/34/34	0/0/3/3
7	XAN	B	1780[A]	-	-	0/0/0/0	0/0/2/2
7	XAN	B	1780[B]	-	-	0/0/0/0	0/0/2/2
8	MOM	B	1781	5	-	0/0/0/0	0/0/0/0
3	FES	C	1463	1	-	0/0/4/4	0/0/1/1
3	FES	C	1464	1	-	0/0/4/4	0/0/1/1
4	FAD	C	1465	-	-	0/34/50/50	0/1/6/6
5	MPN	D	1778	8	1/1/6/8	0/6/34/34	0/0/3/3
7	XAN	D	1780[A]	-	-	0/0/0/0	0/0/2/2
7	XAN	D	1780[B]	-	-	0/0/0/0	0/0/2/2
8	MOM	D	1781	5	-	0/0/0/0	0/0/0/0
3	FES	E	1463	1	-	0/0/4/4	0/0/1/1
3	FES	E	1464	1	-	0/0/4/4	0/0/1/1
4	FAD	E	1465	-	-	0/34/50/50	0/1/6/6
5	MPN	F	1778	8	1/1/6/8	0/6/34/34	0/0/3/3
7	XAN	F	1780[A]	-	-	0/0/0/0	0/0/2/2
7	XAN	F	1780[B]	-	-	0/0/0/0	0/0/2/2
8	MOM	F	1781	5	-	0/0/0/0	0/0/0/0
3	FES	G	1463	1	-	0/0/4/4	0/0/1/1
3	FES	G	1464	1	-	0/0/4/4	0/0/1/1
4	FAD	G	1465	-	-	0/34/50/50	0/1/6/6
5	MPN	H	1778	8	1/1/6/8	0/6/34/34	0/0/3/3
7	XAN	H	1780[A]	-	-	0/0/0/0	0/0/2/2
7	XAN	H	1780[B]	-	-	0/0/0/0	0/0/2/2
8	MOM	H	1781	5	-	0/0/0/0	0/0/0/0

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1778	MPN	C1'-C2'	-39.30	1.31	1.42
5	D	1778	MPN	C1'-C2'	-37.15	1.32	1.42
5	H	1778	MPN	C1'-C2'	-31.87	1.34	1.42
5	B	1778	MPN	C1'-C2'	-30.94	1.34	1.42
5	F	1778	MPN	C6-C1'	-19.08	1.34	1.51
5	H	1778	MPN	C6-C1'	-18.77	1.34	1.51
5	D	1778	MPN	C6-C1'	-18.25	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1778	MPN	C6-C1'	-18.19	1.34	1.51
5	F	1778	MPN	C4'-C3'	-13.05	1.32	1.52
5	B	1778	MPN	C4'-C3'	-12.46	1.33	1.52
5	D	1778	MPN	C4'-C3'	-12.31	1.33	1.52
5	H	1778	MPN	C4'-C3'	-10.90	1.35	1.52
5	H	1778	MPN	C9-C10	9.11	1.48	1.40
5	B	1778	MPN	C9-C10	8.70	1.47	1.40
5	D	1778	MPN	C9-C10	8.10	1.47	1.40
5	D	1778	MPN	C6-N5	-8.05	1.33	1.45
5	F	1778	MPN	C6-N5	-7.83	1.34	1.45
5	H	1778	MPN	C6-N5	-7.82	1.34	1.45
5	B	1778	MPN	C6-N5	-7.68	1.34	1.45
5	F	1778	MPN	C9-C10	7.61	1.46	1.40
4	G	1465	FAD	O4B-C1B	5.68	1.50	1.41
4	A	1465	FAD	C1'-C2'	5.61	1.56	1.51
4	E	1465	FAD	O4B-C1B	5.12	1.49	1.41
7	D	1780[B]	XAN	C6-C5	5.09	1.49	1.41
7	H	1780[B]	XAN	C6-C5	5.05	1.49	1.41
7	F	1780[B]	XAN	C6-C5	5.01	1.49	1.41
7	B	1780[B]	XAN	C6-C5	4.94	1.49	1.41
7	F	1780[A]	XAN	C6-C5	4.93	1.49	1.41
7	B	1780[A]	XAN	C6-C5	4.74	1.49	1.41
5	F	1778	MPN	C3'-C2'	-4.72	1.44	1.51
7	H	1780[A]	XAN	C6-C5	4.67	1.48	1.41
5	B	1778	MPN	C3'-C2'	-4.53	1.45	1.51
5	D	1778	MPN	C4-C9	4.44	1.49	1.41
5	D	1778	MPN	C3'-C2'	-4.43	1.45	1.51
4	A	1465	FAD	O4B-C1B	4.29	1.47	1.41
7	D	1780[A]	XAN	C6-C5	4.27	1.48	1.41
5	H	1778	MPN	C4-C9	4.11	1.48	1.41
5	B	1778	MPN	C4-C9	3.97	1.48	1.41
5	F	1778	MPN	C4-C9	3.97	1.48	1.41
4	C	1465	FAD	C10-N1	3.67	1.42	1.35
7	B	1780[B]	XAN	C5-C4	3.57	1.48	1.40
4	G	1465	FAD	C1'-C2'	3.56	1.55	1.51
4	C	1465	FAD	C9A-N10	3.55	1.44	1.38
7	H	1780[B]	XAN	C5-C4	3.48	1.48	1.40
7	B	1780[A]	XAN	C5-C4	3.35	1.48	1.40
4	C	1465	FAD	O4B-C1B	3.35	1.46	1.41
7	H	1780[A]	XAN	C5-C4	3.31	1.48	1.40
7	D	1780[A]	XAN	C5-C4	3.30	1.47	1.40
7	F	1780[B]	XAN	C5-C4	3.28	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1780[A]	XAN	C5-C4	3.26	1.47	1.40
4	E	1465	FAD	C5X-N5	3.25	1.40	1.35
4	E	1465	FAD	C10-N1	3.24	1.41	1.35
4	G	1465	FAD	C10-N1	3.20	1.41	1.35
4	C	1465	FAD	C2'-C3'	-3.19	1.46	1.53
4	C	1465	FAD	C4A-N9A	-3.18	1.33	1.37
4	A	1465	FAD	C5X-N5	3.18	1.40	1.35
7	D	1780[B]	XAN	C5-C4	3.15	1.47	1.40
5	H	1778	MPN	C3'-C2'	-2.98	1.47	1.51
4	E	1465	FAD	C4A-N9A	-2.92	1.33	1.37
4	A	1465	FAD	C10-N1	2.88	1.40	1.35
4	C	1465	FAD	C1'-C2'	2.87	1.54	1.51
4	C	1465	FAD	C4-N3	2.84	1.42	1.37
4	E	1465	FAD	C1'-C2'	2.82	1.54	1.51
4	C	1465	FAD	C2B-C1B	-2.81	1.49	1.53
4	A	1465	FAD	C1'-N10	2.80	1.51	1.48
4	G	1465	FAD	C4A-N9A	-2.78	1.33	1.37
4	A	1465	FAD	C9A-N10	2.74	1.42	1.38
4	A	1465	FAD	C4X-N5	2.74	1.41	1.36
4	E	1465	FAD	C9A-N10	2.74	1.42	1.38
4	G	1465	FAD	C5X-N5	2.70	1.39	1.35
4	C	1465	FAD	C5X-N5	2.46	1.39	1.35
4	C	1465	FAD	C2-N1	2.44	1.42	1.35
4	C	1465	FAD	P-O3P	2.42	1.64	1.59
4	E	1465	FAD	C4X-N5	2.41	1.41	1.36
4	A	1465	FAD	C4-N3	2.37	1.41	1.37
7	D	1780[B]	XAN	C4-N3	-2.32	1.34	1.37
7	B	1780[A]	XAN	C4-N3	-2.32	1.34	1.37
7	B	1780[B]	XAN	C4-N3	-2.31	1.34	1.37
4	G	1465	FAD	C4-N3	2.31	1.41	1.37
7	F	1780[A]	XAN	C4-N3	-2.29	1.34	1.37
7	D	1780[A]	XAN	C4-N3	-2.28	1.34	1.37
4	A	1465	FAD	C4A-N9A	-2.22	1.34	1.37
5	F	1778	MPN	C2-N2	2.21	1.35	1.32
7	H	1780[B]	XAN	C4-N3	-2.20	1.34	1.37
7	F	1780[B]	XAN	C4-N3	-2.19	1.34	1.37
7	H	1780[A]	XAN	C4-N3	-2.18	1.34	1.37
4	E	1465	FAD	C5B-C4B	2.18	1.58	1.51
4	G	1465	FAD	C2-N1	2.12	1.41	1.35
5	F	1778	MPN	C2-N3	2.12	1.36	1.33
5	H	1778	MPN	C9-N5	2.10	1.45	1.38

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1780[A]	XAN	N9-C4-N3	24.95	135.25	126.41
7	F	1780[B]	XAN	N9-C4-N3	24.83	135.21	126.41
7	H	1780[A]	XAN	N9-C4-N3	24.64	135.14	126.41
7	H	1780[B]	XAN	N9-C4-N3	24.49	135.09	126.41
7	D	1780[A]	XAN	N9-C4-N3	24.46	135.08	126.41
7	B	1780[A]	XAN	N9-C4-N3	24.36	135.04	126.41
7	D	1780[B]	XAN	N9-C4-N3	24.32	135.03	126.41
7	B	1780[B]	XAN	N9-C4-N3	24.11	134.95	126.41
7	D	1780[B]	XAN	C6-C5-N7	17.98	136.56	134.14
7	F	1780[B]	XAN	C6-C5-N7	16.79	136.40	134.14
7	H	1780[B]	XAN	C6-C5-N7	16.05	136.30	134.14
7	B	1780[B]	XAN	C6-C5-N7	14.67	136.12	134.14
7	F	1780[A]	XAN	C6-C5-N7	13.58	135.97	134.14
4	C	1465	FAD	O4B-C1B-N9A	-12.47	96.85	108.44
7	H	1780[A]	XAN	C6-C5-N7	11.50	135.69	134.14
4	G	1465	FAD	O4B-C1B-N9A	-11.21	98.01	108.44
7	B	1780[A]	XAN	C6-C5-N7	10.84	135.60	134.14
7	D	1780[A]	XAN	C6-C5-N7	9.82	135.46	134.14
4	G	1465	FAD	N3A-C2A-N1A	-9.30	120.93	128.71
4	E	1465	FAD	N3A-C2A-N1A	-8.86	121.30	128.71
4	A	1465	FAD	N3A-C2A-N1A	-8.48	121.62	128.71
5	B	1778	MPN	C7-C6-N5	8.08	118.72	108.44
5	D	1778	MPN	C7-C6-N5	7.66	118.17	108.44
5	H	1778	MPN	C4'-C3'-C2'	7.64	124.77	111.55
5	H	1778	MPN	C7-C6-N5	7.49	117.97	108.44
4	C	1465	FAD	N3A-C2A-N1A	-7.37	122.54	128.71
5	F	1778	MPN	O3'-C3'-C2'	7.22	123.13	109.83
5	D	1778	MPN	O3'-C3'-C2'	6.96	122.66	109.83
4	A	1465	FAD	O4B-C1B-N9A	-6.82	102.09	108.44
5	F	1778	MPN	C7-C6-N5	6.57	116.79	108.44
4	E	1465	FAD	O4B-C1B-N9A	6.55	114.54	108.44
5	B	1778	MPN	O3'-C3'-C2'	6.25	121.36	109.83
4	E	1465	FAD	C2-N1-C10	5.95	120.98	114.98
4	A	1465	FAD	C2-N1-C10	5.88	120.90	114.98
4	G	1465	FAD	C2-N1-C10	5.36	120.38	114.98
5	H	1778	MPN	O4'-C4'-C3'	5.28	122.18	108.53
5	D	1778	MPN	O4'-C4'-C3'	5.17	121.92	108.53
5	D	1778	MPN	C4-N3-C2	5.16	122.48	116.91
5	H	1778	MPN	C6-C7-N8	5.12	117.00	110.01
5	B	1778	MPN	C6-C7-N8	5.06	116.92	110.01
5	H	1778	MPN	C4-N3-C2	5.05	122.37	116.91
4	A	1465	FAD	N3A-C4A-N9A	4.92	134.32	125.43
5	F	1778	MPN	C7-C6-C1'	4.92	118.74	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1778	MPN	C4-N3-C2	4.91	122.22	116.91
4	C	1465	FAD	C4X-N5-C5X	4.84	122.13	116.69
5	B	1778	MPN	C7-C6-C1'	4.83	118.60	110.47
5	D	1778	MPN	C7-C6-C1'	4.80	118.54	110.47
5	F	1778	MPN	O3'-C3'-C4'	4.73	121.01	108.81
5	F	1778	MPN	O4'-C4'-C3'	4.67	120.61	108.53
5	B	1778	MPN	O4'-C4'-C3'	4.66	120.59	108.53
4	C	1465	FAD	C2-N1-C10	4.65	119.66	114.98
5	D	1778	MPN	O3'-C3'-C4'	4.58	120.63	108.81
4	E	1465	FAD	N3A-C4A-N9A	4.55	133.64	125.43
4	E	1465	FAD	C4X-N5-C5X	4.50	121.74	116.69
4	C	1465	FAD	N3A-C4A-N9A	4.47	133.50	125.43
4	G	1465	FAD	N3A-C4A-N9A	4.44	133.46	125.43
5	B	1778	MPN	C4'-C3'-C2'	4.42	119.20	111.55
4	E	1465	FAD	C4X-C10-N1	-4.40	118.33	122.73
5	H	1778	MPN	C1'-C6-N5	4.39	120.42	111.32
5	F	1778	MPN	C4-N3-C2	4.10	121.34	116.91
4	G	1465	FAD	C2B-C1B-N9A	4.09	123.75	113.27
5	H	1778	MPN	O3'-C3'-C2'	4.06	117.31	109.83
5	D	1778	MPN	C6-C7-N8	4.00	115.47	110.01
4	A	1465	FAD	C5X-C9A-N10	3.99	120.73	116.80
5	B	1778	MPN	O3'-C3'-C4'	3.96	119.02	108.81
4	A	1465	FAD	P-O3P-PA	-3.88	120.30	131.68
5	H	1778	MPN	C7-C6-C1'	3.81	116.88	110.47
4	A	1465	FAD	C9A-N10-C10	-3.75	118.08	121.77
4	A	1465	FAD	C4X-C10-N1	-3.75	118.98	122.73
5	F	1778	MPN	N8-C10-N1	3.70	123.27	118.22
5	F	1778	MPN	C6-C7-N8	3.66	115.01	110.01
5	H	1778	MPN	C9-C4-N3	-3.65	117.78	124.14
5	D	1778	MPN	C1'-C6-N5	3.65	118.89	111.32
5	D	1778	MPN	C9-C4-N3	-3.58	117.91	124.14
4	G	1465	FAD	C4X-N5-C5X	3.55	120.68	116.69
7	D	1780[B]	XAN	C4-C5-N7	-3.51	106.52	109.93
5	H	1778	MPN	O3'-C3'-C4'	3.51	117.85	108.81
4	E	1465	FAD	C5X-C9A-N10	3.50	120.25	116.80
4	G	1465	FAD	C4X-C10-N1	-3.45	119.28	122.73
5	B	1778	MPN	O2P-P-O4'	-3.44	97.16	106.65
5	B	1778	MPN	C9-C4-N3	-3.35	118.30	124.14
5	B	1778	MPN	C1'-C6-N5	3.33	118.22	111.32
4	C	1465	FAD	C1'-N10-C9A	3.29	122.07	118.87
4	E	1465	FAD	P-O3P-PA	-3.20	122.31	131.68
7	B	1780[B]	XAN	C4-C5-N7	-3.17	106.85	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1780[B]	XAN	C4-C5-N7	-3.15	106.87	109.93
5	F	1778	MPN	O2P-P-O3P	3.15	119.86	107.61
7	F	1780[B]	XAN	C4-C5-N7	-3.08	106.94	109.93
5	F	1778	MPN	O2P-P-O4'	-3.07	98.18	106.65
4	A	1465	FAD	C5A-C4A-N3A	-3.06	119.04	125.70
4	C	1465	FAD	C5A-C4A-N3A	-3.04	119.08	125.70
4	G	1465	FAD	P-O3P-PA	-3.01	122.86	131.68
4	C	1465	FAD	C4X-C10-N10	-2.96	119.03	120.51
5	F	1778	MPN	C9-C4-N3	-2.92	119.05	124.14
4	E	1465	FAD	C5A-C4A-N3A	-2.90	119.38	125.70
4	C	1465	FAD	C4A-C5A-N7A	-2.90	107.03	109.52
5	B	1778	MPN	O3'-C7-N8	-2.89	105.46	109.22
4	A	1465	FAD	C2B-C1B-N9A	2.89	120.68	113.27
4	G	1465	FAD	C4A-C5A-N7A	-2.88	107.06	109.52
4	C	1465	FAD	P-O3P-PA	-2.87	123.27	131.68
4	C	1465	FAD	C2B-C1B-N9A	2.86	120.61	113.27
5	F	1778	MPN	C4-C9-C10	2.85	117.20	114.56
4	G	1465	FAD	C5A-C4A-N3A	-2.83	119.54	125.70
5	F	1778	MPN	C1'-C6-N5	2.82	117.17	111.32
4	C	1465	FAD	C4'-C3'-C2'	-2.79	106.94	113.25
7	F	1780[A]	XAN	C4-C5-N7	-2.77	107.23	109.93
4	G	1465	FAD	C4-N3-C2	-2.76	119.73	125.39
4	C	1465	FAD	O2'-C2'-C3'	-2.74	102.21	109.05
4	C	1465	FAD	C4X-C10-N1	-2.73	120.00	122.73
5	D	1778	MPN	O2P-P-O4'	-2.71	99.18	106.65
7	B	1780[A]	XAN	C4-C5-N7	-2.71	107.30	109.93
4	E	1465	FAD	C4-N3-C2	-2.70	119.84	125.39
4	G	1465	FAD	C5X-C9A-N10	2.70	119.46	116.80
5	D	1778	MPN	N8-C10-N1	2.69	121.89	118.22
5	D	1778	MPN	O2P-P-O3P	2.62	117.82	107.61
4	A	1465	FAD	C4-N3-C2	-2.62	120.02	125.39
4	G	1465	FAD	C9A-N10-C10	-2.61	119.20	121.77
7	H	1780[A]	XAN	C4-C5-N7	-2.57	107.43	109.93
4	A	1465	FAD	C4X-N5-C5X	2.53	119.54	116.69
4	G	1465	FAD	C2A-N3A-C4A	2.52	121.17	114.01
4	E	1465	FAD	C2A-N3A-C4A	2.50	121.12	114.01
4	C	1465	FAD	C2A-N3A-C4A	2.47	121.04	114.01
7	D	1780[A]	XAN	C4-C5-N7	-2.47	107.53	109.93
4	C	1465	FAD	C5X-C9A-N10	2.43	119.20	116.80
4	C	1465	FAD	C4-C4X-C10	2.42	120.86	116.95
4	C	1465	FAD	O4B-C1B-C2B	-2.40	103.09	106.77
4	A	1465	FAD	C4A-C5A-N7A	-2.39	107.47	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1778	MPN	C4-C9-C10	2.39	116.77	114.56
4	C	1465	FAD	C4-N3-C2	-2.35	120.56	125.39
4	E	1465	FAD	C9A-N10-C10	-2.31	119.50	121.77
5	B	1778	MPN	O2P-P-O3P	2.30	116.56	107.61
4	C	1465	FAD	O3'-C3'-C4'	2.28	114.49	108.74
4	A	1465	FAD	C4-C4X-C10	2.26	120.60	116.95
4	A	1465	FAD	C2A-N3A-C4A	2.25	120.42	114.01
4	G	1465	FAD	C8A-N9A-C4A	2.23	108.61	106.90
4	G	1465	FAD	C4-C4X-C10	2.24	120.56	116.95
5	D	1778	MPN	O3'-C7-C6	2.21	112.51	109.50
4	E	1465	FAD	C4-C4X-C10	2.19	120.48	116.95
4	E	1465	FAD	C9A-C5X-N5	-2.15	119.06	122.37
4	E	1465	FAD	N1-C10-N10	2.15	121.63	115.97
4	E	1465	FAD	C1'-N10-C9A	2.14	120.96	118.87
5	H	1778	MPN	C10-N8-C7	-2.14	121.00	124.35
4	G	1465	FAD	O3B-C3B-C4B	-2.12	104.83	111.08
4	E	1465	FAD	C6-C5X-C9A	2.12	121.95	119.02
4	C	1465	FAD	O2'-C2'-C1'	2.11	114.95	109.71
4	E	1465	FAD	O3'-C3'-C4'	2.10	114.04	108.74
5	D	1778	MPN	C9-N5-C6	2.06	123.97	118.60
5	F	1778	MPN	P-O4'-C4'	-2.03	112.31	118.19
4	A	1465	FAD	O4'-C4'-C3'	2.01	114.05	109.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	1778	MPN	C3'
5	D	1778	MPN	C3'
5	B	1778	MPN	C3'
5	H	1778	MPN	C3'

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	450/462 (97%)	0.13	22 (4%) 28 25	25, 49, 66, 70	0
1	C	450/462 (97%)	-0.10	5 (1%) 77 79	22, 47, 66, 70	0
1	E	450/462 (97%)	0.03	19 (4%) 35 31	25, 48, 66, 71	0
1	G	450/462 (97%)	0.13	28 (6%) 20 17	26, 49, 66, 70	0
2	B	760/777 (97%)	-0.37	3 (0%) 90 91	21, 35, 50, 59	0
2	D	760/777 (97%)	-0.37	3 (0%) 90 91	20, 34, 49, 59	0
2	F	760/777 (97%)	-0.43	1 (0%) 93 95	21, 34, 49, 59	0
2	H	760/777 (97%)	-0.43	5 (0%) 84 86	22, 35, 50, 59	0
All	All	4840/4956 (97%)	-0.23	86 (1%) 65 64	20, 39, 62, 71	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	166	LEU	4.5
1	G	374	GLY	4.0
1	A	411	ILE	4.0
2	B	777	ALA	3.8
1	A	377	ILE	3.6
1	A	376	LYS	3.4
1	A	413	ALA	3.3
1	G	239	ASP	3.3
1	E	406	PHE	3.2
1	G	218	ASP	3.1
2	D	777	ALA	3.1
1	A	378	GLU	3.1
1	G	410	THR	3.1
2	H	398	LYS	3.0
1	A	403	GLY	3.0
1	A	310	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	166	LEU	3.0
1	E	302	GLY	2.9
1	A	239	ASP	2.9
1	E	403	GLY	2.9
1	C	15	ARG	2.9
1	G	191	ASP	2.9
1	G	411	ILE	2.9
1	C	166	LEU	2.9
1	G	240	GLY	2.9
1	E	373	LYS	2.8
1	A	312	GLU	2.8
1	G	165	THR	2.8
1	A	166	LEU	2.7
1	E	238	PRO	2.7
1	E	218	ASP	2.7
2	H	564	ARG	2.7
1	A	406	PHE	2.7
1	G	377	ILE	2.7
1	G	312	GLU	2.6
1	E	219	LEU	2.6
1	G	378	GLU	2.6
2	H	561	CYS	2.6
2	F	398	LYS	2.6
1	G	190	ALA	2.6
1	G	402	ILE	2.5
1	G	194	LEU	2.5
2	B	398	LYS	2.5
1	E	372	LEU	2.4
1	A	373	LYS	2.4
1	E	165	THR	2.4
1	G	310	GLY	2.4
2	B	399	LYS	2.4
1	A	332	PRO	2.4
1	G	413	ALA	2.4
2	H	399	LYS	2.4
1	E	194	LEU	2.4
1	E	181	PHE	2.4
1	E	239	ASP	2.4
1	G	235	ARG	2.4
2	H	560	GLY	2.3
1	A	220	PRO	2.3
1	G	19	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	374	GLY	2.3
1	E	220	PRO	2.3
1	G	238	PRO	2.3
1	A	379	THR	2.3
1	E	15	ARG	2.3
2	D	398	LYS	2.3
1	A	238	PRO	2.3
1	G	220	PRO	2.2
1	A	165	THR	2.2
1	C	239	ASP	2.2
1	G	195	ALA	2.2
1	G	373	LYS	2.2
1	G	406	PHE	2.1
1	A	417	LEU	2.1
1	G	403	GLY	2.1
1	G	15	ARG	2.1
1	E	198	GLU	2.1
1	C	218	ASP	2.1
1	A	401	LEU	2.1
1	E	407	ARG	2.1
2	D	399	LYS	2.1
1	G	372	LEU	2.1
1	G	401	LEU	2.1
1	E	312	GLU	2.1
1	E	378	GLU	2.1
1	A	240	GLY	2.1
1	A	331	ARG	2.0
1	C	402	ILE	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
7	XAN	F	1780[B]	11/11	0.28	9.12	61,62,62,62	11
7	XAN	F	1780[A]	11/11	0.28	9.12	62,62,62,62	11
7	XAN	H	1780[A]	11/11	0.28	9.01	62,62,62,62	11
7	XAN	H	1780[B]	11/11	0.28	5.73	61,62,62,62	11
7	XAN	D	1780[B]	11/11	0.19	4.45	61,62,62,62	11
7	XAN	D	1780[A]	11/11	0.19	4.45	62,62,62,62	11
5	MPN	H	1778	24/24	0.26	4.30	33,38,41,43	24
7	XAN	B	1780[B]	11/11	0.24	4.14	61,62,62,62	11
7	XAN	B	1780[A]	11/11	0.24	4.14	62,62,62,62	11
5	MPN	B	1778	24/24	0.31	3.80	27,36,42,43	24
5	MPN	F	1778	24/24	0.26	3.17	22,29,34,36	24
5	MPN	D	1778	24/24	0.25	2.69	9,25,32,33	24
6	CA	F	1779	1/1	0.24	1.86	56,56,56,56	0
3	FES	G	1464	4/4	0.20	1.69	39,40,42,42	0
3	FES	E	1464	4/4	0.18	1.62	38,38,40,42	0
3	FES	E	1463	4/4	0.16	0.90	26,27,30,31	0
3	FES	C	1464	4/4	0.18	0.52	33,35,35,37	0
3	FES	A	1463	4/4	0.19	0.49	25,28,29,30	0
6	CA	D	1779	1/1	0.17	0.29	49,49,49,49	0
3	FES	A	1464	4/4	0.18	0.06	35,35,36,36	0
6	CA	H	1779	1/1	0.19	-0.03	58,58,58,58	0
4	FAD	G	1465	53/53	0.15	-0.06	41,50,63,64	0
3	FES	C	1463	4/4	0.17	-0.16	19,19,21,22	0
4	FAD	A	1465	53/53	0.14	-0.17	38,48,56,56	0
3	FES	G	1463	4/4	0.14	-0.18	29,32,32,33	0
4	FAD	E	1465	53/53	0.14	-0.36	35,45,53,53	0
8	MOM	F	1781	4/4	0.12	-1.14	35,35,36,37	3
4	FAD	C	1465	53/53	0.13	-1.17	16,27,35,37	0
8	MOM	B	1781	4/4	0.10	-1.29	44,45,45,47	3
6	CA	B	1779	1/1	0.17	-1.42	48,48,48,48	0
8	MOM	H	1781	4/4	0.12	-1.54	44,44,44,45	3
8	MOM	D	1781	4/4	0.10	-2.29	34,34,34,37	3

6.5 Other polymers ⓘ

There are no such residues in this entry.