



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:48 am GMT

PDB ID : 2W54  
Title : Crystal Structure of Xanthine Dehydrogenase from Rhodobacter capsulatus in Complex with Bound Inhibitor Pterin-6-aldehyde  
Authors : Doebbler, J.A.; Truglio, J.J.; Leimkuhler, S.; Kisker, C.  
Deposited on : 2008-12-04  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

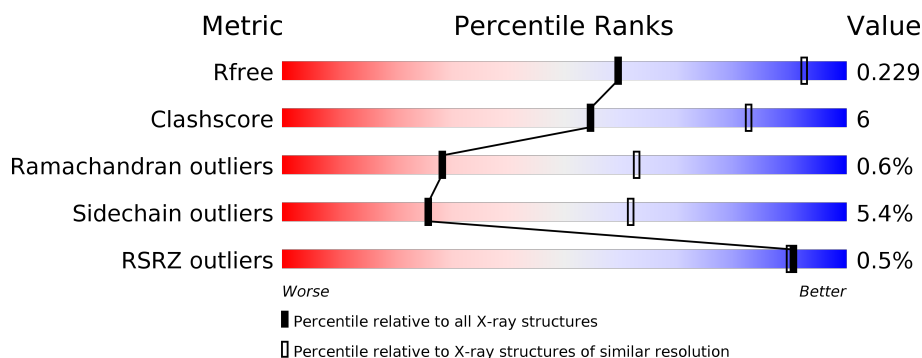
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	462	<div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	E	462	<div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	G	462	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>
2	B	777	<div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div>
2	D	777	<div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	777	 80% 17% ..
2	H	777	 79% 18% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	E	1464	-	-	-	X
5	XAX	B	1778	X	-	-	X
5	XAX	D	1778	X	-	-	-
5	XAX	F	1778	-	-	-	X
5	XAX	H	1778	-	-	-	X
7	HHR	B	1780	-	-	-	X
7	HHR	D	1780	-	-	-	X
7	HHR	H	1780	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36788 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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

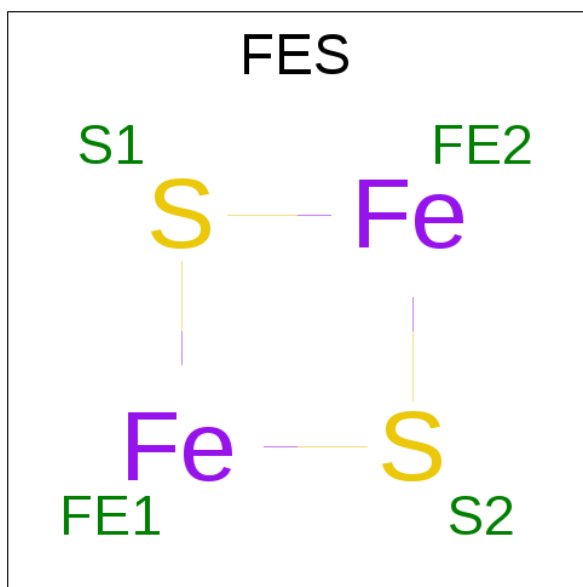
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

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:

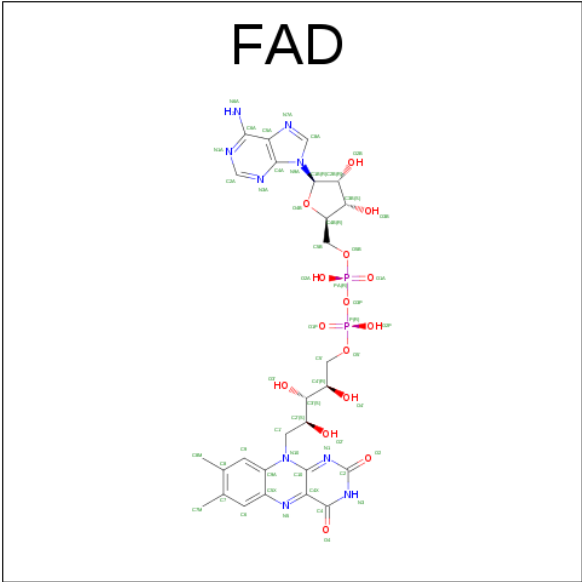
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	CONFLICT	UNP O54051
D	772	ARG	GLY	CONFLICT	UNP O54051
F	772	ARG	GLY	CONFLICT	UNP O54051
H	772	ARG	GLY	CONFLICT	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



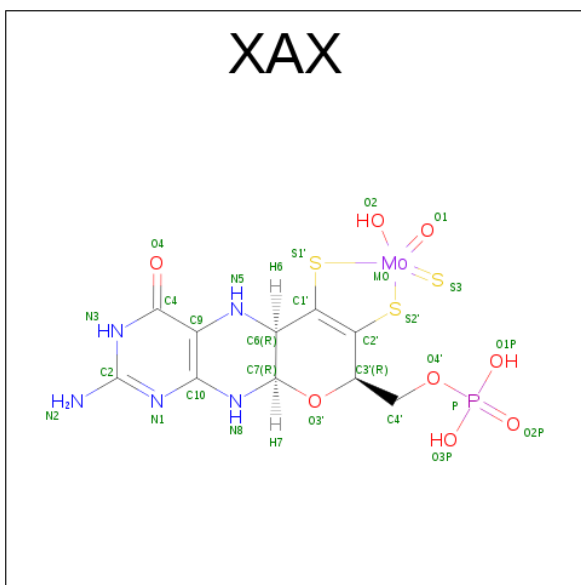
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0

- 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 {[ (5AR,8R,9AR)-2-AMINO-4-OXO-6,7-DI(SULFANYL-KAPPAS)-3,5,5A,8,9A,10-HEXAHYDRO-4H-PYRANO[3,2-G]PTERIDIN-8-YL]METHYL DIHYDROGENATO(2-) PHOSPHATE}(HYDROXY)OXO(THIOXO)MOLYBDENUM (three-letter code: XAX) (formula: C<sub>10</sub>H<sub>13</sub>MoN<sub>5</sub>O<sub>8</sub>PS<sub>3</sub>).

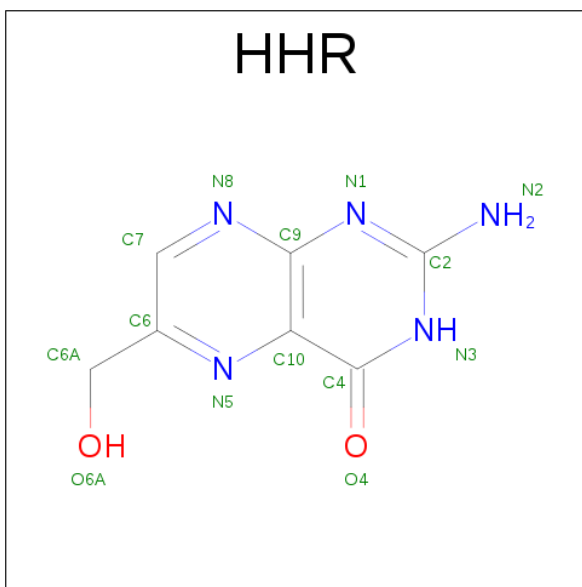


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
5	D	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
5	F	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
5	H	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0

- Molecule 6 is BARIUM ION (three-letter code: BA) (formula: Ba).

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

- Molecule 7 is 6-HYDROXYMETHYLPTERIN (three-letter code: HHR) (formula: C<sub>7</sub>H<sub>7</sub>N<sub>5</sub>O<sub>2</sub>).



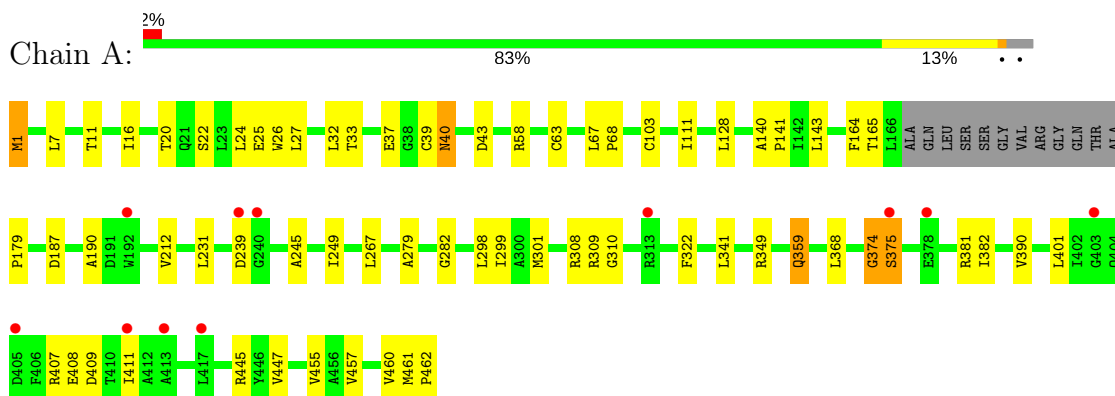
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	7	5	2		
7	D	1	Total	C	N	O	0	0
			14	7	5	2		
7	F	1	Total	C	N	O	0	0
			14	7	5	2		
7	H	1	Total	C	N	O	0	0
			14	7	5	2		



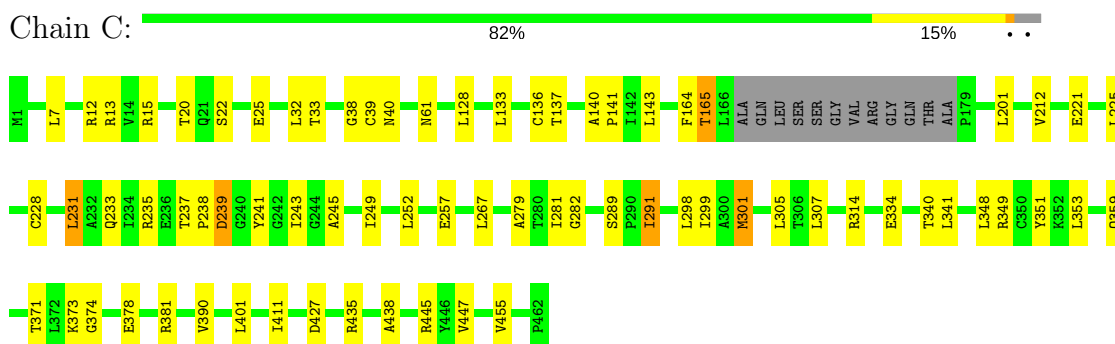
### 3 Residue-property plots [i](#)

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

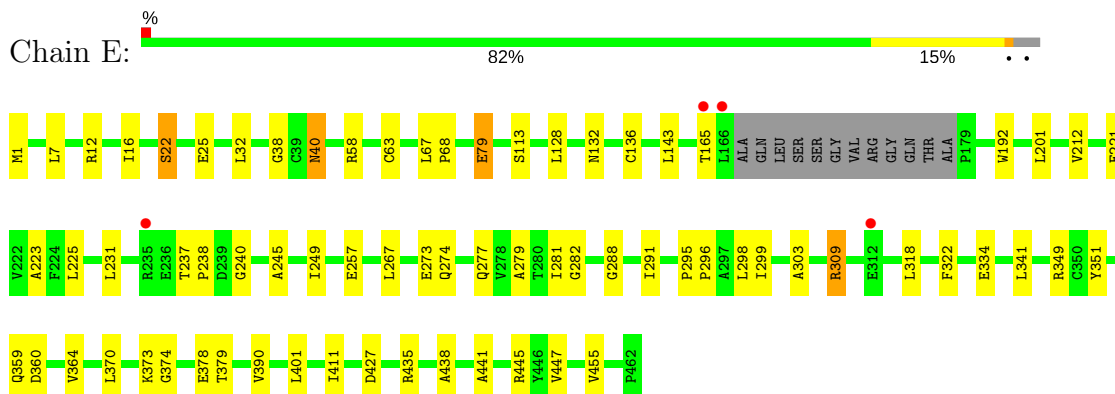
#### • Molecule 1: XANTHINE DEHYDROGENASE



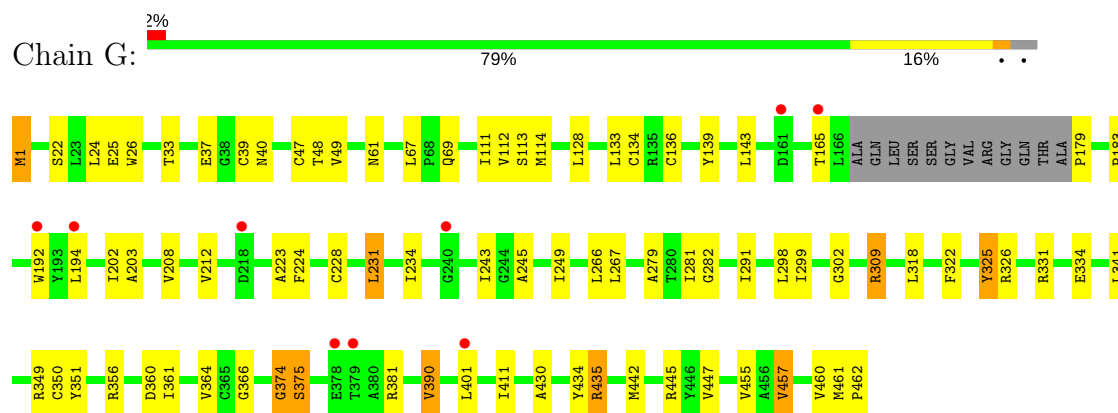
#### • Molecule 1: XANTHINE DEHYDROGENASE



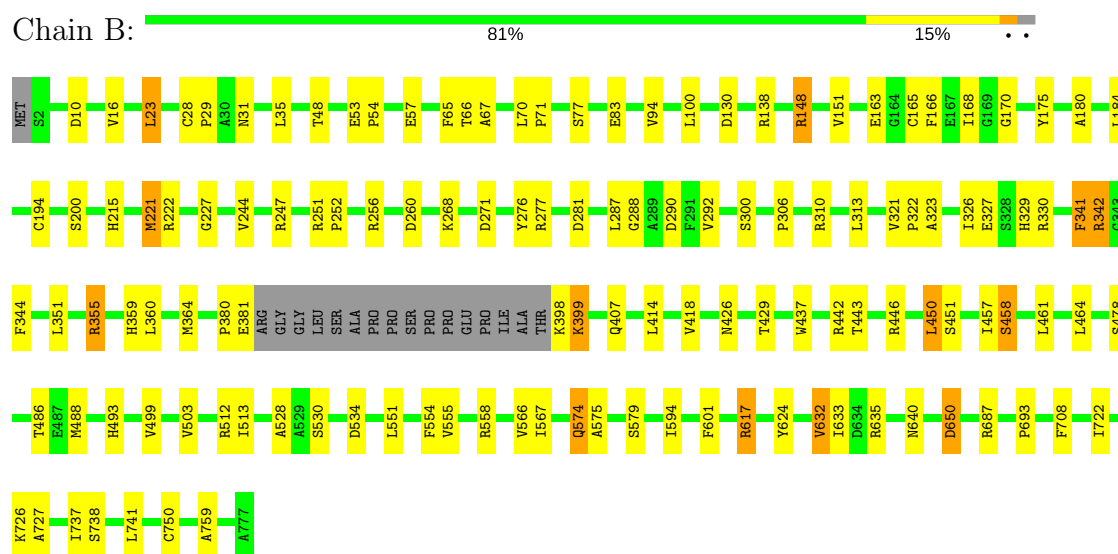
#### • Molecule 1: XANTHINE DEHYDROGENASE



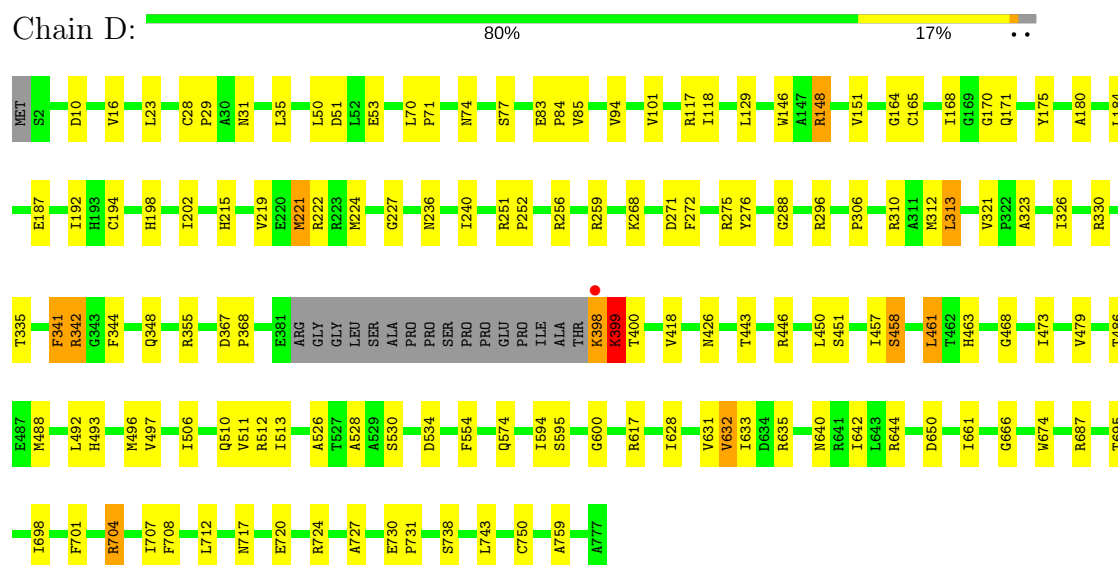
• Molecule 1: XANTHINE DEHYDROGENASE



• Molecule 2: XANTHINE DEHYDROGENASE

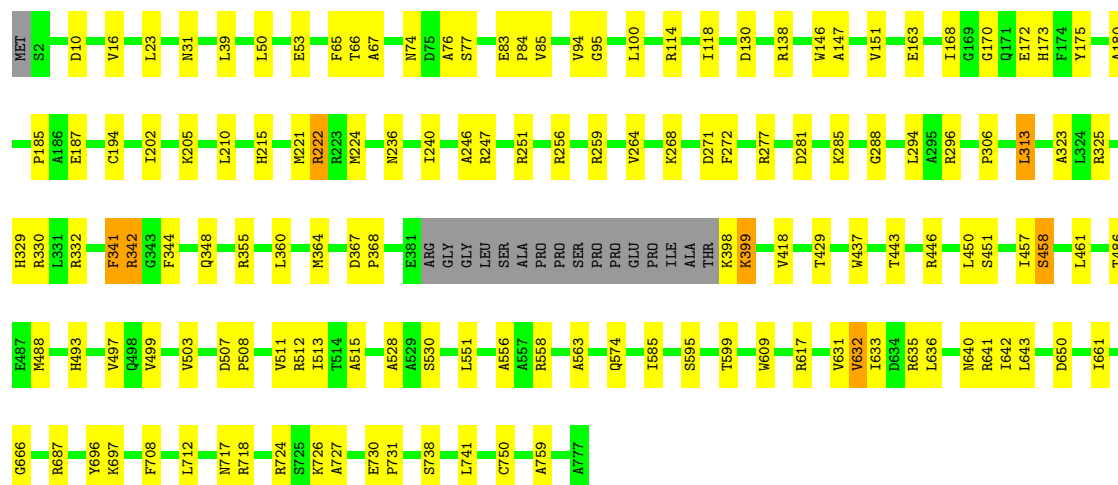


• Molecule 2: XANTHINE DEHYDROGENASE

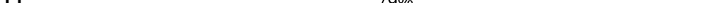


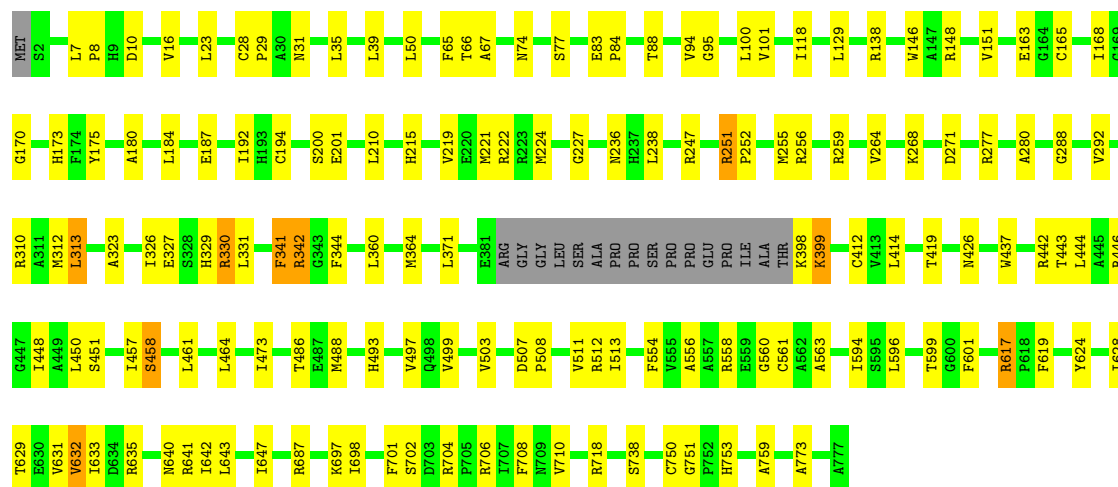
- Molecule 2: XANTHINE DEHYDROGENASE

Chain F:  80% 17% ..



- Molecule 2: XANTHINE DEHYDROGENASE

Chain H:  79% 18% 3%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.57Å 140.69Å 157.86Å 109.63° 105.83° 101.23°	Depositor
Resolution (Å)	50.00 – 3.30 49.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.30) 85.2 (49.82-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, $R_{free}$	0.186 , 0.224 0.193 , 0.229	Depositor DCC
$R_{free}$ test set	5185 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	36788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAX, HHR, BA, FAD, FES

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	0.33	0/3439	0.49	0/4659
1	C	0.33	0/3439	0.51	0/4659
1	E	0.33	0/3439	0.50	0/4659
1	G	0.32	0/3439	0.50	0/4659
2	B	0.32	0/5845	0.50	0/7942
2	D	0.32	0/5845	0.50	0/7942
2	F	0.33	0/5845	0.50	0/7942
2	H	0.33	0/5845	0.50	0/7942
All	All	0.32	0/37136	0.50	0/50404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3367	32	0
1	C	3376	0	3367	35	0
1	E	3376	0	3367	38	0
1	G	3376	0	3368	44	0
2	B	5717	0	5631	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5717	0	5631	72	0
2	F	5717	0	5631	70	0
2	H	5717	0	5631	85	0
3	A	8	0	0	0	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	3	0
4	C	53	0	31	2	0
4	E	53	0	31	3	0
4	G	53	0	31	3	0
5	B	28	0	8	6	0
5	D	28	0	8	6	0
5	F	28	0	8	7	0
5	H	28	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	14	0	6	1	0
7	D	14	0	6	0	0
7	F	14	0	6	0	0
7	H	14	0	6	1	0
All	All	36788	0	36173	439	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.61	0.83
1:C:411:ILE:HG13	1:C:447:VAL:HG21	1.61	0.81
1:C:445:ARG:HG3	1:C:455:VAL:HG11	1.61	0.81
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.65	0.78
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.68	0.76
2:F:360:LEU:HG	2:F:364:MET:HE3	1.68	0.75
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.67	0.75
1:C:252:LEU:HD22	1:C:281:ILE:HD12	1.70	0.74
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.72	0.71
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HB2	1:G:179:PRO:HG2	1.71	0.70
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.74	0.69
2:D:451:SER:HB3	2:D:738:SER:HB3	1.72	0.69
2:H:77:SER:HB2	2:H:83:GLU:HB3	1.75	0.69
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.74	0.69
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.72	0.69
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.75	0.69
1:G:22:SER:OG	1:G:25:GLU:HG2	1.92	0.69
2:H:635:ARG:HD3	2:H:750:CYS:SG	2.33	0.69
2:H:163:GLU:HG2	2:H:277:ARG:HG2	1.74	0.69
5:H:1778:XAX:S3	5:H:1778:XAX:MO	2.05	0.68
5:F:1778:XAX:S3	5:F:1778:XAX:MO	2.04	0.67
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.24	0.67
5:B:1778:XAX:S3	5:B:1778:XAX:MO	2.05	0.67
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.76	0.67
5:D:1778:XAX:MO	5:D:1778:XAX:S3	2.05	0.67
1:G:455:VAL:HG13	2:H:443:THR:HG21	1.77	0.66
2:D:50:LEU:HD12	2:D:118:ILE:HG12	1.79	0.65
2:B:31:ASN:HB2	2:B:251:ARG:HH11	1.61	0.65
1:G:325:TYR:O	1:G:326:ARG:HB2	1.96	0.65
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.77	0.64
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.79	0.63
2:H:641:ARG:HH21	2:H:706:ARG:HE	1.45	0.63
2:H:94:VAL:HG11	2:H:687:ARG:HG2	1.78	0.63
1:C:401:LEU:HD11	1:C:411:ILE:HD13	1.80	0.63
2:H:210:LEU:HD22	2:H:247:ARG:HD3	1.81	0.63
2:B:94:VAL:HG11	2:B:687:ARG:HG2	1.79	0.63
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	1.81	0.63
5:D:1778:XAX:MO	5:D:1778:XAX:O1	1.70	0.62
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.82	0.62
5:H:1778:XAX:O2	5:H:1778:XAX:MO	1.71	0.61
1:C:243:ILE:HD12	1:C:341:LEU:HG	1.83	0.61
5:F:1778:XAX:O2	5:F:1778:XAX:MO	1.70	0.61
1:E:237:THR:OG1	1:E:238:PRO:HD2	1.99	0.61
2:F:650:ASP:OD2	2:F:726:LYS:HD2	2.01	0.61
5:B:1778:XAX:O2	5:B:1778:XAX:MO	1.70	0.61
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.83	0.61
2:F:147:ALA:HB2	2:F:325:ARG:HG3	1.82	0.60
2:D:635:ARG:HD3	2:D:750:CYS:SG	2.40	0.60
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.83	0.60
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:LEU:HD22	2:H:180:ALA:HB1	1.83	0.59
2:H:702:SER:HB2	2:H:706:ARG:HH22	1.67	0.59
1:A:22:SER:OG	1:A:25:GLU:HG2	2.01	0.59
2:H:280:ALA:HB2	2:H:360:LEU:HD21	1.85	0.59
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.83	0.59
1:E:445:ARG:HE	1:E:455:VAL:HG12	1.67	0.59
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.17	0.58
1:E:455:VAL:HG13	2:F:443:THR:HG21	1.85	0.58
2:D:221:MET:HE2	2:D:486:THR:HB	1.86	0.58
2:F:163:GLU:HG2	2:F:277:ARG:HG2	1.86	0.58
1:A:460:VAL:HG11	2:B:632:VAL:HG11	1.87	0.57
2:B:457:ILE:O	2:B:458:SER:HB2	2.05	0.57
1:G:281:ILE:HD11	1:G:298:LEU:HD11	1.86	0.57
2:F:221:MET:HE2	2:F:486:THR:HB	1.86	0.57
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.87	0.57
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.40	0.57
2:B:554:PHE:HB2	2:B:594:ILE:HD13	1.87	0.56
1:C:281:ILE:HD11	1:C:298:LEU:HD11	1.87	0.56
2:F:50:LEU:HD12	2:F:118:ILE:HG12	1.87	0.56
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.45	0.56
1:G:360:ASP:OD1	2:H:697:LYS:HE3	2.05	0.56
1:G:374:GLY:O	1:G:375:SER:HB3	2.06	0.56
2:F:661:ILE:HD11	2:F:712:LEU:HG	1.88	0.56
1:A:245:ALA:HB1	1:A:282:GLY:HA3	1.87	0.56
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.88	0.56
2:F:528:ALA:HA	5:F:1778:XAX:S2'	2.46	0.55
1:G:245:ALA:HB1	1:G:282:GLY:HA3	1.89	0.55
1:G:291:ILE:HD12	1:G:361:ILE:HG21	1.87	0.55
2:H:292:VAL:HG22	2:H:327:GLU:HB3	1.88	0.55
2:H:129:LEU:HD12	2:H:331:LEU:HD12	1.87	0.55
2:H:35:LEU:HB2	2:H:255:MET:HB2	1.88	0.55
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.87	0.55
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.40	0.55
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.88	0.55
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.54	0.55
1:C:289:SER:OG	1:C:291:ILE:HG13	2.06	0.55
1:C:299:ILE:O	1:C:381:ARG:NH1	2.38	0.54
5:B:1778:XAX:S3	5:B:1778:XAX:O2	2.65	0.54
2:D:720:GLU:HG2	2:D:724:ARG:HH21	1.72	0.54
1:E:22:SER:OG	1:E:25:GLU:HG2	2.08	0.54
1:C:228:CYS:HB3	1:C:231:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:O	1:A:381:ARG:NH1	2.37	0.54
2:B:77:SER:HB2	2:B:83:GLU:HB3	1.89	0.54
1:C:237:THR:HG23	1:C:239:ASP:H	1.73	0.54
2:D:198:HIS:ND1	2:D:526:ALA:HB2	2.22	0.54
5:F:1778:XAX:S3	5:F:1778:XAX:O2	2.66	0.54
1:G:445:ARG:HE	1:G:455:VAL:HG12	1.72	0.54
2:B:457:ILE:O	2:B:458:SER:CB	2.55	0.54
2:H:437:TRP:CZ3	2:H:446:ARG:HG3	2.43	0.54
2:B:380:PRO:O	2:B:381:GLU:HB2	2.09	0.53
1:C:455:VAL:HG13	2:D:443:THR:HG21	1.88	0.53
1:C:136:CYS:O	2:D:666:GLY:HA3	2.08	0.53
1:C:22:SER:OG	1:C:25:GLU:HG2	2.07	0.53
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.74	0.53
5:H:1778:XAX:S3	5:H:1778:XAX:O2	2.66	0.53
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.44	0.53
2:B:71:PRO:HG3	2:B:247:ARG:NH1	2.24	0.53
2:B:170:GLY:N	2:B:271:ASP:HB3	2.24	0.53
4:C:1465:FAD:H2'	4:C:1465:FAD:N1	2.24	0.53
2:D:457:ILE:O	2:D:458:SER:CB	2.57	0.53
2:B:70:LEU:HD23	2:B:244:VAL:HG11	1.90	0.52
2:H:641:ARG:HH21	2:H:706:ARG:NE	2.07	0.52
2:D:730:GLU:N	2:D:731:PRO:CD	2.72	0.52
1:A:374:GLY:O	1:A:375:SER:HB3	2.10	0.52
1:A:445:ARG:HE	1:A:455:VAL:HG12	1.75	0.52
2:B:66:THR:HG22	2:B:67:ALA:N	2.25	0.52
1:E:441:ALA:HB1	2:F:636:LEU:HB3	1.92	0.52
2:D:171:GLN:NE2	2:D:674:TRP:HB2	2.25	0.52
2:D:35:LEU:HA	2:D:101:VAL:O	2.10	0.52
2:D:717:ASN:O	2:D:724:ARG:HD2	2.10	0.52
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.25	0.52
2:F:222:ARG:HD2	2:F:515:ALA:HB2	1.92	0.52
5:D:1778:XAX:S3	5:D:1778:XAX:O1	2.68	0.51
2:H:556:ALA:HB1	2:H:561:CYS:O	2.11	0.51
2:F:507:ASP:OD1	2:F:508:PRO:HD2	2.10	0.51
2:H:31:ASN:HB2	2:H:251:ARG:HH11	1.76	0.51
2:B:281:ASP:HB3	2:B:287:LEU:HD21	1.92	0.51
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.91	0.51
1:C:301:MET:HB3	1:C:348:LEU:HD22	1.91	0.51
1:G:302:GLY:HA2	1:G:381:ARG:NH1	2.25	0.51
1:E:240:GLY:HA3	1:E:341:LEU:O	2.10	0.51
2:H:95:GLY:HA3	2:H:264:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:CD2	1:C:281:ILE:HD12	2.39	0.51
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.46	0.51
1:A:43:ASP:HB2	2:B:693:PRO:HB2	1.93	0.51
2:D:497:VAL:HG13	2:D:511:VAL:HB	1.92	0.51
2:F:717:ASN:O	2:F:724:ARG:HD2	2.11	0.51
1:C:305:LEU:HD21	1:C:307:LEU:HD21	1.93	0.50
2:D:554:PHE:HB2	2:D:594:ILE:CD1	2.41	0.50
2:F:599:THR:HG23	2:H:599:THR:HG23	1.94	0.50
2:D:165:CYS:HB2	2:D:275:ARG:HG3	1.92	0.50
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.46	0.50
2:H:560:GLY:O	2:H:561:CYS:HB3	2.11	0.50
1:G:364:VAL:HG22	1:G:435:ARG:HG2	1.93	0.50
2:B:251:ARG:HB2	2:B:252:PRO:HD2	1.92	0.50
2:B:574:GLN:HG3	2:B:579:SER:HB3	1.92	0.50
2:F:451:SER:HB3	2:F:738:SER:HB3	1.94	0.50
2:H:65:PHE:HB2	2:H:100:LEU:HB3	1.92	0.50
2:H:457:ILE:O	2:H:458:SER:CB	2.60	0.50
2:B:184:LEU:HD23	2:B:252:PRO:HB3	1.94	0.50
5:D:1778:XAX:S3	5:D:1778:XAX:O2	2.70	0.50
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.47	0.50
2:H:192:ILE:HB	2:H:219:VAL:HG22	1.94	0.50
2:H:238:LEU:HD23	2:H:255:MET:HG2	1.94	0.50
1:A:16:ILE:HD13	1:A:68:PRO:HG3	1.94	0.49
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.94	0.49
2:H:28:CYS:HB2	2:H:29:PRO:CD	2.42	0.49
1:C:411:ILE:HG13	1:C:447:VAL:CG2	2.37	0.49
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.61	0.49
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.92	0.49
2:B:221:MET:HE2	2:B:486:THR:HB	1.94	0.49
1:E:201:LEU:HD22	1:E:225:LEU:HD21	1.94	0.49
2:D:457:ILE:O	2:D:458:SER:HB2	2.13	0.49
2:D:398:LYS:O	2:D:399:LYS:HD2	2.12	0.49
1:E:16:ILE:HD13	1:E:68:PRO:HG3	1.95	0.49
2:F:138:ARG:NH2	2:F:329:HIS:ND1	2.60	0.49
2:F:457:ILE:O	2:F:458:SER:CB	2.60	0.49
2:H:457:ILE:O	2:H:458:SER:HB2	2.12	0.49
2:D:168:ILE:HA	2:D:759:ALA:HB3	1.95	0.48
2:F:632:VAL:HG13	2:F:643:LEU:HD11	1.95	0.48
1:E:364:VAL:HG21	1:E:438:ALA:HB3	1.95	0.48
2:F:288:GLY:HA2	2:F:323:ALA:O	2.13	0.48
2:D:528:ALA:HA	5:D:1778:XAX:S2'	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.96	0.48
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.44	0.48
1:C:38:GLY:O	2:D:259:ARG:HD2	2.14	0.48
2:B:163:GLU:HG2	2:B:277:ARG:HG2	1.95	0.48
2:D:251:ARG:HB2	2:D:252:PRO:CD	2.44	0.48
1:E:309:ARG:HB2	1:E:334:GLU:HG3	1.96	0.48
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.96	0.48
2:F:202:ILE:HD13	2:F:236:ASN:HD22	1.79	0.48
2:F:66:THR:HG22	2:F:67:ALA:N	2.28	0.48
2:B:292:VAL:HG22	2:B:327:GLU:HB3	1.96	0.48
2:D:554:PHE:HB2	2:D:594:ILE:HD13	1.96	0.48
2:H:23:LEU:CD2	2:H:180:ALA:HB1	2.44	0.48
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.14	0.48
1:E:373:LYS:HB2	1:E:378:GLU:HG2	1.95	0.48
1:G:194:LEU:HD13	1:G:309:ARG:HD3	1.95	0.48
1:A:298:LEU:HA	1:A:301:MET:HG2	1.95	0.47
2:D:74:ASN:O	2:D:84:PRO:HA	2.14	0.47
2:F:294:LEU:HD23	2:F:329:HIS:HB2	1.94	0.47
2:B:341:PHE:O	2:B:342:ARG:C	2.51	0.47
2:D:306:PRO:HB2	2:D:344:PHE:HE2	1.79	0.47
2:F:718:ARG:HE	2:F:718:ARG:HB3	1.58	0.47
2:F:221:MET:HE1	2:F:224:MET:HG3	1.96	0.47
1:G:48:THR:HG21	1:G:113:SER:OG	2.14	0.47
2:H:341:PHE:O	2:H:342:ARG:C	2.52	0.47
2:F:306:PRO:HB2	2:F:344:PHE:HE2	1.79	0.47
1:G:430:ALA:HB1	1:G:434:TYR:HD2	1.79	0.47
2:B:53:GLU:HB3	2:B:54:PRO:HD3	1.96	0.47
5:H:1778:XAX:S3	5:H:1778:XAX:O1	2.73	0.47
1:E:40:ASN:ND2	1:E:63:CYS:HB2	2.29	0.47
1:E:401:LEU:HD11	1:E:411:ILE:HD13	1.97	0.47
2:B:566:VAL:HG13	2:B:575:ALA:HB2	1.96	0.47
2:B:635:ARG:HD3	2:B:750:CYS:SG	2.55	0.47
1:E:411:ILE:HG13	1:E:447:VAL:HG21	1.97	0.47
1:G:24:LEU:HD21	1:G:37:GLU:HB2	1.96	0.47
1:G:356:ARG:NH1	2:H:698:ILE:O	2.44	0.47
1:G:322:PHE:HB3	1:G:390:VAL:HG22	1.97	0.47
1:G:411:ILE:HG13	1:G:447:VAL:HG21	1.97	0.47
1:G:26:TRP:CD1	1:G:67:LEU:HD11	2.50	0.47
1:A:455:VAL:HG13	2:B:443:THR:HG21	1.96	0.46
1:E:192:TRP:CZ3	1:E:223:ALA:HB2	2.50	0.46
2:F:493:HIS:CG	2:F:513:ILE:HG12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.98	0.46
2:D:170:GLY:N	2:D:271:ASP:HB3	2.29	0.46
2:D:450:LEU:HB2	2:D:628:ILE:HG12	1.97	0.46
2:H:632:VAL:HG13	2:H:643:LEU:HD11	1.97	0.46
2:B:288:GLY:HA2	2:B:323:ALA:O	2.15	0.46
2:B:451:SER:HB3	2:B:738:SER:HB3	1.97	0.46
1:E:360:ASP:HA	2:F:697:LYS:HZ1	1.80	0.46
2:F:39:LEU:HB3	2:F:95:GLY:HA2	1.97	0.46
2:F:633:ILE:HG22	2:F:640:ASN:HB3	1.98	0.46
1:A:1:MET:HB2	1:A:179:PRO:HG3	1.97	0.46
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.96	0.46
5:F:1778:XAX:S3	5:F:1778:XAX:O1	2.74	0.46
1:G:228:CYS:HB3	1:G:231:LEU:HB2	1.97	0.46
2:H:74:ASN:O	2:H:84:PRO:HA	2.15	0.46
2:H:50:LEU:HD12	2:H:118:ILE:HG12	1.97	0.46
2:F:205:LYS:HB3	2:F:240:ILE:HD11	1.98	0.46
2:F:272:PHE:CD2	2:F:348:GLN:HG2	2.51	0.46
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.51	0.46
2:D:341:PHE:HD2	2:D:342:ARG:N	2.14	0.46
2:H:35:LEU:HA	2:H:101:VAL:O	2.16	0.46
2:D:493:HIS:CG	2:D:513:ILE:HG12	2.51	0.46
1:A:368:LEU:HG	1:A:382:ILE:HG23	1.98	0.45
2:D:192:ILE:HB	2:D:219:VAL:HG22	1.98	0.45
2:F:77:SER:HB2	2:F:83:GLU:CB	2.43	0.45
2:D:631:VAL:HG12	2:D:642:ILE:HA	1.98	0.45
2:F:185:PRO:HG3	2:F:246:ALA:HB1	1.98	0.45
2:F:595:SER:HB2	2:H:601:PHE:CG	2.52	0.45
2:H:617:ARG:HD3	2:H:619:PHE:O	2.16	0.45
2:F:512:ARG:HA	2:F:512:ARG:HE	1.81	0.45
2:F:631:VAL:HG12	2:F:642:ILE:HA	1.97	0.45
2:F:23:LEU:CD1	2:F:194:CYS:HA	2.47	0.45
1:A:40:ASN:ND2	1:A:63:CYS:HB2	2.32	0.45
1:C:137:THR:HB	1:C:141:PRO:HG2	1.99	0.45
2:F:418:VAL:HG13	2:F:450:LEU:HD21	1.98	0.45
2:F:551:LEU:HD22	2:F:585:ILE:HG22	1.98	0.45
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.99	0.45
4:E:1465:FAD:H9	4:E:1465:FAD:H1'2	1.84	0.45
2:D:23:LEU:CD1	2:D:194:CYS:HA	2.46	0.45
2:D:446:ARG:HG2	2:D:632:VAL:CG1	2.47	0.45
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.32	0.45
2:D:506:ILE:HD12	2:D:510:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:GLU:OE1	2:D:53:GLU:HA	2.17	0.45
2:F:367:ASP:HA	2:F:368:PRO:HD2	1.87	0.45
2:H:556:ALA:HB2	2:H:563:ALA:HA	1.97	0.45
2:D:85:VAL:HG21	2:D:240:ILE:HG21	1.99	0.45
1:E:132:ASN:OD1	1:E:274:GLN:NE2	2.50	0.45
2:F:730:GLU:N	2:F:731:PRO:CD	2.80	0.45
2:H:718:ARG:HE	2:H:718:ARG:HB3	1.62	0.45
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.98	0.44
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.52	0.44
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.99	0.44
1:A:411:ILE:HG13	1:A:447:VAL:CG2	2.44	0.44
5:B:1778:XAX:S3	5:B:1778:XAX:O1	2.74	0.44
2:B:437:TRP:CZ3	2:B:446:ARG:HG3	2.53	0.44
2:F:76:ALA:HB2	2:F:85:VAL:HG22	1.98	0.44
1:A:111:ILE:HD11	2:B:16:VAL:HG22	2.00	0.44
2:B:528:ALA:HA	5:B:1778:XAX:S2'	2.58	0.44
1:E:288:GLY:HA2	1:E:322:PHE:HE2	1.82	0.44
1:G:249:ILE:HG23	1:G:267:LEU:HD22	1.99	0.44
2:H:310:ARG:HD2	2:H:344:PHE:HB3	1.98	0.44
2:B:493:HIS:CG	2:B:513:ILE:HG12	2.51	0.44
2:D:701:PHE:O	2:D:704:ARG:HG2	2.18	0.44
2:D:730:GLU:H	2:D:731:PRO:CD	2.30	0.44
1:E:411:ILE:HG13	1:E:447:VAL:CG2	2.47	0.44
1:G:183:PRO:HD2	1:G:224:PHE:O	2.18	0.44
2:H:633:ILE:HG22	2:H:640:ASN:HB3	2.00	0.44
1:C:249:ILE:HG23	1:C:267:LEU:HD22	1.99	0.44
1:E:281:ILE:HD11	1:E:298:LEU:HD11	2.00	0.44
2:H:554:PHE:HB2	2:H:594:ILE:CD1	2.48	0.44
2:F:172:GLU:HB3	2:F:696:TYR:CZ	2.52	0.44
2:B:488:MET:HG3	5:B:1778:XAX:C4	2.48	0.44
1:C:353:LEU:HD23	1:C:438:ALA:HB1	1.99	0.44
2:F:556:ALA:HB2	2:F:563:ALA:HA	1.99	0.44
1:G:111:ILE:HD13	1:G:114:MET:HE3	2.00	0.44
1:G:299:ILE:HG13	1:G:318:LEU:HD23	2.00	0.44
4:A:1465:FAD:H1'2	4:A:1465:FAD:H9	1.81	0.44
2:B:306:PRO:HB2	2:B:344:PHE:HE2	1.83	0.44
1:C:241:TYR:O	1:C:340:THR:HA	2.17	0.44
1:G:234:ILE:HG12	1:G:243:ILE:HG12	2.00	0.44
1:G:39:CYS:HA	2:H:259:ARG:HB2	2.00	0.44
2:H:168:ILE:HA	2:H:759:ALA:HB3	2.00	0.44
2:B:168:ILE:HA	2:B:759:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:ARG:NH1	2:D:321:VAL:O	2.51	0.43
2:H:499:VAL:O	2:H:503:VAL:HG23	2.17	0.43
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.48	0.43
2:D:312:MET:HG2	2:D:326:ILE:HG21	2.00	0.43
2:H:753:HIS:HB2	2:H:773:ALA:HA	2.00	0.43
1:E:38:GLY:O	2:F:259:ARG:HD2	2.18	0.43
2:F:457:ILE:O	2:F:458:SER:HB2	2.18	0.43
1:C:7:LEU:HD21	1:C:32:LEU:HD11	1.99	0.43
2:F:497:VAL:HG13	2:F:511:VAL:HB	2.01	0.43
2:B:148:ARG:O	2:B:323:ALA:HA	2.17	0.43
2:B:276:TYR:OH	2:B:359:HIS:HD2	2.02	0.43
2:D:224:MET:CE	2:D:488:MET:HB3	2.48	0.43
1:A:359:GLN:O	1:A:359:GLN:HG3	2.18	0.43
1:C:427:ASP:OD1	1:C:435:ARG:NH2	2.47	0.43
2:H:184:LEU:HD23	2:H:252:PRO:HB3	2.01	0.43
2:H:7:LEU:HB3	2:H:8:PRO:HD2	2.00	0.43
1:A:461:MET:HA	1:A:462:PRO:HD3	1.91	0.43
2:B:277:ARG:HB2	2:B:290:ASP:HB3	2.01	0.43
1:C:351:TYR:CE2	1:C:445:ARG:HD3	2.54	0.43
2:D:70:LEU:HA	2:D:71:PRO:HD3	1.91	0.43
2:H:312:MET:CE	2:H:330:ARG:HH12	2.31	0.43
2:H:473:ILE:HB	2:H:596:LEU:HB3	2.01	0.43
2:B:31:ASN:HB2	2:B:251:ARG:NH1	2.32	0.43
2:B:418:VAL:HG13	2:B:450:LEU:HD11	2.00	0.43
2:B:601:PHE:CG	2:D:595:SER:HB2	2.54	0.43
1:G:202:ILE:HG12	1:G:208:VAL:HG11	2.00	0.43
1:G:49:VAL:HA	1:G:112:VAL:HG11	2.00	0.43
2:H:39:LEU:HB3	2:H:95:GLY:HA2	2.00	0.43
2:D:51:ASP:HB3	2:D:117:ARG:HB2	2.00	0.43
2:D:530:SER:HB3	2:D:727:ALA:HB1	2.00	0.43
2:H:451:SER:HB3	2:H:738:SER:HB3	2.01	0.43
2:H:414:LEU:HG	2:H:624:TYR:CD2	2.53	0.43
1:A:249:ILE:HG23	1:A:267:LEU:HD22	2.00	0.42
2:F:499:VAL:O	2:F:503:VAL:HG23	2.18	0.42
2:F:95:GLY:HA3	2:F:264:VAL:HG12	2.01	0.42
2:H:170:GLY:N	2:H:271:ASP:HB3	2.34	0.42
1:E:295:PRO:HB2	1:E:296:PRO:HD3	2.01	0.42
2:H:146:TRP:HZ3	2:H:313:LEU:HD13	1.84	0.42
1:E:136:CYS:O	2:F:666:GLY:HA3	2.20	0.42
2:H:288:GLY:HA2	2:H:323:ALA:O	2.18	0.42
1:A:187:ASP:HA	1:A:308:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ASN:HB2	2:D:251:ARG:HD3	2.01	0.42
2:H:497:VAL:HG13	2:H:511:VAL:HB	2.01	0.42
2:B:530:SER:CB	2:B:727:ALA:HB1	2.49	0.42
2:B:407:GLN:HG3	2:B:617:ARG:HG3	2.01	0.42
1:C:201:LEU:HD22	1:C:225:LEU:HD21	2.00	0.42
2:H:201:GLU:HG2	2:H:236:ASN:HD21	1.85	0.42
1:A:11:THR:HG22	1:A:164:PHE:HE1	1.85	0.42
2:B:650:ASP:OD2	2:B:726:LYS:HD2	2.20	0.42
1:G:322:PHE:HB3	1:G:390:VAL:CG2	2.49	0.42
2:H:364:MET:HE3	2:H:371:LEU:HD11	2.02	0.42
2:H:66:THR:HG22	2:H:67:ALA:H	1.83	0.42
2:B:310:ARG:HD2	2:B:344:PHE:HB3	2.01	0.42
2:D:288:GLY:HA2	2:D:323:ALA:O	2.19	0.42
2:D:492:LEU:O	2:D:496:MET:HG2	2.20	0.42
1:E:58:ARG:HD3	1:E:277:GLN:OE1	2.20	0.42
2:F:168:ILE:HA	2:F:759:ALA:HB3	2.02	0.42
1:A:190:ALA:HB1	1:A:310:GLY:HA2	2.02	0.42
2:B:360:LEU:HG	2:B:364:MET:HE3	2.01	0.42
2:D:271:ASP:OD1	2:D:296:ARG:HB3	2.19	0.42
2:H:35:LEU:HD13	2:H:100:LEU:HD11	2.02	0.42
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.52	0.42
2:B:414:LEU:HG	2:B:624:TYR:CD2	2.54	0.42
2:F:146:TRP:CZ3	2:F:313:LEU:HD13	2.54	0.42
2:D:418:VAL:HG13	2:D:450:LEU:HD21	2.02	0.41
2:D:528:ALA:HB1	5:D:1778:XAX:O2	2.20	0.41
2:D:633:ILE:HG22	2:D:640:ASN:HB3	2.02	0.41
2:F:31:ASN:HB2	2:F:251:ARG:HD3	2.00	0.41
2:H:450:LEU:HB2	2:H:628:ILE:HG12	2.01	0.41
2:B:360:LEU:HG	2:B:364:MET:CE	2.50	0.41
2:F:170:GLY:N	2:F:271:ASP:HB3	2.34	0.41
2:H:341:PHE:HD2	2:H:342:ARG:N	2.19	0.41
1:A:24:LEU:HD21	1:A:37:GLU:HB2	2.01	0.41
2:B:35:LEU:HB3	2:B:100:LEU:HD11	2.02	0.41
4:E:1465:FAD:N1	4:E:1465:FAD:H2'	2.35	0.41
1:E:245:ALA:HB1	1:E:282:GLY:HA3	2.01	0.41
2:F:281:ASP:HB2	2:F:285:LYS:O	2.21	0.41
1:G:351:TYR:CD2	1:G:445:ARG:HD3	2.56	0.41
2:H:647:ILE:HD12	2:H:710:VAL:HG22	2.02	0.41
2:B:530:SER:HB2	2:B:727:ALA:HB1	2.02	0.41
1:C:245:ALA:HB1	1:C:282:GLY:HA3	2.03	0.41
2:D:310:ARG:HD2	2:D:344:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:461:LEU:HD12	2:D:463:HIS:CE1	2.55	0.41
2:F:528:ALA:HB1	5:F:1778:XAX:O1	2.20	0.41
2:F:341:PHE:O	2:F:342:ARG:C	2.58	0.41
4:G:1465:FAD:H1'2	4:G:1465:FAD:H9	1.79	0.41
2:H:28:CYS:HB2	2:H:29:PRO:HD2	2.02	0.41
1:C:140:ALA:N	1:C:141:PRO:HD2	2.35	0.41
2:D:28:CYS:HB2	2:D:29:PRO:CD	2.51	0.41
2:H:221:MET:HE2	2:H:486:THR:HB	2.03	0.41
1:G:136:CYS:HB2	3:G:1463:FES:S2	2.60	0.41
1:G:192:TRP:CZ3	1:G:223:ALA:HB2	2.56	0.41
2:B:321:VAL:HA	2:B:322:PRO:HD3	1.93	0.41
2:B:633:ILE:HG22	2:B:640:ASN:HB3	2.01	0.41
2:B:478:SER:HB2	2:D:215:HIS:ND1	2.35	0.41
2:D:468:GLY:HA2	2:D:600:GLY:O	2.21	0.41
2:F:74:ASN:O	2:F:84:PRO:HA	2.21	0.41
1:G:24:LEU:HD13	1:G:47:CYS:HB2	2.02	0.41
2:F:488:MET:HG3	5:F:1778:XAX:C4	2.50	0.41
2:B:499:VAL:O	2:B:503:VAL:HG23	2.21	0.41
1:C:164:PHE:O	1:C:165:THR:HG22	2.20	0.41
2:D:164:GLY:HA3	2:D:276:TYR:CZ	2.56	0.41
1:E:298:LEU:HB3	1:E:303:ALA:HB3	2.02	0.41
1:E:370:LEU:HA	1:E:379:THR:O	2.21	0.41
1:E:351:TYR:CE2	1:E:445:ARG:HD3	2.56	0.41
2:H:448:ILE:HG13	2:H:629:THR:O	2.20	0.41
1:G:133:LEU:HD13	2:H:698:ILE:HD11	2.02	0.41
1:C:233:GLN:HE21	1:C:235:ARG:HH21	1.69	0.41
1:E:273:GLU:O	1:E:277:GLN:HG2	2.21	0.41
2:F:530:SER:HB3	2:F:727:ALA:HB1	2.01	0.41
1:G:366:GLY:HA3	1:G:442:MET:SD	2.60	0.41
1:G:461:MET:HA	1:G:462:PRO:HD3	1.86	0.41
2:H:446:ARG:HG2	2:H:632:VAL:HG12	2.03	0.41
2:B:464:LEU:CD1	7:B:1780:HHR:H6A1	2.50	0.41
2:F:138:ARG:HA	2:F:332:ARG:H	1.85	0.41
2:F:173:HIS:HA	2:F:341:PHE:CZ	2.57	0.41
2:H:224:MET:HE1	2:H:488:MET:HB3	2.03	0.41
2:D:146:TRP:CZ3	2:D:313:LEU:HD13	2.56	0.40
2:D:473:ILE:HG12	2:D:479:VAL:HG22	2.02	0.40
1:E:298:LEU:HB2	1:E:318:LEU:HD22	2.01	0.40
1:G:457:VAL:HG23	2:H:444:LEU:HD22	2.04	0.40
1:A:7:LEU:HD21	1:A:32:LEU:HD11	2.03	0.40
1:A:407:ARG:HD2	1:A:409:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LEU:O	2:B:555:VAL:HG23	2.21	0.40
1:C:373:LYS:HB2	1:C:378:GLU:HG2	2.03	0.40
2:F:341:PHE:HD2	2:F:342:ARG:N	2.19	0.40
1:G:134:CYS:HB3	1:G:139:TYR:CE2	2.56	0.40
2:H:464:LEU:HD12	7:H:1780:HHR:H6A1	2.03	0.40
2:H:507:ASP:HA	2:H:508:PRO:HD2	1.93	0.40
2:H:702:SER:O	2:H:706:ARG:NH2	2.54	0.40
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.57	0.40
2:D:367:ASP:HA	2:D:368:PRO:HD3	1.96	0.40
2:H:312:MET:HE1	2:H:330:ARG:HH12	1.87	0.40
2:D:184:LEU:HD23	2:D:252:PRO:HB3	2.03	0.40
1:G:331:ARG:HB2	1:G:334:GLU:HB2	2.04	0.40
2:H:701:PHE:O	2:H:704:ARG:HG2	2.21	0.40
2:H:751:GLY:HA3	2:H:773:ALA:O	2.21	0.40
1:A:140:ALA:N	1:A:141:PRO:HD2	2.36	0.40
1:C:133:LEU:HD13	2:D:698:ILE:HD11	2.03	0.40
2:D:296:ARG:HH21	2:D:335:THR:HG21	1.87	0.40
2:D:644:ARG:HG3	2:D:707:ILE:HB	2.02	0.40
2:D:724:ARG:HA	2:D:724:ARG:HD3	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	446/462 (96%)	413 (93%)	30 (7%)	3 (1%)	25 60
1	C	446/462 (96%)	416 (93%)	27 (6%)	3 (1%)	25 60
1	E	446/462 (96%)	423 (95%)	21 (5%)	2 (0%)	38 71
1	G	446/462 (96%)	418 (94%)	25 (6%)	3 (1%)	25 60
2	B	756/777 (97%)	721 (95%)	30 (4%)	5 (1%)	25 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	756/777 (97%)	724 (96%)	27 (4%)	5 (1%)	25	60
2	F	756/777 (97%)	724 (96%)	28 (4%)	4 (0%)	32	66
2	H	756/777 (97%)	730 (97%)	21 (3%)	5 (1%)	25	60
All	All	4808/4956 (97%)	4569 (95%)	209 (4%)	30 (1%)	28	63

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
2	D	187	GLU
2	D	399	LYS
2	D	458	SER
2	F	187	GLU
2	F	458	SER
2	H	187	GLU
2	H	399	LYS
2	H	458	SER
2	B	342	ARG
1	C	374	GLY
2	H	342	ARG
2	D	342	ARG
2	F	342	ARG
1	A	374	GLY
1	A	375	SER
2	B	399	LYS
1	C	39	CYS
1	C	359	GLN
2	F	399	LYS
1	G	203	ALA
1	G	374	GLY
2	H	227	GLY
1	G	375	SER
1	A	39	CYS
1	E	221	GLU
2	B	227	GLY
1	E	374	GLY
2	D	227	GLY
2	B	722	ILE

### 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%)	320 (94%)	19 (6%)	25	60
1	C	339/347 (98%)	319 (94%)	20 (6%)	23	58
1	E	339/347 (98%)	322 (95%)	17 (5%)	28	64
1	G	339/347 (98%)	321 (95%)	18 (5%)	26	62
2	B	571/584 (98%)	533 (93%)	38 (7%)	19	53
2	D	571/584 (98%)	542 (95%)	29 (5%)	28	63
2	F	571/584 (98%)	543 (95%)	28 (5%)	29	65
2	H	571/584 (98%)	543 (95%)	28 (5%)	29	65
All	All	3640/3724 (98%)	3443 (95%)	197 (5%)	26	62

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	20	THR
1	A	27	LEU
1	A	33	THR
1	A	40	ASN
1	A	58	ARG
1	A	103	CYS
1	A	128	LEU
1	A	143	LEU
1	A	165	THR
1	A	212	VAL
1	A	231	LEU
1	A	239	ASP
1	A	309	ARG
1	A	341	LEU
1	A	349	ARG
1	A	359	GLN
1	A	401	LEU
1	A	457	VAL

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Mol	Chain	Res	Type
2	B	10	ASP
2	B	23	LEU
2	B	48	THR
2	B	57	GLU
2	B	130	ASP
2	B	148	ARG
2	B	151	VAL
2	B	165	CYS
2	B	175	TYR
2	B	200	SER
2	B	215	HIS
2	B	221	MET
2	B	222	ARG
2	B	256	ARG
2	B	260	ASP
2	B	268	LYS
2	B	300	SER
2	B	313	LEU
2	B	326	ILE
2	B	330	ARG
2	B	341	PHE
2	B	355	ARG
2	B	398	LYS
2	B	399	LYS
2	B	426	ASN
2	B	429	THR
2	B	450	LEU
2	B	461	LEU
2	B	512	ARG
2	B	534	ASP
2	B	558	ARG
2	B	567	ILE
2	B	574	GLN
2	B	617	ARG
2	B	632	VAL
2	B	650	ASP
2	B	708	PHE
2	B	741	LEU
1	C	12	ARG
1	C	13	ARG
1	C	15	ARG
1	C	20	THR

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Mol	Chain	Res	Type
1	C	33	THR
1	C	40	ASN
1	C	61	ASN
1	C	128	LEU
1	C	143	LEU
1	C	165	THR
1	C	212	VAL
1	C	221	GLU
1	C	231	LEU
1	C	239	ASP
1	C	257	GLU
1	C	291	ILE
1	C	301	MET
1	C	349	ARG
1	C	371	THR
1	C	390	VAL
2	D	10	ASP
2	D	16	VAL
2	D	129	LEU
2	D	148	ARG
2	D	151	VAL
2	D	175	TYR
2	D	221	MET
2	D	222	ARG
2	D	256	ARG
2	D	268	LYS
2	D	313	LEU
2	D	330	ARG
2	D	341	PHE
2	D	355	ARG
2	D	398	LYS
2	D	399	LYS
2	D	400	THR
2	D	426	ASN
2	D	461	LEU
2	D	512	ARG
2	D	534	ASP
2	D	574	GLN
2	D	617	ARG
2	D	632	VAL
2	D	650	ASP
2	D	695	THR

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Mol	Chain	Res	Type
2	D	704	ARG
2	D	708	PHE
2	D	743	LEU
1	E	1	MET
1	E	12	ARG
1	E	22	SER
1	E	40	ASN
1	E	67	LEU
1	E	79	GLU
1	E	113	SER
1	E	128	LEU
1	E	143	LEU
1	E	165	THR
1	E	212	VAL
1	E	231	LEU
1	E	257	GLU
1	E	291	ILE
1	E	309	ARG
1	E	349	ARG
1	E	359	GLN
2	F	10	ASP
2	F	16	VAL
2	F	53	GLU
2	F	114	ARG
2	F	130	ASP
2	F	151	VAL
2	F	175	TYR
2	F	215	HIS
2	F	222	ARG
2	F	256	ARG
2	F	268	LYS
2	F	296	ARG
2	F	313	LEU
2	F	330	ARG
2	F	341	PHE
2	F	355	ARG
2	F	398	LYS
2	F	399	LYS
2	F	429	THR
2	F	461	LEU
2	F	558	ARG
2	F	574	GLN

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Mol	Chain	Res	Type
2	F	609	TRP
2	F	617	ARG
2	F	632	VAL
2	F	641	ARG
2	F	708	PHE
2	F	741	LEU
1	G	1	MET
1	G	33	THR
1	G	40	ASN
1	G	61	ASN
1	G	69	GLN
1	G	128	LEU
1	G	143	LEU
1	G	165	THR
1	G	212	VAL
1	G	231	LEU
1	G	309	ARG
1	G	325	TYR
1	G	341	LEU
1	G	349	ARG
1	G	390	VAL
1	G	401	LEU
1	G	435	ARG
1	G	457	VAL
2	H	10	ASP
2	H	16	VAL
2	H	88	THR
2	H	148	ARG
2	H	151	VAL
2	H	165	CYS
2	H	175	TYR
2	H	200	SER
2	H	215	HIS
2	H	222	ARG
2	H	251	ARG
2	H	256	ARG
2	H	268	LYS
2	H	313	LEU
2	H	326	ILE
2	H	330	ARG
2	H	341	PHE
2	H	398	LYS

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Mol	Chain	Res	Type
2	H	399	LYS
2	H	419	THR
2	H	426	ASN
2	H	442	ARG
2	H	461	LEU
2	H	512	ARG
2	H	558	ARG
2	H	617	ARG
2	H	632	VAL
2	H	708	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	260	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
2	B	691	HIS
2	B	744	HIS
1	C	40	ASN
1	C	61	ASN
1	C	233	GLN
2	D	236	ASN
2	D	426	ASN
2	D	463	HIS
2	D	574	GLN
2	D	744	HIS
1	E	40	ASN
1	E	61	ASN
2	F	236	ASN
2	F	441	ASN
2	F	744	HIS
1	G	40	ASN
1	G	61	ASN
1	G	69	GLN
1	G	118	HIS
2	H	208	HIS

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Mol	Chain	Res	Type
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	426	ASN
2	H	463	HIS
2	H	572	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	-	51,58,58	1.65	6 (11%)	54,89,89	1.74	6 (11%)
5	XAX	B	1778	-	23,31,31	3.79	7 (30%)	20,52,52	2.12	6 (30%)
7	HHR	B	1780	-	14,15,15	2.02	3 (21%)	17,21,21	2.71	9 (52%)
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	C	1465	-	51,58,58	1.66	6 (11%)	54,89,89	1.69	5 (9%)
5	XAX	D	1778	-	23,31,31	3.77	7 (30%)	20,52,52	2.14	6 (30%)
7	HHR	D	1780	-	14,15,15	1.97	3 (21%)	17,21,21	2.65	9 (52%)
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	-	51,58,58	1.66	6 (11%)	54,89,89	1.74	6 (11%)
5	XAX	F	1778	-	23,31,31	3.73	7 (30%)	20,52,52	2.16	6 (30%)
7	HHR	F	1780	-	14,15,15	1.99	3 (21%)	17,21,21	2.70	9 (52%)
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	-	51,58,58	1.67	6 (11%)	54,89,89	1.72	7 (12%)
5	XAX	H	1778	-	23,31,31	3.87	7 (30%)	20,52,52	2.14	5 (25%)
7	HHR	H	1780	-	14,15,15	2.03	3 (21%)	17,21,21	2.78	9 (52%)

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	0/1/1/1
3	FES	A	1464	1	-	0/0/4/4	0/1/1/1
4	FAD	A	1465	-	-	0/28/50/50	0/6/6/6
5	XAX	B	1778	-	1/1/7/9	0/6/46/46	0/4/4/4
7	HHR	B	1780	-	-	0/2/2/2	0/2/2/2
3	FES	C	1463	1	-	0/0/4/4	0/1/1/1
3	FES	C	1464	1	-	0/0/4/4	0/1/1/1
4	FAD	C	1465	-	-	0/28/50/50	0/6/6/6
5	XAX	D	1778	-	1/1/7/9	0/6/46/46	0/4/4/4
7	HHR	D	1780	-	-	0/2/2/2	0/2/2/2
3	FES	E	1463	1	-	0/0/4/4	0/1/1/1
3	FES	E	1464	1	-	0/0/4/4	0/1/1/1
4	FAD	E	1465	-	-	0/28/50/50	0/6/6/6
5	XAX	F	1778	-	-	0/6/46/46	0/4/4/4
7	HHR	F	1780	-	-	0/2/2/2	0/2/2/2
3	FES	G	1463	1	-	0/0/4/4	0/1/1/1
3	FES	G	1464	1	-	0/0/4/4	0/1/1/1
4	FAD	G	1465	-	-	0/28/50/50	0/6/6/6
5	XAX	H	1778	-	-	0/6/46/46	0/4/4/4
7	HHR	H	1780	-	-	0/2/2/2	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1778	XAX	C4'-C3'	-13.11	1.33	1.52
5	B	1778	XAX	C4'-C3'	-12.43	1.34	1.52
5	D	1778	XAX	C4'-C3'	-12.24	1.34	1.52
5	F	1778	XAX	C4'-C3'	-11.96	1.34	1.52
5	H	1778	XAX	C6-N5	-8.44	1.34	1.45
5	F	1778	XAX	C6-N5	-8.41	1.34	1.45
5	B	1778	XAX	C6-N5	-8.38	1.34	1.45
5	D	1778	XAX	C6-N5	-8.31	1.34	1.45
5	D	1778	XAX	C2'-S2'	-5.14	1.65	1.76
5	H	1778	XAX	C2'-S2'	-4.96	1.66	1.76
5	B	1778	XAX	C2'-S2'	-4.93	1.66	1.76
5	F	1778	XAX	C2'-S2'	-4.85	1.66	1.76
5	H	1778	XAX	C1'-S1'	-4.39	1.67	1.76
5	B	1778	XAX	C1'-S1'	-4.33	1.67	1.76
5	D	1778	XAX	C1'-S1'	-4.24	1.67	1.76
7	B	1780	HHR	O6A-C6A	-4.18	1.23	1.41
7	F	1780	HHR	O6A-C6A	-4.17	1.23	1.41
7	D	1780	HHR	O6A-C6A	-4.17	1.23	1.41
5	F	1778	XAX	C1'-S1'	-4.17	1.68	1.76
7	H	1780	HHR	O6A-C6A	-4.16	1.23	1.41
4	E	1465	FAD	C9A-N10	2.06	1.41	1.38
4	G	1465	FAD	C9A-N10	2.18	1.41	1.38
4	C	1465	FAD	C9A-N10	2.52	1.42	1.38
4	A	1465	FAD	C9A-N10	2.55	1.42	1.38
5	H	1778	XAX	C9-C10	2.96	1.47	1.41
5	D	1778	XAX	C9-C10	3.00	1.47	1.41
5	F	1778	XAX	C9-C10	3.00	1.47	1.41
5	B	1778	XAX	C9-C10	3.02	1.47	1.41
5	H	1778	XAX	C9-N5	3.15	1.44	1.37
4	E	1465	FAD	C5X-N5	3.21	1.40	1.35
7	F	1780	HHR	C2-N3	3.23	1.41	1.35
7	H	1780	HHR	C2-N3	3.24	1.41	1.35
5	F	1778	XAX	C9-N5	3.24	1.45	1.37
7	D	1780	HHR	C2-N3	3.25	1.41	1.35
5	B	1778	XAX	C9-N5	3.27	1.45	1.37
4	C	1465	FAD	C5X-N5	3.32	1.40	1.35
5	D	1778	XAX	C9-N5	3.38	1.45	1.37
7	B	1780	HHR	C2-N3	3.42	1.41	1.35
4	G	1465	FAD	C5X-N5	3.55	1.40	1.35
4	A	1465	FAD	C5X-N5	3.57	1.40	1.35
4	A	1465	FAD	O4B-C1B	3.74	1.46	1.41
4	G	1465	FAD	O4B-C1B	4.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1780	HHR	C4-N3	4.19	1.40	1.33
7	F	1780	HHR	C4-N3	4.27	1.40	1.33
7	B	1780	HHR	C4-N3	4.34	1.40	1.33
7	H	1780	HHR	C4-N3	4.38	1.41	1.33
4	A	1465	FAD	C4-N3	4.42	1.41	1.33
4	G	1465	FAD	C4-N3	4.43	1.41	1.33
4	E	1465	FAD	O4B-C1B	4.45	1.47	1.41
4	C	1465	FAD	C4-N3	4.56	1.41	1.33
4	E	1465	FAD	C4-N3	4.63	1.41	1.33
4	C	1465	FAD	C4X-N5	4.83	1.40	1.33
4	C	1465	FAD	O4B-C1B	4.99	1.48	1.41
4	E	1465	FAD	C4X-N5	5.10	1.40	1.33
4	C	1465	FAD	C10-N1	5.30	1.40	1.33
4	G	1465	FAD	C4X-N5	5.36	1.41	1.33
4	A	1465	FAD	C4X-N5	5.42	1.41	1.33
5	H	1778	XAX	C4-C9	5.49	1.47	1.41
4	A	1465	FAD	C10-N1	5.58	1.41	1.33
4	E	1465	FAD	C10-N1	5.62	1.41	1.33
4	G	1465	FAD	C10-N1	5.64	1.41	1.33
5	B	1778	XAX	C4-C9	5.71	1.48	1.41
5	D	1778	XAX	C4-C9	5.85	1.48	1.41
5	F	1778	XAX	C4-C9	6.04	1.48	1.41

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1465	FAD	N3A-C2A-N1A	-8.86	121.14	128.86
4	A	1465	FAD	N3A-C2A-N1A	-8.80	121.19	128.86
4	G	1465	FAD	N3A-C2A-N1A	-8.62	121.35	128.86
4	C	1465	FAD	N3A-C2A-N1A	-8.10	121.81	128.86
7	H	1780	HHR	N1-C2-N3	-4.78	120.47	127.46
7	B	1780	HHR	N1-C2-N3	-4.77	120.49	127.46
7	F	1780	HHR	N1-C2-N3	-4.66	120.65	127.46
7	D	1780	HHR	N1-C2-N3	-4.55	120.81	127.46
7	D	1780	HHR	C10-C4-N3	-3.53	118.45	123.48
7	B	1780	HHR	C10-C4-N3	-3.50	118.50	123.48
7	F	1780	HHR	C10-C4-N3	-3.41	118.63	123.48
7	H	1780	HHR	C10-C4-N3	-3.29	118.80	123.48
7	D	1780	HHR	C6-C7-N8	-3.21	119.83	123.09
7	B	1780	HHR	C6-C7-N8	-3.04	120.01	123.09
7	H	1780	HHR	C6-C7-N8	-2.98	120.07	123.09
7	F	1780	HHR	C6-C7-N8	-2.90	120.15	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1465	FAD	C4X-C4-N3	-2.69	119.66	123.48
4	E	1465	FAD	C4X-C4-N3	-2.35	120.14	123.48
4	G	1465	FAD	C4X-C4-N3	-2.33	120.16	123.48
4	A	1465	FAD	C4X-C4-N3	-2.32	120.17	123.48
5	F	1778	XAX	O1P-P-O4'	-2.08	101.20	106.73
4	G	1465	FAD	C4A-C5A-N7A	-2.04	107.44	109.41
5	B	1778	XAX	N3-C2-N1	-2.03	122.16	125.45
4	E	1465	FAD	C4A-C5A-N7A	-2.02	107.46	109.41
5	D	1778	XAX	N3-C2-N1	-2.00	122.20	125.45
7	B	1780	HHR	C4-C10-N5	2.05	120.92	118.68
7	D	1780	HHR	C4-C10-N5	2.05	120.93	118.68
4	G	1465	FAD	C1'-N10-C10	2.09	120.65	118.50
7	F	1780	HHR	C4-C10-N5	2.14	121.02	118.68
7	H	1780	HHR	C4-C10-N5	2.18	121.07	118.68
7	F	1780	HHR	C4-N3-C2	2.23	119.27	116.06
7	H	1780	HHR	C4-N3-C2	2.25	119.29	116.06
4	A	1465	FAD	C1'-N10-C9A	2.28	120.44	118.35
7	D	1780	HHR	C4-N3-C2	2.29	119.36	116.06
5	D	1778	XAX	C4-C9-C10	2.32	116.67	114.56
5	H	1778	XAX	N8-C10-N1	2.34	121.43	116.90
7	B	1780	HHR	C4-N3-C2	2.34	119.43	116.06
5	B	1778	XAX	N8-C10-N1	2.38	121.51	116.90
5	D	1778	XAX	N8-C10-N1	2.40	121.55	116.90
4	G	1465	FAD	C5X-C9A-N10	2.43	119.47	117.66
5	F	1778	XAX	N8-C10-N1	2.44	121.62	116.90
7	B	1780	HHR	N8-C9-N1	2.54	119.32	116.04
4	E	1465	FAD	C5X-C9A-N10	2.61	119.60	117.66
4	A	1465	FAD	C5X-C9A-N10	2.62	119.60	117.66
7	H	1780	HHR	N8-C9-N1	2.65	119.46	116.04
5	B	1778	XAX	C4-C9-C10	2.68	116.99	114.56
7	D	1780	HHR	N8-C9-N1	2.69	119.51	116.04
7	F	1780	HHR	N8-C9-N1	2.70	119.53	116.04
5	H	1778	XAX	C4-C9-C10	3.00	117.28	114.56
4	C	1465	FAD	C1'-N10-C9A	3.00	121.10	118.35
5	H	1778	XAX	C2-N1-C10	3.03	121.34	114.51
5	D	1778	XAX	C2-N1-C10	3.04	121.37	114.51
5	F	1778	XAX	C4-C9-C10	3.05	117.33	114.56
5	B	1778	XAX	C2-N1-C10	3.07	121.43	114.51
5	F	1778	XAX	C2-N1-C10	3.11	121.51	114.51
4	E	1465	FAD	C4X-N5-C5X	3.25	120.19	116.76
4	G	1465	FAD	C4X-N5-C5X	3.38	120.33	116.76
4	A	1465	FAD	C4X-N5-C5X	3.46	120.42	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1780	HHR	C6A-C6-N5	3.50	119.57	115.39
4	C	1465	FAD	C4X-N5-C5X	3.73	120.70	116.76
7	F	1780	HHR	C6A-C6-N5	3.81	119.94	115.39
7	D	1780	HHR	O6A-C6A-C6	3.82	120.79	112.18
7	B	1780	HHR	O6A-C6A-C6	3.84	120.83	112.18
7	F	1780	HHR	O6A-C6A-C6	3.86	120.87	112.18
7	B	1780	HHR	C6A-C6-N5	3.89	120.04	115.39
5	F	1778	XAX	C4-N3-C2	3.96	121.76	116.06
5	H	1778	XAX	C4-N3-C2	3.97	121.77	116.06
7	H	1780	HHR	O6A-C6A-C6	4.05	121.31	112.18
5	D	1778	XAX	C4-N3-C2	4.06	121.90	116.06
5	B	1778	XAX	C4-N3-C2	4.07	121.92	116.06
7	H	1780	HHR	C6A-C6-N5	4.29	120.52	115.39
5	F	1778	XAX	O3'-C7-C6	4.94	112.26	108.96
7	D	1780	HHR	C2-N1-C9	4.96	120.95	115.16
7	B	1780	HHR	C2-N1-C9	5.09	121.10	115.16
5	B	1778	XAX	O3'-C7-C6	5.15	112.40	108.96
7	H	1780	HHR	C2-N1-C9	5.19	121.22	115.16
7	F	1780	HHR	C2-N1-C9	5.21	121.24	115.16
4	C	1465	FAD	C4-N3-C2	5.35	119.84	115.16
4	A	1465	FAD	C4-N3-C2	5.43	119.91	115.16
5	H	1778	XAX	O3'-C7-C6	5.44	112.59	108.96
4	E	1465	FAD	C4-N3-C2	5.47	119.94	115.16
4	G	1465	FAD	C4-N3-C2	5.56	120.02	115.16
5	D	1778	XAX	O3'-C7-C6	5.58	112.68	108.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1778	XAX	C3'
5	D	1778	XAX	C3'

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1465	FAD	3	0
5	B	1778	XAX	6	0
7	B	1780	HHR	1	0
4	C	1465	FAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1778	XAX	6	0
4	E	1465	FAD	3	0
5	F	1778	XAX	7	0
3	G	1463	FES	1	0
4	G	1465	FAD	3	0
5	H	1778	XAX	4	0
7	H	1780	HHR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	450/462 (97%)	0.05	11 (2%) 59 56	21, 23, 24, 26	0
1	C	450/462 (97%)	-0.29	0 100 100	21, 23, 24, 26	0
1	E	450/462 (97%)	-0.06	4 (0%) 84 83	21, 23, 24, 26	0
1	G	450/462 (97%)	0.06	9 (2%) 65 63	21, 23, 24, 26	0
2	B	760/777 (97%)	-0.32	0 100 100	20, 23, 25, 28	0
2	D	760/777 (97%)	-0.39	1 (0%) 95 96	20, 23, 25, 28	0
2	F	760/777 (97%)	-0.44	0 100 100	20, 23, 25, 28	0
2	H	760/777 (97%)	-0.37	0 100 100	20, 23, 25, 28	0
All	All	4840/4956 (97%)	-0.26	25 (0%) 90 90	20, 23, 25, 28	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	166	LEU	4.1
2	D	398	LYS	3.1
1	G	194	LEU	3.0
1	A	413	ALA	2.8
1	E	165	THR	2.8
1	G	192	TRP	2.7
1	A	240	GLY	2.7
1	G	378	GLU	2.6
1	A	375	SER	2.5
1	A	239	ASP	2.5
1	A	378	GLU	2.5
1	A	403	GLY	2.4
1	E	312	GLU	2.3
1	A	313	ARG	2.3
1	G	401	LEU	2.3
1	A	411	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	240	GLY	2.2
1	G	379	THR	2.1
1	A	417	LEU	2.1
1	E	235	ARG	2.1
1	A	192	TRP	2.1
1	G	161	ASP	2.1
1	G	218	ASP	2.1
1	A	405	ASP	2.0
1	G	165	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	HHR	H	1780	14/14	0.77	0.34	7.88	84,84,84,85	0
7	HHR	D	1780	14/14	0.82	0.33	4.79	76,76,76,76	0
3	FES	E	1464	4/4	0.99	0.23	3.51	49,49,49,50	0
5	XAX	B	1778	28/28	0.97	0.34	3.36	31,33,39,40	28
5	XAX	F	1778	28/28	0.98	0.26	3.08	26,29,32,33	28
5	XAX	H	1778	28/28	0.97	0.24	2.42	34,36,43,44	28
7	HHR	B	1780	14/14	0.85	0.24	2.17	83,83,83,84	0
3	FES	G	1464	4/4	0.99	0.24	1.93	51,52,52,52	0
7	HHR	F	1780	14/14	0.86	0.23	1.90	81,81,82,82	0
3	FES	G	1463	4/4	0.98	0.24	1.79	57,57,58,58	0
3	FES	A	1464	4/4	0.98	0.25	1.71	51,52,52,53	0
3	FES	E	1463	4/4	0.99	0.20	1.47	36,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	XAX	D	1778	28/28	0.98	0.23	1.39	21,25,29,31	28
3	FES	C	1464	4/4	0.99	0.23	1.29	34,34,34,34	0
3	FES	C	1463	4/4	0.99	0.21	0.71	25,26,26,26	0
3	FES	A	1463	4/4	0.99	0.24	0.42	31,32,32,32	0
4	FAD	A	1465	53/53	0.93	0.19	-0.23	57,59,61,62	0
4	FAD	G	1465	53/53	0.92	0.18	-0.37	63,66,72,72	0
4	FAD	C	1465	53/53	0.96	0.17	-0.48	27,29,35,36	0
4	FAD	E	1465	53/53	0.93	0.17	-0.60	48,52,63,64	0
6	BA	F	1779	1/1	0.93	0.12	-1.63	161,161,161,161	0
6	BA	H	1779	1/1	0.98	0.09	-2.86	168,168,168,168	0
6	BA	D	1779	1/1	0.93	0.12	-3.39	160,160,160,160	0
6	BA	B	1779	1/1	0.96	0.09	-5.37	154,154,154,154	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.