Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:11 AM GMT

PDB ID	:	2W55
Title	:	Crystal Structure of Xanthine Dehydrogenase (E232Q variant) from Rhodobacter capsulatus in Complex with Hypoxanthine
Authors	:	Doebbler, J.A.; Truglio, J.J.; Leimkuhler, S.; Kisker, C.
Deposited on	:	2008-12-04
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

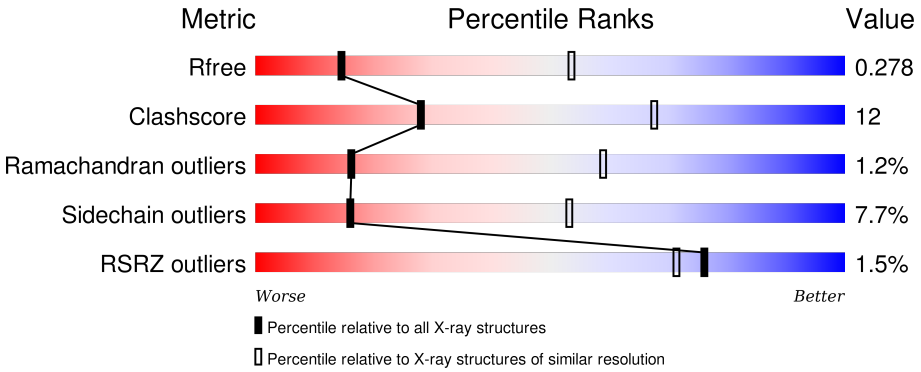
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	6% 71% 25%
1	C	462	% 73% 21%
1	E	462	3% 72% 23%
1	G	462	5% 68% 27%
2	B	777	69% 25%

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Mol	Chain	Length	Quality of chain
2	D	777	68% 27%
2	F	777	68% 27%
2	H	777	69% 25%

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	A	1464	-	-	-	X
3	FES	G	1464	-	-	-	X
5	XAX	B	1778	X	-	-	X
5	XAX	D	1778	X	-	-	-
5	XAX	F	1778	X	-	-	X
5	XAX	H	1778	X	-	-	-
7	HPA	D	1780	-	-	-	X
7	HPA	H	1780	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36807 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
			3375	2115	608	627	25			
1	C	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	E	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	25			
1	G	450	Total	C	N	O	S	0	0	0
			3375	2115	608	627	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

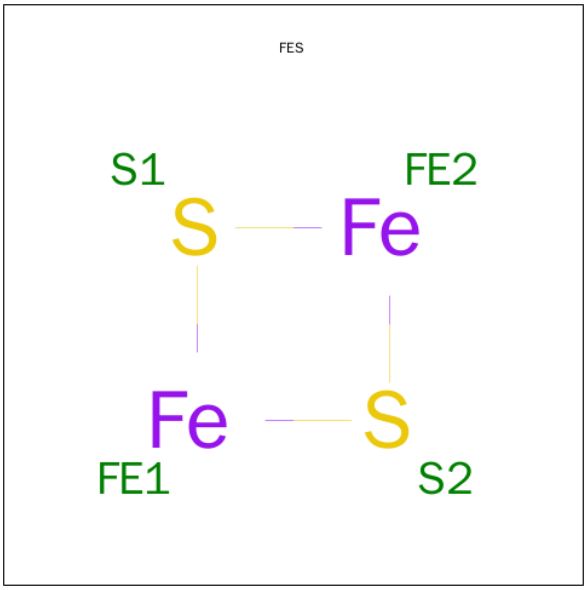
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	D	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	F	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			
2	H	760	Total	C	N	O	S	0	0	0
			5716	3581	1057	1052	26			

There are 8 discrepancies between the modelled and reference sequences:

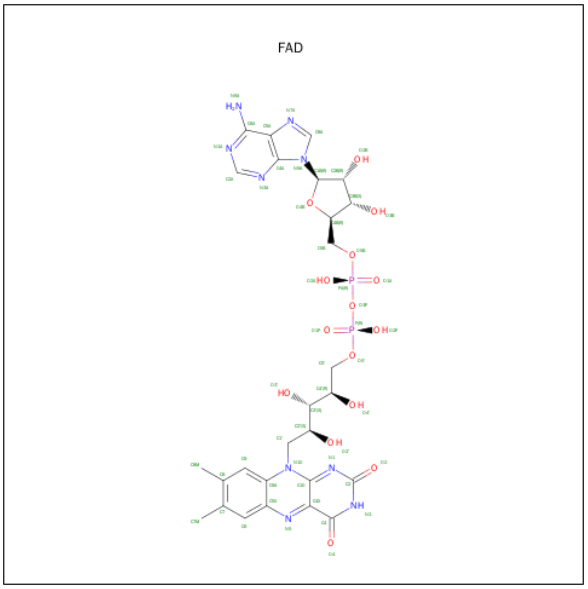
Chain	Residue	Modelled	Actual	Comment	Reference
B	232	GLN	GLU	ENGINEERED MUTATION	UNP O54051
B	772	ARG	GLY	CONFLICT	UNP O54051
D	232	GLN	GLU	ENGINEERED MUTATION	UNP O54051
D	772	ARG	GLY	CONFLICT	UNP O54051
F	232	GLN	GLU	ENGINEERED MUTATION	UNP O54051
F	772	ARG	GLY	CONFLICT	UNP O54051
H	232	GLN	GLU	ENGINEERED MUTATION	UNP O54051
H	772	ARG	GLY	CONFLICT	UNP O54051

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



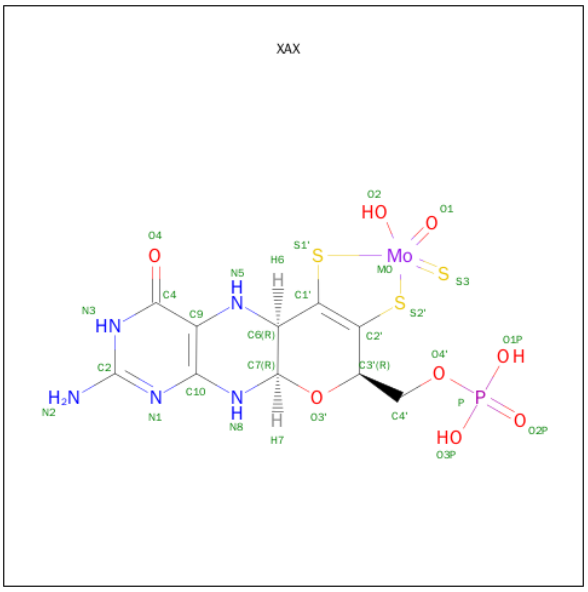
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	E	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0
3	G	1	Total Fe S 4 2 2	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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: $C_{10}H_{13}MoN_5O_8PS_3$).

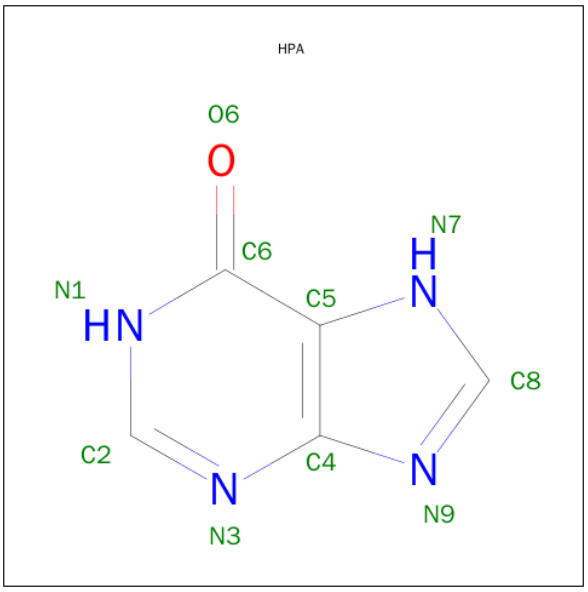


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	F	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
5	H	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- 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 HYPOXANTHINE (three-letter code: HPA) (formula: $C_5H_4N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 10 5 4 1	0	0
7	D	1	Total C N O 10 5 4 1	0	0
7	F	1	Total C N O 10 5 4 1	0	0
7	H	1	Total C N O 10 5 4 1	0	0

- Molecule 8 is water.

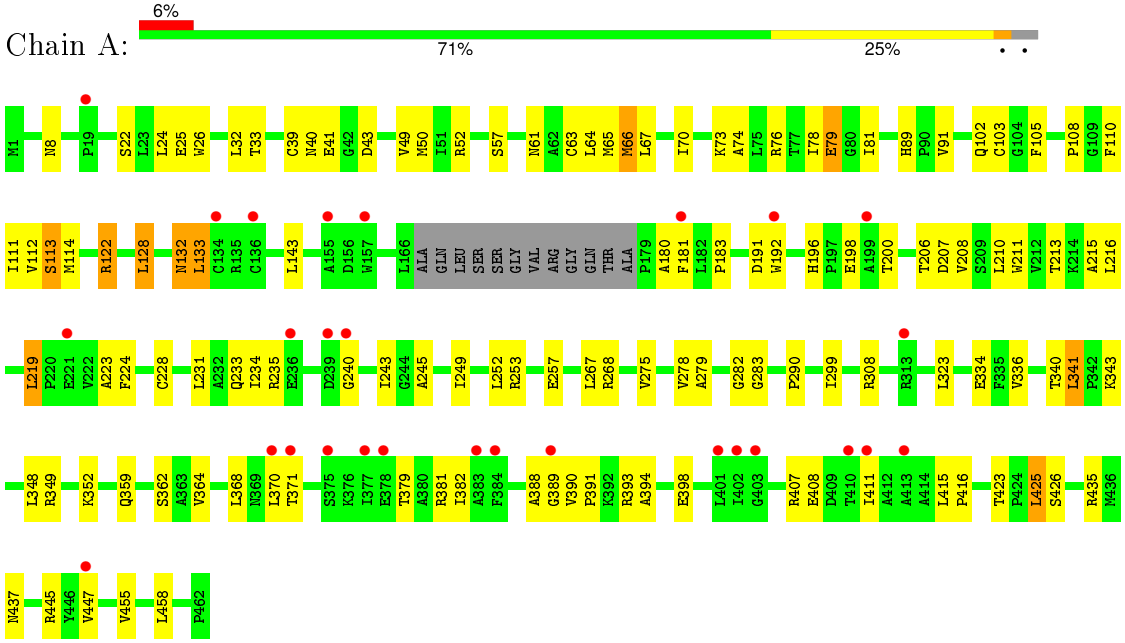
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total O 4 4	0	0
8	B	8	Total O 8 8	0	0
8	C	3	Total O 3 3	0	0
8	D	11	Total O 11 11	0	0
8	E	1	Total O 1 1	0	0
8	F	12	Total O 12 12	0	0
8	G	1	Total O 1 1	0	0
8	H	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

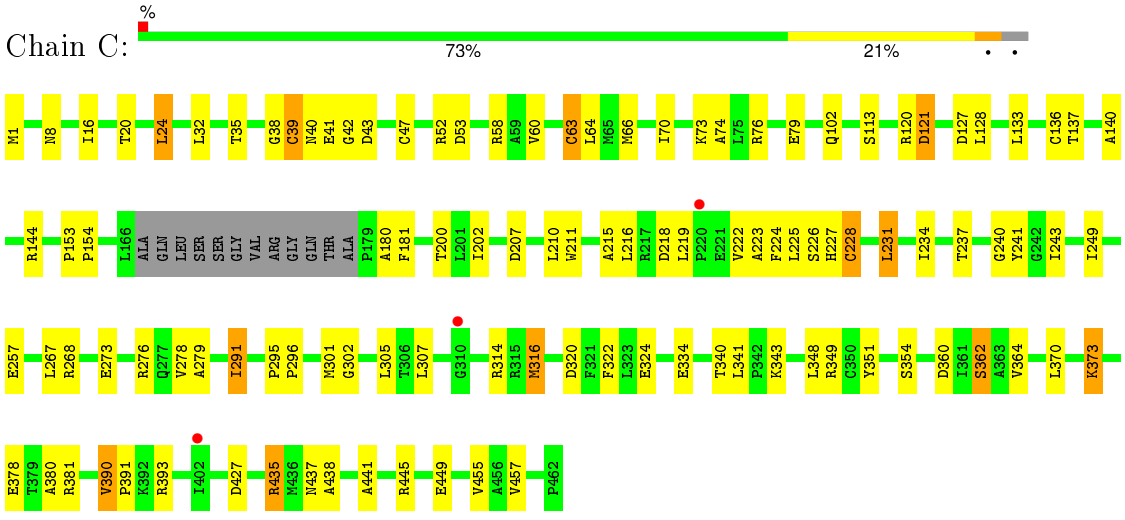
- Molecule 1: XANTHINE DEHYDROGENASE

Chain A:



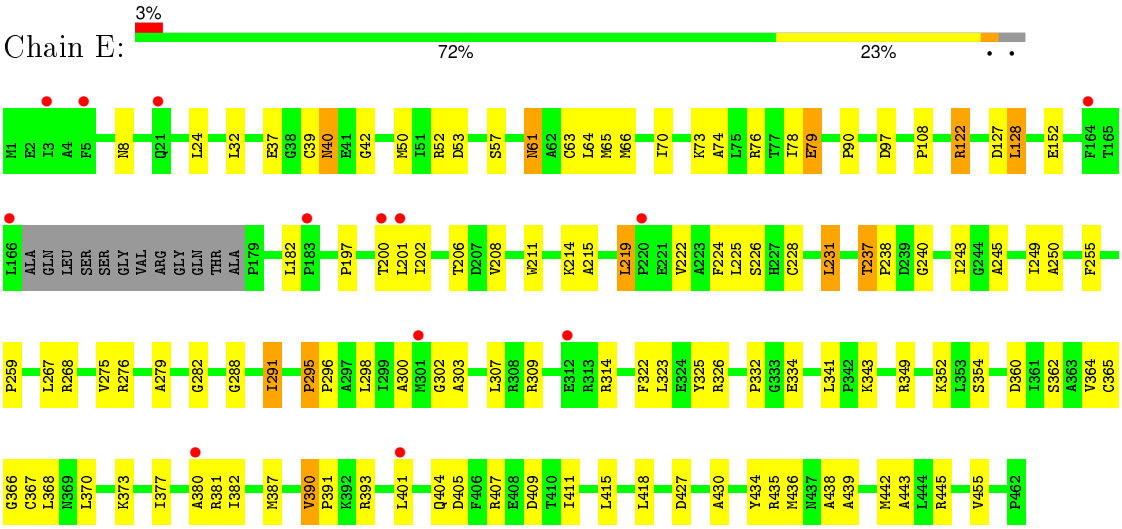
- Molecule 1: XANTHINE DEHYDROGENASE

Chain C:



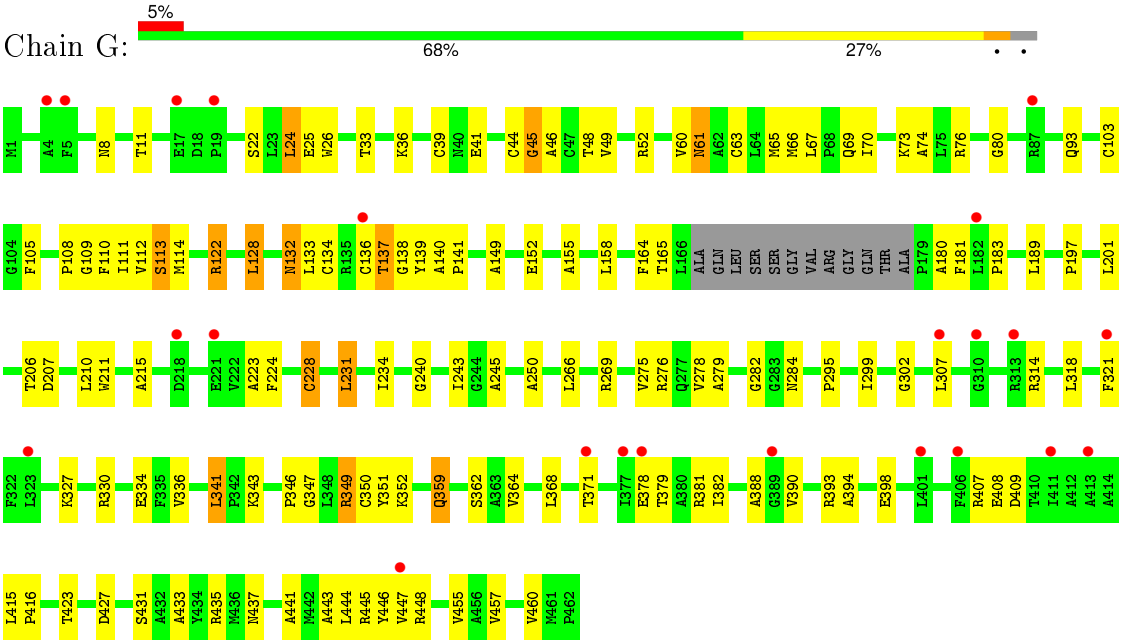
- Molecule 1: XANTHINE DEHYDROGENASE

Chain E:



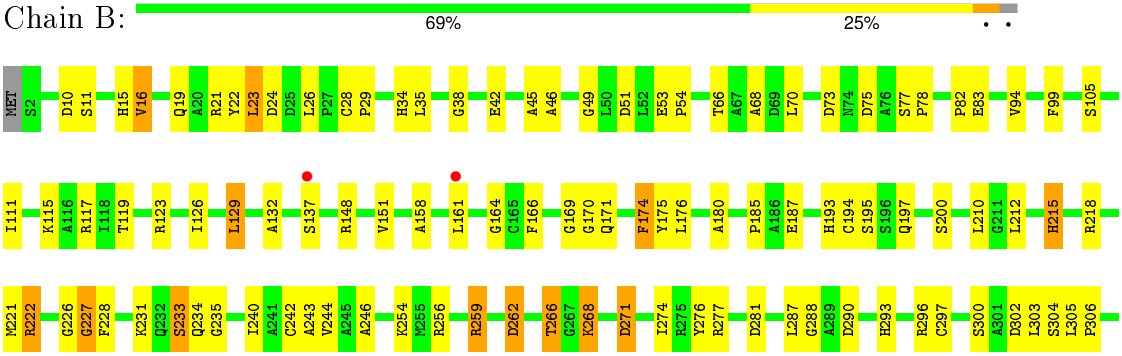
• Molecule 1: XANTHINE DEHYDROGENASE

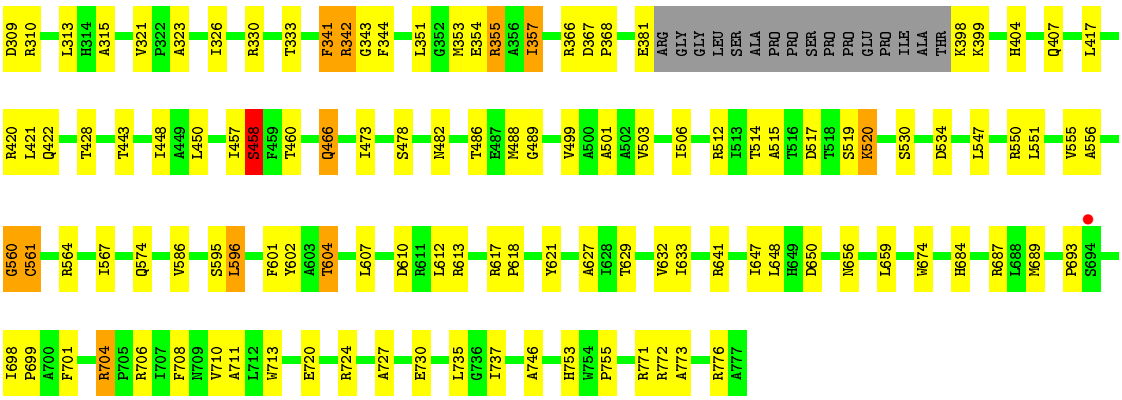
Chain G:



• Molecule 2: XANTHINE DEHYDROGENASE

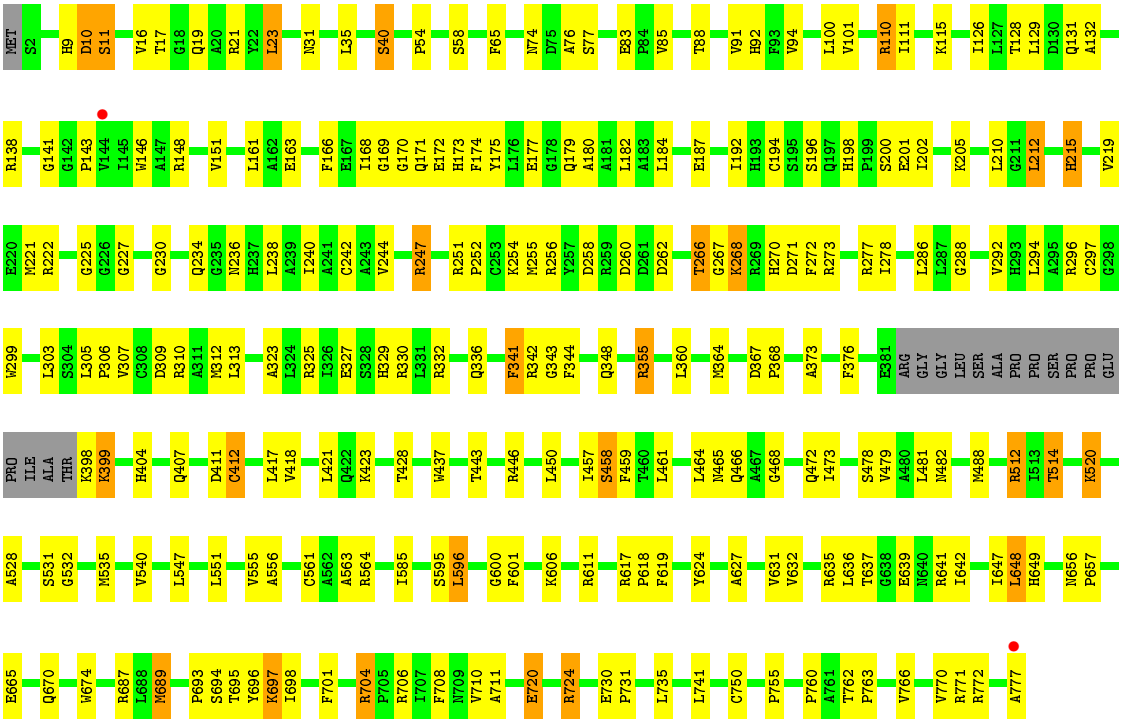
Chain B:





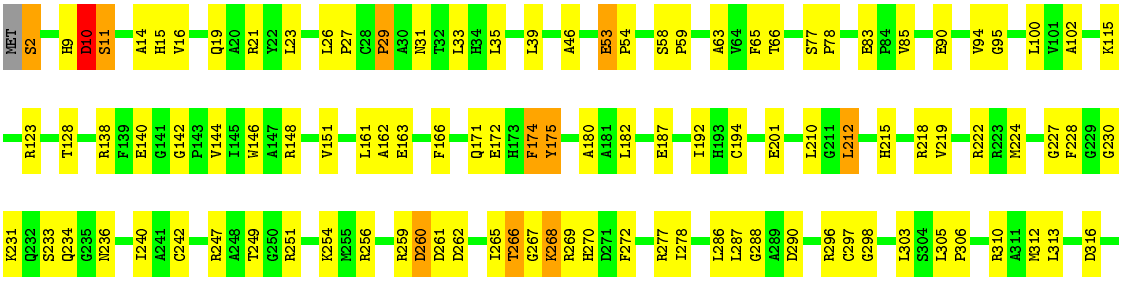
• Molecule 2: XANTHINE DEHYDROGENASE

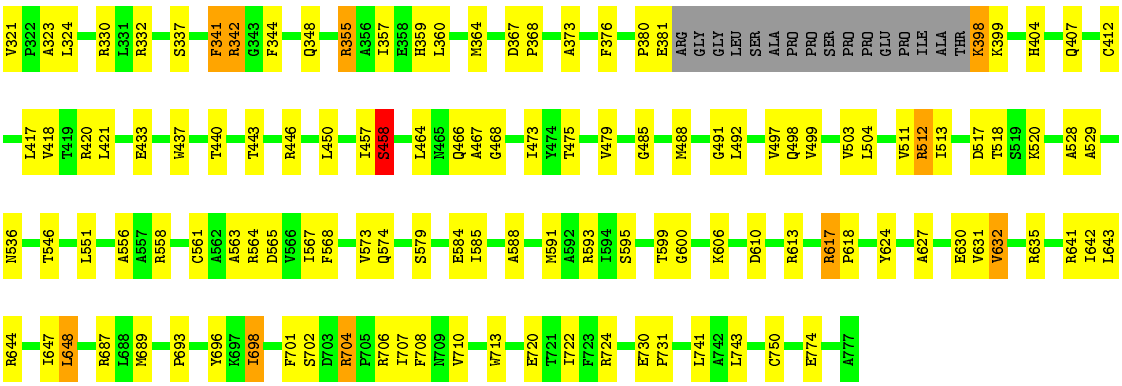
Chain D:



• Molecule 2: XANTHINE DEHYDROGENASE

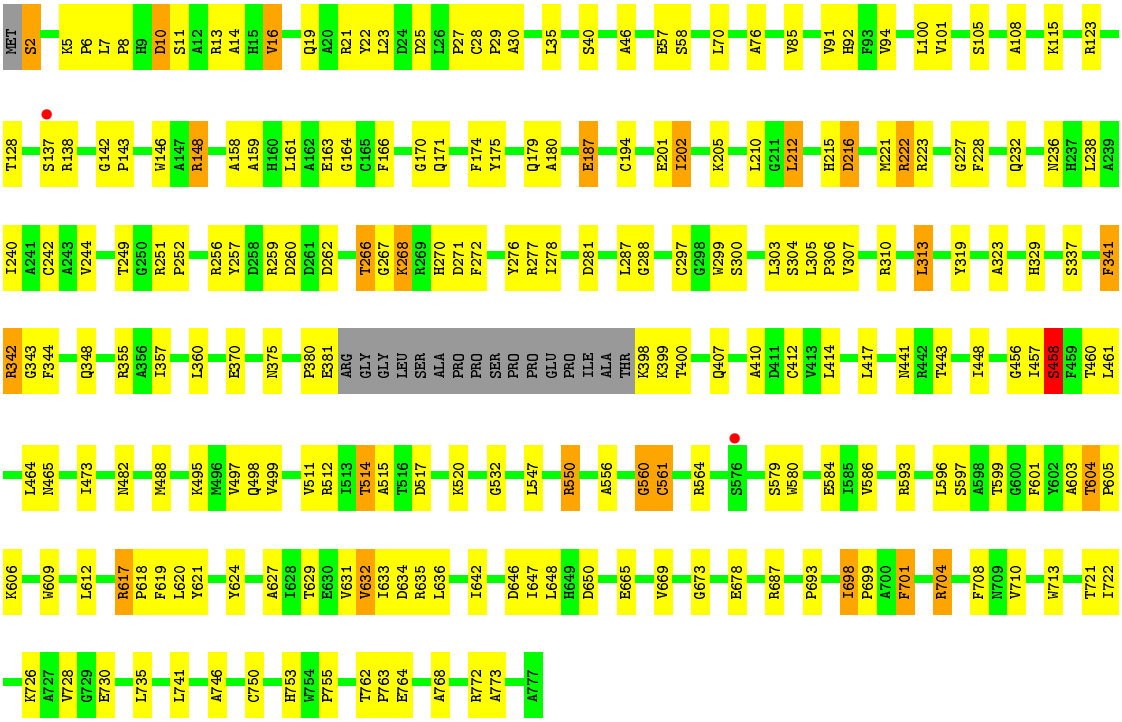
Chain F:





• Molecule 2: XANTHINE DEHYDROGENASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.74Å 140.57Å 157.61Å 109.45° 106.10° 101.09°	Depositor
Resolution (Å)	50.00 – 3.40 49.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.40) 70.5 (49.83-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.221 , 0.270 0.225 , 0.278	Depositor DCC
R_{free} test set	3708 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 73280 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	36807	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.94 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.7034e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAX, HPA, 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	0.36	0/3438	0.54	0/4658
1	C	0.35	0/3438	0.54	0/4658
1	E	0.35	0/3438	0.53	0/4658
1	G	0.36	0/3438	0.55	0/4658
2	B	0.35	0/5844	0.53	0/7941
2	D	0.36	0/5844	0.55	0/7941
2	F	0.37	0/5844	0.56	0/7941
2	H	0.36	0/5844	0.53	0/7941
All	All	0.36	0/37128	0.54	0/50396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	3368	69	0
1	C	3375	0	3368	64	0
1	E	3375	0	3369	72	0
1	G	3375	0	3371	87	0
2	B	5716	0	5633	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5716	0	5633	155	0
2	F	5716	0	5633	145	0
2	H	5716	0	5633	142	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	6	0
4	C	53	0	31	5	0
4	E	53	0	31	3	0
4	G	53	0	31	8	0
5	B	28	0	8	4	0
5	D	28	0	8	7	0
5	F	28	0	8	8	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	10	0	4	0	0
7	D	10	0	4	3	0
7	F	10	0	4	1	0
7	H	10	0	4	7	0
8	A	4	0	0	0	0
8	B	8	0	0	1	0
8	C	3	0	0	1	0
8	D	11	0	0	0	0
8	E	1	0	0	0	0
8	F	12	0	0	0	0
8	G	1	0	0	0	0
8	H	3	0	0	0	0
All	All	36807	0	36180	851	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 12.

All (851) 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)
5:F:1778:XAX:O1	7:F:1780:HPA:H2	1.49	1.12
2:D:179:GLN:HB3	2:D:238:LEU:HD11	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ARG:HG3	1:C:455:VAL:HG11	1.50	0.94
2:H:457:ILE:O	2:H:458:SER:HB2	1.62	0.93
2:F:138:ARG:HD3	2:F:142:GLY:H	1.34	0.92
1:E:387:MET:CE	1:E:439:ALA:HB2	1.99	0.91
1:G:243:ILE:HD13	1:G:341:LEU:HD21	1.52	0.91
1:A:24:LEU:HD12	1:A:63:CYS:HB3	1.53	0.91
2:F:407:GLN:OE1	2:F:618:PRO:HD2	1.71	0.91
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.53	0.90
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.55	0.89
1:C:40:ASN:ND2	1:C:63:CYS:HB2	1.87	0.88
2:D:179:GLN:HB3	2:D:238:LEU:CD1	2.04	0.87
2:F:210:LEU:HB3	2:F:212:LEU:HD21	1.58	0.85
2:B:457:ILE:O	2:B:458:SER:HB2	1.75	0.85
2:H:755:PRO:O	2:H:772:ARG:HD2	1.76	0.85
2:B:701:PHE:O	2:B:704:ARG:HG2	1.76	0.84
2:H:465:ASN:HB3	2:H:604:THR:OG1	1.77	0.84
1:E:237:THR:OG1	1:E:238:PRO:HD2	1.78	0.83
2:D:247:ARG:HH11	2:D:247:ARG:HG2	1.41	0.83
2:H:701:PHE:O	2:H:704:ARG:HG2	1.79	0.82
2:B:129:LEU:H	2:B:129:LEU:HD12	1.44	0.82
2:D:443:THR:HG23	2:D:636:LEU:HD13	1.61	0.81
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.63	0.80
1:C:200:THR:HB	1:C:222:VAL:HG12	1.63	0.80
2:D:701:PHE:O	2:D:704:ARG:HG2	1.84	0.78
1:C:249:ILE:HG23	1:C:267:LEU:HD22	1.65	0.78
2:H:259:ARG:HG2	2:H:693:PRO:HD3	1.65	0.78
2:D:31:ASN:HB2	2:D:251:ARG:HD3	1.66	0.77
1:C:133:LEU:HD13	2:D:698:ILE:HD11	1.67	0.77
2:F:272:PHE:CD2	2:F:348:GLN:HG2	2.21	0.76
1:G:41:GLU:HA	1:G:210:LEU:HD21	1.67	0.76
2:D:151:VAL:HG21	2:D:325:ARG:HB2	1.67	0.76
1:C:322:PHE:HB3	1:C:390:VAL:HG22	1.67	0.75
1:G:24:LEU:HD12	1:G:63:CYS:HB3	1.69	0.75
2:B:75:ASP:OD2	2:B:82:PRO:HA	1.87	0.74
1:G:455:VAL:HG13	2:H:443:THR:HG21	1.69	0.74
2:F:288:GLY:HA2	2:F:323:ALA:O	1.87	0.74
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.70	0.74
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.70	0.73
2:F:497:VAL:HG13	2:F:511:VAL:HB	1.70	0.73
2:F:457:ILE:O	2:F:458:SER:HB2	1.85	0.73
1:G:352:LYS:HG3	1:G:362:SER:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:637:THR:OG1	2:D:639:GLU:HG3	1.89	0.72
1:C:40:ASN:HD22	1:C:63:CYS:HB2	1.52	0.71
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.71	0.71
1:A:133:LEU:HD13	2:B:698:ILE:HD11	1.71	0.71
2:H:163:GLU:HG2	2:H:277:ARG:HG2	1.71	0.71
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.71	0.71
1:A:394:ALA:O	1:A:398:GLU:HB2	1.90	0.71
2:F:31:ASN:HB2	2:F:251:ARG:HD3	1.73	0.70
1:E:455:VAL:HG13	2:F:443:THR:HG21	1.73	0.70
2:D:360:LEU:HG	2:D:364:MET:HE3	1.71	0.70
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.71	0.70
2:F:58:SER:HB2	2:F:115:LYS:HD2	1.73	0.70
2:H:13:ARG:HH11	2:H:13:ARG:HG2	1.55	0.70
2:H:232:GLN:HE22	7:H:1780:HPA:H2	1.56	0.70
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.73	0.70
2:H:753:HIS:HB2	2:H:773:ALA:HA	1.73	0.69
1:G:382:ILE:HD12	1:G:398:GLU:HG3	1.73	0.69
2:F:144:VAL:CG2	2:F:330:ARG:HH12	2.05	0.69
1:A:455:VAL:HG13	2:B:443:THR:HG21	1.74	0.69
2:B:720:GLU:HA	2:B:724:ARG:NH2	2.08	0.69
2:F:701:PHE:O	2:F:704:ARG:HG2	1.93	0.68
2:F:303:LEU:O	2:F:306:PRO:HD2	1.92	0.68
2:H:482:ASN:HD22	2:H:514:THR:HB	1.57	0.68
2:B:610:ASP:HB3	2:B:613:ARG:HB2	1.75	0.68
2:F:641:ARG:NH2	2:F:706:ARG:HD3	2.09	0.68
2:B:755:PRO:O	2:B:772:ARG:HD2	1.93	0.68
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.29	0.68
2:B:77:SER:HB2	2:B:83:GLU:HB3	1.75	0.68
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.76	0.68
5:F:1778:XAX:S3	5:F:1778:XAX:MO	2.04	0.68
2:B:259:ARG:HG2	2:B:693:PRO:HD3	1.76	0.67
2:H:11:SER:OG	2:H:223:ARG:NH2	2.27	0.67
1:E:24:LEU:HD21	1:E:37:GLU:HG2	1.77	0.67
2:B:70:LEU:HD23	2:B:244:VAL:HG11	1.77	0.67
5:D:1778:XAX:S3	5:D:1778:XAX:MO	2.05	0.67
2:F:635:ARG:NH1	2:F:750:CYS:HB3	2.10	0.66
1:A:105:PHE:O	1:A:108:PRO:HD2	1.95	0.66
5:H:1778:XAX:S3	5:H:1778:XAX:MO	2.06	0.66
2:F:27:PRO:HB2	2:H:29:PRO:HG3	1.76	0.66
1:E:322:PHE:HB3	1:E:390:VAL:HG22	1.77	0.66
2:F:9:HIS:CD2	2:F:15:HIS:HE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD13	1:A:243:ILE:HG13	1.76	0.66
5:B:1778:XAX:S3	5:B:1778:XAX:MO	2.06	0.66
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.78	0.66
2:B:650:ASP:HA	2:B:713:TRP:HB3	1.78	0.66
1:E:387:MET:HE2	1:E:439:ALA:HB2	1.78	0.66
1:A:122:ARG:HB3	1:A:128:LEU:HD21	1.76	0.65
1:A:352:LYS:HG3	1:A:362:SER:HB3	1.77	0.65
2:H:92:HIS:HB2	2:H:299:TRP:CE3	2.30	0.65
2:B:641:ARG:HH21	2:B:706:ARG:HH21	1.43	0.65
1:E:387:MET:HE3	1:E:439:ALA:HB2	1.79	0.65
1:G:183:PRO:HG3	1:G:189:LEU:HD13	1.77	0.65
2:F:29:PRO:HG3	2:H:27:PRO:HB2	1.78	0.65
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.79	0.65
2:D:163:GLU:HG2	2:D:277:ARG:HG2	1.79	0.65
2:B:586:VAL:HG13	2:B:596:LEU:HD22	1.77	0.64
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.27	0.64
2:H:380:PRO:O	2:H:381:GLU:HB2	1.96	0.64
2:F:144:VAL:HG22	2:F:330:ARG:HH12	1.63	0.64
2:F:420:ARG:HE	2:F:713:TRP:HZ3	1.46	0.64
2:B:78:PRO:HD2	2:B:302:ASP:HA	1.80	0.64
2:D:341:PHE:HD2	2:D:342:ARG:H	1.44	0.64
2:D:247:ARG:NH1	2:D:247:ARG:HG2	2.08	0.64
2:D:179:GLN:NE2	2:D:234:GLN:HB2	2.13	0.63
1:A:243:ILE:HD13	1:A:341:LEU:HD21	1.80	0.63
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.12	0.63
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.98	0.63
2:B:720:GLU:HA	2:B:724:ARG:HH21	1.62	0.63
2:F:9:HIS:HD2	2:F:15:HIS:HE1	1.46	0.63
2:F:556:ALA:HB2	2:F:563:ALA:HA	1.81	0.63
2:B:262:ASP:O	2:B:266:THR:HG23	1.99	0.63
1:G:364:VAL:HG22	1:G:435:ARG:HG3	1.79	0.63
1:G:371:THR:HB	1:G:378:GLU:HB3	1.81	0.63
2:F:148:ARG:HD2	2:F:404:HIS:HA	1.81	0.63
2:D:341:PHE:HD2	2:D:342:ARG:N	1.96	0.63
1:A:382:ILE:HD12	1:A:398:GLU:HG3	1.80	0.62
5:H:1778:XAX:O2	5:H:1778:XAX:MO	1.70	0.62
2:D:418:VAL:HG13	2:D:450:LEU:HD11	1.82	0.62
5:F:1778:XAX:O2	5:F:1778:XAX:MO	1.71	0.62
2:D:730:GLU:H	2:D:731:PRO:HD2	1.64	0.62
5:D:1778:XAX:O2	5:D:1778:XAX:MO	1.70	0.62
2:F:467:ALA:HB1	2:F:536:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:CYS:SG	1:C:41:GLU:HB2	2.40	0.62
1:E:211:TRP:HA	1:E:215:ALA:HB3	1.81	0.62
1:G:8:ASN:HA	1:G:76:ARG:HD2	1.80	0.62
1:C:1:MET:HE2	1:C:16:ILE:HG13	1.81	0.62
2:D:210:LEU:HD22	2:D:247:ARG:HD3	1.81	0.61
4:C:1465:FAD:N1	4:C:1465:FAD:H2'	2.15	0.61
2:D:461:LEU:HD12	7:D:1780:HPA:H8	1.82	0.61
5:B:1778:XAX:O2	5:B:1778:XAX:MO	1.71	0.61
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.82	0.61
2:H:560:GLY:O	2:H:561:CYS:HB3	2.00	0.61
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.81	0.61
2:F:210:LEU:HB3	2:F:212:LEU:CD2	2.29	0.61
2:D:201:GLU:HG2	2:D:236:ASN:HD21	1.66	0.61
1:A:426:SER:H	2:F:574:GLN:HE22	1.47	0.61
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.82	0.61
5:D:1778:XAX:O1	7:D:1780:HPA:H2	2.01	0.61
1:A:22:SER:OG	1:A:25:GLU:HG2	2.00	0.61
2:F:35:LEU:HD11	2:F:242:CYS:HA	1.81	0.61
2:D:512:ARG:HE	2:D:512:ARG:HA	1.64	0.61
1:A:216:LEU:HD13	2:B:111:ILE:HG13	1.83	0.61
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.82	0.61
2:H:310:ARG:HD2	2:H:344:PHE:HB3	1.81	0.61
1:C:234:ILE:HD13	1:C:243:ILE:HG13	1.82	0.61
2:B:46:ALA:HB2	2:B:123:ARG:HH21	1.66	0.61
2:D:179:GLN:CB	2:D:238:LEU:HD11	2.27	0.61
2:D:730:GLU:N	2:D:731:PRO:HD2	2.16	0.60
2:D:417:LEU:HG	2:D:648:LEU:HD23	1.82	0.60
2:H:457:ILE:O	2:H:458:SER:CB	2.43	0.60
1:C:373:LYS:HB2	1:C:378:GLU:HG3	1.82	0.60
2:D:482:ASN:HD22	2:D:514:THR:HB	1.65	0.60
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.84	0.60
2:B:227:GLY:HA2	2:B:231:LYS:HG3	1.84	0.60
2:B:422:GLN:HE21	2:B:450:LEU:HD13	1.66	0.60
1:A:283:GLY:HA2	4:A:1465:FAD:C8A	2.32	0.60
2:D:459:PHE:H	2:D:465:ASN:HD21	1.50	0.60
2:H:297:CYS:SG	2:H:304:SER:HB3	2.42	0.60
1:C:32:LEU:HD12	1:C:79:GLU:HG3	1.84	0.60
1:C:302:GLY:HA2	1:C:381:ARG:NH1	2.16	0.60
2:F:269:ARG:HD3	2:F:348:GLN:HE22	1.67	0.59
2:F:144:VAL:HG22	2:F:330:ARG:NH1	2.17	0.59
1:C:427:ASP:OD1	1:C:435:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:LEU:HD12	2:D:711:ALA:HB3	1.84	0.59
2:D:240:ILE:O	2:D:244:VAL:HG23	2.01	0.59
2:B:720:GLU:HG2	2:B:724:ARG:HH22	1.66	0.59
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.84	0.59
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.32	0.59
1:A:70:ILE:HA	1:A:73:LYS:HG3	1.84	0.59
2:B:49:GLY:HA3	2:B:119:THR:OG1	2.01	0.59
2:D:35:LEU:HD11	2:D:242:CYS:HA	1.84	0.59
2:H:550:ARG:HH12	2:H:597:SER:H	1.49	0.59
1:A:245:ALA:HB2	1:A:336:VAL:HG12	1.85	0.59
1:G:245:ALA:HB1	1:G:282:GLY:HA3	1.84	0.59
2:D:77:SER:HB2	2:D:83:GLU:CB	2.30	0.59
2:H:460:THR:H	7:H:1780:HPA:H8	1.67	0.59
2:F:201:GLU:HG2	2:F:236:ASN:HD21	1.68	0.59
2:D:421:LEU:HD13	2:D:648:LEU:HB2	1.84	0.58
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.85	0.58
2:F:528:ALA:HA	5:F:1778:XAX:S2'	2.42	0.58
2:F:262:ASP:O	2:F:266:THR:HG23	2.03	0.58
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.85	0.58
1:E:201:LEU:HD22	1:E:225:LEU:HD21	1.84	0.58
2:H:698:ILE:HB	2:H:699:PRO:HD2	1.86	0.58
2:F:606:LYS:O	2:F:617:ARG:HD2	2.03	0.58
2:B:70:LEU:CD2	2:B:244:VAL:HG11	2.33	0.58
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.83	0.58
2:B:310:ARG:HD2	2:B:344:PHE:HB3	1.86	0.58
1:C:301:MET:HB3	1:C:348:LEU:HD22	1.85	0.58
2:D:58:SER:HB2	2:D:115:LYS:HD2	1.86	0.58
1:C:52:ARG:HB3	1:C:74:ALA:HB3	1.86	0.58
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.85	0.58
2:D:17:THR:OG1	2:D:19:GLN:HG3	2.03	0.58
1:G:138:GLY:HA2	2:H:669:VAL:HG21	1.84	0.58
1:E:250:ALA:HB2	1:E:276:ARG:HB3	1.85	0.58
2:B:753:HIS:HB2	2:B:773:ALA:HA	1.85	0.58
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.39	0.58
2:D:54:PRO:HB2	2:D:115:LYS:O	2.04	0.57
2:B:11:SER:HB2	2:B:15:HIS:CD2	2.39	0.57
2:D:262:ASP:O	2:D:266:THR:HG23	2.04	0.57
1:G:415:LEU:N	1:G:416:PRO:HD2	2.19	0.57
1:G:445:ARG:HE	1:G:455:VAL:HG12	1.69	0.57
2:F:9:HIS:HD2	2:F:15:HIS:CE1	2.22	0.57
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:PRO:HB2	2:F:115:LYS:O	2.05	0.57
2:H:148:ARG:O	2:H:323:ALA:HA	2.04	0.57
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.05	0.57
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.86	0.57
1:G:22:SER:OG	1:G:25:GLU:HG2	2.04	0.57
2:F:2:SER:HB3	2:F:498:GLN:HG2	1.86	0.57
2:B:547:LEU:HD23	2:B:550:ARG:HH11	1.69	0.57
2:B:601:PHE:CG	2:D:595:SER:HB2	2.40	0.57
2:D:40:SER:HB2	2:D:91:VAL:HG11	1.86	0.57
2:H:262:ASP:O	2:H:266:THR:HG23	2.04	0.57
2:H:460:THR:H	7:H:1780:HPA:C8	2.18	0.57
2:F:473:ILE:HG23	2:F:479:VAL:HG12	1.87	0.57
2:H:161:LEU:HD21	2:H:163:GLU:OE2	2.04	0.57
1:G:330:ARG:HH21	4:G:1465:FAD:C2A	2.18	0.56
2:F:224:MET:CE	2:F:488:MET:HB3	2.35	0.56
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.86	0.56
2:F:730:GLU:N	2:F:731:PRO:HD2	2.20	0.56
1:E:295:PRO:HB2	1:E:296:PRO:CD	2.31	0.56
2:H:232:GLN:NE2	7:H:1780:HPA:H2	2.20	0.56
2:H:23:LEU:HD22	2:H:180:ALA:HB1	1.86	0.56
2:B:171:GLN:O	2:B:268:LYS:HB3	2.05	0.56
2:H:35:LEU:HB3	2:H:100:LEU:HD11	1.86	0.56
2:D:556:ALA:HB1	2:D:561:CYS:O	2.05	0.56
2:F:46:ALA:HB2	2:F:123:ARG:HH21	1.69	0.56
2:D:459:PHE:HB2	2:D:465:ASN:ND2	2.21	0.56
2:H:170:GLY:N	2:H:271:ASP:HB3	2.21	0.56
2:H:46:ALA:HB2	2:H:123:ARG:HH21	1.71	0.56
2:D:76:ALA:HA	2:D:205:LYS:HD2	1.87	0.56
1:E:8:ASN:HA	1:E:76:ARG:HD2	1.86	0.56
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.39	0.56
2:F:417:LEU:HD21	2:F:648:LEU:O	2.06	0.55
2:F:163:GLU:HG2	2:F:277:ARG:HG2	1.88	0.55
2:F:573:VAL:HB	2:F:585:ILE:HG13	1.88	0.55
1:C:305:LEU:HD21	1:C:307:LEU:HD21	1.89	0.55
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.87	0.55
1:G:299:ILE:HG13	1:G:318:LEU:HD23	1.88	0.55
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.89	0.55
2:B:51:ASP:HB3	2:B:117:ARG:HB3	1.88	0.55
2:D:35:LEU:HA	2:D:101:VAL:O	2.07	0.55
2:F:9:HIS:ND1	2:F:491:GLY:HA2	2.21	0.55
2:B:148:ARG:HD2	2:B:404:HIS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:GLY:O	2:B:561:CYS:HB3	2.07	0.55
2:B:262:ASP:O	2:B:266:THR:CG2	2.55	0.55
1:A:233:GLN:HG3	1:A:235:ARG:HH22	1.72	0.55
1:E:228:CYS:HB3	1:E:231:LEU:HB2	1.89	0.55
2:F:720:GLU:HG3	2:F:724:ARG:NH2	2.22	0.55
2:B:151:VAL:HG11	2:B:290:ASP:HB2	1.89	0.55
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.88	0.54
2:D:148:ARG:HD2	2:D:404:HIS:HA	1.89	0.54
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.88	0.54
5:H:1778:XAX:O1	5:H:1778:XAX:S3	2.65	0.54
1:C:249:ILE:CG2	1:C:267:LEU:HD22	2.34	0.54
2:F:270:HIS:CD2	2:F:297:CYS:HA	2.43	0.54
2:H:58:SER:HB2	2:H:115:LYS:HD2	1.89	0.54
2:B:197:GLN:HG3	2:B:231:LYS:HB2	1.88	0.54
2:H:35:LEU:HA	2:H:101:VAL:O	2.07	0.54
2:B:277:ARG:HB2	2:B:290:ASP:HB3	1.90	0.54
1:E:200:THR:HB	1:E:222:VAL:HG12	1.89	0.54
2:H:665:GLU:O	2:H:669:VAL:HG23	2.08	0.54
2:B:517:ASP:HB3	2:B:520:LYS:HB2	1.89	0.54
2:B:194:CYS:O	2:B:221:MET:HG2	2.07	0.54
2:F:162:ALA:HB1	2:F:359:HIS:CD2	2.43	0.54
2:D:138:ARG:HA	2:D:332:ARG:H	1.72	0.54
1:E:307:LEU:HB2	1:E:314:ARG:HB2	1.88	0.54
2:D:169:GLY:HA3	2:D:760:PRO:HD3	1.89	0.54
5:B:1778:XAX:S3	5:B:1778:XAX:O2	2.66	0.54
1:G:371:THR:OG1	1:G:379:THR:HB	2.07	0.54
2:H:586:VAL:HG13	2:H:596:LEU:HD22	1.90	0.54
2:B:417:LEU:HG	2:B:648:LEU:HD23	1.90	0.54
1:G:444:LEU:O	1:G:448:ARG:HG3	2.07	0.54
2:F:174:PHE:HZ	2:F:693:PRO:HB3	1.73	0.54
1:C:370:LEU:HD22	1:C:380:ALA:HA	1.90	0.54
2:H:370:GLU:HA	2:H:370:GLU:OE2	2.08	0.53
1:G:134:CYS:SG	1:G:137:THR:HG23	2.48	0.53
2:B:129:LEU:CD1	2:B:129:LEU:H	2.20	0.53
5:D:1778:XAX:S3	5:D:1778:XAX:O2	2.66	0.53
1:G:70:ILE:HA	1:G:73:LYS:HG3	1.90	0.53
2:D:310:ARG:HD2	2:D:344:PHE:HD2	1.73	0.53
2:D:177:GLU:HB3	2:D:225:GLY:HA3	1.90	0.53
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.43	0.53
2:D:627:ALA:HB2	2:D:735:LEU:HD22	1.90	0.53
2:D:184:LEU:HD23	2:D:252:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:556:ALA:HB2	2:D:563:ALA:HA	1.89	0.53
2:D:288:GLY:HA2	2:D:323:ALA:O	2.07	0.53
2:D:468:GLY:HA2	2:D:600:GLY:O	2.08	0.53
2:H:580:TRP:HB3	2:H:584:GLU:HB2	1.89	0.53
1:E:405:ASP:HB3	1:E:407:ARG:HG2	1.89	0.53
1:A:290:PRO:HA	1:A:391:PRO:HD3	1.91	0.53
2:D:457:ILE:O	2:D:458:SER:HB2	2.08	0.53
1:G:207:ASP:HB2	4:G:1465:FAD:H52A	1.90	0.53
2:F:321:VAL:HB	2:F:324:LEU:HD12	1.91	0.53
1:G:234:ILE:HD13	1:G:243:ILE:HG13	1.91	0.53
1:A:200:THR:HG21	1:A:219:LEU:HD13	1.91	0.53
2:H:2:SER:HB3	2:H:498:GLN:O	2.08	0.53
2:F:698:ILE:H	2:F:698:ILE:HD13	1.73	0.53
2:H:547:LEU:HD23	2:H:550:ARG:HH11	1.74	0.53
2:D:171:GLN:O	2:D:268:LYS:HB3	2.09	0.53
2:D:143:PRO:HB3	2:D:329:HIS:ND1	2.24	0.53
2:B:771:ARG:HG3	2:B:776:ARG:HB2	1.89	0.53
1:C:66:MET:HE2	1:C:202:ILE:HD13	1.91	0.53
2:D:771:ARG:NH2	2:D:777:ALA:HB2	2.24	0.53
1:G:111:ILE:HD11	2:H:16:VAL:HG22	1.91	0.53
2:D:23:LEU:CD2	2:D:180:ALA:HB1	2.39	0.52
1:G:441:ALA:HB1	2:H:636:LEU:HB3	1.91	0.52
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.91	0.52
2:H:461:LEU:HB2	2:H:464:LEU:HD12	1.89	0.52
2:B:228:PHE:O	2:B:341:PHE:HA	2.09	0.52
2:F:78:PRO:HG3	2:F:233:SER:HB2	1.91	0.52
2:F:146:TRP:CZ3	2:F:312:MET:HB3	2.44	0.52
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.43	0.52
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.91	0.52
1:G:206:THR:HG21	1:G:275:VAL:HG13	1.91	0.52
1:C:316:MET:HG3	1:C:320:ASP:HB2	1.92	0.52
1:E:390:VAL:HG22	1:E:391:PRO:HD2	1.91	0.52
2:F:174:PHE:CZ	2:F:693:PRO:HB3	2.45	0.52
2:B:218:ARG:CD	8:B:2004:HOH:O	2.58	0.52
2:D:128:THR:HG23	2:D:131:GLN:H	1.74	0.52
2:D:720:GLU:HG3	2:D:724:ARG:NH2	2.24	0.52
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.92	0.52
2:F:171:GLN:O	2:F:268:LYS:HB3	2.10	0.51
2:B:421:LEU:HD13	2:B:648:LEU:HB2	1.92	0.51
2:D:641:ARG:HH21	2:D:706:ARG:HH21	1.59	0.51
2:F:398:LYS:N	2:F:398:LYS:HE3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:OD2	2:B:693:PRO:HG2	2.10	0.51
1:E:200:THR:HG21	1:E:219:LEU:HD13	1.92	0.51
1:G:164:PHE:O	1:G:165:THR:HG22	2.10	0.51
2:H:232:GLN:HE22	7:H:1780:HPA:C2	2.22	0.51
2:H:11:SER:HB2	2:H:14:ALA:HB3	1.93	0.51
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.11	0.51
2:H:473:ILE:HB	2:H:596:LEU:HB3	1.91	0.51
1:E:32:LEU:HD12	1:E:79:GLU:HG3	1.92	0.51
2:F:21:ARG:HD3	2:F:26:LEU:HD23	1.93	0.51
2:H:617:ARG:HD3	2:H:619:PHE:O	2.11	0.51
1:G:351:TYR:CE2	1:G:445:ARG:HD3	2.46	0.51
2:H:40:SER:HB2	2:H:91:VAL:HG11	1.93	0.51
1:C:144:ARG:NH2	2:D:665:GLU:OE2	2.41	0.51
2:D:762:THR:HB	2:D:763:PRO:HD2	1.93	0.51
2:H:417:LEU:HD21	2:H:648:LEU:O	2.10	0.51
2:F:192:ILE:HB	2:F:219:VAL:HG22	1.92	0.51
2:F:227:GLY:HA2	2:F:231:LYS:HG3	1.93	0.51
1:G:201:LEU:HD12	1:G:330:ARG:HH22	1.75	0.51
1:C:140:ALA:O	1:C:144:ARG:HG3	2.11	0.51
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.93	0.51
1:C:351:TYR:CE2	1:C:445:ARG:HD3	2.46	0.51
2:D:443:THR:HG23	2:D:636:LEU:CD1	2.38	0.51
2:B:586:VAL:HG13	2:B:596:LEU:CD2	2.41	0.51
1:C:216:LEU:HD13	2:D:111:ILE:HG12	1.92	0.51
2:F:151:VAL:HG11	2:F:290:ASP:HB2	1.91	0.51
2:F:730:GLU:H	2:F:731:PRO:HD2	1.76	0.50
2:D:457:ILE:O	2:D:458:SER:CB	2.59	0.50
2:D:182:LEU:HD13	2:D:254:LYS:HB2	1.92	0.50
2:B:226:GLY:O	2:B:231:LYS:HE3	2.10	0.50
1:C:70:ILE:HA	1:C:73:LYS:HG3	1.93	0.50
1:G:122:ARG:HB3	1:G:128:LEU:HD21	1.92	0.50
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.27	0.50
1:C:43:ASP:HB3	2:D:693:PRO:HB2	1.92	0.50
2:B:627:ALA:HB2	2:B:735:LEU:HD22	1.91	0.50
2:D:309:ASP:CG	2:D:611:ARG:HE	2.14	0.50
2:H:13:ARG:HH11	2:H:13:ARG:CG	2.22	0.50
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.47	0.50
1:G:48:THR:O	1:G:112:VAL:HB	2.11	0.50
1:A:111:ILE:HD11	2:B:16:VAL:HG22	1.94	0.50
2:D:360:LEU:HG	2:D:364:MET:CE	2.41	0.50
2:B:604:THR:HB	2:B:607:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:ARG:HB3	1:G:74:ALA:HB3	1.93	0.50
1:G:368:LEU:HG	1:G:382:ILE:HG23	1.93	0.50
1:A:183:PRO:HD2	1:A:224:PHE:O	2.11	0.50
1:G:394:ALA:O	1:G:398:GLU:HB2	2.11	0.50
2:D:551:LEU:HD22	2:D:585:ILE:HG22	1.94	0.50
2:F:488:MET:CE	5:F:1778:XAX:H4'	2.41	0.50
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.25	0.50
2:B:132:ALA:HA	2:B:137:SER:HB3	1.93	0.50
2:F:647:ILE:HB	2:F:710:VAL:HG22	1.94	0.50
2:F:551:LEU:HD22	2:F:585:ILE:HG22	1.94	0.50
2:B:499:VAL:O	2:B:503:VAL:HG23	2.12	0.50
2:B:473:ILE:HB	2:B:596:LEU:HB3	1.94	0.49
2:F:418:VAL:HG13	2:F:450:LEU:HD11	1.93	0.49
2:D:171:GLN:NE2	2:D:674:TRP:HB2	2.26	0.49
2:D:9:HIS:CD2	2:D:11:SER:H	2.30	0.49
2:H:171:GLN:O	2:H:268:LYS:HB3	2.12	0.49
2:B:633:ILE:HG12	2:B:746:ALA:HB1	1.94	0.49
2:F:11:SER:HB2	2:F:14:ALA:HB3	1.94	0.49
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.47	0.49
2:D:210:LEU:HB3	2:D:212:LEU:HD21	1.93	0.49
2:B:78:PRO:HG3	2:B:233:SER:HB2	1.94	0.49
1:C:66:MET:HG3	1:C:224:PHE:HE2	1.77	0.49
2:F:380:PRO:HD3	2:F:412:CYS:O	2.12	0.49
1:E:368:LEU:HG	1:E:382:ILE:HG23	1.94	0.49
2:H:407:GLN:OE1	2:H:618:PRO:HD2	2.13	0.49
1:G:433:ALA:O	1:G:437:ASN:HB2	2.12	0.49
2:H:158:ALA:HA	2:H:287:LEU:HD22	1.93	0.49
1:E:90:PRO:HB3	1:E:152:GLU:HB2	1.95	0.49
1:A:8:ASN:HA	1:A:76:ARG:HD2	1.95	0.49
1:E:206:THR:O	4:E:1465:FAD:HM81	2.13	0.49
2:F:224:MET:HE1	2:F:488:MET:HB3	1.94	0.49
1:C:302:GLY:HA2	1:C:381:ARG:HH11	1.76	0.49
5:D:1778:XAX:S3	5:D:1778:XAX:O1	2.71	0.49
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.78	0.49
1:C:211:TRP:HA	1:C:215:ALA:HB3	1.95	0.49
2:B:174:PHE:HZ	2:B:693:PRO:HB3	1.78	0.48
2:H:166:PHE:HB3	2:H:355:ARG:NH2	2.28	0.48
1:E:430:ALA:HB1	1:E:434:TYR:HD2	1.78	0.48
5:F:1778:XAX:O2	5:F:1778:XAX:S3	2.71	0.48
1:A:206:THR:OG1	4:A:1465:FAD:O1P	2.28	0.48
2:H:267:GLY:HA2	2:H:268:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:SER:HB3	1:C:362:SER:HA	1.94	0.48
1:E:354:SER:HB2	1:E:360:ASP:OD2	2.13	0.48
2:F:172:GLU:HB3	2:F:696:TYR:CZ	2.49	0.48
2:D:310:ARG:NH2	2:D:619:PHE:HE2	2.11	0.48
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.29	0.48
2:B:417:LEU:HD21	2:B:648:LEU:O	2.13	0.48
1:A:50:MET:HE2	1:A:57:SER:HB2	1.96	0.48
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.95	0.48
2:F:23:LEU:CD2	2:F:180:ALA:HB1	2.42	0.48
2:D:85:VAL:HG21	2:D:240:ILE:HG21	1.94	0.48
1:G:299:ILE:O	1:G:381:ARG:NH1	2.39	0.48
2:B:698:ILE:HB	2:B:699:PRO:HD2	1.96	0.48
2:D:482:ASN:ND2	2:D:514:THR:HB	2.29	0.48
2:D:110:ARG:HH22	2:D:260:ASP:HB2	1.78	0.48
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.29	0.48
2:B:148:ARG:O	2:B:323:ALA:HA	2.14	0.48
1:C:8:ASN:HA	1:C:76:ARG:HD2	1.96	0.48
2:D:531:SER:HB2	2:D:535:MET:HG3	1.96	0.48
2:H:547:LEU:HD23	2:H:550:ARG:HD3	1.95	0.48
1:A:50:MET:CE	1:A:57:SER:HB2	2.44	0.48
1:E:300:ALA:HB2	1:E:367:CYS:HB3	1.95	0.48
2:H:673:GLY:O	2:H:678:GLU:HB2	2.14	0.48
2:F:138:ARG:HD3	2:F:142:GLY:N	2.16	0.48
2:F:46:ALA:HB2	2:F:123:ARG:NH2	2.29	0.48
2:D:641:ARG:NH2	2:D:706:ARG:HE	2.12	0.48
1:E:42:GLY:HA3	1:E:64:LEU:HD11	1.95	0.48
2:H:497:VAL:HG13	2:H:511:VAL:HB	1.96	0.48
2:B:448:ILE:HA	2:B:629:THR:O	2.14	0.48
2:H:762:THR:HB	2:H:763:PRO:HD2	1.96	0.48
1:A:426:SER:N	2:F:574:GLN:HE22	2.12	0.47
2:D:292:VAL:HG22	2:D:327:GLU:HB3	1.96	0.47
2:B:530:SER:O	2:B:727:ALA:HB1	2.13	0.47
2:H:76:ALA:HA	2:H:205:LYS:HD2	1.95	0.47
1:G:245:ALA:HB2	1:G:336:VAL:HG12	1.96	0.47
1:G:346:PRO:O	1:G:349:ARG:NH2	2.46	0.47
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.95	0.47
2:D:481:LEU:HD11	2:D:540:VAL:HG22	1.95	0.47
1:E:237:THR:OG1	1:E:238:PRO:CD	2.57	0.47
2:F:635:ARG:NH1	2:F:774:GLU:OE2	2.47	0.47
1:E:322:PHE:HB3	1:E:390:VAL:CG2	2.44	0.47
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:PRO:HB2	2:D:344:PHE:CZ	2.50	0.47
1:C:41:GLU:HA	1:C:210:LEU:HD21	1.95	0.47
2:B:94:VAL:HG11	2:B:687:ARG:HG2	1.96	0.47
1:C:127:ASP:OD1	1:C:268:ARG:HD3	2.14	0.47
2:B:567:ILE:HG13	2:B:574:GLN:HB2	1.94	0.47
1:G:26:TRP:CD1	1:G:67:LEU:HD11	2.49	0.47
2:F:85:VAL:HG21	2:F:240:ILE:HG21	1.96	0.47
1:G:359:GLN:NE2	4:G:1465:FAD:HM73	2.28	0.47
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.95	0.47
2:H:380:PRO:O	2:H:381:GLU:CB	2.61	0.47
2:H:179:GLN:HB2	2:H:257:TYR:CD1	2.49	0.47
1:G:113:SER:HB2	1:G:132:ASN:HD21	1.79	0.47
2:H:70:LEU:HD22	2:H:244:VAL:HG11	1.97	0.47
2:H:22:TYR:O	2:H:25:ASP:HB2	2.14	0.47
2:H:460:THR:OG1	7:H:1780:HPA:H8	2.14	0.47
1:G:66:MET:HG3	1:G:224:PHE:HE2	1.79	0.47
1:C:38:GLY:O	1:C:39:CYS:HB3	2.14	0.47
2:B:341:PHE:O	2:B:342:ARG:C	2.52	0.47
2:H:201:GLU:HG2	2:H:236:ASN:HD21	1.80	0.47
2:B:34:HIS:HD2	2:B:105:SER:HA	1.80	0.47
2:H:300:SER:HB2	2:H:337:SER:HB2	1.97	0.47
2:F:316:ASP:HB3	2:F:404:HIS:ND1	2.29	0.47
2:F:473:ILE:HG12	2:F:479:VAL:HG12	1.96	0.47
2:H:605:PRO:HB2	2:H:606:LYS:HG3	1.97	0.47
1:E:70:ILE:HA	1:E:73:LYS:HG3	1.96	0.47
1:G:108:PRO:O	1:G:112:VAL:HG23	2.14	0.47
1:C:42:GLY:HA3	1:C:64:LEU:HD11	1.95	0.47
1:E:245:ALA:HB1	1:E:282:GLY:HA3	1.97	0.47
5:B:1778:XAX:S3	5:B:1778:XAX:O1	2.72	0.47
1:G:228:CYS:HB3	1:G:231:LEU:HB2	1.97	0.47
2:B:501:ALA:HB1	2:B:506:ILE:O	2.15	0.47
1:E:401:LEU:O	1:E:404:GLN:HB2	2.15	0.47
1:C:35:THR:CG2	1:C:47:CYS:HB2	2.45	0.47
1:C:120:ARG:O	1:C:121:ASP:C	2.53	0.47
2:H:448:ILE:HA	2:H:629:THR:O	2.15	0.47
2:D:606:LYS:O	2:D:617:ARG:HD2	2.14	0.47
2:D:551:LEU:O	2:D:555:VAL:HG23	2.16	0.46
1:G:155:ALA:HB3	1:G:158:LEU:HD12	1.97	0.46
1:A:252:LEU:HD23	1:A:267:LEU:HD11	1.96	0.46
1:G:45:GLY:N	3:G:1464:FES:S2	2.87	0.46
1:E:418:LEU:HB3	1:E:436:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HA	1:A:112:VAL:HG11	1.97	0.46
2:H:35:LEU:HD11	2:H:242:CYS:HA	1.97	0.46
2:H:105:SER:OG	2:H:108:ALA:HB2	2.15	0.46
1:E:370:LEU:HD23	1:E:380:ALA:HA	1.98	0.46
2:D:196:SER:O	2:D:221:MET:HG3	2.14	0.46
2:H:303:LEU:O	2:H:307:VAL:HG23	2.15	0.46
1:G:347:GLY:O	1:G:446:TYR:OH	2.26	0.46
2:B:185:PRO:HG3	2:B:246:ALA:HB1	1.97	0.46
1:G:352:LYS:HE3	1:G:362:SER:HB3	1.98	0.46
1:G:427:ASP:OD1	1:G:435:ARG:NH2	2.48	0.46
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.97	0.46
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.50	0.46
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.56	0.46
4:A:1465:FAD:H1'2	4:A:1465:FAD:H9	1.84	0.46
2:B:520:LYS:HE2	2:D:520:LYS:HD2	1.98	0.46
2:F:14:ALA:HA	2:F:19:GLN:HB2	1.98	0.46
1:A:249:ILE:HG23	1:A:267:LEU:HD22	1.96	0.46
1:G:250:ALA:HB2	1:G:276:ARG:HB3	1.98	0.46
2:D:399:LYS:HD2	2:D:399:LYS:C	2.36	0.46
2:F:266:THR:O	2:F:268:LYS:HE2	2.15	0.46
1:E:24:LEU:CD1	1:E:63:CYS:HB3	2.46	0.46
1:G:11:THR:HG22	1:G:164:PHE:HE1	1.81	0.46
2:D:488:MET:CE	5:D:1778:XAX:H4'	2.46	0.46
1:E:377:ILE:HD13	1:E:401:LEU:HG	1.98	0.46
2:D:166:PHE:CZ	2:D:168:ILE:HD11	2.51	0.46
2:B:240:ILE:O	2:B:244:VAL:HG23	2.16	0.45
2:B:215:HIS:ND1	2:D:478:SER:HB2	2.31	0.45
1:G:136:CYS:HB3	2:H:228:PHE:CZ	2.51	0.45
2:D:267:GLY:HA2	2:D:336:GLN:HB3	1.97	0.45
1:A:113:SER:HB2	1:A:132:ASN:HD21	1.79	0.45
1:G:211:TRP:HA	1:G:215:ALA:HB3	1.98	0.45
2:D:473:ILE:HG23	2:D:479:VAL:HG12	1.98	0.45
5:F:1778:XAX:O1	5:F:1778:XAX:S3	2.75	0.45
2:D:31:ASN:ND2	2:D:252:PRO:CD	2.80	0.45
2:B:158:ALA:HA	2:B:287:LEU:HD22	1.97	0.45
2:D:262:ASP:O	2:D:266:THR:CG2	2.63	0.45
1:A:370:LEU:HA	1:A:379:THR:O	2.16	0.45
1:A:41:GLU:HA	1:A:210:LEU:HD21	1.99	0.45
2:B:647:ILE:HD12	2:B:710:VAL:HG22	1.98	0.45
1:E:366:GLY:HA3	1:E:442:MET:SD	2.57	0.45
2:F:249:THR:C	2:F:251:ARG:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:HG21	1:E:275:VAL:HG13	1.98	0.45
2:H:288:GLY:HA2	2:H:323:ALA:O	2.17	0.45
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.81	0.45
2:H:174:PHE:CZ	2:H:693:PRO:HB3	2.52	0.45
2:B:23:LEU:HA	2:B:26:LEU:HD12	1.97	0.45
2:H:341:PHE:O	2:H:342:ARG:C	2.54	0.45
2:B:482:ASN:HD22	2:B:514:THR:HB	1.82	0.45
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.81	0.45
2:B:595:SER:HB2	2:D:601:PHE:CG	2.52	0.45
2:B:551:LEU:O	2:B:555:VAL:HG23	2.16	0.45
2:B:366:ARG:HH11	2:B:366:ARG:HB3	1.82	0.45
1:G:113:SER:CB	1:G:132:ASN:HD21	2.30	0.45
2:H:517:ASP:HB3	2:H:520:LYS:HB2	1.99	0.45
2:F:599:THR:HG23	2:H:599:THR:HG23	1.98	0.45
2:H:460:THR:N	7:H:1780:HPA:H8	2.31	0.45
2:F:641:ARG:HH22	2:F:706:ARG:HD3	1.79	0.45
2:F:9:HIS:CD2	2:F:15:HIS:CE1	2.99	0.45
2:F:182:LEU:HD13	2:F:254:LYS:HB2	1.98	0.45
2:H:650:ASP:HA	2:H:713:TRP:HB3	1.99	0.45
2:B:534:ASP:OD2	2:B:621:TYR:OH	2.30	0.45
1:G:330:ARG:HH21	4:G:1465:FAD:H2A	1.82	0.45
2:H:281:ASP:HB3	2:H:287:LEU:HD11	1.97	0.45
1:E:50:MET:CE	1:E:57:SER:HB2	2.47	0.45
2:F:631:VAL:HG12	2:F:642:ILE:HA	1.98	0.45
2:H:635:ARG:HH11	2:H:750:CYS:HB3	1.82	0.45
1:G:431:SER:OG	2:H:764:GLU:OE1	2.28	0.45
2:F:267:GLY:HA3	2:F:337:SER:O	2.17	0.45
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.45
2:F:166:PHE:CZ	2:F:355:ARG:HG3	2.51	0.45
5:H:1778:XAX:O2	5:H:1778:XAX:S3	2.75	0.44
1:G:66:MET:O	1:G:69:GLN:HB2	2.17	0.44
2:D:341:PHE:HE2	2:D:670:GLN:HE22	1.65	0.44
2:D:343:GLY:H	2:D:730:GLU:HG2	1.82	0.44
1:A:211:TRP:HA	1:A:215:ALA:HB3	1.99	0.44
2:D:74:ASN:ND2	2:D:88:THR:HG23	2.32	0.44
1:A:388:ALA:O	1:A:390:VAL:N	2.36	0.44
2:B:288:GLY:HA2	2:B:321:VAL:HG13	1.99	0.44
1:G:61:ASN:H	1:G:61:ASN:ND2	2.15	0.44
2:F:278:ILE:HD11	2:F:286:LEU:HD22	1.98	0.44
1:A:181:PHE:O	1:A:223:ALA:HA	2.17	0.44
2:F:485:GLY:HA3	2:F:492:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:ARG:HB2	1:E:334:GLU:HG2	1.99	0.44
1:G:41:GLU:O	4:G:1465:FAD:HM82	2.17	0.44
2:B:478:SER:HB2	2:D:215:HIS:ND1	2.32	0.44
1:A:66:MET:HG2	1:A:66:MET:H	1.65	0.44
4:C:1465:FAD:H9	4:C:1465:FAD:H1'2	1.76	0.44
2:D:649:HIS:CE1	2:D:731:PRO:HB2	2.53	0.44
1:G:134:CYS:SG	1:G:137:THR:CG2	3.06	0.44
2:D:92:HIS:HB2	2:D:299:TRP:CE3	2.52	0.44
2:F:306:PRO:HB2	2:F:344:PHE:CZ	2.52	0.44
2:F:144:VAL:CG2	2:F:330:ARG:NH1	2.77	0.44
2:H:650:ASP:OD2	2:H:726:LYS:NZ	2.41	0.44
2:B:38:GLY:HA3	2:B:99:PHE:CE2	2.53	0.44
1:A:425:LEU:HG	2:F:579:SER:HB2	1.99	0.44
2:H:319:TYR:HA	2:H:375:ASN:O	2.18	0.44
2:H:92:HIS:HB2	2:H:299:TRP:HE3	1.78	0.44
2:B:556:ALA:HB1	2:B:561:CYS:O	2.18	0.44
2:B:222:ARG:HD2	2:B:222:ARG:HA	1.82	0.44
2:F:373:ALA:HA	2:F:376:PHE:CE1	2.52	0.44
2:D:303:LEU:O	2:D:307:VAL:HG23	2.18	0.44
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.53	0.44
2:D:635:ARG:NH1	2:D:750:CYS:HB3	2.32	0.44
2:D:173:HIS:HA	2:D:341:PHE:CZ	2.53	0.44
1:A:64:LEU:HD13	1:A:206:THR:HG22	1.99	0.44
1:A:8:ASN:OD1	1:A:76:ARG:HA	2.17	0.44
2:F:360:LEU:HG	2:F:364:MET:HE3	2.00	0.44
1:A:253:ARG:HH21	1:A:268:ARG:HG3	1.83	0.44
2:F:35:LEU:HB3	2:F:100:LEU:HD11	1.99	0.44
1:G:318:LEU:O	1:G:321:PHE:HB3	2.18	0.44
1:A:240:GLY:HA2	1:A:343:LYS:HG2	1.99	0.44
2:F:446:ARG:HD3	2:F:630:GLU:OE2	2.18	0.44
1:G:36:LYS:HB3	1:G:105:PHE:CZ	2.52	0.44
1:G:110:PHE:O	1:G:114:MET:HE2	2.17	0.44
2:H:305:LEU:HB3	2:H:306:PRO:CD	2.48	0.44
2:F:488:MET:HE1	5:F:1778:XAX:H4'	1.98	0.44
2:H:29:PRO:HG2	2:H:252:PRO:HG3	1.99	0.44
2:H:7:LEU:HB3	2:H:8:PRO:CD	2.47	0.44
2:B:195:SER:O	2:B:231:LYS:HD2	2.17	0.44
1:A:245:ALA:HB1	1:A:282:GLY:HA3	1.99	0.44
1:G:284:ASN:OD1	1:G:295:PRO:HD3	2.18	0.44
1:E:182:LEU:HG	1:E:224:PHE:HB2	2.00	0.44
2:B:35:LEU:HD11	2:B:242:CYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:528:ALA:HA	5:D:1778:XAX:S2'	2.58	0.43
2:D:266:THR:O	2:D:268:LYS:HE2	2.18	0.43
1:G:149:ALA:O	1:G:152:GLU:HB2	2.18	0.43
2:D:755:PRO:O	2:D:772:ARG:HD2	2.18	0.43
1:C:24:LEU:HD12	1:C:63:CYS:HB3	2.01	0.43
2:D:128:THR:HG22	2:D:131:GLN:CD	2.39	0.43
1:E:127:ASP:OD2	1:E:268:ARG:HD3	2.18	0.43
1:G:388:ALA:C	1:G:390:VAL:H	2.21	0.43
2:B:656:ASN:HB3	2:B:659:LEU:HB2	2.00	0.43
1:C:291:ILE:H	1:C:291:ILE:HG12	1.69	0.43
2:H:194:CYS:O	2:H:221:MET:HG2	2.17	0.43
2:D:192:ILE:HB	2:D:219:VAL:HG22	2.00	0.43
2:B:126:ILE:HG22	2:B:333:THR:HG22	1.99	0.43
2:H:222:ARG:HD2	2:H:515:ALA:HA	2.01	0.43
2:D:31:ASN:ND2	2:D:252:PRO:HD3	2.34	0.43
1:G:8:ASN:OD1	1:G:80:GLY:HA3	2.18	0.43
4:E:1465:FAD:H2'	4:E:1465:FAD:N1	2.32	0.43
1:C:102:GLN:HB2	1:C:136:CYS:HB3	2.00	0.43
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.54	0.43
2:D:648:LEU:HA	2:D:711:ALA:O	2.18	0.43
1:E:407:ARG:O	1:E:411:ILE:HG12	2.18	0.43
1:G:109:GLY:O	1:G:113:SER:HB2	2.19	0.43
2:H:278:ILE:HG23	2:H:360:LEU:HD13	2.00	0.43
1:C:364:VAL:HG21	1:C:438:ALA:HB3	1.98	0.43
1:A:198:GLU:HG3	1:A:198:GLU:O	2.17	0.43
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.99	0.43
2:D:9:HIS:HD2	2:D:11:SER:H	1.66	0.43
2:F:261:ASP:HB3	2:F:265:ILE:CD1	2.48	0.43
2:H:94:VAL:HG11	2:H:687:ARG:HG2	2.01	0.43
1:G:181:PHE:O	1:G:223:ALA:HA	2.17	0.43
1:A:102:GLN:O	2:B:489:GLY:HA2	2.18	0.43
1:E:78:ILE:HD13	1:E:108:PRO:HA	2.00	0.43
2:F:53:GLU:HB3	2:F:54:PRO:HD3	2.00	0.43
2:F:641:ARG:HH21	2:F:706:ARG:HD3	1.84	0.43
2:H:270:HIS:CD2	2:H:297:CYS:HA	2.54	0.43
2:D:656:ASN:HA	2:D:657:PRO:HD2	1.90	0.43
1:G:240:GLY:HA2	1:G:343:LYS:HG3	2.00	0.43
1:C:441:ALA:O	2:D:636:LEU:HD23	2.19	0.43
4:C:1465:FAD:N1	4:C:1465:FAD:C2'	2.81	0.43
2:F:556:ALA:HB1	2:F:561:CYS:O	2.19	0.43
2:D:730:GLU:N	2:D:731:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ASP:HB3	2:B:287:LEU:HD11	2.00	0.43
2:F:261:ASP:HB3	2:F:265:ILE:HD12	2.01	0.43
1:A:32:LEU:HD12	1:A:79:GLU:HG3	2.00	0.43
2:D:631:VAL:HG12	2:D:642:ILE:HA	2.01	0.43
2:F:23:LEU:HD13	2:F:194:CYS:HA	2.01	0.43
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.54	0.43
2:B:297:CYS:SG	2:B:304:SER:HB3	2.59	0.43
1:A:299:ILE:O	1:A:381:ARG:NH1	2.45	0.43
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.54	0.43
1:G:44:CYS:HA	1:G:133:LEU:HG	2.01	0.43
2:F:528:ALA:O	2:F:529:ALA:HB3	2.19	0.42
1:C:207:ASP:HB2	4:C:1465:FAD:O1A	2.19	0.42
2:B:309:ASP:OD1	2:B:330:ARG:NH2	2.52	0.42
1:A:364:VAL:HG22	1:A:435:ARG:HG2	2.00	0.42
2:B:170:GLY:N	2:B:271:ASP:HB3	2.34	0.42
1:G:307:LEU:HB2	1:G:314:ARG:HB2	2.01	0.42
2:B:648:LEU:HD12	2:B:711:ALA:HB3	2.01	0.42
2:H:456:GLY:HA3	2:H:619:PHE:CD1	2.54	0.42
2:F:631:VAL:HG21	2:F:743:LEU:HA	2.01	0.42
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.54	0.42
2:D:367:ASP:HA	2:D:368:PRO:HD3	1.90	0.42
1:E:249:ILE:CG2	1:E:267:LEU:HD22	2.42	0.42
4:G:1465:FAD:H9	4:G:1465:FAD:H1'2	1.77	0.42
1:A:368:LEU:HG	1:A:382:ILE:HG23	2.01	0.42
1:C:1:MET:N	8:C:2001:HOH:O	2.53	0.42
2:D:35:LEU:HB2	2:D:255:MET:HE3	2.01	0.42
2:F:298:GLY:HA3	2:F:337:SER:HA	2.00	0.42
2:B:519:SER:O	2:D:472:GLN:NE2	2.50	0.42
2:H:272:PHE:CD2	2:H:348:GLN:HG2	2.54	0.42
1:A:89:HIS:ND1	1:A:91:VAL:HB	2.35	0.42
2:H:159:ALA:HB3	2:H:281:ASP:HA	2.01	0.42
1:A:110:PHE:C	1:A:114:MET:HE2	2.40	0.42
1:E:24:LEU:HD13	1:E:40:ASN:HD21	1.82	0.42
2:B:422:GLN:NE2	2:B:450:LEU:HD13	2.34	0.42
2:B:420:ARG:HD2	2:B:648:LEU:HD21	2.02	0.42
1:G:443:ALA:O	1:G:447:VAL:HG23	2.18	0.42
2:F:9:HIS:O	2:F:10:ASP:C	2.58	0.42
1:A:415:LEU:N	1:A:416:PRO:CD	2.83	0.42
2:F:595:SER:HB2	2:H:601:PHE:CG	2.54	0.42
1:A:40:ASN:HD22	1:A:213:THR:CG2	2.33	0.42
1:E:66:MET:HE3	1:E:202:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:TYR:N	2:B:22:TYR:CD1	2.88	0.42
1:E:415:LEU:HD21	1:E:443:ALA:HB3	2.02	0.42
2:F:39:LEU:HB3	2:F:95:GLY:HA2	2.01	0.42
2:D:641:ARG:HH21	2:D:706:ARG:HE	1.67	0.42
2:F:437:TRP:HA	2:F:440:THR:HG22	2.00	0.42
1:C:228:CYS:HB3	1:C:231:LEU:HB2	2.01	0.42
1:E:122:ARG:HG2	1:E:128:LEU:HD11	2.02	0.42
2:D:170:GLY:N	2:D:271:ASP:HB3	2.34	0.42
2:F:588:ALA:O	2:F:591:MET:HB2	2.20	0.42
2:D:547:LEU:HD21	2:D:596:LEU:C	2.39	0.42
2:D:179:GLN:NE2	2:D:230:GLY:O	2.53	0.42
2:F:138:ARG:HA	2:F:332:ARG:H	1.84	0.42
2:F:23:LEU:HD11	2:F:182:LEU:HB3	2.02	0.42
2:H:228:PHE:O	2:H:341:PHE:HA	2.20	0.42
1:A:40:ASN:HD22	1:A:213:THR:HG21	1.85	0.42
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.54	0.42
1:A:308:ARG:O	1:A:334:GLU:HA	2.19	0.42
2:B:24:ASP:HA	2:B:254:LYS:NZ	2.35	0.42
2:F:722:ILE:HG23	2:F:722:ILE:O	2.20	0.42
1:A:78:ILE:HA	1:A:81:ILE:HG12	2.02	0.42
2:F:512:ARG:HG3	2:F:513:ILE:N	2.35	0.42
2:B:302:ASP:OD1	2:B:303:LEU:N	2.53	0.42
1:E:364:VAL:HG21	1:E:438:ALA:HB3	2.01	0.42
1:C:240:GLY:HA2	1:C:343:LYS:HG2	2.01	0.42
1:G:65:MET:CE	1:G:278:VAL:HG11	2.50	0.42
1:E:61:ASN:H	1:E:61:ASN:ND2	2.17	0.42
2:D:179:GLN:HE22	2:D:234:GLN:HB2	1.84	0.42
2:D:309:ASP:O	2:D:313:LEU:HB2	2.19	0.42
2:F:468:GLY:HA2	2:F:600:GLY:O	2.20	0.42
2:B:684:HIS:HE2	2:F:565:ASP:HA	1.85	0.42
2:H:495:LYS:O	2:H:499:VAL:HG23	2.19	0.42
1:A:41:GLU:HA	1:A:210:LEU:CD2	2.50	0.41
2:H:85:VAL:HG21	2:H:240:ILE:HG21	2.01	0.41
2:F:63:ALA:HB3	2:F:102:ALA:HB3	2.02	0.41
2:H:627:ALA:HB2	2:H:735:LEU:HD22	2.02	0.41
2:D:172:GLU:HB3	2:D:696:TYR:CZ	2.55	0.41
2:D:461:LEU:CD1	7:D:1780:HPA:H8	2.49	0.41
1:G:183:PRO:HD2	1:G:224:PHE:O	2.19	0.41
2:H:380:PRO:HD3	2:H:412:CYS:O	2.20	0.41
2:D:110:ARG:HH21	2:D:258:ASP:HB2	1.85	0.41
1:C:241:TYR:O	1:C:340:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:THR:HG22	2:B:68:ALA:H	1.85	0.41
2:B:42:GLU:HG2	2:B:45:ALA:HB2	2.01	0.41
1:A:65:MET:CE	1:A:278:VAL:HG11	2.50	0.41
2:D:270:HIS:CD2	2:D:297:CYS:HA	2.55	0.41
2:H:606:LYS:HE3	2:H:617:ARG:HH22	1.86	0.41
2:F:360:LEU:O	2:F:364:MET:HG2	2.20	0.41
1:G:314:ARG:NH1	1:G:334:GLU:OE2	2.53	0.41
2:D:146:TRP:CZ3	2:D:312:MET:HB3	2.55	0.41
1:E:291:ILE:H	1:E:291:ILE:HD13	1.85	0.41
2:H:560:GLY:O	2:H:561:CYS:CB	2.67	0.41
2:F:166:PHE:CE1	2:F:355:ARG:HG3	2.56	0.41
2:F:610:ASP:HB3	2:F:613:ARG:HB2	2.01	0.41
2:H:249:THR:C	2:H:251:ARG:H	2.24	0.41
2:D:126:ILE:HG21	2:D:132:ALA:HA	2.01	0.41
2:D:766:VAL:O	2:D:770:VAL:HG23	2.19	0.41
1:G:49:VAL:HG23	1:G:60:VAL:HG23	2.01	0.41
1:C:295:PRO:HB2	1:C:296:PRO:HD3	2.01	0.41
2:D:310:ARG:HD2	2:D:344:PHE:CD2	2.54	0.41
2:F:421:LEU:HD13	2:F:648:LEU:HB2	2.01	0.41
2:D:373:ALA:HA	2:D:376:PHE:CE1	2.56	0.41
2:H:647:ILE:HD12	2:H:710:VAL:HG22	2.00	0.41
2:B:564:ARG:H	2:B:564:ARG:HG3	1.65	0.41
2:H:465:ASN:HB3	2:H:604:THR:HG1	1.82	0.41
2:H:414:LEU:HG	2:H:624:TYR:CD2	2.55	0.41
2:B:23:LEU:CD1	2:B:193:HIS:O	2.68	0.41
1:E:352:LYS:HE3	1:E:362:SER:HB3	2.01	0.41
1:E:352:LYS:HG3	1:E:362:SER:HB3	2.01	0.41
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.21	0.41
1:E:52:ARG:HB3	1:E:74:ALA:HB3	2.03	0.41
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.96	0.41
2:H:174:PHE:HZ	2:H:693:PRO:HB3	1.85	0.41
1:G:351:TYR:CZ	1:G:445:ARG:HG2	2.56	0.41
2:B:266:THR:O	2:B:268:LYS:HE2	2.21	0.41
2:D:177:GLU:CB	2:D:225:GLY:HA3	2.51	0.41
2:F:450:LEU:HA	2:F:627:ALA:O	2.21	0.41
2:H:179:GLN:HB3	2:H:238:LEU:HD11	2.02	0.41
2:H:212:LEU:CD1	2:H:216:ASP:HB3	2.50	0.41
1:G:140:ALA:N	1:G:141:PRO:CD	2.84	0.41
2:F:175:TYR:HE2	2:F:230:GLY:HA3	1.84	0.41
2:H:400:THR:HG21	2:H:410:ALA:HB2	2.02	0.41
1:C:225:LEU:C	1:C:227:HIS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:633:ILE:HG12	2:H:746:ALA:HB1	2.03	0.41
2:B:53:GLU:HB3	2:B:54:PRO:HD3	2.01	0.41
1:A:111:ILE:HD11	2:B:16:VAL:CG2	2.51	0.41
1:G:136:CYS:HB3	2:H:228:PHE:HZ	1.84	0.41
2:F:499:VAL:O	2:F:503:VAL:HG23	2.21	0.41
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.54	0.41
2:F:269:ARG:HB2	2:F:341:PHE:CD1	2.56	0.41
2:D:278:ILE:HG23	2:D:360:LEU:HD13	2.02	0.41
2:B:233:SER:C	2:B:235:GLY:H	2.24	0.41
2:B:233:SER:O	2:B:235:GLY:N	2.54	0.41
2:H:635:ARG:HD3	2:H:750:CYS:SG	2.61	0.41
1:C:102:GLN:HG3	1:C:137:THR:HG22	2.03	0.41
2:B:169:GLY:C	2:B:271:ASP:HB3	2.42	0.41
1:E:202:ILE:HG12	1:E:208:VAL:HG11	2.03	0.41
1:C:237:THR:HG23	1:C:240:GLY:H	1.86	0.41
2:B:210:LEU:HD11	2:B:243:ALA:HB1	2.01	0.41
2:B:343:GLY:H	2:B:730:GLU:HG2	1.86	0.41
1:E:214:LYS:HD2	2:F:260:ASP:OD1	2.21	0.41
1:C:60:VAL:HG11	1:C:278:VAL:HG13	2.03	0.41
2:H:138:ARG:HD3	2:H:142:GLY:H	1.86	0.41
1:C:181:PHE:O	1:C:223:ALA:HA	2.21	0.41
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.55	0.41
1:C:455:VAL:HG13	2:D:443:THR:HG21	2.02	0.41
1:E:387:MET:HE3	1:E:439:ALA:CB	2.48	0.41
2:F:632:VAL:HG13	2:F:643:LEU:HD11	2.02	0.41
2:B:315:ALA:O	2:B:353:MET:HE2	2.21	0.41
2:B:367:ASP:HA	2:B:368:PRO:HD3	1.99	0.41
2:D:689:MET:HA	2:D:689:MET:CE	2.51	0.41
2:H:768:ALA:O	2:H:772:ARG:HG3	2.20	0.40
2:H:14:ALA:HA	2:H:19:GLN:HB2	2.03	0.40
2:D:198:HIS:CD2	2:D:201:GLU:H	2.39	0.40
1:G:138:GLY:O	1:G:139:TYR:HB2	2.21	0.40
2:H:341:PHE:HD2	2:H:342:ARG:N	2.19	0.40
2:F:644:ARG:HB2	2:F:707:ILE:HB	2.03	0.40
2:D:273:ARG:HB3	2:D:294:LEU:HD12	2.02	0.40
2:B:466:GLN:HA	2:B:602:TYR:O	2.22	0.40
2:D:647:ILE:HB	2:D:710:VAL:HG22	2.03	0.40
2:F:341:PHE:O	2:F:342:ARG:C	2.59	0.40
1:A:108:PRO:O	1:A:112:VAL:HG23	2.22	0.40
1:C:1:MET:CE	1:C:16:ILE:HG13	2.47	0.40
1:A:208:VAL:HG22	4:A:1465:FAD:H3B	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	2.03	0.40
2:B:222:ARG:HD2	2:B:515:ALA:HA	2.04	0.40
2:H:212:LEU:HD13	2:H:216:ASP:HB3	2.04	0.40
2:F:466:GLN:NE2	2:H:593:ARG:HG2	2.37	0.40
1:E:298:LEU:HB3	1:E:303:ALA:HB3	2.03	0.40
2:F:33:LEU:HG	2:F:251:ARG:HD2	2.02	0.40
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.21	0.40
2:B:221:MET:HE2	2:B:486:THR:HB	2.03	0.40
2:H:222:ARG:HA	2:H:222:ARG:HD2	1.88	0.40
1:A:65:MET:HE1	1:A:278:VAL:HG11	2.03	0.40
2:F:367:ASP:HA	2:F:368:PRO:HD2	1.78	0.40
1:A:192:TRP:O	1:A:196:HIS:HD2	2.04	0.40
2:F:593:ARG:HD2	2:H:603:ALA:HB1	2.04	0.40
2:H:5:LYS:HA	2:H:6:PRO:HD3	1.97	0.40
1:E:243:ILE:HD11	1:E:255:PHE:CE2	2.55	0.40
1:E:255:PHE:O	1:E:259:PRO:HD2	2.21	0.40
2:F:310:ARG:HD2	2:F:344:PHE:HB3	2.04	0.40
1:G:269:ARG:HH12	1:G:352:LYS:HB3	1.86	0.40
2:H:194:CYS:SG	2:H:202:ILE:HD12	2.61	0.40
1:G:44:CYS:O	1:G:46:ALA:N	2.55	0.40
2:F:504:LEU:O	2:F:568:PHE:HB3	2.22	0.40
1:E:288:GLY:HA2	1:E:322:PHE:HE2	1.86	0.40
2:H:473:ILE:HD11	2:H:547:LEU:HD13	2.03	0.40
2:H:262:ASP:O	2:H:266:THR:CG2	2.68	0.40
2:B:478:SER:HB2	2:D:215:HIS:CE1	2.56	0.40
2:H:343:GLY:H	2:H:730:GLU:HG2	1.86	0.40
2:B:354:GLU:HA	2:B:357:ILE:HG22	2.03	0.40
1:E:325:TYR:CZ	1:E:326:ARG:HD2	2.57	0.40
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.51	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%)	394 (88%)	47 (10%)	5 (1%)	17	61
1	C	446/462 (96%)	405 (91%)	37 (8%)	4 (1%)	21	65
1	E	446/462 (96%)	406 (91%)	34 (8%)	6 (1%)	15	57
1	G	446/462 (96%)	393 (88%)	47 (10%)	6 (1%)	15	57
2	B	756/777 (97%)	707 (94%)	39 (5%)	10 (1%)	15	57
2	D	756/777 (97%)	685 (91%)	65 (9%)	6 (1%)	24	67
2	F	756/777 (97%)	690 (91%)	58 (8%)	8 (1%)	17	61
2	H	756/777 (97%)	699 (92%)	46 (6%)	11 (2%)	13	54
All	All	4808/4956 (97%)	4379 (91%)	373 (8%)	56 (1%)	16	59

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
1	C	39	CYS
2	D	187	GLU
2	D	458	SER
2	D	532	GLY
2	F	10	ASP
2	F	187	GLU
2	H	187	GLU
2	H	458	SER
1	A	39	CYS
1	A	389	GLY
2	B	73	ASP
2	B	187	GLU
2	B	234	GLN
2	B	342	ARG
1	C	121	ASP
2	D	10	ASP
1	E	39	CYS
2	F	342	ARG
2	F	458	SER
1	G	45	GLY
2	H	10	ASP
2	H	560	GLY
2	H	561	CYS
1	A	257	GLU
2	B	561	CYS
1	C	180	ALA

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Mol	Chain	Res	Type
1	E	197	PRO
1	E	226	SER
2	F	29	PRO
2	F	140	GLU
2	F	228	PHE
2	H	342	ARG
2	H	701	PHE
1	A	180	ALA
1	C	226	SER
2	D	227	GLY
1	E	323	LEU
1	G	39	CYS
2	B	115	LYS
2	B	560	GLY
1	E	332	PRO
2	F	260	ASP
1	G	359	GLN
2	H	30	ALA
1	A	359	GLN
2	B	233	SER
1	E	295	PRO
1	G	180	ALA
2	B	227	GLY
2	H	722	ILE
2	D	141	GLY
1	G	302	GLY
2	H	532	GLY
2	H	227	GLY
1	G	197	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	339/347 (98%)	310 (91%)	29 (9%)	13 48
1	C	339/347 (98%)	316 (93%)	23 (7%)	20 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	339/347 (98%)	321 (95%)	18 (5%)	28 67
1	G	339/347 (98%)	318 (94%)	21 (6%)	23 63
2	B	571/584 (98%)	526 (92%)	45 (8%)	15 52
2	D	571/584 (98%)	523 (92%)	48 (8%)	14 49
2	F	571/584 (98%)	521 (91%)	50 (9%)	12 46
2	H	571/584 (98%)	524 (92%)	47 (8%)	14 50
All	All	3640/3724 (98%)	3359 (92%)	281 (8%)	16 53

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	61	ASN
1	A	66	MET
1	A	79	GLU
1	A	103	CYS
1	A	113	SER
1	A	122	ARG
1	A	128	LEU
1	A	132	ASN
1	A	133	LEU
1	A	143	LEU
1	A	191	ASP
1	A	207	ASP
1	A	219	LEU
1	A	228	CYS
1	A	231	LEU
1	A	323	LEU
1	A	340	THR
1	A	341	LEU
1	A	348	LEU
1	A	349	ARG
1	A	371	THR
1	A	393	ARG
1	A	407	ARG
1	A	408	GLU
1	A	423	THR
1	A	425	LEU
1	A	437	ASN
1	A	458	LEU

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Mol	Chain	Res	Type
2	B	10	ASP
2	B	16	VAL
2	B	19	GLN
2	B	21	ARG
2	B	23	LEU
2	B	129	LEU
2	B	161	LEU
2	B	174	PHE
2	B	175	TYR
2	B	176	LEU
2	B	200	SER
2	B	212	LEU
2	B	215	HIS
2	B	222	ARG
2	B	256	ARG
2	B	259	ARG
2	B	262	ASP
2	B	266	THR
2	B	268	LYS
2	B	271	ASP
2	B	296	ARG
2	B	300	SER
2	B	313	LEU
2	B	326	ILE
2	B	341	PHE
2	B	355	ARG
2	B	357	ILE
2	B	381	GLU
2	B	398	LYS
2	B	399	LYS
2	B	428	THR
2	B	458	SER
2	B	460	THR
2	B	466	GLN
2	B	488	MET
2	B	512	ARG
2	B	520	LYS
2	B	596	LEU
2	B	604	THR
2	B	612	LEU
2	B	617	ARG
2	B	632	VAL

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Mol	Chain	Res	Type
2	B	689	MET
2	B	704	ARG
2	B	708	PHE
1	C	20	THR
1	C	24	LEU
1	C	63	CYS
1	C	113	SER
1	C	128	LEU
1	C	218	ASP
1	C	219	LEU
1	C	228	CYS
1	C	231	LEU
1	C	257	GLU
1	C	291	ILE
1	C	316	MET
1	C	324	GLU
1	C	341	LEU
1	C	349	ARG
1	C	362	SER
1	C	373	LYS
1	C	390	VAL
1	C	393	ARG
1	C	435	ARG
1	C	437	ASN
1	C	449	GLU
1	C	457	VAL
2	D	10	ASP
2	D	11	SER
2	D	16	VAL
2	D	21	ARG
2	D	23	LEU
2	D	40	SER
2	D	110	ARG
2	D	129	LEU
2	D	161	LEU
2	D	174	PHE
2	D	175	TYR
2	D	200	SER
2	D	202	ILE
2	D	212	LEU
2	D	215	HIS
2	D	222	ARG

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Mol	Chain	Res	Type
2	D	247	ARG
2	D	256	ARG
2	D	266	THR
2	D	268	LYS
2	D	296	ARG
2	D	330	ARG
2	D	341	PHE
2	D	355	ARG
2	D	398	LYS
2	D	399	LYS
2	D	411	ASP
2	D	412	CYS
2	D	423	LYS
2	D	428	THR
2	D	464	LEU
2	D	466	GLN
2	D	512	ARG
2	D	514	THR
2	D	520	LYS
2	D	564	ARG
2	D	596	LEU
2	D	632	VAL
2	D	648	LEU
2	D	689	MET
2	D	694	SER
2	D	695	THR
2	D	697	LYS
2	D	704	ARG
2	D	708	PHE
2	D	720	GLU
2	D	724	ARG
2	D	741	LEU
1	E	40	ASN
1	E	61	ASN
1	E	65	MET
1	E	79	GLU
1	E	97	ASP
1	E	122	ARG
1	E	128	LEU
1	E	219	LEU
1	E	231	LEU
1	E	237	THR

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Mol	Chain	Res	Type
1	E	291	ILE
1	E	341	LEU
1	E	349	ARG
1	E	365	CYS
1	E	373	LYS
1	E	390	VAL
1	E	393	ARG
1	E	409	ASP
2	F	2	SER
2	F	10	ASP
2	F	11	SER
2	F	16	VAL
2	F	53	GLU
2	F	59	PRO
2	F	66	THR
2	F	90	GLU
2	F	128	THR
2	F	161	LEU
2	F	174	PHE
2	F	175	TYR
2	F	212	LEU
2	F	215	HIS
2	F	222	ARG
2	F	234	GLN
2	F	256	ARG
2	F	259	ARG
2	F	266	THR
2	F	268	LYS
2	F	287	LEU
2	F	296	ARG
2	F	313	LEU
2	F	341	PHE
2	F	355	ARG
2	F	357	ILE
2	F	381	GLU
2	F	398	LYS
2	F	399	LYS
2	F	433	GLU
2	F	458	SER
2	F	464	LEU
2	F	475	THR
2	F	512	ARG

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Mol	Chain	Res	Type
2	F	518	THR
2	F	520	LYS
2	F	546	THR
2	F	558	ARG
2	F	564	ARG
2	F	567	ILE
2	F	584	GLU
2	F	617	ARG
2	F	632	VAL
2	F	648	LEU
2	F	689	MET
2	F	698	ILE
2	F	702	SER
2	F	704	ARG
2	F	708	PHE
2	F	741	LEU
1	G	24	LEU
1	G	33	THR
1	G	61	ASN
1	G	93	GLN
1	G	103	CYS
1	G	113	SER
1	G	122	ARG
1	G	128	LEU
1	G	132	ASN
1	G	137	THR
1	G	228	CYS
1	G	231	LEU
1	G	327	LYS
1	G	341	LEU
1	G	349	ARG
1	G	393	ARG
1	G	407	ARG
1	G	408	GLU
1	G	409	ASP
1	G	423	THR
1	G	457	VAL
2	H	2	SER
2	H	10	ASP
2	H	16	VAL
2	H	21	ARG
2	H	57	GLU

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Mol	Chain	Res	Type
2	H	128	THR
2	H	137	SER
2	H	148	ARG
2	H	175	TYR
2	H	187	GLU
2	H	202	ILE
2	H	210	LEU
2	H	212	LEU
2	H	215	HIS
2	H	216	ASP
2	H	222	ARG
2	H	256	ARG
2	H	260	ASP
2	H	266	THR
2	H	268	LYS
2	H	313	LEU
2	H	341	PHE
2	H	357	ILE
2	H	398	LYS
2	H	399	LYS
2	H	441	ASN
2	H	458	SER
2	H	488	MET
2	H	512	ARG
2	H	514	THR
2	H	550	ARG
2	H	564	ARG
2	H	579	SER
2	H	604	THR
2	H	609	TRP
2	H	612	LEU
2	H	617	ARG
2	H	620	LEU
2	H	632	VAL
2	H	634	ASP
2	H	646	ASP
2	H	698	ILE
2	H	704	ARG
2	H	708	PHE
2	H	721	THR
2	H	728	VAL
2	H	741	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	61	ASN
1	A	93	GLN
1	A	132	ASN
1	A	196	HIS
1	A	359	GLN
1	A	440	GLN
2	B	19	GLN
2	B	34	HIS
2	B	208	HIS
2	B	236	ASN
2	B	237	HIS
2	B	293	HIS
2	B	422	GLN
2	B	466	GLN
2	B	572	GLN
2	B	744	HIS
1	C	40	ASN
1	C	61	ASN
1	C	260	HIS
1	C	437	ASN
2	D	9	HIS
2	D	179	GLN
2	D	193	HIS
2	D	198	HIS
2	D	232	GLN
2	D	236	ASN
2	D	422	GLN
2	D	426	ASN
2	D	465	ASN
2	D	466	GLN
2	D	482	ASN
2	D	649	HIS
2	D	744	HIS
2	D	753	HIS
1	E	40	ASN
1	E	61	ASN
1	E	93	GLN
1	E	260	HIS
2	F	9	HIS
2	F	15	HIS

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Mol	Chain	Res	Type
2	F	236	ASN
2	F	237	HIS
2	F	441	ASN
2	F	465	ASN
2	F	574	GLN
2	F	649	HIS
1	G	40	ASN
1	G	61	ASN
1	G	93	GLN
1	G	132	ASN
1	G	260	HIS
1	G	359	GLN
2	H	106	HIS
2	H	232	GLN
2	H	236	ASN
2	H	293	HIS
2	H	441	ASN
2	H	466	GLN
2	H	482	ASN
2	H	744	HIS

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	-	48,58,58	1.66	8 (16%)	54,89,89	1.87	6 (11%)
5	XAX	B	1778	-	22,31,31	2.44	5 (22%)	19,52,52	2.23	6 (31%)
7	HPA	B	1780	-	8,11,11	2.21	3 (37%)	4,15,15	5.56	3 (75%)
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	-	48,58,58	1.55	5 (10%)	54,89,89	2.01	8 (14%)
5	XAX	D	1778	-	22,31,31	2.62	6 (27%)	19,52,52	2.01	5 (26%)
7	HPA	D	1780	-	8,11,11	2.01	3 (37%)	4,15,15	5.75	3 (75%)
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	-	48,58,58	1.61	5 (10%)	54,89,89	1.90	7 (12%)
5	XAX	F	1778	-	22,31,31	2.54	6 (27%)	19,52,52	2.09	6 (31%)
7	HPA	F	1780	-	8,11,11	2.13	3 (37%)	4,15,15	5.33	2 (50%)
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	-	48,58,58	1.65	6 (12%)	54,89,89	1.94	9 (16%)
5	XAX	H	1778	-	22,31,31	2.44	5 (22%)	19,52,52	2.23	6 (31%)
7	HPA	H	1780	-	8,11,11	2.07	3 (37%)	4,15,15	5.71	2 (50%)

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	-	-	0/30/50/50	0/6/6/6
5	XAX	B	1778	-	1/1/7/9	0/6/46/46	0/4/4/4
7	HPA	B	1780	-	-	0/0/0/0	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	-	-	0/30/50/50	0/6/6/6
5	XAX	D	1778	-	1/1/7/9	0/6/46/46	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HPA	D	1780	-	-	0/0/0/0	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	-	-	0/30/50/50	0/6/6/6
5	XAX	F	1778	-	1/1/7/9	0/6/46/46	0/4/4/4
7	HPA	F	1780	-	-	0/0/0/0	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	-	-	0/30/50/50	0/6/6/6
5	XAX	H	1778	-	1/1/7/9	0/6/46/46	0/4/4/4
7	HPA	H	1780	-	-	0/0/0/0	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1778	XAX	C6-N5	-8.50	1.33	1.45
5	D	1778	XAX	C6-N5	-8.32	1.33	1.45
5	H	1778	XAX	C6-N5	-7.94	1.34	1.45
5	B	1778	XAX	C6-N5	-7.84	1.34	1.45
5	D	1778	XAX	C2'-S2'	-5.45	1.65	1.76
5	H	1778	XAX	C2'-S2'	-4.85	1.66	1.76
5	F	1778	XAX	C2'-S2'	-4.82	1.66	1.76
5	B	1778	XAX	C2'-S2'	-4.70	1.67	1.76
5	B	1778	XAX	C1'-S1'	-4.46	1.67	1.76
5	F	1778	XAX	C1'-S1'	-4.39	1.67	1.76
5	H	1778	XAX	C1'-S1'	-4.30	1.67	1.76
5	D	1778	XAX	C1'-S1'	-4.29	1.67	1.76
5	D	1778	XAX	C7-C6	-2.83	1.51	1.53
5	F	1778	XAX	C7-C6	-2.03	1.52	1.53
5	F	1778	XAX	C9-C10	2.49	1.46	1.41
4	A	1465	FAD	C1'-N10	2.55	1.51	1.48
7	H	1780	HPA	C2-N1	2.55	1.38	1.33
5	B	1778	XAX	C9-C10	2.63	1.47	1.41
4	G	1465	FAD	C10-N10	2.64	1.42	1.39
7	D	1780	HPA	C2-N1	2.70	1.39	1.33
5	H	1778	XAX	C9-C10	2.72	1.47	1.41
5	D	1778	XAX	C9-C10	2.78	1.47	1.41
5	F	1778	XAX	C9-N5	2.89	1.44	1.38
7	B	1780	HPA	C2-N1	2.91	1.39	1.33
4	A	1465	FAD	C10-N10	2.97	1.42	1.39
7	F	1780	HPA	C2-N1	2.97	1.39	1.33
5	D	1778	XAX	C9-N5	2.99	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1465	FAD	C5X-N5	3.07	1.40	1.35
5	H	1778	XAX	C9-N5	3.09	1.45	1.38
4	E	1465	FAD	C5X-N5	3.09	1.40	1.35
7	D	1780	HPA	C6-N1	3.10	1.38	1.33
4	A	1465	FAD	C5X-N5	3.16	1.40	1.35
5	B	1778	XAX	C9-N5	3.18	1.45	1.38
4	C	1465	FAD	C10-N1	3.18	1.40	1.35
4	A	1465	FAD	C9A-N10	3.20	1.43	1.38
7	F	1780	HPA	C6-N1	3.26	1.39	1.33
4	E	1465	FAD	C10-N1	3.26	1.41	1.35
4	G	1465	FAD	C10-N1	3.30	1.41	1.35
7	H	1780	HPA	C6-N1	3.30	1.39	1.33
4	A	1465	FAD	C10-N1	3.47	1.41	1.35
4	G	1465	FAD	C5X-N5	3.74	1.41	1.35
7	B	1780	HPA	C6-N1	3.74	1.40	1.33
7	D	1780	HPA	C2-N3	3.77	1.38	1.32
7	H	1780	HPA	C2-N3	3.94	1.39	1.32
7	F	1780	HPA	C2-N3	4.00	1.39	1.32
7	B	1780	HPA	C2-N3	4.04	1.39	1.32
4	A	1465	FAD	C4-N3	4.17	1.40	1.33
4	C	1465	FAD	O4B-C1B	4.25	1.46	1.41
4	G	1465	FAD	C4-N3	4.39	1.41	1.33
4	E	1465	FAD	C4-N3	4.45	1.41	1.33
4	A	1465	FAD	C4X-N5	4.65	1.40	1.33
4	A	1465	FAD	O4B-C1B	4.76	1.47	1.41
4	E	1465	FAD	C4X-N5	4.76	1.40	1.33
4	C	1465	FAD	C4-N3	4.80	1.42	1.33
4	C	1465	FAD	C4X-N5	4.94	1.41	1.33
4	G	1465	FAD	O4B-C1B	5.03	1.47	1.41
4	G	1465	FAD	C4X-N5	5.27	1.41	1.33
4	E	1465	FAD	O4B-C1B	5.62	1.48	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1780	HPA	N3-C2-N1	-10.96	120.50	128.89
7	H	1780	HPA	N3-C2-N1	-10.95	120.51	128.89
7	B	1780	HPA	N3-C2-N1	-10.61	120.77	128.89
7	F	1780	HPA	N3-C2-N1	-10.18	121.10	128.89
4	G	1465	FAD	N3A-C2A-N1A	-9.98	121.25	128.89
4	A	1465	FAD	N3A-C2A-N1A	-9.87	121.34	128.89
4	C	1465	FAD	N3A-C2A-N1A	-9.83	121.37	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1465	FAD	N3A-C2A-N1A	-9.73	121.44	128.89
4	C	1465	FAD	P-O3P-PA	-3.50	122.89	132.73
4	A	1465	FAD	P-O3P-PA	-3.50	122.91	132.73
4	E	1465	FAD	P-O3P-PA	-3.28	123.53	132.73
4	C	1465	FAD	O4B-C1B-N9A	-3.05	101.71	108.10
4	G	1465	FAD	P-O3P-PA	-2.95	124.45	132.73
4	C	1465	FAD	C4X-C4-N3	-2.79	119.77	123.59
4	G	1465	FAD	C4X-C4-N3	-2.71	119.88	123.59
4	G	1465	FAD	C4A-C5A-N7A	-2.47	107.21	109.48
5	D	1778	XAX	O4'-P-O2P	-2.44	100.93	107.14
4	E	1465	FAD	C4X-C4-N3	-2.44	120.25	123.59
5	F	1778	XAX	O4'-P-O2P	-2.38	101.07	107.14
5	B	1778	XAX	N3-C2-N1	-2.34	121.69	125.53
7	B	1780	HPA	C4-C5-N7	-2.31	107.36	109.48
4	A	1465	FAD	C4X-C4-N3	-2.22	120.56	123.59
5	H	1778	XAX	N3-C2-N1	-2.10	122.10	125.53
4	E	1465	FAD	C2B-C1B-N9A	-2.06	111.15	114.29
7	D	1780	HPA	C4-C5-N7	-2.02	107.62	109.48
4	G	1465	FAD	C4-C4X-N5	2.07	121.23	118.72
5	B	1778	XAX	C4-C9-C10	2.13	116.49	114.56
4	G	1465	FAD	C2B-C1B-N9A	2.16	117.59	114.29
7	B	1780	HPA	C2-N1-C6	2.19	119.36	116.04
4	E	1465	FAD	C5X-C9A-N10	2.22	119.31	117.62
7	H	1780	HPA	C2-N1-C6	2.24	119.43	116.04
7	F	1780	HPA	C2-N1-C6	2.33	119.57	116.04
7	D	1780	HPA	C2-N1-C6	2.61	120.00	116.04
5	H	1778	XAX	C4-C9-C10	2.71	117.02	114.56
5	H	1778	XAX	N8-C10-N1	2.80	121.09	116.62
5	D	1778	XAX	C4-C9-C10	2.84	117.13	114.56
4	G	1465	FAD	C5X-C9A-N10	2.93	119.85	117.62
5	B	1778	XAX	N8-C10-N1	2.94	121.31	116.62
5	D	1778	XAX	C2-N1-C10	2.97	121.20	114.54
5	H	1778	XAX	C2-N1-C10	3.01	121.31	114.54
4	C	1465	FAD	C5X-C9A-N10	3.03	119.92	117.62
4	A	1465	FAD	C5X-C9A-N10	3.10	119.98	117.62
5	F	1778	XAX	C2-N1-C10	3.13	121.58	114.54
5	F	1778	XAX	O3'-C7-C6	3.16	111.12	108.96
4	A	1465	FAD	C4X-N5-C5X	3.16	120.40	116.76
4	G	1465	FAD	C4X-N5-C5X	3.17	120.41	116.76
5	B	1778	XAX	C2-N1-C10	3.28	121.91	114.54
5	F	1778	XAX	N8-C10-N1	3.30	121.88	116.62
4	C	1465	FAD	C4X-N5-C5X	3.33	120.60	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1778	XAX	C4-C9-C10	3.45	117.69	114.56
5	D	1778	XAX	N8-C10-N1	3.51	122.20	116.62
4	C	1465	FAD	C2B-C1B-N9A	3.64	119.85	114.29
4	E	1465	FAD	C4X-N5-C5X	3.84	121.18	116.76
5	F	1778	XAX	C4-N3-C2	3.93	121.40	115.94
5	B	1778	XAX	C4-N3-C2	4.12	121.66	115.94
5	D	1778	XAX	C4-N3-C2	4.31	121.92	115.94
5	H	1778	XAX	C4-N3-C2	4.47	122.14	115.94
4	E	1465	FAD	C4-N3-C2	4.92	119.50	115.25
4	A	1465	FAD	C4-N3-C2	5.01	119.58	115.25
5	H	1778	XAX	O3'-C7-C6	5.26	112.56	108.96
4	C	1465	FAD	C4-N3-C2	5.38	119.89	115.25
5	B	1778	XAX	O3'-C7-C6	5.45	112.69	108.96
4	G	1465	FAD	C4-N3-C2	5.69	120.16	115.25

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1465	FAD	6	0
5	B	1778	XAX	4	0
4	C	1465	FAD	5	0
5	D	1778	XAX	7	0
7	D	1780	HPA	3	0
4	E	1465	FAD	3	0
5	F	1778	XAX	8	0
7	F	1780	HPA	1	0
3	G	1464	FES	1	0
4	G	1465	FAD	8	0
5	H	1778	XAX	4	0
7	H	1780	HPA	7	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	450/462 (97%)	0.38	28 (6%) 24 22	41, 43, 44, 45	0
1	C	450/462 (97%)	-0.05	3 (0%) 89 85	41, 43, 44, 45	0
1	E	450/462 (97%)	0.20	13 (2%) 55 50	41, 43, 44, 45	0
1	G	450/462 (97%)	0.30	23 (5%) 32 28	42, 43, 44, 45	0
2	B	760/777 (97%)	-0.07	3 (0%) 93 91	40, 43, 44, 46	0
2	D	760/777 (97%)	-0.24	2 (0%) 94 92	41, 43, 44, 46	0
2	F	760/777 (97%)	-0.24	0 100 100	41, 43, 44, 46	0
2	H	760/777 (97%)	-0.17	2 (0%) 94 92	41, 43, 44, 46	0
All	All	4840/4956 (97%)	-0.04	74 (1%) 76 71	40, 43, 44, 46	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	17	GLU	4.3
1	G	378	GLU	3.8
1	G	411	ILE	3.8
1	A	413	ALA	3.8
1	A	240	GLY	3.6
1	A	377	ILE	3.5
2	H	137	SER	3.4
1	A	378	GLU	3.4
1	A	239	ASP	3.3
1	G	323	LEU	3.3
1	A	313	ARG	3.2
1	E	220	PRO	3.2
1	G	4	ALA	3.1
1	A	192	TRP	3.1
1	G	389	GLY	3.1
1	G	401	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	181	PHE	3.0
1	G	371	THR	3.0
1	G	5	PHE	2.9
1	A	19	PRO	2.9
1	G	313	ARG	2.8
1	A	401	LEU	2.8
1	E	312	GLU	2.8
1	G	218	ASP	2.7
1	A	199	ALA	2.7
1	G	310	GLY	2.7
1	E	5	PHE	2.7
2	D	777	ALA	2.7
1	A	410	THR	2.7
1	A	375	SER	2.7
1	G	19	PRO	2.7
1	A	136	CYS	2.6
1	E	301	MET	2.6
2	B	694	SER	2.6
1	A	383	ALA	2.5
1	E	380	ALA	2.5
1	E	164	PHE	2.5
1	E	401	LEU	2.5
1	A	411	ILE	2.5
1	G	136	CYS	2.5
1	E	166	LEU	2.5
1	E	201	LEU	2.4
1	G	87	ARG	2.4
2	D	144	VAL	2.4
1	C	310	GLY	2.4
1	C	402	ILE	2.4
1	G	377	ILE	2.3
2	B	137	SER	2.3
1	E	200	THR	2.3
2	B	161	LEU	2.3
1	E	21	GLN	2.3
1	G	406	PHE	2.3
1	A	370	LEU	2.3
1	A	447	VAL	2.3
1	G	447	VAL	2.2
1	A	157	TRP	2.2
1	A	403	GLY	2.2
1	G	413	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	3	ILE	2.2
1	A	389	GLY	2.2
1	A	134	CYS	2.2
1	C	220	PRO	2.2
1	A	384	PHE	2.2
1	A	371	THR	2.1
1	G	182	LEU	2.1
1	A	236	GLU	2.1
1	E	183	PRO	2.1
2	H	576	SER	2.1
1	G	221	GLU	2.1
1	A	221	GLU	2.1
1	G	307	LEU	2.1
1	G	321	PHE	2.0
1	A	155	ALA	2.0
1	A	402	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FES	A	1464	4/4	0.98	0.42	3.02	84,84,84,85	4
3	FES	G	1464	4/4	0.97	0.29	2.70	66,66,66,66	4
5	XAX	B	1778	28/28	0.96	0.37	2.18	52,55,60,61	28
5	XAX	F	1778	28/28	0.98	0.28	2.10	39,41,47,49	28
7	HPA	D	1780	10/10	0.89	0.26	2.01	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FES	E	1464	4/4	0.94	0.28	1.91	97,98,98,99	4
3	FES	C	1463	4/4	0.99	0.29	1.89	24,25,25,25	4
5	XAX	D	1778	28/28	0.98	0.28	1.70	37,42,47,49	28
3	FES	C	1464	4/4	0.96	0.27	1.34	107,108,108,108	4
5	XAX	H	1778	28/28	0.97	0.24	0.89	52,55,62,63	28
3	FES	E	1463	4/4	0.99	0.27	0.83	32,32,32,33	4
3	FES	A	1463	4/4	0.99	0.33	0.47	29,30,30,30	4
3	FES	G	1463	4/4	0.99	0.29	0.16	44,45,45,46	4
4	FAD	C	1465	53/53	0.94	0.18	-0.59	46,51,55,55	0
4	FAD	E	1465	53/53	0.93	0.18	-0.64	62,66,78,78	0
4	FAD	A	1465	53/53	0.93	0.17	-0.71	72,74,76,76	0
7	HPA	H	1780	10/10	0.91	0.17	-0.74	43,43,43,43	0
4	FAD	G	1465	53/53	0.92	0.17	-0.99	74,76,79,80	0
7	HPA	F	1780	10/10	0.94	0.16	-1.08	43,43,43,43	0
7	HPA	B	1780	10/10	0.95	0.14	-1.67	43,43,43,43	0
6	BA	B	1779	1/1	0.99	0.07	-3.52	108,108,108,108	0
6	BA	H	1779	1/1	0.99	0.08	-3.93	115,115,115,115	0
6	BA	D	1779	1/1	0.99	0.05	-6.07	105,105,105,105	0
6	BA	F	1779	1/1	0.99	0.06	-6.78	98,98,98,98	0

6.5 Other polymers (i)

There are no such residues in this entry.