



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:11 AM GMT

PDB ID : 3HHD  
Title : Structure of the Human Fatty Acid Synthase KS-MAT Didomain as a Framework for Inhibitor Design.  
Authors : Pappenberger, G.M.; Benz, J.; Thoma, R.; Rudolph, M.G.  
Deposited on : 2009-05-15  
Resolution : 2.15 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 (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

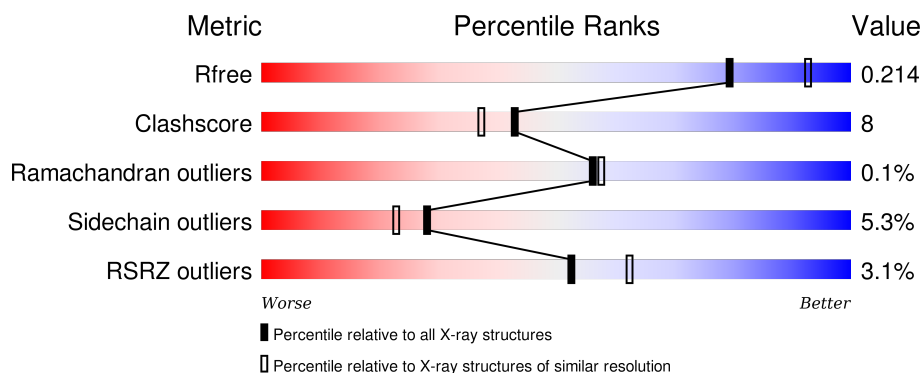
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	965	<div> <div>2%</div> <div>72% 15% • 12%</div> </div>
1	B	965	<div> <div>4%</div> <div>71% 15% • 12%</div> </div>
1	C	965	<div> <div>2%</div> <div>73% 14% • 11%</div> </div>
1	D	965	<div> <div>3%</div> <div>72% 14% • 12%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27836 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	2	0
			6497	4119	1144	1200	34			
1	B	852	Total	C	N	O	S	0	3	0
			6505	4125	1147	1199	34			
1	C	855	Total	C	N	O	S	0	1	0
			6512	4127	1147	1204	34			
1	D	854	Total	C	N	O	S	0	2	0
			6512	4129	1146	1203	34			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P49327
A	0	THR	-	EXPRESSION TAG	UNP P49327
A	1	GLY	-	EXPRESSION TAG	UNP P49327
B	-1	SER	-	EXPRESSION TAG	UNP P49327
B	0	THR	-	EXPRESSION TAG	UNP P49327
B	1	GLY	-	EXPRESSION TAG	UNP P49327
C	-1	SER	-	EXPRESSION TAG	UNP P49327
C	0	THR	-	EXPRESSION TAG	UNP P49327
C	1	GLY	-	EXPRESSION TAG	UNP P49327
D	-1	SER	-	EXPRESSION TAG	UNP P49327
D	0	THR	-	EXPRESSION TAG	UNP P49327
D	1	GLY	-	EXPRESSION TAG	UNP P49327

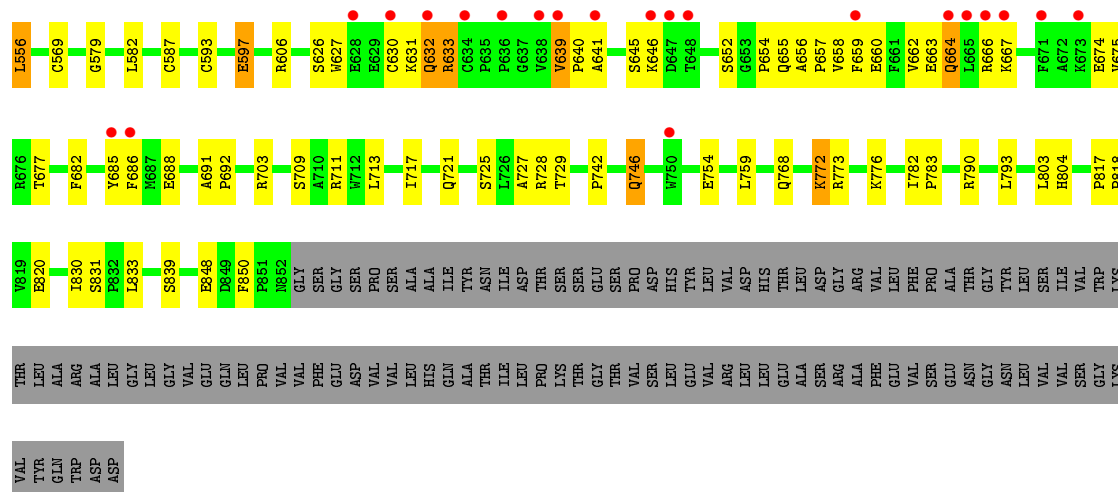
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

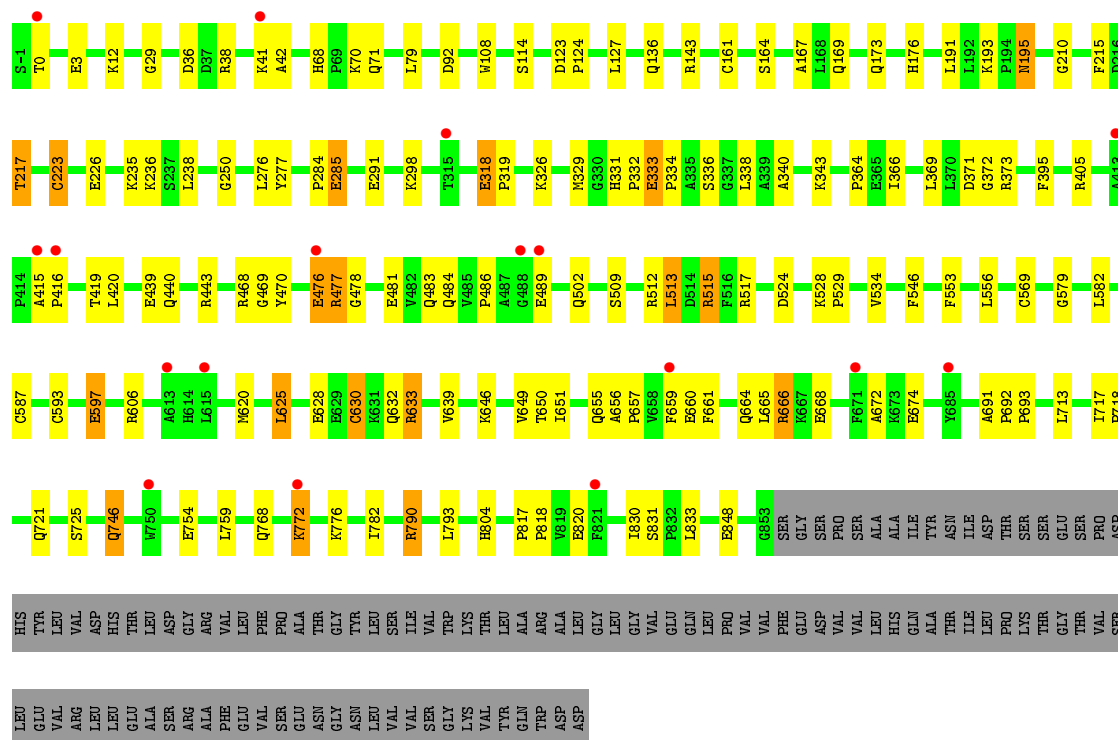
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	561	Total 561	O 561	0	0
3	B	371	Total 371	O 371	0	0
3	C	437	Total 437	O 437	0	0
3	D	439	Total 439	O 439	0	0

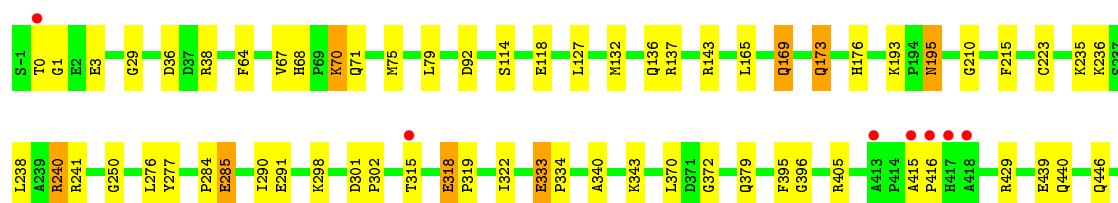




• Molecule 1: Fatty acid synthase



• Molecule 1: Fatty acid synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.62Å 91.16Å 132.11Å 73.84° 86.83° 62.54°	Depositor
Resolution (Å)	45.64 – 2.15 45.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.64-2.15) 88.0 (45.64-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.14Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, $R_{free}$	0.169 , 0.211 0.171 , 0.214	Depositor DCC
$R_{free}$ test set	9150 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 182506 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% 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, 0.375 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: CL

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	0.68	1/6662 (0.0%)	0.68	0/9058
1	B	0.61	1/6673 (0.0%)	0.66	1/9074 (0.0%)
1	C	0.63	2/6674 (0.0%)	0.67	1/9075 (0.0%)
1	D	0.62	1/6678 (0.0%)	0.68	2/9083 (0.0%)
All	All	0.64	5/26687 (0.0%)	0.67	4/36290 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	593	CYS	CB-SG	-7.10	1.70	1.82
1	A	593	CYS	CB-SG	-5.64	1.72	1.81
1	D	223	CYS	CB-SG	-5.36	1.73	1.81
1	B	593	CYS	CB-SG	-5.31	1.73	1.81
1	C	161	CYS	CB-SG	-5.06	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	333	GLU	C-N-CD	5.47	139.88	128.40
1	C	468	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	802	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	6497	0	6477	106	0
1	B	6505	0	6491	119	0
1	C	6512	0	6491	94	0
1	D	6512	0	6487	117	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	561	0	0	8	0
3	B	371	0	0	11	0
3	C	437	0	0	13	0
3	D	439	0	0	15	0
All	All	27836	0	25946	427	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 8.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.45	0.95
1:D:656:ALA:HB3	1:D:657:PRO:HD3	1.50	0.94
1:A:42:ALA:HB1	1:A:49:ARG:HD2	1.56	0.87
1:A:67:VAL:HG11	1:A:75:MET:HE1	1.56	0.85
1:D:556:LEU:HD23	1:D:582:LEU:HD23	1.62	0.81
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.68	0.75
1:C:333:GLU:HB2	1:C:334:PRO:HD2	1.68	0.75
1:D:626:SER:OG	1:D:629:GLU:HB2	1.88	0.72
1:B:639:VAL:HG22	1:B:640:PRO:HD2	1.70	0.72
1:A:790:ARG:H	1:A:790:ARG:CD	2.01	0.72
1:C:790:ARG:CD	1:C:790:ARG:H	2.03	0.69
1:B:728:ARG:HG2	1:B:729:THR:HG23	1.73	0.69
1:D:633:ARG:NH2	1:D:668:GLU:OE1	2.25	0.69
1:B:368:ALA:HA	1:B:371:ASP:OD1	1.92	0.69
1:D:790:ARG:CD	1:D:790:ARG:H	2.03	0.69
1:C:848:GLU:HG2	3:C:1008:HOH:O	1.93	0.69
1:B:440:GLN:OE1	1:B:443:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLN:OE1	1:A:443:ARG:NH1	2.26	0.69
1:D:786:LYS:NZ	3:D:1096:HOH:O	2.24	0.68
1:A:477:ARG:NH1	1:A:789:HIS:HE2	1.91	0.68
1:C:440:GLN:HG3	1:C:833:LEU:HD22	1.76	0.68
1:D:440:GLN:HG3	1:D:833:LEU:HD22	1.76	0.68
1:B:655:GLN:HG3	1:B:659:PHE:CE2	2.30	0.67
1:D:291:GLU:HG2	1:D:340:ALA:HB1	1.78	0.66
1:A:209:GLU:OE2	1:A:213:LYS:NZ	2.27	0.66
1:C:3:GLU:OE2	1:C:236:LYS:HD2	1.96	0.66
1:D:515:ARG:HB2	3:D:1250:HOH:O	1.95	0.65
1:C:477:ARG:HG3	1:C:478:GLY:H	1.61	0.65
1:D:656:ALA:CB	1:D:657:PRO:HD3	2.25	0.65
1:C:193:LYS:HE3	1:C:195:ASN:HB2	1.79	0.65
3:A:1712:HOH:O	1:C:41:LYS:HD3	1.96	0.65
1:B:656:ALA:O	1:B:660:GLU:HG2	1.97	0.64
1:D:68[A]:HIS:HB3	1:D:71:GLN:OE1	1.97	0.64
1:A:3:GLU:OE2	1:A:236:LYS:HD2	1.98	0.64
1:A:663:GLU:HA	1:A:663:GLU:OE1	1.96	0.64
1:D:768:GLN:O	1:D:772:LYS:HD2	1.98	0.63
1:A:768:GLN:O	1:A:772:LYS:HD2	1.98	0.63
1:B:68:HIS:CE1	1:B:70:LYS:HG3	2.33	0.63
1:A:68:HIS:CE1	1:A:70:LYS:HG3	2.33	0.63
1:C:333:GLU:HB2	1:C:334:PRO:CD	2.29	0.63
1:D:290:ILE:HG23	1:D:322:ILE:HG22	1.80	0.63
1:A:363:ASN:HB3	1:A:366:ILE:HD12	1.80	0.63
1:B:768:GLN:O	1:B:772:LYS:HD2	1.99	0.62
1:A:515:ARG:HB2	3:A:1251:HOH:O	1.99	0.62
1:C:217:THR:HG23	1:C:364:PRO:CD	2.28	0.62
1:C:666:ARG:NH1	1:C:672:ALA:O	2.32	0.62
1:C:318:GLU:HG2	3:C:1794:HOH:O	1.98	0.62
1:D:71:GLN:HB3	3:D:1519:HOH:O	2.00	0.62
1:A:786:LYS:NZ	3:A:1091:HOH:O	2.29	0.62
1:A:664:GLN:O	1:A:667:LYS:HB2	1.99	0.62
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.82	0.62
1:C:768:GLN:O	1:C:772:LYS:HD2	1.99	0.62
1:A:139:MET:HE3	1:D:395:PHE:CE1	2.34	0.61
1:B:703:ARG:NH2	3:B:1065:HOH:O	2.29	0.61
1:C:285:GLU:HB3	3:C:1536:HOH:O	1.99	0.61
1:B:645:SER:HA	1:B:746:GLN:CG	2.29	0.61
1:D:285:GLU:O	1:D:285:GLU:HG3	2.00	0.61
1:D:547:ASP:OD1	1:D:676:ARG:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:HB2	1:D:334:PRO:HD2	1.82	0.61
1:D:804:HIS:HB2	3:D:1053:HOH:O	2.00	0.61
1:A:68:HIS:HE1	1:A:70:LYS:HG3	1.65	0.61
1:B:645:SER:HA	1:B:746:GLN:HG2	1.81	0.61
1:C:556:LEU:HD23	1:C:582:LEU:HD23	1.82	0.61
1:D:67:VAL:HG11	1:D:75:MET:HE1	1.83	0.61
1:B:333:GLU:HB2	1:B:334:PRO:HD2	1.83	0.61
1:B:3:GLU:OE2	1:B:236:LYS:HD2	2.01	0.61
1:A:790:ARG:H	1:A:790:ARG:NE	1.98	0.61
1:B:68:HIS:HE1	1:B:70:LYS:HG3	1.64	0.61
1:C:691:ALA:HB3	1:C:692:PRO:HD3	1.83	0.60
1:D:3:GLU:OE2	1:D:236:LYS:HD2	2.01	0.60
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.82	0.60
1:D:193:LYS:HE3	1:D:195:ASN:HB2	1.82	0.60
1:A:333:GLU:HB2	1:A:334:PRO:HD2	1.82	0.60
1:C:661:PHE:O	1:C:665:LEU:HG	2.02	0.60
1:D:790:ARG:NE	1:D:790:ARG:H	1.99	0.60
1:B:746:GLN:HE21	1:B:746:GLN:CA	2.15	0.60
1:B:641:ALA:HB2	1:B:652:SER:HB2	1.84	0.60
1:A:193:LYS:HE3	1:A:195:ASN:HB2	1.84	0.60
1:B:285:GLU:HG3	1:B:285:GLU:O	1.99	0.60
1:A:417:HIS:ND1	1:A:422:ARG:NH2	2.49	0.60
1:D:754:GLU:HG2	1:D:776:LYS:HD3	1.84	0.60
1:C:790:ARG:H	1:C:790:ARG:NE	2.00	0.59
1:B:531:GLY:HA2	3:B:1230:HOH:O	2.02	0.59
1:B:476:GLU:HB2	3:B:1353:HOH:O	2.01	0.59
1:B:75:MET:HE1	1:B:79:LEU:HG	1.85	0.59
1:B:664:GLN:O	1:B:667:LYS:HB2	2.03	0.59
1:C:285:GLU:O	1:C:285:GLU:HG3	2.00	0.59
1:B:193:LYS:HE3	1:B:195:ASN:HB2	1.84	0.58
1:B:627:TRP:CD1	1:B:631:LYS:HE2	2.37	0.58
1:B:632:GLN:HG3	1:B:633:ARG:HG2	1.84	0.58
1:C:754:GLU:HG2	1:C:776:LYS:HD3	1.84	0.58
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.36	0.58
1:D:290:ILE:CG2	1:D:322:ILE:HG22	2.34	0.58
1:B:79:LEU:HD21	1:B:143[A]:ARG:HG3	1.86	0.58
1:C:42:ALA:HA	3:C:1704:HOH:O	2.04	0.58
1:A:499:MET:HE2	1:A:553:PHE:HE1	1.68	0.58
1:D:470:TYR:CZ	1:D:481:GLU:HG3	2.39	0.58
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.85	0.58
1:C:405:ARG:NH1	3:C:1194:HOH:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.87	0.57
1:A:627:TRP:CD1	1:A:631:LYS:HE2	2.38	0.57
1:B:685:TYR:O	1:B:688:GLU:HB2	2.03	0.57
1:C:0:THR:HG23	1:C:176:HIS:HE1	1.69	0.57
1:C:477:ARG:CG	1:C:478:GLY:H	2.15	0.57
1:D:703:ARG:NH1	3:D:1142:HOH:O	2.38	0.57
1:B:504[B]:ARG:NH2	1:B:543:GLU:OE1	2.38	0.57
1:A:625:LEU:HD12	1:A:629:GLU:HB3	1.87	0.56
1:C:291:GLU:HG2	1:C:340:ALA:HB1	1.86	0.56
1:B:139:MET:HE3	1:C:395:PHE:CE1	2.39	0.56
1:B:293:HIS:O	1:B:326:LYS:HE2	2.04	0.56
1:A:285:GLU:HG3	1:A:285:GLU:O	2.06	0.56
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.86	0.56
1:B:363:ASN:HB3	1:B:366:ILE:HD12	1.88	0.56
1:B:658:VAL:O	1:B:662:VAL:HG23	2.06	0.55
1:C:502:GLN:HG3	1:C:546:PHE:HB3	1.88	0.55
1:D:639:VAL:HG22	1:D:640:PRO:N	2.21	0.55
1:D:440:GLN:HG3	1:D:833:LEU:CD2	2.36	0.55
1:D:509:SER:O	1:D:512:ARG:HD3	2.06	0.54
1:A:754:GLU:HG2	1:A:776:LYS:HD3	1.89	0.54
1:B:440:GLN:HG2	1:B:833:LEU:HD11	1.89	0.54
1:C:217:THR:HG23	1:C:364:PRO:HD2	1.88	0.54
1:C:440:GLN:HG3	1:C:833:LEU:CD2	2.37	0.54
1:B:235:LYS:HE2	1:B:238:LEU:HD13	1.89	0.54
1:D:627:TRP:HA	1:D:649:VAL:HG21	1.89	0.54
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.89	0.54
1:D:319:PRO:HB3	1:D:372:GLY:O	2.08	0.54
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.89	0.54
1:D:333:GLU:CB	1:D:334:PRO:CD	2.85	0.54
1:B:502:GLN:HG3	1:B:546:PHE:HB3	1.90	0.54
1:B:556:LEU:HD22	1:B:582:LEU:HD23	1.90	0.54
1:C:332:PRO:HG2	1:C:336:SER:HA	1.89	0.53
1:A:685:TYR:O	1:A:688:GLU:HB2	2.08	0.53
1:A:499:MET:CE	1:A:553:PHE:CE1	2.91	0.53
1:A:285:GLU:HB3	3:A:1073:HOH:O	2.07	0.53
1:B:509:SER:O	1:B:512:ARG:HD3	2.09	0.53
1:C:333:GLU:CB	1:C:334:PRO:CD	2.87	0.53
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.90	0.53
1:A:440:GLN:HG2	1:A:833:LEU:HD11	1.91	0.53
1:B:746:GLN:C	1:B:746:GLN:HE21	2.11	0.53
1:A:502:GLN:HG3	1:A:546:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:HD22	1:A:582:LEU:HD23	1.89	0.52
1:A:509:SER:O	1:A:512:ARG:HD3	2.09	0.52
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.38	0.52
1:D:550:VAL:HG23	1:D:611:LYS:HD2	1.92	0.52
1:A:240:ARG:NH1	1:A:821:PHE:CE2	2.78	0.52
1:A:319:PRO:HB3	1:A:372:GLY:O	2.09	0.52
1:C:656:ALA:HB3	1:C:657:PRO:CD	2.40	0.52
1:A:79:LEU:HD21	1:A:143[A]:ARG:HG3	1.92	0.52
1:D:649:VAL:CG1	1:D:650:THR:N	2.73	0.52
1:B:365:GLU:O	1:B:367:PRO:HD3	2.09	0.52
1:B:663:GLU:OE1	1:B:663:GLU:HA	2.09	0.52
1:B:68:HIS:HE1	1:B:70:LYS:CG	2.22	0.52
1:D:622:ALA:HB3	1:D:673:LYS:HG2	1.92	0.52
1:C:579:GLY:HA3	1:C:587:CYS:SG	2.50	0.52
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.92	0.51
1:C:92:ASP:HB2	1:C:831:SER:HB3	1.91	0.51
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.90	0.51
1:B:522:ARG:HD2	3:B:1105:HOH:O	2.10	0.51
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.92	0.51
1:C:509:SER:O	1:C:512:ARG:HD3	2.10	0.51
1:C:524:ASP:OD1	1:C:534:VAL:N	2.43	0.51
1:B:639:VAL:CG2	1:B:640:PRO:HD2	2.41	0.51
1:A:549:ILE:HD11	1:A:553:PHE:CZ	2.45	0.51
1:C:486:PRO:HD2	3:C:1576:HOH:O	2.11	0.51
1:B:656:ALA:CB	1:B:657:PRO:HD3	2.28	0.51
1:C:235:LYS:HE2	1:C:238:LEU:HD13	1.92	0.51
1:A:235:LYS:HE2	1:A:238:LEU:HD13	1.92	0.51
1:D:333:GLU:CB	1:D:334:PRO:HD2	2.41	0.51
1:A:68:HIS:HE1	1:A:70:LYS:CG	2.24	0.50
1:D:671:PHE:CZ	1:D:673:LYS:HB3	2.45	0.50
1:B:331:HIS:CD2	1:B:333:GLU:H	2.29	0.50
1:B:92:ASP:HB2	1:B:831:SER:HB3	1.93	0.50
1:A:524:ASP:OD1	1:A:534:VAL:N	2.44	0.50
1:D:405:ARG:NH1	3:D:1100:HOH:O	2.35	0.50
1:B:319:PRO:HB3	1:B:372:GLY:O	2.11	0.50
1:D:92:ASP:HB2	1:D:831:SER:HB3	1.92	0.50
1:C:173:GLN:HG3	3:C:992:HOH:O	2.11	0.50
1:D:852:ASN:C	1:D:852:ASN:HD22	2.15	0.50
1:D:493:TRP:CD2	1:D:576:GLY:HA3	2.46	0.50
1:C:0:THR:HG23	1:C:176:HIS:CE1	2.46	0.49
1:D:639:VAL:CG2	1:D:640:PRO:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ARG:NH1	1:A:668:GLU:OE1	2.45	0.49
1:D:675:VAL:HG12	1:D:676:ARG:N	2.28	0.49
1:C:484:GLN:OE1	3:C:1480:HOH:O	2.19	0.49
1:D:524:ASP:OD1	1:D:534:VAL:N	2.46	0.49
1:B:597:GLU:CD	1:B:597:GLU:H	2.16	0.49
1:B:499:MET:HE3	1:B:682:PHE:CD2	2.47	0.49
1:A:499:MET:HE1	1:A:553:PHE:CE1	2.47	0.49
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.95	0.49
1:A:92:ASP:HB2	1:A:831:SER:HB3	1.93	0.49
1:A:333:GLU:CB	1:A:334:PRO:CD	2.90	0.49
1:D:627:TRP:CA	1:D:649:VAL:HG21	2.43	0.48
1:A:200:PHE:CZ	1:D:132:MET:HE1	2.48	0.48
1:D:719:GLU:HG3	1:D:722:TRP:CE3	2.48	0.48
1:A:71:GLN:HB2	3:A:1037:HOH:O	2.12	0.48
1:B:139:MET:CE	1:C:395:PHE:CE1	2.96	0.48
1:A:139:MET:CE	1:D:395:PHE:CE1	2.95	0.48
1:D:235:LYS:HE2	1:D:238:LEU:HD13	1.94	0.48
1:A:416:PRO:O	1:A:419:THR:OG1	2.31	0.48
1:B:656:ALA:HB3	1:B:657:PRO:CD	2.29	0.48
1:D:627:TRP:HE1	1:D:631:LYS:NZ	2.12	0.48
1:D:627:TRP:CE3	1:D:643:HIS:HB2	2.48	0.48
1:B:754:GLU:HG2	1:B:776:LYS:HD2	1.94	0.48
1:B:524:ASP:OD1	1:B:534:VAL:N	2.46	0.48
1:D:597:GLU:CD	1:D:597:GLU:H	2.17	0.48
1:A:417:HIS:HE1	3:A:1365:HOH:O	1.97	0.48
1:D:549:ILE:HG23	1:D:678:GLY:HA3	1.95	0.48
1:C:29:GLY:HA2	3:C:1031:HOH:O	2.14	0.48
1:B:75:MET:HE3	1:B:79:LEU:HD23	1.95	0.48
1:A:675:VAL:HG12	1:A:676:ARG:N	2.29	0.48
1:A:597:GLU:H	1:A:597:GLU:CD	2.17	0.48
1:D:515:ARG:CB	3:D:1250:HOH:O	2.56	0.47
1:D:79:LEU:HD21	1:D:143:ARG:HG3	1.97	0.47
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.43	0.47
1:A:170:ASN:HA	1:A:173:GLN:HG3	1.96	0.47
1:B:804:HIS:HB2	3:B:1104:HOH:O	2.14	0.47
1:C:319:PRO:HB3	1:C:372:GLY:O	2.13	0.47
1:A:499:MET:CE	1:A:553:PHE:HE1	2.28	0.47
1:D:664:GLN:HG2	1:D:664:GLN:O	2.10	0.47
1:C:513:LEU:HD22	1:C:793:LEU:HD13	1.97	0.47
1:A:493:TRP:CD2	1:A:576:GLY:HA3	2.50	0.47
1:B:675:VAL:HG12	1:B:677:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:LEU:HD23	1:C:782:ILE:HB	1.97	0.47
1:D:318:GLU:HG2	3:D:984:HOH:O	2.15	0.47
1:C:597:GLU:H	1:C:597:GLU:CD	2.18	0.47
1:C:68:HIS:HB2	1:C:71:GLN:OE1	2.15	0.47
1:D:634:CYS:SG	1:D:638:VAL:HG12	2.55	0.47
1:D:0:THR:HG23	1:D:176:HIS:HE1	1.80	0.47
1:A:75:MET:HB2	1:A:75:MET:HE2	1.76	0.46
1:B:711:ARG:NE	3:B:1120:HOH:O	2.47	0.46
1:B:36:ASP:OD1	1:B:38:ARG:HB2	2.15	0.46
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.50	0.46
1:D:0:THR:HG23	1:D:176:HIS:CE1	2.50	0.46
1:B:515:ARG:HB2	3:B:988:HOH:O	2.15	0.46
1:B:536:GLN:NE2	3:B:1011:HOH:O	2.47	0.46
1:B:645:SER:HA	1:B:746:GLN:HG3	1.97	0.46
1:B:675:VAL:HG12	1:B:677:THR:CG2	2.45	0.46
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.98	0.46
1:D:240:ARG:NE	3:D:1005:HOH:O	2.47	0.46
1:D:241:ARG:HB2	1:D:453:MET:HE1	1.97	0.46
1:A:67:VAL:HG11	1:A:75:MET:CE	2.38	0.46
1:D:68[A]:HIS:CE1	1:D:70:LYS:HG3	2.51	0.46
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.97	0.46
1:A:241:ARG:HB2	1:A:453:MET:HE1	1.96	0.46
1:A:68:HIS:CE1	1:A:70:LYS:CG	2.98	0.46
1:D:36:ASP:OD1	1:D:38:ARG:HB2	2.16	0.46
1:C:477:ARG:HD3	1:C:477:ARG:HA	1.48	0.46
1:A:528:LYS:N	1:A:529:PRO:CD	2.79	0.46
1:C:470:TYR:CZ	1:C:481:GLU:HG3	2.50	0.46
1:B:68:HIS:CE1	1:B:70:LYS:CG	2.96	0.46
1:B:75:MET:HE2	1:B:80:ARG:HG2	1.98	0.46
1:B:315:THR:HG23	1:B:315:THR:O	2.15	0.46
1:B:210:GLY:C	1:B:223:CYS:HB2	2.36	0.46
1:A:513:LEU:HD22	1:A:793:LEU:HD13	1.97	0.46
1:C:692:PRO:HB2	1:C:693:PRO:HD3	1.98	0.46
1:A:72:ALA:HA	1:A:75:MET:HE3	1.97	0.46
1:D:627:TRP:CD1	1:D:627:TRP:C	2.90	0.46
1:C:371:ASP:OD2	1:C:373:ARG:NH2	2.47	0.46
1:B:333:GLU:CB	1:B:334:PRO:CD	2.94	0.45
1:A:208:PRO:HD2	1:A:220:ASN:ND2	2.31	0.45
1:C:664:GLN:O	1:C:668:GLU:HG3	2.16	0.45
1:C:439:GLU:HB2	3:C:1046:HOH:O	2.16	0.45
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:LEU:CD1	1:C:630:CYS:SG	3.04	0.45
1:C:649:VAL:CG1	1:C:650:THR:N	2.79	0.45
1:D:654:PRO:O	1:D:658:VAL:HG23	2.16	0.45
1:D:502[A]:GLN:CG	1:D:676:ARG:NH2	2.80	0.45
1:C:660:GLU:O	1:C:664:GLN:HG3	2.17	0.45
1:D:708:ARG:HG2	1:D:712:TRP:CZ3	2.52	0.45
1:D:513:LEU:HD22	1:D:793:LEU:HD13	1.99	0.45
1:C:36:ASP:OD1	1:C:38:ARG:HB2	2.17	0.45
1:A:200:PHE:CE2	1:D:132:MET:HE1	2.52	0.45
1:D:717:ILE:HA	1:D:718:PRO:HD3	1.87	0.45
1:B:332:PRO:HG2	1:B:336:SER:HA	1.99	0.45
1:B:528:LYS:N	1:B:529:PRO:CD	2.79	0.45
1:C:528:LYS:HB3	1:C:529:PRO:HD3	1.99	0.45
1:C:655:GLN:HG3	1:C:659:PHE:CE2	2.52	0.45
1:C:329:MET:HE2	1:C:332:PRO:HD3	1.98	0.45
1:A:200:PHE:CZ	1:D:132:MET:CE	3.00	0.45
1:D:528:LYS:N	1:D:529:PRO:CD	2.80	0.45
1:D:127:LEU:C	1:D:127:LEU:HD12	2.37	0.45
1:C:79:LEU:HD21	1:C:143:ARG:HG3	1.99	0.45
1:D:556:LEU:HD23	1:D:582:LEU:CD2	2.40	0.45
1:D:708:ARG:HD2	1:D:712:TRP:CZ3	2.52	0.45
1:D:169:GLN:O	1:D:173:GLN:HG2	2.16	0.45
1:C:633:ARG:HB3	1:C:633:ARG:HE	1.70	0.45
1:C:553:PHE:CD1	1:C:582:LEU:HD22	2.52	0.44
1:C:528:LYS:N	1:C:529:PRO:CD	2.80	0.44
1:B:817:PRO:HA	1:B:818:PRO:HD3	1.88	0.44
1:D:759:LEU:HD23	1:D:782:ILE:HB	1.99	0.44
1:C:476:GLU:O	1:C:477:ARG:HB2	2.17	0.44
1:C:579:GLY:CA	1:C:587:CYS:SG	3.05	0.44
1:B:92:ASP:HA	1:B:830:ILE:HB	1.99	0.44
1:D:564:ILE:HD13	1:D:590:ALA:HB2	1.99	0.44
1:A:620:MET:HA	1:A:651:ILE:O	2.18	0.44
1:A:641:ALA:HB2	1:A:652:SER:HB2	1.99	0.44
1:A:115:GLU:HA	1:A:118:GLU:HG3	1.98	0.44
1:A:582:LEU:HD13	1:A:606:ARG:HD3	1.99	0.44
1:B:343:LYS:C	1:B:343:LYS:HD3	2.38	0.44
1:A:168:LEU:HD12	1:A:185:VAL:HG21	1.99	0.44
1:B:641:ALA:O	1:B:742:PRO:HA	2.18	0.44
1:D:301:ASP:HB2	1:D:302:PRO:HD3	1.99	0.44
1:D:626:SER:HG	1:D:629:GLU:HB2	1.81	0.44
1:B:499:MET:CE	1:B:682:PHE:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD21	1:B:143[B]:ARG:HG2	1.99	0.44
1:A:36:ASP:OD1	1:A:38:ARG:HB2	2.17	0.44
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.99	0.44
1:A:490:ARG:HA	1:A:491:PRO:HD2	1.90	0.44
1:D:654:PRO:HB2	1:D:657:PRO:HD2	2.00	0.43
1:C:620:MET:HA	1:C:651:ILE:O	2.17	0.43
1:D:468:ARG:HD2	1:D:485:VAL:HG21	2.00	0.43
1:A:301:ASP:CB	1:A:302:PRO:HD3	2.49	0.43
1:A:638:VAL:HG11	1:A:651:ILE:HD12	2.00	0.43
1:C:804:HIS:HB2	3:C:1176:HOH:O	2.18	0.43
1:C:210:GLY:C	1:C:223:CYS:HB2	2.37	0.43
1:C:582:LEU:HD13	1:C:606:ARG:HD3	2.00	0.43
1:D:649:VAL:HG12	1:D:650:THR:N	2.33	0.43
1:B:343:LYS:O	1:B:343:LYS:HD3	2.18	0.43
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.53	0.43
1:C:515:ARG:HD3	1:C:569:CYS:SG	2.59	0.43
1:B:29:GLY:HA2	3:B:1085:HOH:O	2.18	0.43
1:C:250:GLY:HA3	1:C:276:LEU:HD21	2.01	0.43
1:C:416:PRO:O	1:C:419:THR:OG1	2.36	0.43
1:B:416:PRO:O	1:B:419:THR:OG1	2.35	0.43
1:B:513:LEU:HD22	1:B:793:LEU:HD13	2.00	0.43
1:B:633:ARG:HE	1:B:633:ARG:HB3	1.49	0.43
1:B:582:LEU:HD13	1:B:606:ARG:HD3	1.99	0.43
1:D:502[A]:GLN:HG2	1:D:676:ARG:NH2	2.34	0.43
1:B:49:ARG:H	1:B:49:ARG:HG2	1.68	0.43
1:A:210:GLY:C	1:A:223:CYS:HB2	2.38	0.43
1:B:75:MET:CE	1:B:79:LEU:HG	2.48	0.43
1:C:517:ARG:HD2	3:C:1631:HOH:O	2.17	0.43
1:C:477:ARG:CG	1:C:478:GLY:N	2.80	0.43
1:C:326:LYS:HE3	1:C:331:HIS:CD2	2.54	0.43
1:B:191:LEU:HG	1:B:226:GLU:HG2	2.01	0.43
1:D:29:GLY:HA2	3:D:1089:HOH:O	2.18	0.43
1:C:692:PRO:HB2	1:C:693:PRO:CD	2.48	0.42
1:C:108:TRP:HB3	1:C:167:ALA:HB1	2.01	0.42
1:D:439:GLU:HB2	3:D:1126:HOH:O	2.19	0.42
1:A:804:HIS:HB2	3:A:1291:HOH:O	2.19	0.42
1:B:196:THR:HA	1:B:199:GLN:HE21	1.84	0.42
1:C:123:ASP:HA	1:C:124:PRO:HD2	1.94	0.42
1:D:92:ASP:HA	1:D:830:ILE:HB	2.01	0.42
1:C:164:SER:HB2	1:C:338:LEU:HG	2.01	0.42
1:C:127:LEU:HD12	1:C:127:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:THR:O	1:D:315:THR:HG23	2.18	0.42
1:D:633:ARG:O	1:D:635:PRO:HD3	2.20	0.42
1:C:469:GLY:HA2	1:C:481:GLU:O	2.19	0.42
1:B:211:THR:CG2	1:B:358:HIS:CD2	3.02	0.42
1:C:420:LEU:HD21	1:C:512:ARG:HB3	2.00	0.42
1:C:277:TYR:CZ	1:C:284:PRO:HG3	2.55	0.42
1:C:746:GLN:HE21	1:C:746:GLN:HB3	1.61	0.42
1:B:803:LEU:HA	1:B:803:LEU:HD12	1.82	0.42
1:D:0:THR:HG23	1:D:1:GLY:N	2.35	0.42
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.01	0.42
1:A:633:ARG:HH12	1:A:668:GLU:CD	2.23	0.42
1:D:528:LYS:HB3	1:D:529:PRO:HD3	2.02	0.42
1:A:431:PRO:HG2	1:B:839:SER:HB2	2.01	0.42
1:B:240:ARG:HA	1:B:240:ARG:HD2	1.86	0.42
1:D:550:VAL:HG23	1:D:611:LYS:CD	2.49	0.42
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.02	0.42
1:B:241:ARG:HB2	1:B:453:MET:HE1	2.01	0.42
1:D:665:LEU:HD23	1:D:665:LEU:HA	1.82	0.42
1:D:75:MET:HE2	1:D:75:MET:HB2	1.82	0.41
1:B:782:ILE:HA	1:B:783:PRO:HD2	1.93	0.41
1:B:185:VAL:HG12	1:B:338:LEU:HD11	2.01	0.41
1:C:191:LEU:HG	1:C:226:GLU:HG2	2.02	0.41
1:C:817:PRO:HA	1:C:818:PRO:HD3	1.91	0.41
1:B:579:GLY:HA3	1:B:587:CYS:SG	2.60	0.41
1:D:277:TYR:CZ	1:D:284:PRO:HG3	2.55	0.41
1:A:692:PRO:HB2	1:A:693:PRO:HD3	2.02	0.41
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.55	0.41
1:A:92:ASP:HA	1:A:830:ILE:HB	2.02	0.41
1:D:165:LEU:HD12	1:D:165:LEU:HA	1.90	0.41
1:C:12:LYS:HE3	3:C:1180:HOH:O	2.19	0.41
1:B:71:GLN:O	1:B:75:MET:HG3	2.21	0.41
1:B:75:MET:HE2	1:B:80:ARG:CG	2.50	0.41
1:A:196:THR:HA	1:A:199:GLN:HE21	1.85	0.41
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.86	0.41
1:D:493:TRP:CE2	1:D:576:GLY:HA3	2.56	0.41
1:B:499:MET:HE1	1:B:682:PHE:CG	2.56	0.41
3:A:1238:HOH:O	1:B:839:SER:HA	2.18	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.55	0.41
1:D:817:PRO:HA	1:D:818:PRO:HD3	1.91	0.41
1:D:746:GLN:HE21	1:D:746:GLN:HB3	1.64	0.41
1:D:379:GLN:HG3	3:D:1343:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ALA:CB	1:B:657:PRO:CD	2.96	0.41
1:B:848:GLU:OE2	3:B:1055:HOH:O	2.22	0.41
1:D:415:ALA:HB1	1:D:416:PRO:HD2	2.03	0.41
1:B:277:TYR:CZ	1:B:284:PRO:HG3	2.56	0.41
1:B:682:PHE:HB3	3:B:1187:HOH:O	2.20	0.41
1:D:64:PHE:CD1	1:D:429:ARG:HD3	2.56	0.41
1:D:671:PHE:HZ	1:D:673:LYS:HD2	1.86	0.41
1:D:210:GLY:HA2	3:D:1012:HOH:O	2.20	0.41
1:A:277:TYR:CZ	1:A:284:PRO:HG3	2.55	0.41
1:A:717:ILE:HD13	1:A:727:ALA:HB2	2.02	0.41
1:B:118:GLU:HG2	1:B:850:PHE:CE1	2.56	0.41
1:D:67:VAL:HG11	1:D:75:MET:CE	2.49	0.41
1:A:169:GLN:O	1:A:173:GLN:HG2	2.20	0.41
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.84	0.41
1:D:250:GLY:HA3	1:D:276:LEU:HD21	2.02	0.41
1:D:579:GLY:HA3	1:D:587:CYS:SG	2.61	0.41
1:B:746:GLN:HA	1:B:746:GLN:HE21	1.84	0.40
1:B:552:SER:O	1:B:556:LEU:HB2	2.20	0.40
1:A:552:SER:O	1:A:556:LEU:HB2	2.21	0.40
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.98	0.40
1:B:123:ASP:HA	1:B:124:PRO:HD2	1.93	0.40
1:D:654:PRO:HG3	1:D:686:PHE:CZ	2.56	0.40
1:A:417:HIS:H	1:A:417:HIS:CD2	2.39	0.40
1:B:363:ASN:OD1	1:B:364:PRO:HD2	2.22	0.40
1:C:92:ASP:HA	1:C:830:ILE:HB	2.02	0.40
1:D:240:ARG:CD	3:D:1005:HOH:O	2.69	0.40
1:C:415:ALA:HB1	1:C:416:PRO:HD2	2.03	0.40
1:C:717:ILE:HA	1:C:718:PRO:HD3	1.92	0.40
1:A:712:TRP:C	1:A:712:TRP:CD1	2.94	0.40
1:C:754:GLU:HG2	1:C:776:LYS:CD	2.50	0.40
1:A:185:VAL:HG12	1:A:338:LEU:HD11	2.03	0.40
1:A:164:SER:HB2	1:A:338:LEU:HG	2.03	0.40
1:B:579:GLY:CA	1:B:587:CYS:SG	3.09	0.40
1:A:142:ASN:HD22	1:D:396:GLY:HA3	1.85	0.40
1:D:820:GLU:HB2	3:D:1042:HOH:O	2.20	0.40
1:A:817:PRO:HA	1:A:818:PRO:HD3	1.91	0.40
1:D:670:VAL:HG12	1:D:671:PHE:N	2.36	0.40
1:B:499:MET:HG2	1:B:499:MET:H	1.70	0.40
1:D:610:ILE:HD13	1:D:682:PHE:HE1	1.87	0.40
1:A:687:MET:HB2	1:A:740:VAL:HG12	2.04	0.40
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.57	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	852/965 (88%)	837 (98%)	14 (2%)	1 (0%)	56	57
1	B	853/965 (88%)	836 (98%)	16 (2%)	1 (0%)	56	57
1	C	854/965 (88%)	840 (98%)	13 (2%)	1 (0%)	56	57
1	D	854/965 (88%)	837 (98%)	16 (2%)	1 (0%)	56	57
All	All	3413/3860 (88%)	3350 (98%)	59 (2%)	4 (0%)	56	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	B	333	GLU
1	C	333	GLU
1	D	333	GLU

### 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	698/792 (88%)	666 (95%)	32 (5%)	33	29
1	B	698/792 (88%)	658 (94%)	40 (6%)	25	19
1	C	699/792 (88%)	663 (95%)	36 (5%)	29	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	699/792 (88%)	658 (94%)	41 (6%)	24	18
All	All	2794/3168 (88%)	2645 (95%)	149 (5%)	28	23

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	70	LYS
1	A	75	MET
1	A	114	SER
1	A	136	GLN
1	A	173	GLN
1	A	195	ASN
1	A	285	GLU
1	A	298	LYS
1	A	318	GLU
1	A	343	LYS
1	A	384	ARG
1	A	476	GLU
1	A	477	ARG
1	A	489	GLU
1	A	499	MET
1	A	513	LEU
1	A	515	ARG
1	A	536	GLN
1	A	556	LEU
1	A	597	GLU
1	A	625	LEU
1	A	630	CYS
1	A	646	LYS
1	A	663	GLU
1	A	713	LEU
1	A	721	GLN
1	A	746	GLN
1	A	772	LYS
1	A	790	ARG
1	A	820	GLU
1	A	852	ASN
1	B	49	ARG
1	B	70	LYS
1	B	114	SER
1	B	118	GLU

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	169	GLN
1	B	195	ASN
1	B	215	PHE
1	B	223	CYS
1	B	285	GLU
1	B	298	LYS
1	B	318	GLU
1	B	343	LYS
1	B	476	GLU
1	B	489	GLU
1	B	499	MET
1	B	513	LEU
1	B	515	ARG
1	B	536	GLN
1	B	556	LEU
1	B	569	CYS
1	B	597	GLU
1	B	626	SER
1	B	630	CYS
1	B	632	GLN
1	B	633	ARG
1	B	639	VAL
1	B	646	LYS
1	B	664	GLN
1	B	666	ARG
1	B	674	GLU
1	B	709	SER
1	B	713	LEU
1	B	721	GLN
1	B	725	SER
1	B	746	GLN
1	B	772	LYS
1	B	773	ARG
1	B	790	ARG
1	B	820	GLU
1	C	70	LYS
1	C	114	SER
1	C	136	GLN
1	C	169	GLN
1	C	195	ASN
1	C	215	PHE

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Mol	Chain	Res	Type
1	C	217	THR
1	C	223	CYS
1	C	285	GLU
1	C	298	LYS
1	C	318	GLU
1	C	343	LYS
1	C	443	ARG
1	C	476	GLU
1	C	477	ARG
1	C	483	GLN
1	C	489	GLU
1	C	513	LEU
1	C	515	ARG
1	C	597	GLU
1	C	625	LEU
1	C	628	GLU
1	C	630	CYS
1	C	632	GLN
1	C	633	ARG
1	C	639	VAL
1	C	646	LYS
1	C	666	ARG
1	C	674	GLU
1	C	713	LEU
1	C	721	GLN
1	C	725	SER
1	C	746	GLN
1	C	772	LYS
1	C	790	ARG
1	C	820	GLU
1	D	70	LYS
1	D	114	SER
1	D	118	GLU
1	D	136	GLN
1	D	169	GLN
1	D	173	GLN
1	D	195	ASN
1	D	215	PHE
1	D	240	ARG
1	D	285	GLU
1	D	298	LYS
1	D	318	GLU

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Mol	Chain	Res	Type
1	D	343	LYS
1	D	370	LEU
1	D	446	GLN
1	D	489	GLU
1	D	502[A]	GLN
1	D	502[B]	GLN
1	D	513	LEU
1	D	515	ARG
1	D	522	ARG
1	D	569	CYS
1	D	593	CYS
1	D	597	GLU
1	D	629	GLU
1	D	631	LYS
1	D	664	GLN
1	D	667	LYS
1	D	673	LYS
1	D	676	ARG
1	D	709	SER
1	D	713	LEU
1	D	721	GLN
1	D	725	SER
1	D	728	ARG
1	D	746	GLN
1	D	772	LYS
1	D	790	ARG
1	D	802	ARG
1	D	820	GLU
1	D	852	ASN

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	142	ASN
1	A	179	GLN
1	A	199	GLN
1	A	271	GLN
1	A	375	GLN
1	A	746	GLN
1	A	852	ASN
1	B	169	GLN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	179	GLN
1	B	199	GLN
1	B	271	GLN
1	B	331	HIS
1	B	375	GLN
1	B	483	GLN
1	B	536	GLN
1	B	723	HIS
1	B	746	GLN
1	C	136	GLN
1	C	169	GLN
1	C	170	ASN
1	C	173	GLN
1	C	199	GLN
1	C	271	GLN
1	C	331	HIS
1	C	375	GLN
1	C	483	GLN
1	C	746	GLN
1	D	199	GLN
1	D	271	GLN
1	D	331	HIS
1	D	746	GLN
1	D	852	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	852/965 (88%)	-0.27	23 (2%) 58 67	8, 22, 56, 78	0
1	B	852/965 (88%)	-0.07	37 (4%) 39 49	15, 31, 63, 91	0
1	C	855/965 (88%)	-0.22	17 (1%) 68 75	13, 28, 60, 78	0
1	D	854/965 (88%)	-0.19	30 (3%) 48 58	10, 27, 60, 85	0
All	All	3413/3860 (88%)	-0.19	107 (3%) 52 62	8, 27, 60, 91	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ALA	8.3
1	B	416	PRO	7.7
1	A	415	ALA	7.1
1	D	415	ALA	6.8
1	A	414	PRO	6.4
1	D	630	CYS	5.9
1	B	478	GLY	5.7
1	B	632	GLN	5.4
1	D	627	TRP	5.0
1	B	750	TRP	5.0
1	C	415	ALA	4.9
1	A	413	ALA	4.8
1	C	489	GLU	4.8
1	D	671	PHE	4.7
1	D	416	PRO	4.6
1	C	488	GLY	4.4
1	C	416	PRO	4.3
1	B	413	ALA	4.3
1	A	665	LEU	4.1
1	C	476	GLU	4.1
1	D	476	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	487	ALA	4.1
1	C	821	PHE	4.1
1	D	750	TRP	4.0
1	C	685	TYR	4.0
1	C	750	TRP	3.9
1	A	416	PRO	3.8
1	D	659	PHE	3.8
1	B	414	PRO	3.8
1	B	417	HIS	3.8
1	D	315	THR	3.8
1	D	662	VAL	3.8
1	A	42	ALA	3.8
1	B	418	ALA	3.7
1	D	418	ALA	3.7
1	A	417	HIS	3.7
1	D	685	TYR	3.6
1	D	821	PHE	3.6
1	B	671	PHE	3.6
1	D	634	CYS	3.5
1	D	669	GLY	3.5
1	D	663	GLU	3.4
1	D	666	ARG	3.4
1	A	418	ALA	3.3
1	D	489	GLU	3.3
1	C	0	THR	3.2
1	B	648	THR	3.2
1	B	636	PRO	3.2
1	C	671	PHE	3.2
1	D	647	ASP	3.1
1	A	647	ASP	3.1
1	B	412	PRO	3.1
1	C	615	LEU	3.0
1	A	412	PRO	3.0
1	D	487	ALA	3.0
1	B	317	GLN	3.0
1	A	659	PHE	2.9
1	B	641	ALA	2.9
1	D	667	LYS	2.9
1	D	648	THR	2.9
1	B	638	VAL	2.8
1	C	659	PHE	2.8
1	B	659	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	661	PHE	2.7
1	B	628	GLU	2.7
1	D	670	VAL	2.6
1	A	686	PHE	2.6
1	B	665	LEU	2.6
1	B	639	VAL	2.6
1	D	629	GLU	2.5
1	B	315	THR	2.5
1	A	648	THR	2.5
1	C	413	ALA	2.5
1	B	673	LYS	2.4
1	A	634	CYS	2.4
1	D	615	LEU	2.4
1	B	489	GLU	2.4
1	C	41	LYS	2.4
1	B	685	TYR	2.4
1	D	413	ALA	2.3
1	D	0	THR	2.3
1	A	632	GLN	2.3
1	B	488	GLY	2.3
1	B	667	LYS	2.3
1	B	686	PHE	2.3
1	B	666	ARG	2.2
1	B	419	THR	2.2
1	A	669	GLY	2.2
1	B	647	ASP	2.2
1	A	676	ARG	2.2
1	D	488	GLY	2.2
1	B	379	GLN	2.2
1	A	315	THR	2.1
1	A	419	THR	2.1
1	B	664	GLN	2.1
1	A	667	LYS	2.1
1	D	417	HIS	2.1
1	B	361	SER	2.1
1	A	750	TRP	2.1
1	B	646	LYS	2.1
1	C	315	THR	2.1
1	D	636	PRO	2.1
1	A	477	ARG	2.1
1	B	630	CYS	2.1
1	C	772	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	613	ALA	2.0
1	B	634	CYS	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( $\text{\AA}^2$ )	Q<0.9
2	CL	D	964	1/1	0.92	0.11	-	66,66,66,66	0
2	CL	C	964	1/1	0.94	0.15	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.