Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 12:52 pm BST

PDB ID	:	2XAQ
Title	:	Crystal structure of LSD1-CoREST in complex with a tranylcypromine derivative (MC2584, 13b)
Authors	:	Binda, C.; Valente, S.; Romanenghi, M.; Pilotto, S.; Cirilli, R.; Karytinos, A.; Ciossani, G.; Botrugno, O.A.; Forneris, F.; Tardugno, M.; Edmondson, D.E.; Minucci, S.; Mattevi, A.; Mai, A.
Deposited on	:	2010-03-31
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/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:

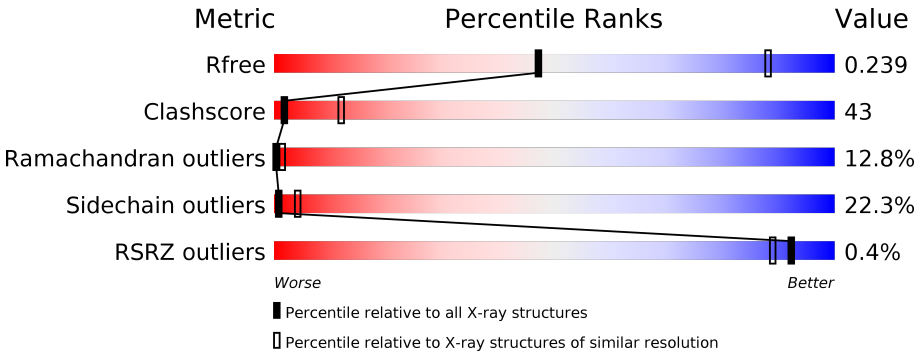
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. 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	852	26% 36% 14% • 22%
2	B	482	9% 16% • 72%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6365 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.

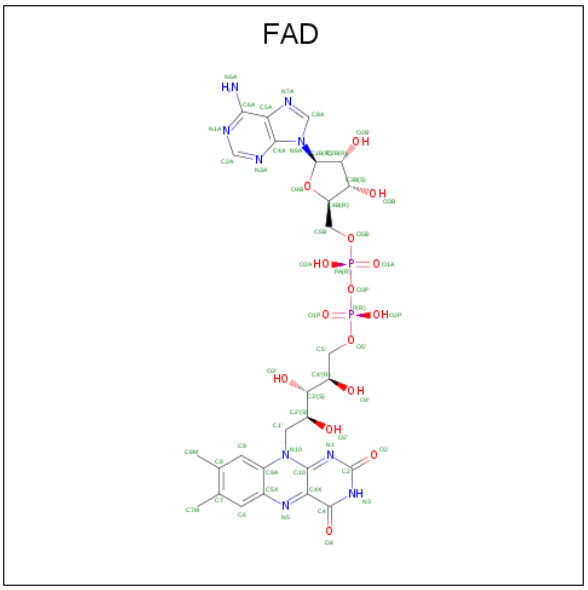
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

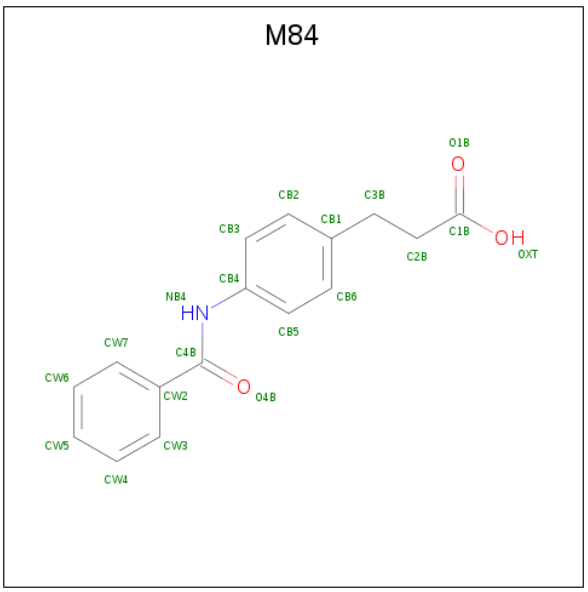
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 3-{4-[(PHENYLCARBONYL)AMINO]PHENYL}PROPANOIC ACID

(three-letter code: M84) (formula: $C_{16}H_{15}NO_3$).



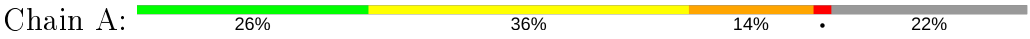
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	19	16	1	2	0	0

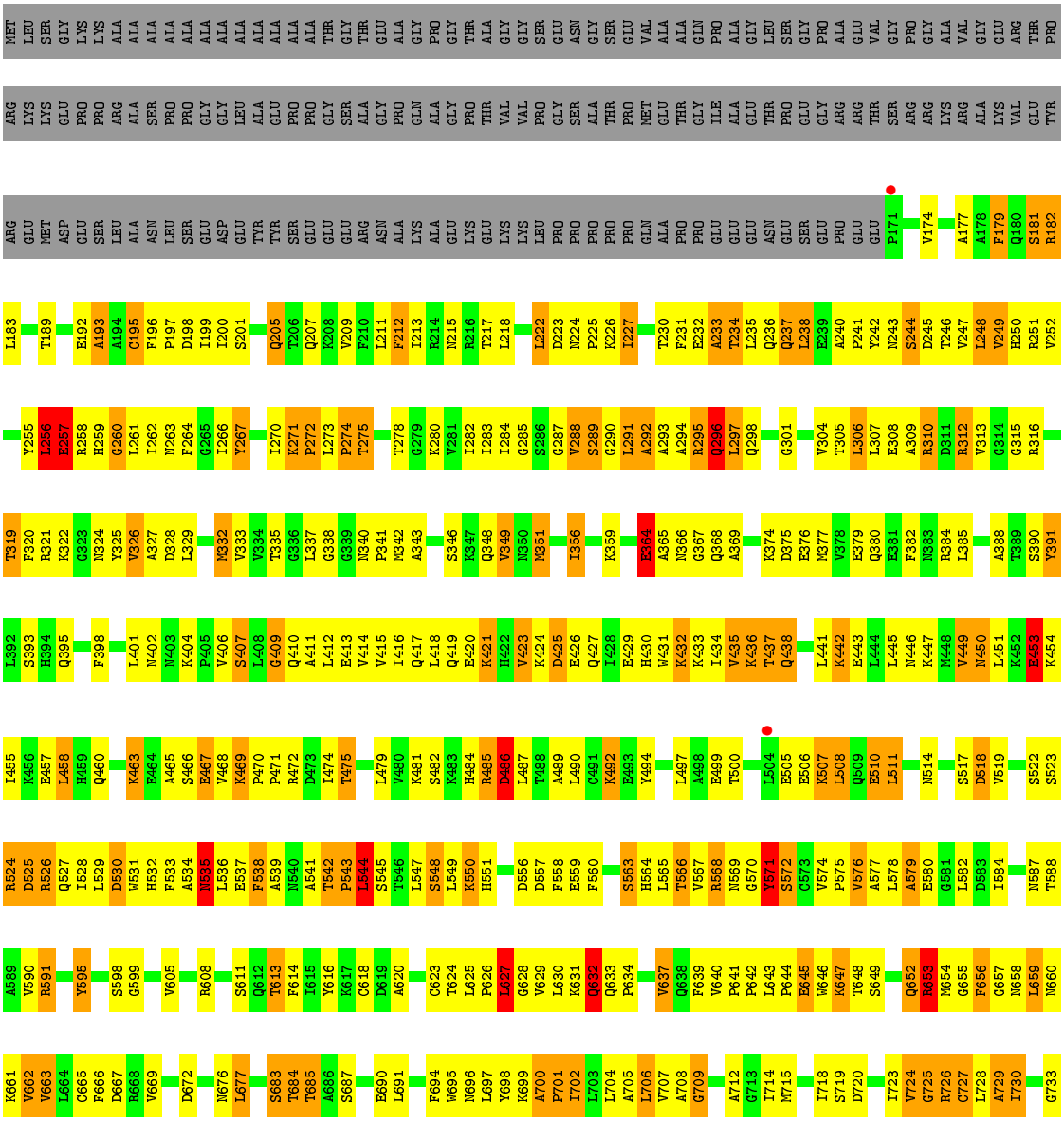
3 Residue-property plots (i)

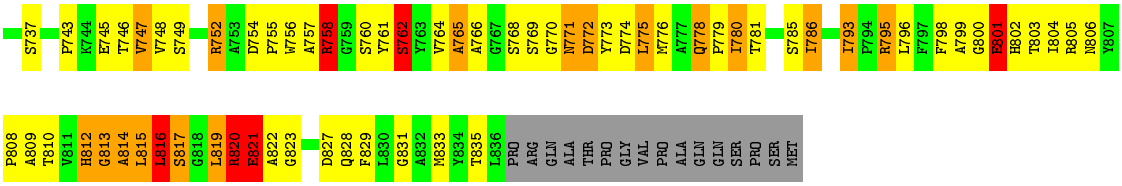
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1

Chain A:

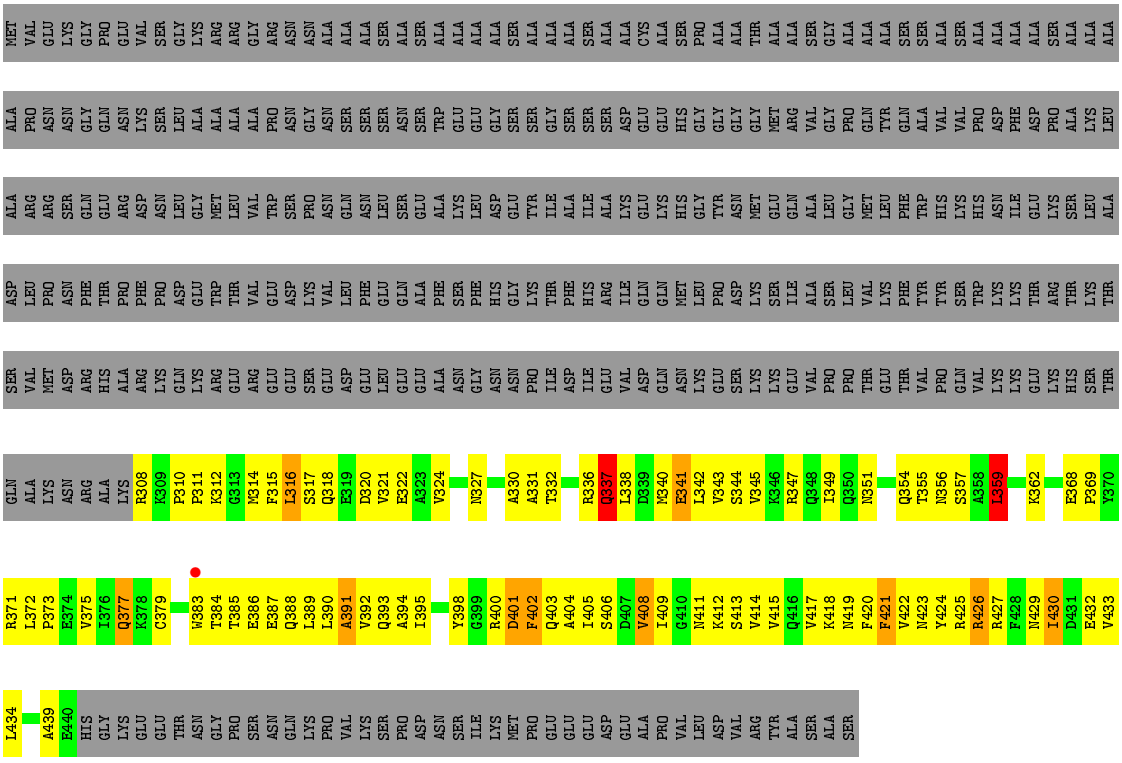






- Molecule 2: REST COREPRESSOR 1

Chain B: 9% 16% 72%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.10Å 180.35Å 235.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.96 – 3.20 99.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.96-3.20) 100.0 (99.96-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.264 0.217 , 0.239	Depositor DCC
R_{free} test set	822 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: M84, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.91	3/5331 (0.1%)	1.01	7/7232 (0.1%)
2	B	0.66	0/1091	0.79	1/1471 (0.1%)
All	All	0.87	3/6422 (0.0%)	0.98	8/8703 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	GLU	CD-OE1	7.15	1.33	1.25
1	A	821	GLU	CD-OE2	6.54	1.32	1.25
1	A	814	ALA	CA-CB	5.22	1.63	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	LEU	CA-CB-CG	9.50	137.16	115.30
1	A	774	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	291	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	820	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	691	LEU	CA-CB-CG	-5.33	103.04	115.30
1	A	796	LEU	CA-CB-CG	5.32	127.53	115.30
2	B	359	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	816	LEU	CB-CG-CD1	5.11	119.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	627	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	492	0
2	B	1076	0	1091	68	0
3	A	53	0	31	6	0
4	A	19	0	14	6	0
All	All	6365	0	6388	544	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 43.

All (544) 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:A:801:GLU:CG	1:A:809:ALA:HA	1.63	1.25
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.24	1.15
1:A:316:ARG:HH21	1:A:626:PRO:HB3	1.02	1.13
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.05	1.11
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.13	1.11
1:A:316:ARG:NH2	1:A:626:PRO:HB3	1.64	1.10
1:A:801:GLU:HG2	1:A:809:ALA:CA	1.82	1.09
1:A:659:LEU:HD12	1:A:660:ASN:N	1.66	1.09
1:A:801:GLU:HG2	1:A:809:ALA:HA	1.17	1.07
1:A:559:GLU:HG3	4:A:901:M84:CW4	1.84	1.06
1:A:559:GLU:CG	4:A:901:M84:HW4	1.84	1.06
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.51	1.03
3:A:900:FAD:C4X	4:A:901:M84:H3B2	1.92	0.99
1:A:231:PHE:CE1	1:A:249:VAL:HG12	1.97	0.98
1:A:658:ASN:HD22	1:A:752:ARG:HB2	1.28	0.98
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:HB	1:A:572:SER:HB3	1.46	0.96
1:A:656:PHE:HE1	1:A:761:TYR:HA	1.29	0.95
1:A:306:LEU:HD12	1:A:306:LEU:H	1.31	0.95
1:A:799:ALA:HB1	1:A:817:SER:OG	1.67	0.94
1:A:558:PHE:CE2	1:A:806:ASN:ND2	2.35	0.94
1:A:342:MET:HE3	1:A:342:MET:HA	1.51	0.93
2:B:317:SER:O	2:B:321:VAL:HG23	1.68	0.93
1:A:758:ARG:HH11	1:A:758:ARG:HG2	1.34	0.92
1:A:658:ASN:ND2	1:A:752:ARG:HB2	1.85	0.91
1:A:659:LEU:C	1:A:659:LEU:HD12	1.85	0.91
1:A:435:VAL:HG23	1:A:436:LYS:H	1.33	0.91
1:A:525:ASP:O	1:A:527:GLN:N	2.05	0.89
2:B:425:ARG:HA	2:B:430:ILE:CG1	2.02	0.88
2:B:388:GLN:O	2:B:391:ALA:HB3	1.73	0.88
1:A:415:VAL:O	1:A:419:GLN:HG2	1.72	0.88
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.42	0.88
1:A:544:LEU:H	1:A:544:LEU:HD23	1.37	0.87
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.54	0.86
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.92	0.85
1:A:656:PHE:CE1	1:A:761:TYR:HA	2.11	0.85
1:A:435:VAL:HG23	1:A:436:LYS:N	1.90	0.84
1:A:310:ARG:HH12	1:A:756:TRP:HB2	1.43	0.84
1:A:653:ARG:HH11	1:A:653:ARG:HG3	1.43	0.83
2:B:429:ASN:HB3	2:B:432:GLU:OE2	1.78	0.83
1:A:544:LEU:HD23	1:A:544:LEU:N	1.94	0.83
1:A:695:TRP:HB2	1:A:704:LEU:HB2	1.58	0.83
1:A:231:PHE:HE1	1:A:249:VAL:CG1	1.88	0.83
1:A:506:GLU:O	1:A:508:LEU:N	2.13	0.82
1:A:663:VAL:CG2	1:A:747:VAL:HG23	2.10	0.81
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.15	0.81
1:A:484:HIS:HD2	2:B:372:LEU:HD13	1.46	0.81
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.27	0.80
2:B:418:LYS:O	2:B:421:PHE:HB2	1.82	0.80
1:A:595:TYR:CE1	1:A:641:PRO:HD2	2.16	0.80
1:A:654:MET:CE	1:A:773:TYR:CE1	2.65	0.79
1:A:700:ALA:HB1	1:A:701:PRO:CD	2.13	0.79
1:A:319:THR:OG1	1:A:328:ASP:OD1	2.01	0.78
1:A:659:LEU:CD1	1:A:660:ASN:N	2.46	0.78
1:A:548:SER:HB2	1:A:766:ALA:HA	1.63	0.78
1:A:366:ASN:OD1	1:A:367:GLY:N	2.15	0.78
1:A:316:ARG:HH21	1:A:626:PRO:CB	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:C	1:A:508:LEU:H	1.86	0.77
1:A:306:LEU:N	1:A:306:LEU:HD12	1.99	0.76
1:A:308:GLU:OE1	3:A:900:FAD:O3B	2.04	0.76
1:A:663:VAL:HG21	1:A:747:VAL:HG23	1.68	0.76
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.05	0.75
1:A:758:ARG:NH1	1:A:758:ARG:HG2	2.02	0.75
1:A:801:GLU:HG2	1:A:809:ALA:N	2.00	0.75
1:A:510:GLU:HG3	1:A:511:LEU:CD2	2.11	0.74
1:A:308:GLU:OE2	1:A:309:ALA:N	2.21	0.73
1:A:599:GLY:N	1:A:795:ARG:HH21	1.85	0.73
1:A:720:ASP:O	1:A:724:VAL:HG23	1.88	0.73
1:A:658:ASN:OD1	1:A:659:LEU:N	2.22	0.73
1:A:198:ASP:OD2	1:A:199:ILE:HG13	1.89	0.72
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.55	0.72
1:A:445:LEU:HB3	2:B:359:LEU:HD12	1.71	0.72
1:A:284:ILE:O	1:A:624:THR:OG1	2.06	0.72
1:A:793:ILE:HD12	1:A:793:ILE:H	1.52	0.72
1:A:485:ARG:O	1:A:487:LEU:N	2.23	0.72
1:A:654:MET:HE1	1:A:773:TYR:HE1	1.53	0.72
1:A:222:LEU:O	1:A:224:ASN:N	2.23	0.72
1:A:654:MET:HE3	1:A:773:TYR:CE1	2.25	0.72
1:A:644:PRO:CB	1:A:646:TRP:NE1	2.53	0.71
1:A:297:LEU:HD23	1:A:822:ALA:HB1	1.72	0.71
1:A:654:MET:HE1	1:A:773:TYR:CE1	2.26	0.71
1:A:624:THR:HA	1:A:799:ALA:O	1.91	0.71
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.55	0.71
1:A:649:SER:O	1:A:653:ARG:NH1	2.24	0.70
1:A:310:ARG:NH1	1:A:756:TRP:HB2	2.06	0.70
1:A:578:LEU:O	1:A:580:GLU:N	2.24	0.70
1:A:598:SER:C	1:A:795:ARG:HH21	1.95	0.70
1:A:644:PRO:HB2	1:A:646:TRP:NE1	2.06	0.69
1:A:393:SER:HB2	1:A:549:LEU:HD21	1.74	0.69
1:A:661:LYS:N	1:A:749:SER:OG	2.21	0.69
1:A:435:VAL:O	1:A:437:THR:N	2.26	0.69
1:A:632:GLN:HG3	1:A:758:ARG:HD2	1.73	0.69
1:A:196:PHE:N	1:A:197:PRO:HD3	2.08	0.69
1:A:200:ILE:HA	1:A:207:GLN:HE21	1.56	0.69
1:A:435:VAL:CG2	1:A:436:LYS:H	2.03	0.69
1:A:419:GLN:HE22	2:B:315:PHE:H	1.41	0.69
1:A:525:ASP:C	1:A:527:GLN:H	1.96	0.68
2:B:400:ARG:O	2:B:402:PHE:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:ND2	1:A:227:ILE:HD11	2.07	0.68
1:A:652:GLN:O	1:A:654:MET:N	2.26	0.68
1:A:445:LEU:CB	2:B:359:LEU:HD12	2.23	0.68
1:A:563:SER:O	1:A:565:LEU:HD12	1.93	0.68
1:A:572:SER:O	1:A:576:VAL:HG23	1.94	0.68
1:A:258:ARG:NH1	1:A:827:ASP:OD1	2.26	0.68
1:A:659:LEU:CD1	1:A:659:LEU:C	2.60	0.68
1:A:248:LEU:O	1:A:249:VAL:C	2.31	0.68
1:A:256:LEU:O	1:A:258:ARG:N	2.26	0.68
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.76	0.68
1:A:342:MET:CA	1:A:342:MET:HE3	2.22	0.67
2:B:386:GLU:O	2:B:390:LEU:HD12	1.94	0.67
1:A:660:ASN:OD1	1:A:749:SER:O	2.13	0.66
1:A:296:GLN:OE1	1:A:296:GLN:CA	2.42	0.66
1:A:595:TYR:HD1	1:A:595:TYR:H	1.41	0.66
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.63	0.66
1:A:411:ALA:O	1:A:415:VAL:HG23	1.96	0.66
1:A:655:GLY:O	1:A:762:SER:HA	1.95	0.66
1:A:291:LEU:O	1:A:293:ALA:N	2.28	0.65
2:B:406:SER:OG	2:B:412:LYS:O	2.14	0.65
1:A:665:CYS:HB2	1:A:745:GLU:O	1.95	0.65
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.79	0.65
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.96	0.65
1:A:312:ARG:NH2	1:A:315:GLY:O	2.29	0.65
1:A:266:ILE:N	1:A:348:GLN:OE1	2.27	0.64
1:A:205:GLN:O	1:A:209:VAL:HG23	1.98	0.64
1:A:799:ALA:HA	1:A:803:THR:HG21	1.79	0.64
1:A:528:ILE:O	1:A:531:TRP:N	2.18	0.64
1:A:718:ILE:HG22	1:A:719:SER:O	1.95	0.64
1:A:595:TYR:N	1:A:595:TYR:CD1	2.60	0.63
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.13	0.63
1:A:694:PHE:HA	1:A:704:LEU:O	1.98	0.63
1:A:195:CYS:C	1:A:197:PRO:HD3	2.18	0.63
1:A:644:PRO:HB2	1:A:646:TRP:CD1	2.34	0.63
1:A:801:GLU:HG2	1:A:809:ALA:H	1.63	0.63
1:A:662:VAL:HG13	1:A:748:VAL:CG2	2.28	0.63
1:A:653:ARG:HH11	1:A:653:ARG:CG	2.10	0.63
1:A:342:MET:HA	1:A:342:MET:CE	2.27	0.63
1:A:726:ARG:O	1:A:730:ILE:HG13	1.99	0.63
1:A:773:TYR:HD1	1:A:802:HIS:O	1.81	0.63
1:A:666:PHE:O	1:A:701:PRO:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:OG	1:A:290:GLY:N	2.31	0.62
1:A:296:GLN:HA	1:A:296:GLN:OE1	1.98	0.62
1:A:724:VAL:HG11	1:A:746:THR:HG21	1.81	0.62
1:A:656:PHE:HD1	1:A:762:SER:N	1.98	0.62
1:A:828:GLN:HG3	1:A:829:PHE:CE2	2.34	0.62
1:A:288:VAL:O	1:A:289:SER:C	2.38	0.62
1:A:793:ILE:HG22	1:A:828:GLN:OE1	1.99	0.62
2:B:384:THR:O	2:B:387:GLU:N	2.32	0.62
1:A:322:LYS:O	1:A:325:TYR:HB2	1.99	0.61
1:A:700:ALA:HB1	1:A:701:PRO:HD3	1.81	0.61
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.81	0.61
1:A:595:TYR:HD1	1:A:595:TYR:N	1.96	0.61
1:A:647:LYS:NZ	1:A:775:LEU:O	2.33	0.61
1:A:658:ASN:ND2	1:A:752:ARG:CB	2.60	0.61
1:A:310:ARG:CG	1:A:310:ARG:HH11	2.13	0.61
1:A:656:PHE:CD1	1:A:762:SER:N	2.68	0.61
1:A:760:SER:O	1:A:761:TYR:HB3	1.99	0.61
1:A:666:PHE:CE1	1:A:743:PRO:HB3	2.35	0.61
3:A:900:FAD:O5'	3:A:900:FAD:O2A	2.18	0.61
1:A:288:VAL:HG12	1:A:289:SER:N	2.15	0.60
1:A:182:ARG:HG3	1:A:182:ARG:HH11	1.65	0.60
1:A:437:THR:HG22	1:A:508:LEU:HD12	1.84	0.60
1:A:196:PHE:HD2	1:A:199:ILE:HD12	1.66	0.60
1:A:527:GLN:NE2	1:A:683:SER:O	2.27	0.60
2:B:341:GLU:O	2:B:345:VAL:HG23	2.01	0.60
1:A:640:VAL:HG12	1:A:640:VAL:O	2.01	0.60
1:A:684:THR:HG22	1:A:685:THR:H	1.65	0.60
2:B:320:ASP:O	2:B:324:VAL:HG23	2.01	0.60
1:A:256:LEU:O	1:A:257:GLU:C	2.40	0.59
1:A:454:LYS:O	1:A:458:LEU:HB2	2.02	0.59
1:A:537:GLU:OE2	1:A:544:LEU:HD23	2.03	0.59
1:A:570:GLY:O	1:A:572:SER:N	2.35	0.59
1:A:614:PHE:HB3	1:A:616:TYR:HE1	1.67	0.59
1:A:558:PHE:CE2	1:A:806:ASN:CG	2.76	0.59
1:A:618:CYS:SG	1:A:620:ALA:O	2.47	0.59
1:A:310:ARG:HG3	1:A:310:ARG:HH11	1.67	0.59
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.85	0.59
1:A:321:ARG:HG2	1:A:326:VAL:HG22	1.85	0.59
1:A:801:GLU:CG	1:A:809:ALA:CA	2.52	0.59
2:B:400:ARG:O	2:B:402:PHE:CD2	2.56	0.59
1:A:424:LYS:O	1:A:426:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PHE:HD1	1:A:659:LEU:CD2	2.16	0.58
1:A:263:ASN:HB3	1:A:267:TYR:CE1	2.38	0.58
1:A:663:VAL:HG23	1:A:747:VAL:HG23	1.85	0.58
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.67	0.58
1:A:649:SER:HB3	1:A:653:ARG:HH12	1.68	0.58
1:A:544:LEU:CD2	1:A:544:LEU:N	2.65	0.58
1:A:248:LEU:O	1:A:250:HIS:N	2.36	0.58
1:A:195:CYS:HB3	1:A:196:PHE:CD1	2.39	0.58
1:A:506:GLU:C	1:A:508:LEU:N	2.54	0.58
2:B:401:ASP:O	2:B:403:GLN:N	2.37	0.58
1:A:259:HIS:O	1:A:261:LEU:N	2.36	0.57
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.84	0.57
1:A:656:PHE:CE1	1:A:761:TYR:CA	2.86	0.57
1:A:385:LEU:O	1:A:388:ALA:HB3	2.05	0.57
1:A:485:ARG:HD2	2:B:404:ALA:HB1	1.86	0.57
1:A:531:TRP:CE3	1:A:532:HIS:ND1	2.73	0.57
1:A:568:ARG:HH12	1:A:699:LYS:HG3	1.70	0.57
1:A:648:THR:OG1	1:A:649:SER:N	2.38	0.57
1:A:366:ASN:OD1	1:A:368:GLN:HG3	2.04	0.57
1:A:760:SER:HB2	3:A:900:FAD:HM83	1.87	0.57
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.87	0.57
1:A:263:ASN:C	1:A:267:TYR:HE1	2.09	0.57
1:A:530:ASP:OD2	1:A:685:THR:HA	2.04	0.56
1:A:248:LEU:O	1:A:251:ARG:N	2.37	0.56
1:A:296:GLN:OE1	1:A:296:GLN:N	2.38	0.56
1:A:263:ASN:HB3	1:A:267:TYR:HE1	1.69	0.56
1:A:438:GLN:HA	1:A:438:GLN:HE21	1.69	0.56
1:A:538:PHE:HD1	1:A:659:LEU:HD21	1.71	0.56
2:B:390:LEU:H	2:B:390:LEU:HD12	1.70	0.56
1:A:316:ARG:NH2	1:A:626:PRO:CB	2.55	0.56
1:A:567:VAL:HG11	1:A:571:TYR:HA	1.87	0.56
1:A:695:TRP:HE1	1:A:706:LEU:CD2	2.18	0.56
1:A:548:SER:CB	1:A:765:ALA:O	2.54	0.56
1:A:666:PHE:HE1	1:A:743:PRO:HB3	1.70	0.56
2:B:426:ARG:HB3	2:B:427:ARG:HG3	1.88	0.56
1:A:543:PRO:C	1:A:545:SER:H	2.09	0.56
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.35	0.55
1:A:295:ARG:NH2	1:A:580:GLU:O	2.39	0.55
1:A:804:ILE:O	1:A:806:ASN:N	2.39	0.55
1:A:639:PHE:CD2	1:A:643:LEU:HD21	2.41	0.55
1:A:183:LEU:HD23	1:A:189:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HD12	1:A:577:ALA:HB1	1.87	0.55
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.06	0.55
1:A:431:TRP:C	1:A:433:LYS:H	2.10	0.55
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.42	0.55
1:A:646:TRP:HE3	1:A:775:LEU:CD2	2.20	0.55
1:A:793:ILE:H	1:A:793:ILE:CD1	2.10	0.55
1:A:271:LYS:O	1:A:272:PRO:O	2.25	0.54
1:A:537:GLU:OE2	1:A:544:LEU:CD2	2.54	0.54
1:A:715:MET:SD	1:A:718:ILE:HD12	2.47	0.54
1:A:417:GLN:O	1:A:419:GLN:N	2.40	0.54
1:A:321:ARG:NH2	1:A:569:ASN:O	2.32	0.54
1:A:587:ASN:HD22	1:A:608:ARG:NE	2.05	0.54
1:A:828:GLN:HG3	1:A:829:PHE:CD2	2.42	0.54
2:B:340:MET:O	2:B:342:LEU:N	2.40	0.54
1:A:627:LEU:O	1:A:630:LEU:N	2.40	0.54
1:A:812:HIS:CD2	1:A:813:GLY:H	2.26	0.54
1:A:263:ASN:CA	1:A:267:TYR:HE1	2.20	0.54
1:A:510:GLU:CG	1:A:511:LEU:HD23	2.17	0.54
1:A:626:PRO:HD2	1:A:629:VAL:CG2	2.36	0.54
1:A:568:ARG:NH1	1:A:699:LYS:HG3	2.23	0.54
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.43	0.54
1:A:437:THR:CG2	1:A:508:LEU:HD12	2.36	0.54
1:A:230:THR:O	1:A:234:THR:OG1	2.26	0.53
1:A:260:GLY:O	1:A:264:PHE:CD2	2.61	0.53
1:A:306:LEU:H	1:A:306:LEU:CD1	2.14	0.53
2:B:415:VAL:HG22	2:B:419:ASN:HD21	1.73	0.53
1:A:256:LEU:HB2	1:A:262:ILE:HG12	1.90	0.53
1:A:567:VAL:HG11	1:A:571:TYR:N	2.24	0.53
1:A:644:PRO:HB3	1:A:646:TRP:HE1	1.72	0.53
1:A:449:VAL:HG12	1:A:450:ASN:N	2.21	0.53
1:A:255:TYR:O	1:A:256:LEU:C	2.46	0.53
1:A:421:LYS:HD3	1:A:425:ASP:OD1	2.08	0.53
2:B:391:ALA:O	2:B:394:ALA:N	2.42	0.53
1:A:374:LYS:O	1:A:375:ASP:C	2.47	0.53
1:A:558:PHE:HE2	1:A:806:ASN:CG	2.12	0.53
1:A:240:ALA:HA	1:A:241:PRO:C	2.28	0.53
1:A:424:LYS:O	1:A:425:ASP:C	2.48	0.53
1:A:543:PRO:O	1:A:545:SER:N	2.42	0.52
1:A:431:TRP:O	1:A:433:LYS:N	2.42	0.52
1:A:770:GLY:O	1:A:772:ASP:N	2.43	0.52
1:A:531:TRP:HE3	1:A:532:HIS:ND1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:O	1:A:575:PRO:C	2.45	0.52
1:A:595:TYR:HE2	1:A:780:ILE:CG2	2.23	0.52
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.75	0.52
1:A:773:TYR:CD1	1:A:802:HIS:O	2.63	0.52
1:A:773:TYR:O	1:A:776:MET:N	2.43	0.52
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.45	0.51
1:A:644:PRO:HB3	1:A:646:TRP:NE1	2.25	0.51
1:A:196:PHE:N	1:A:197:PRO:CD	2.74	0.51
1:A:820:ARG:O	1:A:821:GLU:C	2.44	0.51
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.91	0.51
1:A:256:LEU:CB	1:A:262:ILE:HG12	2.40	0.51
1:A:255:TYR:O	1:A:258:ARG:HB3	2.11	0.51
1:A:320:PHE:O	1:A:326:VAL:HA	2.09	0.51
1:A:290:GLY:HA2	1:A:624:THR:HG21	1.93	0.51
1:A:613:THR:C	1:A:614:PHE:HD2	2.14	0.51
1:A:531:TRP:HE3	1:A:532:HIS:HD1	1.55	0.51
1:A:346:SER:O	1:A:349:VAL:O	2.28	0.51
1:A:416:ILE:O	1:A:419:GLN:HB2	2.12	0.51
1:A:548:SER:HB3	1:A:765:ALA:O	2.10	0.51
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.93	0.50
1:A:484:HIS:HD2	2:B:372:LEU:CD1	2.19	0.50
1:A:632:GLN:HG3	1:A:758:ARG:CD	2.40	0.50
1:A:341:PRO:HB2	1:A:815:LEU:HD12	1.93	0.50
1:A:291:LEU:C	1:A:293:ALA:N	2.64	0.50
2:B:368:GLU:N	2:B:369:PRO:HD2	2.26	0.50
1:A:808:PRO:O	1:A:810:THR:HG23	2.12	0.50
2:B:389:LEU:O	2:B:393:GLN:HG3	2.12	0.50
1:A:179:PHE:CD2	1:A:179:PHE:C	2.84	0.50
1:A:431:TRP:O	1:A:434:ILE:N	2.43	0.50
1:A:541:ALA:O	1:A:657:GLY:HA3	2.11	0.50
1:A:525:ASP:O	1:A:528:ILE:N	2.44	0.50
1:A:215:ASN:O	1:A:218:LEU:HB2	2.12	0.50
1:A:284:ILE:HD13	1:A:590:VAL:HG11	1.94	0.50
1:A:614:PHE:HB3	1:A:616:TYR:CE1	2.47	0.50
1:A:685:THR:O	1:A:687:SER:N	2.45	0.50
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.93	0.50
1:A:181:SER:O	1:A:182:ARG:HB2	2.12	0.50
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.93	0.50
1:A:799:ALA:HB2	1:A:821:GLU:HG2	1.94	0.50
1:A:506:GLU:HG2	1:A:507:LYS:H	1.76	0.49
1:A:427:GLN:O	1:A:430:HIS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HG22	1:A:508:LEU:CD1	2.42	0.49
1:A:819:LEU:O	1:A:822:ALA:N	2.27	0.49
1:A:828:GLN:HB3	1:A:829:PHE:HD2	1.78	0.49
2:B:368:GLU:OE1	2:B:371:ARG:NH1	2.45	0.49
1:A:435:VAL:CG2	1:A:436:LYS:N	2.60	0.49
1:A:563:SER:O	1:A:565:LEU:CD1	2.59	0.49
1:A:658:ASN:HD22	1:A:752:ARG:CB	2.12	0.49
1:A:415:VAL:HG13	2:B:316:LEU:HD21	1.93	0.49
1:A:326:VAL:O	1:A:326:VAL:HG12	2.12	0.49
1:A:578:LEU:C	1:A:580:GLU:H	2.16	0.49
1:A:195:CYS:HB3	1:A:196:PHE:HD1	1.78	0.49
1:A:420:GLU:O	1:A:423:VAL:HG12	2.13	0.49
1:A:465:ALA:HB1	1:A:479:LEU:HD23	1.94	0.49
1:A:626:PRO:HD2	1:A:629:VAL:HG23	1.93	0.49
1:A:291:LEU:O	1:A:292:ALA:C	2.50	0.49
1:A:192:GLU:O	1:A:195:CYS:N	2.44	0.48
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.93	0.48
1:A:718:ILE:CG2	1:A:723:ILE:HG13	2.43	0.48
1:A:828:GLN:CG	1:A:829:PHE:CE2	2.97	0.48
1:A:631:LYS:O	1:A:632:GLN:C	2.51	0.48
1:A:645:GLU:O	1:A:647:LYS:N	2.47	0.48
1:A:438:GLN:O	1:A:441:LEU:HB3	2.14	0.48
1:A:467:GLU:O	1:A:469:LYS:N	2.47	0.48
1:A:666:PHE:CD1	1:A:743:PRO:HA	2.48	0.48
1:A:752:ARG:O	1:A:752:ARG:HG3	2.14	0.48
1:A:770:GLY:O	1:A:771:ASN:C	2.52	0.48
1:A:800:GLY:N	1:A:817:SER:OG	2.45	0.48
1:A:295:ARG:O	1:A:296:GLN:C	2.52	0.48
1:A:398:PHE:O	1:A:406:VAL:HG21	2.12	0.48
1:A:329:LEU:O	1:A:661:LYS:HD2	2.13	0.48
1:A:406:VAL:HG12	1:A:407:SER:O	2.13	0.48
1:A:761:TYR:CD1	1:A:761:TYR:O	2.67	0.48
1:A:342:MET:CA	1:A:342:MET:CE	2.89	0.47
1:A:366:ASN:OD1	1:A:368:GLN:N	2.47	0.47
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.95	0.47
1:A:485:ARG:C	1:A:487:LEU:N	2.66	0.47
1:A:232:GLU:O	1:A:234:THR:N	2.47	0.47
1:A:625:LEU:HD13	1:A:637:VAL:HG21	1.96	0.47
1:A:726:ARG:O	1:A:730:ILE:CG1	2.60	0.47
1:A:551:HIS:CD2	1:A:769:SER:HB3	2.49	0.47
1:A:177:ALA:O	1:A:181:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:VAL:N	1:A:705:ALA:O	2.35	0.47
1:A:543:PRO:C	1:A:545:SER:N	2.66	0.47
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.97	0.47
1:A:525:ASP:C	1:A:527:GLN:N	2.62	0.47
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.95	0.47
1:A:364:GLU:OE1	1:A:524:ARG:HG2	2.14	0.47
1:A:209:VAL:HG13	1:A:242:TYR:CD1	2.42	0.47
1:A:306:LEU:O	1:A:307:LEU:HD23	2.15	0.47
1:A:481:LYS:O	1:A:482:SER:C	2.51	0.47
1:A:820:ARG:O	1:A:822:ALA:N	2.48	0.47
1:A:445:LEU:HB2	2:B:359:LEU:HD12	1.97	0.47
1:A:340:ASN:HA	1:A:341:PRO:HD2	1.78	0.47
1:A:542:THR:HA	1:A:543:PRO:HD2	1.65	0.47
1:A:677:LEU:HA	1:A:694:PHE:O	2.15	0.47
2:B:408:VAL:HG12	2:B:409:ILE:N	2.30	0.47
1:A:633:GLN:HA	1:A:634:PRO:C	2.35	0.47
1:A:587:ASN:HD22	1:A:608:ARG:CZ	2.28	0.46
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.50	0.46
1:A:212:PHE:CD2	1:A:212:PHE:C	2.89	0.46
1:A:248:LEU:HB3	1:A:249:VAL:H	1.58	0.46
1:A:758:ARG:NH1	1:A:758:ARG:CG	2.77	0.46
2:B:405:ILE:O	2:B:409:ILE:HG13	2.15	0.46
1:A:745:GLU:OE1	1:A:745:GLU:HA	2.15	0.46
2:B:415:VAL:O	2:B:418:LYS:N	2.49	0.46
1:A:591:ARG:O	1:A:637:VAL:HA	2.15	0.46
1:A:645:GLU:O	1:A:646:TRP:C	2.53	0.46
1:A:551:HIS:O	1:A:764:VAL:HG11	2.16	0.46
1:A:799:ALA:HB1	1:A:817:SER:HG	1.74	0.46
1:A:217:THR:HG23	1:A:234:THR:HG21	1.98	0.46
1:A:393:SER:HB2	1:A:549:LEU:CD2	2.44	0.46
1:A:485:ARG:O	1:A:486:ASP:C	2.52	0.46
1:A:662:VAL:CB	1:A:705:ALA:HB3	2.43	0.46
1:A:720:ASP:OD1	1:A:748:VAL:HB	2.16	0.46
1:A:558:PHE:HE2	1:A:806:ASN:ND2	2.06	0.46
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.80	0.46
1:A:559:GLU:HG3	4:A:901:M84:HW4	0.88	0.46
1:A:441:LEU:HD23	2:B:356:ASN:ND2	2.31	0.46
1:A:662:VAL:HG13	1:A:748:VAL:HG23	1.98	0.46
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.71	0.46
1:A:287:GLY:O	1:A:288:VAL:C	2.54	0.46
1:A:646:TRP:CE3	1:A:775:LEU:HD23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PHE:HE2	1:A:757:ALA:O	1.98	0.46
1:A:665:CYS:SG	1:A:702:ILE:HD11	2.56	0.46
1:A:380:GLN:O	1:A:384:ARG:HG3	2.16	0.45
1:A:417:GLN:C	1:A:419:GLN:H	2.19	0.45
1:A:728:LEU:HD21	1:A:743:PRO:HD3	1.98	0.45
1:A:558:PHE:CD1	1:A:558:PHE:N	2.83	0.45
1:A:779:PRO:C	1:A:780:ILE:HD13	2.37	0.45
1:A:258:ARG:NH1	1:A:827:ASP:N	2.64	0.45
1:A:533:PHE:O	1:A:537:GLU:HG2	2.16	0.45
1:A:384:ARG:NH2	2:B:312:LYS:O	2.47	0.45
1:A:653:ARG:NH1	1:A:653:ARG:CG	2.76	0.45
1:A:244:SER:OG	1:A:245:ASP:N	2.50	0.45
1:A:541:ALA:HB1	1:A:658:ASN:N	2.31	0.45
1:A:310:ARG:NH1	1:A:756:TRP:CD1	2.84	0.45
2:B:401:ASP:OD1	2:B:401:ASP:O	2.34	0.45
1:A:193:ALA:C	1:A:195:CYS:H	2.19	0.45
1:A:506:GLU:HG2	1:A:507:LYS:N	2.32	0.45
1:A:567:VAL:CG1	1:A:571:TYR:N	2.80	0.45
1:A:284:ILE:HD13	1:A:590:VAL:HG21	1.99	0.45
1:A:595:TYR:CE2	1:A:780:ILE:HG21	2.52	0.45
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.17	0.45
1:A:197:PRO:O	1:A:201:SER:OG	2.29	0.45
1:A:263:ASN:CB	1:A:267:TYR:HE1	2.28	0.45
1:A:435:VAL:C	1:A:437:THR:N	2.70	0.45
1:A:799:ALA:HB2	1:A:820:ARG:NH2	2.32	0.45
1:A:312:ARG:HG3	1:A:313:VAL:O	2.17	0.45
1:A:320:PHE:HB3	1:A:327:ALA:O	2.17	0.45
1:A:449:VAL:C	1:A:451:LEU:H	2.19	0.45
1:A:535:ASN:HD22	1:A:535:ASN:HA	1.51	0.45
1:A:542:THR:HG22	1:A:547:LEU:HD21	1.99	0.45
2:B:354:GLN:O	2:B:357:SER:HB3	2.17	0.44
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.97	0.44
1:A:198:ASP:OD1	1:A:251:ARG:NH2	2.47	0.44
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.68	0.44
1:A:793:ILE:CG2	1:A:828:GLN:OE1	2.64	0.44
1:A:419:GLN:NE2	2:B:315:PHE:H	2.13	0.44
1:A:718:ILE:HG21	1:A:723:ILE:HG13	1.99	0.44
1:A:193:ALA:HB2	1:A:200:ILE:HD13	1.99	0.44
1:A:409:GLY:O	1:A:412:LEU:N	2.47	0.44
1:A:431:TRP:C	1:A:433:LYS:N	2.71	0.44
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:OD1	1:A:672:ASP:C	2.56	0.44
1:A:193:ALA:HB2	1:A:200:ILE:CD1	2.47	0.44
1:A:319:THR:HA	1:A:328:ASP:HA	1.99	0.44
1:A:333:VAL:CG1	1:A:564:HIS:HB3	2.47	0.44
1:A:549:LEU:HG	1:A:549:LEU:O	2.17	0.44
1:A:812:HIS:O	1:A:815:LEU:N	2.50	0.44
2:B:420:PHE:CD1	2:B:424:TYR:CD2	3.06	0.44
1:A:290:GLY:CA	1:A:624:THR:HG21	2.47	0.44
1:A:442:LYS:HE3	2:B:355:THR:CG2	2.38	0.44
2:B:413:SER:O	2:B:415:VAL:N	2.51	0.44
1:A:364:GLU:O	1:A:365:ALA:C	2.57	0.43
1:A:624:THR:O	1:A:625:LEU:C	2.56	0.43
1:A:666:PHE:HD1	1:A:743:PRO:HA	1.82	0.43
1:A:754:ASP:O	1:A:756:TRP:N	2.50	0.43
1:A:465:ALA:HB2	1:A:479:LEU:HD23	1.99	0.43
1:A:786:ILE:HD12	1:A:786:ILE:H	1.82	0.43
1:A:435:VAL:O	1:A:436:LYS:C	2.56	0.43
1:A:708:ALA:O	1:A:709:GLY:O	2.37	0.43
1:A:760:SER:OG	1:A:761:TYR:N	2.51	0.43
1:A:217:THR:HG23	1:A:234:THR:CG2	2.48	0.43
1:A:233:ALA:O	1:A:237:GLN:NE2	2.52	0.43
1:A:182:ARG:NH1	1:A:182:ARG:HG3	2.33	0.43
1:A:196:PHE:CD2	1:A:199:ILE:HD12	2.49	0.43
1:A:241:PRO:O	1:A:244:SER:HB3	2.18	0.43
1:A:567:VAL:HG12	1:A:570:GLY:H	1.84	0.43
1:A:639:PHE:CG	1:A:643:LEU:HD21	2.54	0.43
1:A:538:PHE:CD1	1:A:659:LEU:HD21	2.52	0.43
1:A:195:CYS:C	1:A:196:PHE:CD1	2.92	0.43
1:A:255:TYR:O	1:A:258:ARG:N	2.47	0.43
1:A:270:ILE:O	1:A:272:PRO:HD3	2.18	0.43
1:A:518:ASP:C	1:A:518:ASP:OD1	2.57	0.43
2:B:355:THR:O	2:B:359:LEU:HB2	2.19	0.43
1:A:337:LEU:HB3	1:A:343:ALA:HB2	2.00	0.43
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.54	0.43
1:A:349:VAL:HG21	1:A:577:ALA:CB	2.48	0.43
1:A:379:GLU:O	1:A:382:PHE:HB3	2.18	0.43
1:A:643:LEU:O	1:A:644:PRO:C	2.57	0.43
2:B:310:PRO:O	2:B:311:PRO:C	2.57	0.43
2:B:337:GLN:O	2:B:341:GLU:HB2	2.19	0.43
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.54	0.43
1:A:285:GLY:N	1:A:307:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ALA:N	1:A:243:ASN:OD1	2.52	0.42
1:A:595:TYR:HE2	1:A:780:ILE:HG21	1.84	0.42
1:A:232:GLU:CD	1:A:232:GLU:H	2.21	0.42
1:A:417:GLN:C	1:A:419:GLN:N	2.72	0.42
1:A:528:ILE:C	1:A:530:ASP:N	2.73	0.42
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.18	0.42
1:A:538:PHE:O	1:A:539:ALA:C	2.58	0.42
1:A:685:THR:C	1:A:687:SER:H	2.22	0.42
1:A:401:LEU:HA	1:A:401:LEU:HD12	1.65	0.42
2:B:415:VAL:HG22	2:B:419:ASN:ND2	2.34	0.42
1:A:196:PHE:HD2	1:A:199:ILE:CD1	2.29	0.42
1:A:485:ARG:HD2	2:B:404:ALA:CB	2.48	0.42
1:A:209:VAL:HG12	1:A:213:ILE:CD1	2.49	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.81	0.42
1:A:695:TRP:HB2	1:A:704:LEU:CB	2.42	0.42
1:A:183:LEU:CD2	1:A:189:THR:HG21	2.48	0.42
1:A:266:ILE:CD1	1:A:577:ALA:HB1	2.48	0.42
1:A:390:SER:O	1:A:391:TYR:C	2.58	0.42
1:A:728:LEU:O	1:A:729:ALA:C	2.57	0.42
1:A:222:LEU:C	1:A:224:ASN:N	2.74	0.41
1:A:587:ASN:ND2	1:A:608:ARG:NE	2.68	0.41
2:B:336:ARG:O	2:B:338:LEU:N	2.53	0.41
2:B:421:PHE:O	2:B:425:ARG:HB2	2.20	0.41
1:A:424:LYS:C	1:A:426:GLU:N	2.73	0.41
1:A:695:TRP:NE1	1:A:706:LEU:HD22	2.35	0.41
3:A:900:FAD:C10	4:A:901:M84:H3B2	2.46	0.41
1:A:423:VAL:O	1:A:426:GLU:HB2	2.21	0.41
1:A:627:LEU:O	1:A:630:LEU:HB2	2.21	0.41
1:A:548:SER:CB	1:A:766:ALA:HA	2.43	0.41
1:A:595:TYR:CE2	1:A:780:ILE:CG2	3.03	0.41
1:A:804:ILE:O	1:A:804:ILE:HG23	2.19	0.41
1:A:645:GLU:C	1:A:647:LYS:N	2.73	0.41
1:A:725:GLY:C	1:A:727:CYS:H	2.24	0.41
1:A:447:LYS:HE3	1:A:497:LEU:HD21	2.02	0.41
1:A:474:ILE:HG23	1:A:475:THR:N	2.35	0.41
1:A:263:ASN:C	1:A:267:TYR:CE1	2.92	0.41
1:A:356:ILE:HD11	1:A:566:THR:HG23	2.02	0.41
1:A:566:THR:HG21	1:A:697:LEU:HD22	2.02	0.41
1:A:801:GLU:OE2	1:A:809:ALA:HB2	2.19	0.41
1:A:816:LEU:HD23	1:A:816:LEU:HA	1.54	0.41
1:A:470:PRO:HA	1:A:471:PRO:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:HIS:O	1:A:815:LEU:HB3	2.21	0.41
3:A:900:FAD:C4X	4:A:901:M84:C3B	2.76	0.41
1:A:413:GLU:O	1:A:414:VAL:C	2.59	0.41
1:A:535:ASN:O	1:A:538:PHE:N	2.37	0.41
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.51	0.41
1:A:778:GLN:HA	1:A:779:PRO:HD3	1.87	0.41
2:B:411:ASN:CG	2:B:411:ASN:O	2.58	0.41
1:A:306:LEU:HD13	1:A:584:ILE:CG1	2.48	0.41
1:A:332:MET:SD	1:A:661:LYS:NZ	2.72	0.41
1:A:697:LEU:HB2	1:A:698:TYR:CD1	2.56	0.41
1:A:708:ALA:O	1:A:709:GLY:C	2.60	0.41
2:B:318:GLN:O	2:B:322:GLU:HG3	2.20	0.41
1:A:297:LEU:CB	1:A:304:VAL:HG21	2.51	0.41
1:A:761:TYR:HB2	1:A:809:ALA:HB1	2.03	0.41
1:A:815:LEU:O	1:A:816:LEU:C	2.59	0.41
1:A:289:SER:O	1:A:290:GLY:C	2.59	0.40
1:A:391:TYR:C	1:A:391:TYR:CD1	2.94	0.40
1:A:463:LYS:HA	1:A:463:LYS:HD2	1.92	0.40
1:A:485:ARG:C	1:A:487:LEU:H	2.23	0.40
1:A:567:VAL:HG11	1:A:571:TYR:CA	2.50	0.40
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.93	0.40
1:A:351:MET:HG2	1:A:574:VAL:HG23	2.03	0.40
1:A:266:ILE:HD11	1:A:577:ALA:C	2.41	0.40
1:A:349:VAL:HG21	1:A:577:ALA:HB1	2.03	0.40
1:A:576:VAL:O	1:A:579:ALA:HB3	2.21	0.40
2:B:368:GLU:N	2:B:369:PRO:CD	2.84	0.40
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.51	0.40
2:B:417:VAL:O	2:B:420:PHE:HB3	2.21	0.40
1:A:310:ARG:NH1	1:A:310:ARG:CG	2.80	0.40
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.22	0.40
1:A:644:PRO:CB	1:A:646:TRP:HE1	2.26	0.40
1:A:781:THR:HG23	1:A:793:ILE:O	2.20	0.40
1:A:280:LYS:HG3	1:A:618:CYS:HB2	2.02	0.40
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.92	0.40
1:A:676:ASN:O	1:A:696:ASN:N	2.39	0.40
1:A:395:GLN:HE22	2:B:308:ARG:NH1	2.19	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	664/852 (78%)	468 (70%)	110 (17%)	86 (13%)	0 1
2	B	131/482 (27%)	93 (71%)	22 (17%)	16 (12%)	0 2
All	All	795/1334 (60%)	561 (71%)	132 (17%)	102 (13%)	0 1

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	248	LEU
1	A	249	VAL
1	A	260	GLY
1	A	274	PRO
1	A	275	THR
1	A	288	VAL
1	A	292	ALA
1	A	432	LYS
1	A	453	GLU
1	A	468	VAL
1	A	486	ASP
1	A	499	GLU
1	A	507	LYS
1	A	525	ASP
1	A	526	ARG
1	A	560	PHE
1	A	571	TYR
1	A	579	ALA
1	A	628	GLY
1	A	653	ARG
1	A	700	ALA
1	A	762	SER
1	A	805	ARG
1	A	820	ARG

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Mol	Chain	Res	Type
2	B	341	GLU
2	B	401	ASP
1	A	256	LEU
1	A	257	GLU
1	A	272	PRO
1	A	289	SER
1	A	364	GLU
1	A	409	GLY
1	A	425	ASP
1	A	436	LYS
1	A	450	ASN
1	A	485	ARG
1	A	510	GLU
1	A	529	LEU
1	A	544	LEU
1	A	669	VAL
1	A	709	GLY
1	A	758	ARG
1	A	765	ALA
1	A	771	ASN
1	A	813	GLY
1	A	823	GLY
1	A	831	GLY
2	B	331	ALA
2	B	337	GLN
2	B	359	LEU
2	B	379	CYS
2	B	402	PHE
2	B	426	ARG
1	A	182	ARG
1	A	211	LEU
1	A	233	ALA
1	A	252	VAL
1	A	295	ARG
1	A	338	GLY
1	A	410	GLN
1	A	421	LYS
1	A	443	GLU
1	A	460	GLN
1	A	500	THR
1	A	627	LEU
1	A	652	GLN

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Mol	Chain	Res	Type
1	A	690	GLU
1	A	701	PRO
1	A	729	ALA
1	A	733	GLY
1	A	752	ARG
2	B	362	LYS
2	B	373	PRO
2	B	391	ALA
1	A	193	ALA
1	A	236	GLN
1	A	332	MET
1	A	369	ALA
1	A	489	ALA
1	A	535	ASN
1	A	632	GLN
1	A	812	HIS
1	A	816	LEU
1	A	819	LEU
2	B	421	PHE
1	A	391	TYR
1	A	435	VAL
1	A	442	LYS
1	A	492	LYS
1	A	725	GLY
1	A	737	SER
1	A	785	SER
2	B	392	VAL
2	B	414	VAL
1	A	222	LEU
1	A	296	GLN
2	B	439	ALA
1	A	543	PRO
1	A	301	GLY
1	A	225	PRO
2	B	408	VAL

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	566/699 (81%)	430 (76%)	136 (24%)	0 3
2	B	117/395 (30%)	101 (86%)	16 (14%)	3 17
All	All	683/1094 (62%)	531 (78%)	152 (22%)	1 4

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	VAL
1	A	179	PHE
1	A	181	SER
1	A	195	CYS
1	A	205	GLN
1	A	212	PHE
1	A	226	LYS
1	A	227	ILE
1	A	234	THR
1	A	235	LEU
1	A	237	GLN
1	A	238	LEU
1	A	244	SER
1	A	246	THR
1	A	247	VAL
1	A	256	LEU
1	A	257	GLU
1	A	267	TYR
1	A	271	LYS
1	A	275	THR
1	A	278	THR
1	A	282	ILE
1	A	296	GLN
1	A	297	LEU
1	A	298	GLN
1	A	305	THR
1	A	306	LEU
1	A	310	ARG
1	A	312	ARG
1	A	319	THR
1	A	324	ASN
1	A	326	VAL
1	A	335	THR
1	A	349	VAL

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Mol	Chain	Res	Type
1	A	351	MET
1	A	356	ILE
1	A	359	LYS
1	A	364	GLU
1	A	376	GLU
1	A	377	MET
1	A	402	ASN
1	A	404	LYS
1	A	407	SER
1	A	418	LEU
1	A	423	VAL
1	A	429	GLU
1	A	432	LYS
1	A	437	THR
1	A	438	GLN
1	A	449	VAL
1	A	453	GLU
1	A	455	ILE
1	A	457	GLU
1	A	458	LEU
1	A	463	LYS
1	A	466	SER
1	A	467	GLU
1	A	469	LYS
1	A	472	ARG
1	A	475	THR
1	A	486	ASP
1	A	490	LEU
1	A	492	LYS
1	A	505	GLU
1	A	508	LEU
1	A	511	LEU
1	A	514	ASN
1	A	517	SER
1	A	518	ASP
1	A	519	VAL
1	A	522	SER
1	A	523	SER
1	A	524	ARG
1	A	526	ARG
1	A	530	ASP
1	A	535	ASN

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Mol	Chain	Res	Type
1	A	536	LEU
1	A	538	PHE
1	A	542	THR
1	A	544	LEU
1	A	548	SER
1	A	550	LYS
1	A	556	ASP
1	A	557	ASP
1	A	563	SER
1	A	566	THR
1	A	568	ARG
1	A	571	TYR
1	A	572	SER
1	A	576	VAL
1	A	588	THR
1	A	591	ARG
1	A	595	TYR
1	A	605	VAL
1	A	611	SER
1	A	613	THR
1	A	623	CYS
1	A	627	LEU
1	A	632	GLN
1	A	637	VAL
1	A	642	PRO
1	A	645	GLU
1	A	647	LYS
1	A	653	ARG
1	A	656	PHE
1	A	659	LEU
1	A	662	VAL
1	A	663	VAL
1	A	667	ASP
1	A	677	LEU
1	A	683	SER
1	A	684	THR
1	A	685	THR
1	A	702	ILE
1	A	706	LEU
1	A	714	ILE
1	A	724	VAL
1	A	726	ARG

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Mol	Chain	Res	Type
1	A	727	CYS
1	A	730	ILE
1	A	747	VAL
1	A	758	ARG
1	A	762	SER
1	A	768	SER
1	A	772	ASP
1	A	775	LEU
1	A	778	GLN
1	A	780	ILE
1	A	786	ILE
1	A	793	ILE
1	A	795	ARG
1	A	801	GLU
1	A	817	SER
1	A	821	GLU
1	A	833	MET
1	A	835	THR
2	B	314	MET
2	B	316	LEU
2	B	332	THR
2	B	337	GLN
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	351	ASN
2	B	359	LEU
2	B	375	VAL
2	B	377	GLN
2	B	385	THR
2	B	422	VAL
2	B	423	ASN
2	B	430	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	224	ASN
1	A	237	GLN
1	A	395	GLN

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Mol	Chain	Res	Type
1	A	399	ASN
1	A	410	GLN
1	A	419	GLN
1	A	438	GLN
1	A	460	GLN
1	A	484	HIS
1	A	509	GLN
1	A	535	ASN
1	A	540	ASN
1	A	551	HIS
1	A	612	GLN
1	A	812	HIS
2	B	337	GLN
2	B	348	GLN
2	B	419	ASN
2	B	423	ASN

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	M84	A	901	3	20,20,21	0.74	0	25,25,27	0.90	1 (4%)
3	FAD	A	900	4	51,58,58	2.94	10 (19%)	60,89,89	2.73	18 (30%)

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
4	M84	A	901	3	-	4/11/12/13	0/2/2/2
3	FAD	A	900	4	-	6/30/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C2A-N3A	10.80	1.49	1.32
3	A	900	FAD	C4X-N5	10.26	1.47	1.33
3	A	900	FAD	C2A-N1A	8.12	1.49	1.33
3	A	900	FAD	C4X-C10	7.44	1.46	1.38
3	A	900	FAD	O4-C4	4.32	1.35	1.24
3	A	900	FAD	C9A-N10	4.28	1.44	1.38
3	A	900	FAD	C5X-N5	3.37	1.40	1.35
3	A	900	FAD	C4-C4X	3.27	1.47	1.41
3	A	900	FAD	C4A-N3A	-2.42	1.32	1.35
3	A	900	FAD	C2-N3	-2.13	1.33	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	N3A-C2A-N1A	-8.17	115.91	128.68
3	A	900	FAD	C4-C4X-C10	-7.36	115.08	119.95
3	A	900	FAD	C1'-N10-C9A	7.34	124.07	118.29
3	A	900	FAD	C4-N3-C2	6.97	121.03	115.14
3	A	900	FAD	O4B-C1B-C2B	-6.39	97.58	106.93
3	A	900	FAD	P-O3P-PA	-4.87	116.11	132.83
3	A	900	FAD	C4X-C10-N10	-4.31	115.87	120.30
3	A	900	FAD	C1'-N10-C10	-4.27	114.59	118.41
3	A	900	FAD	C9A-N10-C10	-3.57	117.23	121.91
3	A	900	FAD	C5X-C9A-N10	3.54	120.28	117.72
3	A	900	FAD	C5A-C6A-N6A	-3.07	115.69	120.35
3	A	900	FAD	O4'-C4'-C5'	-2.89	103.42	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	C4X-C4-N3	-2.84	119.55	123.43
3	A	900	FAD	O2P-P-O1P	2.66	125.38	112.24
3	A	900	FAD	O5B-PA-O1A	-2.38	99.78	109.07
3	A	900	FAD	O2A-PA-O1A	2.23	123.29	112.24
3	A	900	FAD	N6A-C6A-N1A	2.19	123.12	118.57
4	A	901	M84	C3B-CB1-CB2	-2.13	115.84	121.23
3	A	900	FAD	C4A-C5A-N7A	-2.05	107.26	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	M84	O4B-C4B-NB4-CB4
4	A	901	M84	CW2-C4B-NB4-CB4
3	A	900	FAD	P-O3P-PA-O1A
3	A	900	FAD	O3'-C3'-C4'-C5'
3	A	900	FAD	C2'-C3'-C4'-C5'
3	A	900	FAD	PA-O3P-P-O5'
3	A	900	FAD	P-O3P-PA-O2A
4	A	901	M84	C2B-C3B-CB1-CB6
4	A	901	M84	C2B-C3B-CB1-CB2
3	A	900	FAD	O4B-C4B-C5B-O5B

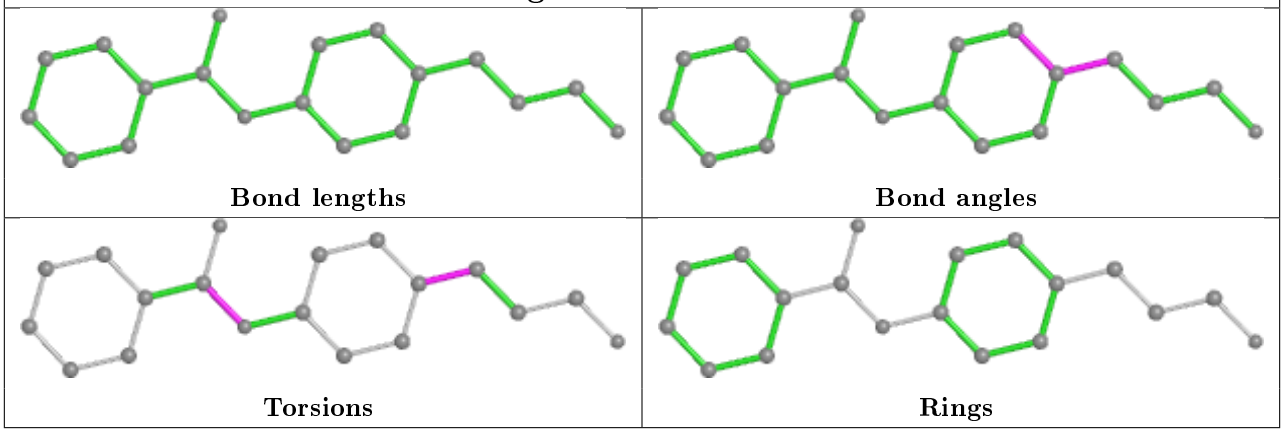
There are no ring outliers.

2 monomers are involved in 9 short contacts:

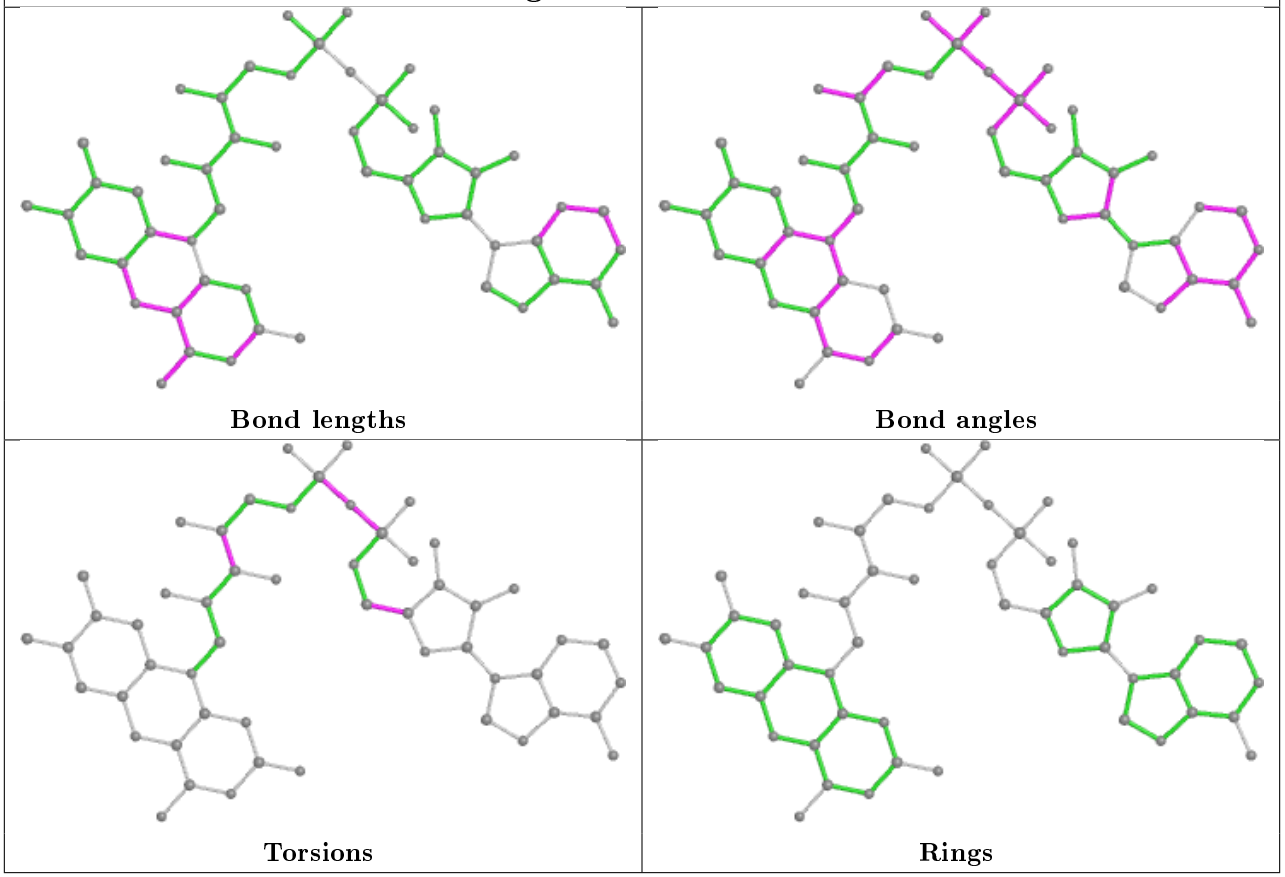
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	M84	6	0
3	A	900	FAD	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand M84 A 901



Ligand FAD A 900



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	666/852 (78%)	0.26	2 (0%)	94	92	43, 88, 117, 139	0
2	B	133/482 (27%)	0.26	1 (0%)	86	78	81, 116, 135, 140	0
All	All	799/1334 (59%)	0.26	3 (0%)	92	89	43, 92, 126, 140	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.0
2	B	383	TRP	2.2
1	A	504	LEU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

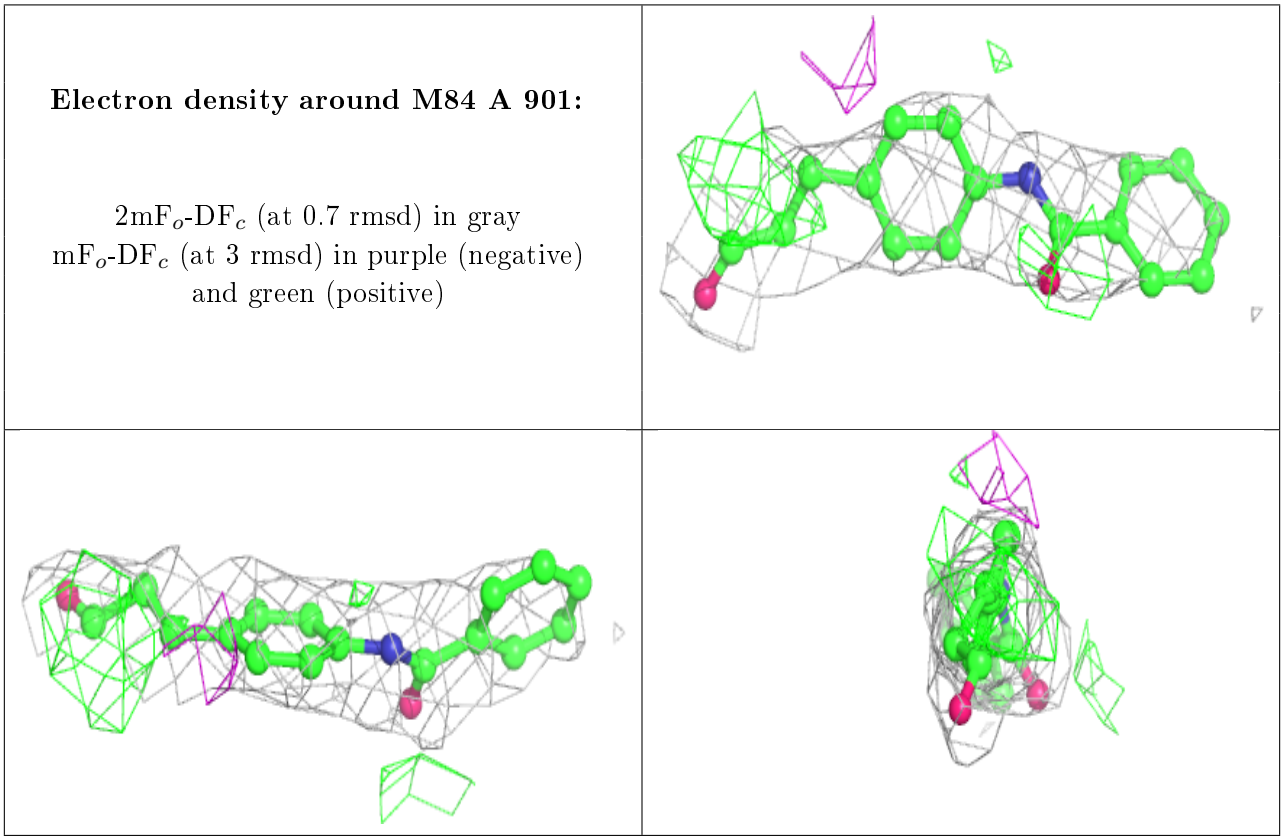
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	M84	A	901	19/20	0.95	0.45	89,108,123,124	0
3	FAD	A	900	53/53	0.98	0.26	50,68,88,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

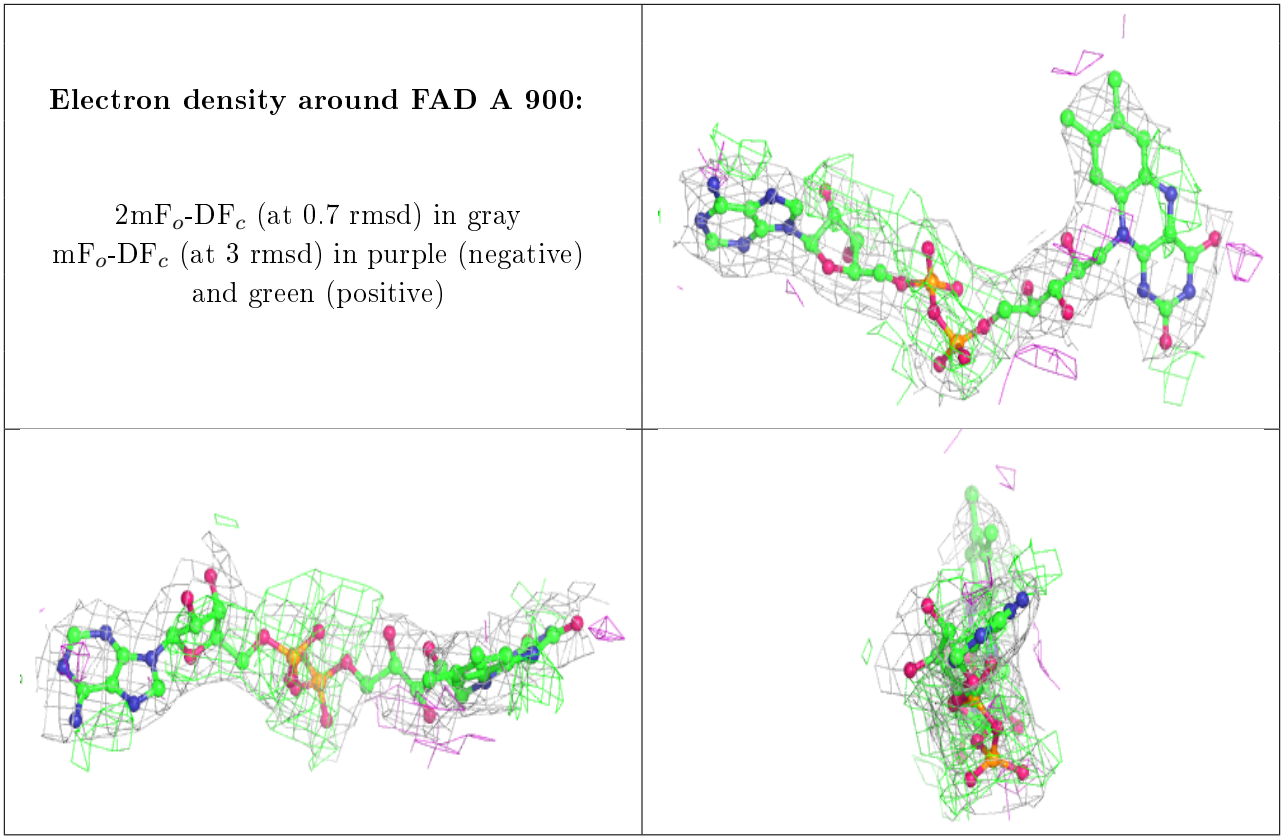
Electron density around M84 A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.