



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:01 AM UTC

PDB ID : 1NDI / pdb_00001ndi
Title : Carnitine Acetyltransferase in complex with CoA
Authors : Jogl, G.; Tong, L.
Deposited on : 2002-12-09
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

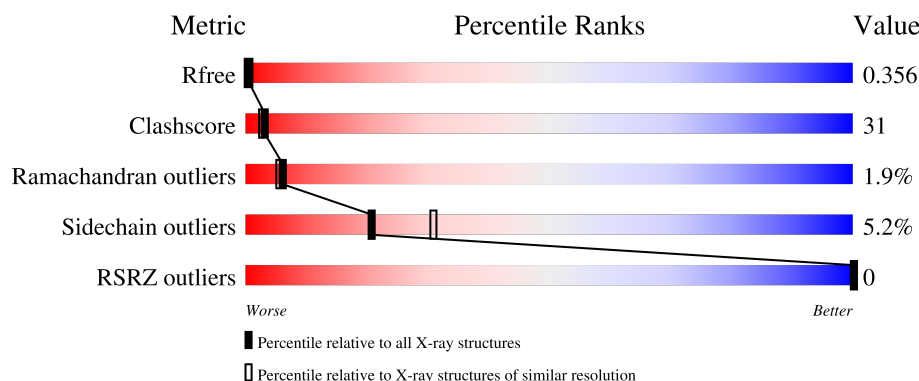
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of 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 $\leq 5\%$. 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	596	
1	B	596	

2 Entry composition ⓘ

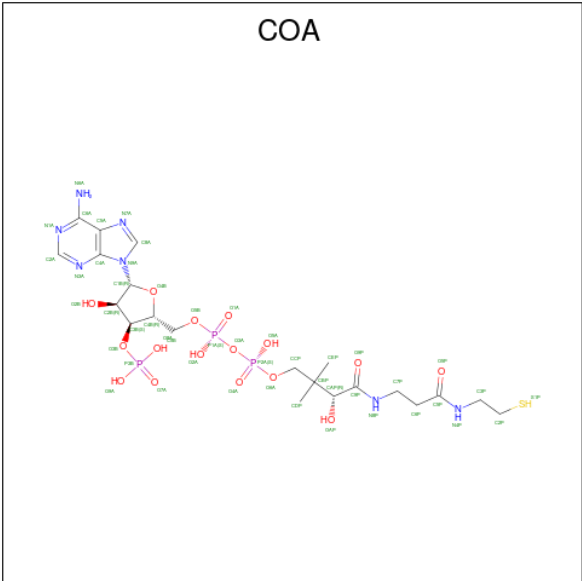
There are 3 unique types of molecules in this entry. The entry contains 10303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carnitine Acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			
1	B	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	B	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

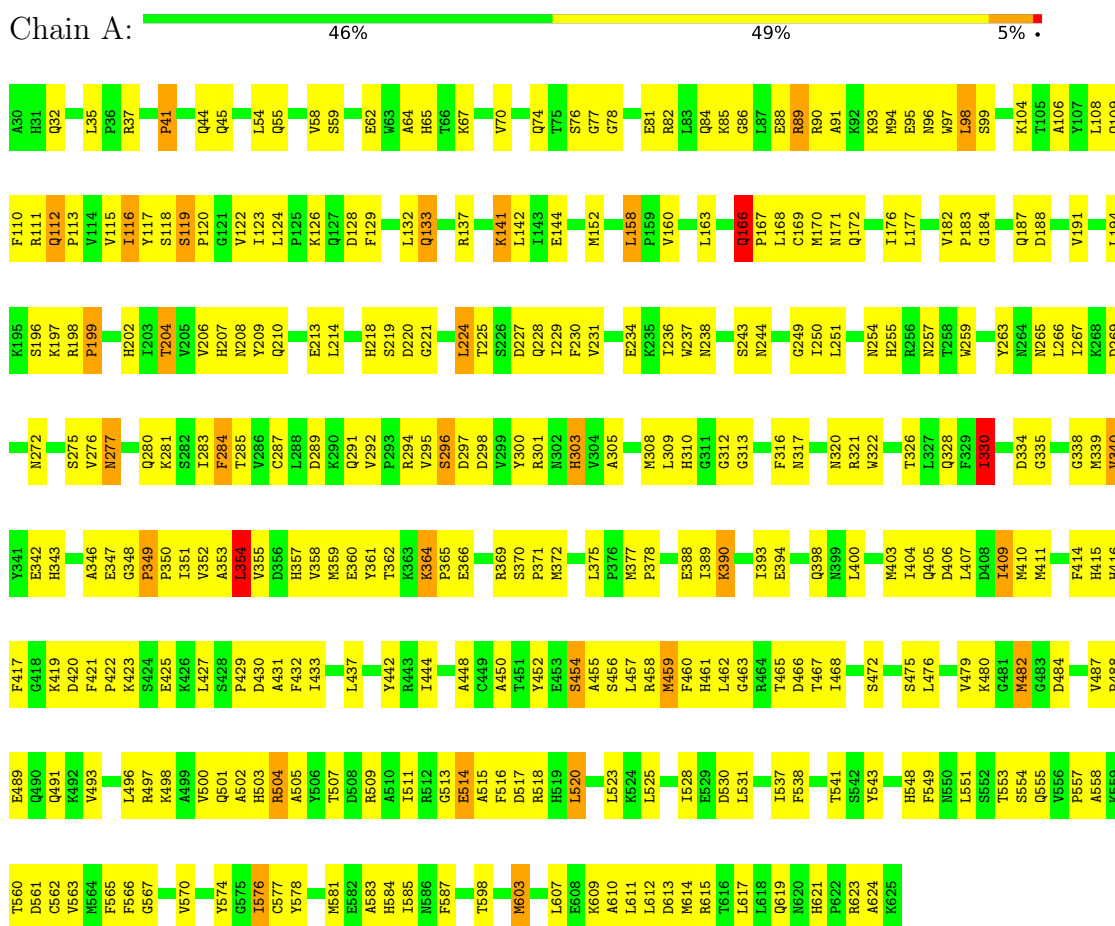
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	342	Total 342	O 342	0	0
3	B	351	Total 351	O 351	0	0

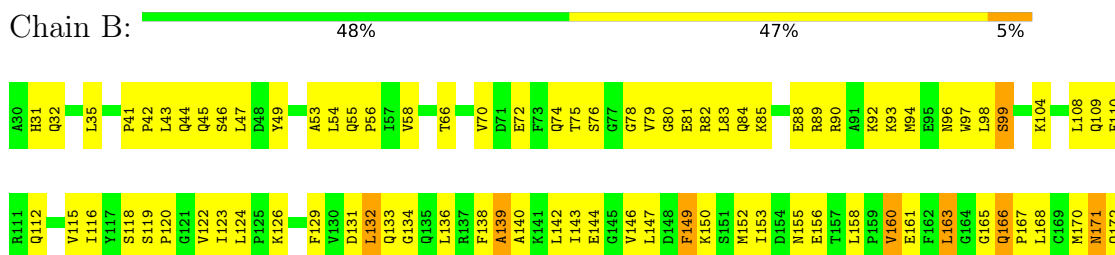
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Carnitine Acetyltransferase



• Molecule 1: Carnitine Acetyltransferase



E582	K492	H415	E342	D269	Y173
T585	V493	H416	H343	K270	Y174
N586	E494	F417	A344	N271	Q175
F587	L495	L496	A345	V272	I176
S588	L496	D420	A346	L177	L177
V589	V500	F421	E347	S178	S178
		P422	G348		
			P349		
			P350		
			P351		
			P352		
			P353		
			P354		
			P355		
			P356		
			P357		
			P358		
			P359		
			P360		
			P361		
			P362		
			P363		
			P364		
			P365		
			P366		
			P367		
			P368		
			P369		
			P370		
			P371		
			P372		
			P373		
			P374		
			P375		
			P376		
			P377		
			P378		
			P379		
			P380		
			P381		
			P382		
			P383		
			P384		
			P385		
			P386		
			P387		
			P388		
			P389		
			P390		
			P391		
			P392		
			P393		
			P394		
			P395		
			P396		
			P397		
			P398		
			P399		
			P400		
			P401		
			P402		
			P403		
			P404		
			P405		
			P406		
			P407		
			P408		
			P409		
			P410		
			P411		
			P412		
			P413		
			P414		
			P415		
			P416		
			P417		
			P418		
			P419		
			P420		
			P421		
			P422		
			P423		
			P424		
			P425		
			P426		
			P427		
			P428		
			P429		
			P430		
			P431		
			P432		
			P433		
			P434		
			P435		
			P436		
			P437		
			P438		
			P439		
			P440		
			P441		
			P442		
			P443		
			P444		
			P445		
			P446		
			P447		
			P448		
			P449		
			P450		
			P451		
			P452		
			P453		
			P454		
			P455		
			P456		
			P457		
			P458		
			P459		
			P460		
			P461		
			P462		
			P463		
			P464		
			P465		
			P466		
			P467		
			P468		
			P469		
			P470		
			P471		
			P472		
			P473		
			P474		
			P475		
			P476		
			P477		
			P478		
			P479		
			P480		
			P481		
			P482		
			P483		
			P484		
			P485		
			P486		
			P487		
			P488		
			P489		
			P490		
			P491		
			P492		
			P493		
			P494		
			P495		
			P496		
			P497		
			P498		
			P499		
			P500		
			P501		
			P502		
			P503		
			P504		
			P505		
			P506		
			P507		
			P508		
			P509		
			P510		
			P511		
			P512		
			P513		
			P514		
			P515		
			P516		
			P517		
			P518		
			P519		
			P520		
			P521		
			P522		
			P523		
			P524		
			P525		
			P526		
			P527		
			P528		
			P529		
			P530		
			P531		
			P532		
			P533		
			P534		
			P535		
			P536		
			P537		
			P538		
			P539		
			P540		
			P541		
			P542		
			P543		
			P544		
			P545		
			P546		
			P547		
			P548		
			P549		
			P550		
			P551		
			P552		
			P553		
			P554		
			P555		
			P556		
			P557		
			P558		
			P559		
			P560		
			P561		
			P562		
			P563		
			P564		
			P565		
			P566		
			P567		
			P568		
			P569		
			P570		
			P571		
			P572		
			P573		
			P574		
			P575		
			P576		
			P577		
			P578		
			P579		
			P580		
			P581		
			P582		
			P583		
			P584		
			P585		
			P586		
			P587		
			P588		
			P589		
			P590		
			P591		
			P592		
			P593		
			P594		
			P595		
			P596		
			P597		
			P598		
			P599		
			P600		
			P601		
			P602		
			P603		
			P604		
			P605		
			P606		
			P607		
			P608		
			P609		
			P610		
			P611		
			P612		
			P613		
			P614		
			P615		
			P616		
			P617		
			P618		
			P619		
			P620		
			P621		
			P622		
			P623		
			P624		
			P625		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.26Å 92.05Å 122.90Å 90.00° 128.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-2.30) 76.6 (30.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.270 , 0.363 0.271 , 0.356	Depositor DCC
R_{free} test set	4090 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10303	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0.57	1/4872 (0.0%)	1.01	19/6600 (0.3%)
1	B	0.61	1/4872 (0.0%)	1.00	19/6600 (0.3%)
All	All	0.59	2/9744 (0.0%)	1.01	38/13200 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	ILE	CA-CB	7.25	1.65	1.54
1	A	41	PRO	CA-C	5.83	1.55	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	-7.87	104.28	114.04
1	B	353	ALA	N-CA-C	-7.37	104.09	113.23
1	A	119	SER	CA-C-N	6.84	127.09	119.90
1	A	119	SER	C-N-CA	6.84	127.09	119.90
1	B	364	LYS	CA-C-N	6.27	126.29	119.89
1	B	364	LYS	C-N-CA	6.27	126.29	119.89
1	B	343	HIS	N-CA-C	6.18	120.08	112.54
1	B	176	ILE	N-CA-C	6.04	116.21	110.53
1	A	353	ALA	N-CA-C	-6.00	106.00	113.15
1	B	578	TYR	N-CA-C	5.91	118.09	108.76
1	A	576	ILE	N-CA-C	5.85	116.42	107.77
1	A	182	VAL	CA-C-N	5.79	127.35	120.23
1	A	182	VAL	C-N-CA	5.79	127.35	120.23
1	B	582	GLU	N-CA-C	5.73	117.99	111.11
1	B	166	GLN	CA-C-N	5.65	125.56	119.85
1	B	166	GLN	C-N-CA	5.65	125.56	119.85
1	B	553	THR	N-CA-C	5.61	118.22	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ILE	N-CA-C	5.53	115.56	107.37
1	A	128	ASP	N-CA-C	5.52	120.02	113.28
1	A	106	ALA	N-CA-C	5.51	118.21	111.82
1	A	343	HIS	N-CA-C	5.47	118.00	111.71
1	B	171	ASN	N-CA-C	5.45	117.98	111.71
1	A	339	MET	N-CA-C	5.40	115.36	108.24
1	B	594	SER	N-CA-C	-5.35	106.45	112.87
1	A	370	SER	CA-C-N	5.34	126.51	119.84
1	A	370	SER	C-N-CA	5.34	126.51	119.84
1	A	364	LYS	CA-C-N	5.33	126.50	119.84
1	A	364	LYS	C-N-CA	5.33	126.50	119.84
1	B	458	ARG	N-CA-C	5.30	119.23	112.87
1	B	466	ASP	N-CA-C	-5.29	102.36	110.14
1	B	539	MET	N-CA-C	-5.25	106.26	113.30
1	A	166	GLN	CA-C-N	5.12	125.03	119.85
1	A	166	GLN	C-N-CA	5.12	125.03	119.85
1	B	153	ILE	N-CA-C	-5.12	106.81	111.67
1	B	550	ASN	N-CA-C	-5.10	105.84	111.71
1	B	149	PHE	N-CA-C	-5.10	105.36	112.45
1	A	346	ALA	N-CA-C	5.08	115.23	108.38
1	B	505	ALA	N-CA-C	-5.01	105.90	111.36

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	4757	0	4733	293	0
1	B	4757	0	4733	299	0
2	A	48	0	32	5	0
2	B	48	0	32	7	0
3	A	342	0	0	31	0
3	B	351	0	0	53	0
All	All	10303	0	9530	595	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 31.

All (595) 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:410:MET:HG2	1:B:601:ALA:HA	1.36	1.05
1:B:585:ILE:HG22	3:B:6421:HOH:O	1.60	1.02
1:A:90:ARG:HD3	1:A:97:TRP:HB2	1.44	0.98
1:A:32:GLN:HE22	1:A:170:MET:H	1.15	0.93
1:A:310:HIS:HD2	1:A:312:GLY:H	1.15	0.90
1:B:132:LEU:HD22	1:B:132:LEU:H	1.37	0.89
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.56	0.88
1:A:287:CYS:HB2	1:A:330:ILE:HG22	1.57	0.86
1:B:398:GLN:HB2	3:B:6312:HOH:O	1.75	0.84
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.58	0.84
1:B:150:LYS:HE3	1:B:283:ILE:HG12	1.61	0.82
1:B:330:ILE:HG23	3:B:6202:HOH:O	1.77	0.82
1:B:202:HIS:ND1	1:B:213:GLU:HG3	1.95	0.81
1:B:348:GLY:H	2:B:6170:COA:H32	1.47	0.79
1:A:414:PHE:CE1	1:A:416:HIS:HD2	1.99	0.79
1:B:96:ASN:HB3	1:B:99:SER:OG	1.81	0.79
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.65	0.79
1:A:450:ALA:HB3	1:A:548:HIS:O	1.84	0.78
1:B:90:ARG:HG2	1:B:94:MET:HE2	1.65	0.77
1:B:451:THR:HG23	1:B:551:LEU:HB3	1.66	0.77
1:B:431:ALA:HB2	3:B:6348:HOH:O	1.85	0.76
1:B:315:LYS:H	1:B:315:LYS:HD3	1.51	0.76
1:B:94:MET:HE3	1:B:97:TRP:HA	1.68	0.76
1:B:410:MET:HB2	3:B:6384:HOH:O	1.85	0.76
1:A:85:LYS:HG3	1:A:89:ARG:HH12	1.52	0.75
1:A:398:GLN:HG3	3:A:5300:HOH:O	1.88	0.74
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.24	0.72
1:B:47:LEU:HD13	1:B:74:GLN:HB3	1.70	0.72
1:B:120:PRO:HB2	1:B:341:TYR:HE2	1.52	0.72
1:A:520:LEU:HD13	1:A:538:PHE:HE2	1.54	0.72
1:B:553:THR:HG22	1:B:576:ILE:HB	1.71	0.72
1:A:309:LEU:HB2	1:A:565:PHE:HE1	1.55	0.71
1:B:177:LEU:HD22	1:B:283:ILE:HG22	1.72	0.71
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.72	0.71
1:A:141:LYS:HD2	1:A:362:THR:HA	1.73	0.70
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.26	0.70
1:B:204:THR:HG21	1:B:279:ILE:HG12	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:HG3	1:B:245:LYS:HE2	1.72	0.70
1:B:602:ARG:HD3	3:B:6287:HOH:O	1.92	0.70
1:B:410:MET:HG2	1:B:601:ALA:CA	2.19	0.69
1:A:221:GLY:HA3	3:A:5189:HOH:O	1.93	0.69
1:B:150:LYS:HD2	1:B:283:ILE:HG21	1.75	0.69
1:A:511:ILE:HD11	2:A:5170:COA:H143	1.72	0.69
1:A:171:ASN:HB2	3:A:5235:HOH:O	1.92	0.69
1:A:204:THR:HB	1:A:285:THR:HG23	1.73	0.69
1:B:394:GLU:O	1:B:398:GLN:HG3	1.92	0.69
1:B:166:GLN:HG2	3:B:6183:HOH:O	1.92	0.69
1:B:340:VAL:HB	3:B:6174:HOH:O	1.92	0.69
1:B:361:TYR:HA	1:B:364:LYS:HD2	1.75	0.69
1:B:120:PRO:HB2	1:B:341:TYR:CE2	2.29	0.68
1:B:225:THR:H	1:B:228:GLN:NE2	1.92	0.68
1:B:171:ASN:ND2	1:B:175:GLN:HE21	1.92	0.67
1:A:225:THR:H	1:A:228:GLN:NE2	1.92	0.67
1:B:322:TRP:H	1:B:328:GLN:NE2	1.93	0.67
1:A:110:PHE:CE2	1:A:112:GLN:HB2	2.30	0.67
1:A:584:HIS:C	1:A:585:ILE:HG13	2.20	0.67
1:B:509:ARG:HB3	1:B:514:GLU:HB2	1.76	0.67
1:A:163:LEU:HB2	1:A:168:LEU:HD21	1.77	0.67
1:B:142:LEU:O	1:B:146:VAL:HG23	1.95	0.67
1:B:308:MET:C	3:B:6174:HOH:O	2.37	0.66
1:B:578:TYR:HB2	3:B:6421:HOH:O	1.94	0.66
1:B:609:LYS:NZ	1:B:613:ASP:OD1	2.28	0.66
1:A:202:HIS:O	1:A:283:ILE:HG13	1.96	0.66
1:B:213:GLU:HB2	1:B:381:LEU:HD21	1.76	0.66
2:B:6170:COA:H141	2:B:6170:COA:O9P	1.95	0.66
1:B:98:LEU:HD21	1:B:518:ARG:HD2	1.77	0.66
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.77	0.66
1:A:295:VAL:HG12	1:A:296:SER:H	1.60	0.66
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.76	0.66
1:A:218:HIS:C	1:A:220:ASP:H	2.05	0.65
1:B:143:ILE:HG13	3:B:6342:HOH:O	1.95	0.65
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.32	0.65
1:B:225:THR:H	1:B:228:GLN:HE21	1.43	0.65
1:B:601:ALA:HB2	3:B:6384:HOH:O	1.96	0.65
1:A:166:GLN:HG3	1:A:459:MET:HE2	1.79	0.65
1:A:117:TYR:CE1	1:A:403:MET:HE3	2.32	0.64
1:A:525:LEU:HD23	1:A:528:ILE:HD12	1.79	0.64
1:B:123:ILE:HD12	1:B:411:MET:HE2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:MET:HE1	1:B:330:ILE:HG21	1.80	0.64
1:B:459:MET:HG2	3:B:6375:HOH:O	1.96	0.64
1:A:54:LEU:O	1:A:58:VAL:HG22	1.98	0.64
1:A:390:LYS:O	1:A:394:GLU:HG2	1.97	0.63
1:B:577:CYS:N	3:B:6224:HOH:O	2.32	0.63
1:A:310:HIS:CD2	1:A:312:GLY:H	2.07	0.63
1:B:528:ILE:HD11	1:B:534:MET:HE1	1.80	0.63
1:B:247:PRO:HB2	1:B:319:GLY:HA3	1.79	0.63
1:B:476:LEU:HG	1:B:480:LYS:HE3	1.79	0.63
1:B:326:THR:HA	1:B:342:GLU:HB2	1.81	0.62
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.64	0.62
1:A:390:LYS:HB2	1:A:390:LYS:NZ	2.15	0.62
1:A:482:MET:HE1	1:A:617:LEU:HD22	1.82	0.62
1:A:198:ARG:HH12	1:A:281:LYS:NZ	1.97	0.62
1:B:231:VAL:HG21	1:B:372:MET:HE3	1.81	0.61
1:B:440:ALA:O	1:B:444:ILE:HG13	1.99	0.61
1:B:271:VAL:HG22	3:B:6326:HOH:O	1.99	0.61
1:B:75:THR:O	1:B:81:GLU:HG3	2.01	0.61
1:B:76:SER:C	1:B:78:GLY:H	2.08	0.61
1:B:178:SER:HA	1:B:282:SER:O	1.99	0.61
1:B:94:MET:SD	3:B:6210:HOH:O	2.56	0.61
1:B:124:LEU:HB2	1:B:337:CYS:SG	2.41	0.61
1:B:202:HIS:O	1:B:283:ILE:HD12	1.99	0.61
1:B:227:ASP:HB3	1:B:372:MET:HE1	1.82	0.61
1:A:85:LYS:CG	1:A:89:ARG:HH12	2.14	0.61
1:A:389:ILE:O	1:A:393:ILE:HG13	2.01	0.61
1:B:90:ARG:CG	1:B:94:MET:HE2	2.31	0.61
1:A:152:MET:HB3	1:A:158:LEU:HD12	1.82	0.61
1:B:206:VAL:HA	1:B:210:GLN:O	2.01	0.61
1:A:294:ARG:HG3	1:A:294:ARG:HH11	1.65	0.61
1:A:420:ASP:OD2	1:A:583:ALA:HA	2.01	0.61
1:B:308:MET:HE1	1:B:330:ILE:CG2	2.31	0.60
1:A:44:GLN:HB3	3:A:5195:HOH:O	2.02	0.60
1:A:421:PHE:CE1	1:A:615:ARG:HG3	2.36	0.60
1:B:161:GLU:H	1:B:170:MET:HE3	1.65	0.60
1:B:322:TRP:H	1:B:328:GLN:HE22	1.48	0.60
1:B:276:VAL:O	1:B:280:GLN:HG3	2.01	0.60
1:A:32:GLN:NE2	1:A:170:MET:H	1.95	0.59
1:A:358:VAL:HG12	1:A:359:MET:HE2	1.83	0.59
1:B:354:LEU:O	1:B:358:VAL:HG23	2.02	0.59
1:A:231:VAL:HG21	1:A:372:MET:HE2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ALA:HB1	3:A:5426:HOH:O	2.01	0.59
1:A:184:GLY:HA3	1:A:187:GLN:O	2.03	0.59
1:A:612:LEU:HD23	1:A:615:ARG:HH21	1.67	0.59
1:A:349:PRO:HB2	1:A:350:PRO:CD	2.31	0.58
1:B:104:LYS:O	1:B:109:GLN:HB2	2.03	0.58
1:A:54:LEU:HD22	1:A:58:VAL:HG11	1.86	0.58
1:B:524:LYS:HG3	1:B:534:MET:SD	2.43	0.58
1:B:133:GLN:HG3	1:B:134:GLY:N	2.17	0.58
1:B:400:LEU:O	1:B:404:ILE:HG13	2.03	0.58
1:A:214:LEU:HB2	1:A:236:ILE:HD11	1.85	0.58
1:A:557:PRO:HB3	3:A:5430:HOH:O	2.03	0.58
1:A:297:ASP:HA	1:A:300:TYR:HB2	1.86	0.58
1:B:242:GLN:HB2	1:B:244:ASN:OD1	2.04	0.58
1:A:561:ASP:OD1	1:A:581:MET:HE2	2.04	0.58
1:B:431:ALA:CB	1:B:500:VAL:HG13	2.34	0.58
1:A:463:GLY:HA2	3:A:5332:HOH:O	2.04	0.57
1:A:59:SER:HB3	1:A:62:GLU:HG3	1.86	0.57
1:A:84:GLN:O	1:A:88:GLU:HG3	2.04	0.57
1:B:407:LEU:HD12	1:B:408:ASP:H	1.69	0.57
1:A:461:HIS:CD2	1:A:462:LEU:HG	2.39	0.57
1:A:598:THR:HG21	3:A:5233:HOH:O	2.03	0.57
1:A:610:ALA:O	1:A:614:MET:HG3	2.04	0.57
1:B:414:PHE:CE1	1:B:608:GLU:HG3	2.40	0.57
1:A:194:LEU:HD22	3:A:5207:HOH:O	2.05	0.57
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.40	0.57
1:A:489:GLU:O	1:A:493:VAL:HG23	2.05	0.57
1:A:530:ASP:O	1:A:531:LEU:HB2	2.04	0.57
1:B:461:HIS:CE1	1:B:462:LEU:HD12	2.40	0.57
2:B:6170:COA:O2A	2:B:6170:COA:H8A	2.05	0.56
1:A:615:ARG:HG2	1:A:619:GLN:NE2	2.20	0.56
1:B:138:PHE:C	1:B:140:ALA:H	2.13	0.56
1:A:454:SER:HB2	1:A:554:SER:HB3	1.87	0.56
1:A:455:ALA:HB2	1:A:468:ILE:CD1	2.35	0.56
1:B:488:PRO:HB3	3:B:6240:HOH:O	2.05	0.56
1:A:472:SER:H	1:A:475:SER:HB3	1.70	0.56
1:B:132:LEU:HD12	1:B:237:TRP:CZ2	2.40	0.56
1:A:501:GLN:HE22	1:A:504:ARG:HD3	1.70	0.56
1:A:78:GLY:HA2	3:A:5240:HOH:O	2.04	0.56
1:B:160:VAL:HG23	3:B:6483:HOH:O	2.06	0.56
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.70	0.56
1:B:609:LYS:NZ	1:B:613:ASP:CG	2.64	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:OE1	1:B:346:ALA:HB1	2.05	0.56
1:A:98:LEU:HD12	1:A:98:LEU:O	2.05	0.55
1:B:377:MET:HE3	1:B:378:PRO:HD2	1.88	0.55
1:B:595:CYS:SG	1:B:598:THR:HG23	2.46	0.55
1:A:218:HIS:HB2	1:A:220:ASP:OD1	2.07	0.55
1:B:295:VAL:HG11	1:B:303:HIS:CD2	2.42	0.55
1:B:414:PHE:HE1	1:B:608:GLU:HG3	1.71	0.55
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.87	0.55
1:B:195:LYS:HB3	3:B:6260:HOH:O	2.06	0.55
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.70	0.55
1:A:351:ILE:O	1:A:355:VAL:HG23	2.06	0.55
1:B:242:GLN:HG3	1:B:245:LYS:CE	2.37	0.55
1:B:122:VAL:HG22	1:B:564:MET:HG3	1.88	0.55
1:B:126:LYS:NZ	1:B:334:ASP:O	2.35	0.55
1:A:431:ALA:HA	1:A:503:HIS:CE1	2.41	0.55
1:B:166:GLN:NE2	1:B:459:MET:HE1	2.22	0.55
1:B:482:MET:HA	1:B:492:LYS:HD3	1.89	0.55
1:B:43:LEU:HD13	1:B:84:GLN:HB2	1.88	0.55
1:B:231:VAL:O	1:B:235:LYS:HG3	2.06	0.55
1:A:85:LYS:HG3	1:A:89:ARG:NH1	2.20	0.54
1:A:122:VAL:O	1:A:308:MET:HG2	2.06	0.54
1:A:227:ASP:HA	3:A:5205:HOH:O	2.06	0.54
1:A:250:ILE:HD11	1:A:400:LEU:HD23	1.90	0.54
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.43	0.54
1:B:354:LEU:C	1:B:354:LEU:HD23	2.33	0.54
1:B:321:ARG:HH21	1:B:330:ILE:HD13	1.72	0.54
1:B:333:GLU:CD	1:B:333:GLU:C	2.76	0.54
1:B:578:TYR:HD2	1:B:580:PRO:HG3	1.73	0.54
1:A:501:GLN:NE2	1:A:504:ARG:HD3	2.23	0.53
1:B:143:ILE:O	1:B:147:LEU:HG	2.07	0.53
1:A:537:ILE:HG23	1:A:538:PHE:N	2.22	0.53
1:B:176:ILE:HA	1:B:326:THR:HG21	1.90	0.53
1:A:313:GLY:H	1:A:404:ILE:HD13	1.72	0.53
1:A:560:THR:HB	3:A:5321:HOH:O	2.08	0.53
1:B:171:ASN:ND2	1:B:175:GLN:NE2	2.56	0.53
1:A:289:ASP:CG	1:A:321:ARG:HH12	2.16	0.53
1:B:89:ARG:HB3	3:B:6356:HOH:O	2.09	0.53
1:B:173:TYR:OH	1:B:350:PRO:HA	2.07	0.53
1:B:401:SER:O	1:B:405:GLN:HG3	2.08	0.53
1:A:198:ARG:HH12	1:A:281:LYS:HZ3	1.56	0.53
1:B:99:SER:HB2	3:B:6250:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:GLU:CD	1:B:170:MET:HE1	2.34	0.53
1:A:461:HIS:NE2	1:A:462:LEU:HG	2.23	0.53
1:B:576:ILE:HG12	1:B:589:VAL:HG22	1.91	0.53
1:A:90:ARG:NE	1:A:97:TRP:O	2.40	0.52
1:B:270:LYS:HG3	1:B:271:VAL:N	2.24	0.52
1:A:496:LEU:HD12	1:A:617:LEU:HD23	1.92	0.52
1:B:31:HIS:HA	3:B:6320:HOH:O	2.09	0.52
1:B:321:ARG:NH2	1:B:330:ILE:HD13	2.24	0.52
1:A:45:GLN:HE22	1:A:514:GLU:HG2	1.75	0.52
1:A:476:LEU:HD11	1:A:480:LYS:HE3	1.91	0.52
1:B:46:SER:HB3	1:B:516:PHE:HB2	1.92	0.52
1:B:269:ASP:OD2	1:B:384:ASN:ND2	2.41	0.52
1:B:272:ASN:O	1:B:276:VAL:HG23	2.09	0.52
1:A:96:ASN:HB3	1:A:99:SER:OG	2.09	0.52
1:A:448:ALA:HB2	1:A:476:LEU:HD13	1.92	0.52
1:B:296:SER:HB3	1:B:298:ASP:OD1	2.10	0.52
2:B:6170:COA:H132	3:B:6354:HOH:O	2.08	0.52
1:A:466:ASP:OD1	1:A:518:ARG:HG2	2.09	0.52
1:B:116:ILE:HD12	1:B:403:MET:HE2	1.91	0.52
1:B:133:GLN:HG3	1:B:134:GLY:H	1.75	0.52
1:A:357:HIS:O	1:A:360:GLU:HB3	2.10	0.52
1:A:615:ARG:O	1:A:619:GLN:HG3	2.10	0.52
1:A:104:LYS:HE3	1:A:187:GLN:HE22	1.74	0.52
1:A:124:LEU:HG	1:A:338:GLY:HA2	1.92	0.52
1:A:228:GLN:HG2	1:A:375:LEU:HD11	1.92	0.52
1:A:554:SER:HB2	2:A:5170:COA:H22	1.92	0.52
1:A:84:GLN:NE2	1:A:523:LEU:HD21	2.25	0.51
1:B:413:THR:N	3:B:6204:HOH:O	2.43	0.51
1:A:255:HIS:CD2	1:A:257:ASN:H	2.28	0.51
1:B:171:ASN:HD21	1:B:175:GLN:NE2	2.08	0.51
1:B:540:ASP:OD2	1:B:541:THR:N	2.44	0.51
1:A:41:PRO:HG3	1:A:513:GLY:O	2.10	0.51
1:A:430:ASP:HB2	1:A:555:GLN:NE2	2.25	0.51
1:A:276:VAL:O	1:A:280:GLN:HG3	2.10	0.51
1:A:287:CYS:HB3	1:A:320:ASN:HD22	1.75	0.51
1:B:212:PHE:CD1	1:B:236:ILE:HG23	2.46	0.51
1:A:227:ASP:O	1:A:231:VAL:HG23	2.10	0.51
1:A:202:HIS:ND1	1:A:213:GLU:HG3	2.25	0.51
1:A:85:LYS:HB3	3:A:5200:HOH:O	2.10	0.51
1:A:208:ASN:OD1	1:A:243:SER:HB2	2.11	0.51
1:A:456:SER:O	1:A:511:ILE:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:PHE:O	1:A:520:LEU:HB2	2.11	0.51
1:A:583:ALA:HB3	3:A:5341:HOH:O	2.09	0.51
1:A:197:LYS:C	1:A:199:PRO:HD3	2.36	0.50
1:B:84:GLN:HG3	1:B:88:GLU:OE1	2.11	0.50
1:B:104:LYS:HG3	1:B:187:GLN:NE2	2.26	0.50
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.93	0.50
1:B:263:TYR:HE1	1:B:276:VAL:HG11	1.76	0.50
1:A:361:TYR:HA	1:A:364:LYS:HE3	1.92	0.50
1:A:574:TYR:CZ	1:A:603:MET:HG3	2.46	0.50
1:A:624:ALA:HA	3:A:5351:HOH:O	2.11	0.50
1:B:287:CYS:HB2	3:B:6202:HOH:O	2.11	0.50
1:A:321:ARG:CZ	1:A:330:ILE:HG21	2.41	0.50
1:A:487:VAL:HG13	1:A:491:GLN:OE1	2.10	0.50
1:B:136:LEU:HD21	1:B:237:TRP:CE3	2.46	0.50
1:A:45:GLN:NE2	1:A:514:GLU:HG2	2.25	0.50
1:B:88:GLU:HG2	3:B:6303:HOH:O	2.11	0.50
1:B:104:LYS:CD	1:B:187:GLN:HE22	2.23	0.50
1:B:456:SER:HB2	2:B:6170:COA:H72	1.93	0.50
1:B:431:ALA:HB3	1:B:500:VAL:HG13	1.94	0.50
1:A:144:GLU:HG2	1:A:361:TYR:CZ	2.47	0.50
1:B:75:THR:HG23	1:B:78:GLY:HA3	1.93	0.50
1:B:586:ASN:C	3:B:6421:HOH:O	2.55	0.50
1:A:104:LYS:HE3	1:A:187:GLN:NE2	2.26	0.49
1:A:263:TYR:HE1	1:A:276:VAL:HG11	1.77	0.49
1:A:496:LEU:HG	1:A:614:MET:HE3	1.93	0.49
1:B:452:TYR:C	1:B:452:TYR:CD2	2.90	0.49
1:A:95:GLU:OE1	1:A:462:LEU:HD11	2.12	0.49
1:A:263:TYR:O	1:A:267:ILE:HG12	2.13	0.49
1:A:366:GLU:HA	1:A:369:ARG:HH21	1.76	0.49
1:A:404:ILE:C	1:A:406:ASP:H	2.20	0.49
1:B:70:VAL:O	1:B:74:GLN:HG2	2.12	0.49
1:A:566:PHE:CE2	1:A:577:CYS:HB2	2.46	0.49
1:A:277:ASN:O	1:A:281:LYS:HG3	2.12	0.49
1:A:410:MET:SD	3:A:5309:HOH:O	2.60	0.49
1:B:209:TYR:CD1	1:B:247:PRO:HB3	2.46	0.49
1:A:93:LYS:O	1:A:94:MET:HG3	2.13	0.49
1:A:230:PHE:O	1:A:234:GLU:HB2	2.13	0.49
1:A:548:HIS:CE1	1:A:570:VAL:HG11	2.48	0.49
1:A:553:THR:HG22	1:A:576:ILE:HB	1.95	0.49
1:B:167:PRO:HD2	3:B:6285:HOH:O	2.12	0.49
1:B:177:LEU:HD22	1:B:283:ILE:CG2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HE1	1:A:357:HIS:CD2	2.47	0.48
1:A:208:ASN:O	1:A:209:TYR:HB2	2.13	0.48
1:A:295:VAL:HG12	1:A:296:SER:N	2.25	0.48
1:A:115:VAL:C	1:A:117:TYR:H	2.20	0.48
1:A:123:ILE:O	1:A:562:CYS:HB2	2.14	0.48
1:A:355:VAL:HG12	3:A:5321:HOH:O	2.12	0.48
1:A:366:GLU:HB3	1:A:369:ARG:HE	1.78	0.48
1:A:86:GLY:HA2	1:A:89:ARG:NH2	2.28	0.48
1:A:296:SER:HB3	1:A:298:ASP:OD1	2.14	0.48
1:B:161:GLU:HB2	1:B:170:MET:HE1	1.95	0.48
1:B:528:ILE:HG22	3:B:6247:HOH:O	2.12	0.48
1:A:110:PHE:CZ	1:A:112:GLN:HB2	2.48	0.48
1:B:66:THR:O	1:B:70:VAL:HG23	2.14	0.48
1:B:270:LYS:HG3	1:B:271:VAL:H	1.76	0.48
1:B:410:MET:HE2	3:B:6334:HOH:O	2.13	0.48
1:B:509:ARG:HG3	3:B:6251:HOH:O	2.14	0.48
1:A:225:THR:H	1:A:228:GLN:HE22	1.62	0.48
1:B:110:PHE:CE2	1:B:112:GLN:HB2	2.49	0.48
1:A:108:LEU:HD22	1:A:188:ASP:O	2.12	0.48
2:A:5170:COA:O2A	2:A:5170:COA:H8A	2.14	0.48
1:B:94:MET:CE	1:B:97:TRP:HA	2.40	0.48
1:B:425:GLU:OE1	1:B:618:LEU:HD22	2.14	0.48
1:B:160:VAL:N	3:B:6263:HOH:O	2.47	0.48
1:B:601:ALA:N	3:B:6384:HOH:O	2.39	0.48
1:B:90:ARG:HB2	3:B:6280:HOH:O	2.14	0.48
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.48	0.48
1:B:453:GLU:HA	1:B:553:THR:O	2.14	0.48
1:A:169:CYS:N	1:A:458:ARG:O	2.32	0.47
1:A:255:HIS:HD2	1:A:257:ASN:H	1.60	0.47
1:B:227:ASP:O	1:B:231:VAL:HG23	2.14	0.47
1:B:310:HIS:CD2	1:B:312:GLY:H	2.31	0.47
1:B:569:VAL:HG23	1:B:570:VAL:N	2.29	0.47
1:A:496:LEU:HD21	1:A:614:MET:CE	2.44	0.47
1:A:520:LEU:CD1	1:A:538:PHE:HE2	2.26	0.47
1:B:171:ASN:N	3:B:6288:HOH:O	2.47	0.47
1:B:407:LEU:HD21	1:B:409:ILE:HD11	1.96	0.47
1:B:469:ARG:NH2	1:B:547:MET:HE2	2.29	0.47
1:A:352:VAL:C	1:A:354:LEU:H	2.22	0.47
1:A:414:PHE:CE2	1:A:611:LEU:HD13	2.49	0.47
1:B:321:ARG:HB3	1:B:328:GLN:HE22	1.78	0.47
1:A:269:ASP:HB3	1:A:272:ASN:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASP:OD1	1:A:317:ASN:HB3	2.15	0.47
1:B:80:GLY:C	1:B:82:ARG:H	2.22	0.47
1:A:65:HIS:CD2	3:A:5274:HOH:O	2.67	0.47
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.28	0.47
1:A:584:HIS:O	1:A:585:ILE:HG13	2.14	0.47
1:A:366:GLU:CB	1:A:369:ARG:HH21	2.27	0.47
1:B:455:ALA:HB2	1:B:468:ILE:CG1	2.43	0.47
1:B:514:GLU:HG2	3:B:6282:HOH:O	2.14	0.47
1:A:291:GLN:HG2	1:A:292:VAL:N	2.29	0.47
1:A:558:ALA:C	1:A:560:THR:H	2.23	0.47
1:A:581:MET:HG3	1:A:584:HIS:CE1	2.50	0.47
1:B:163:LEU:HD23	1:B:168:LEU:HD21	1.95	0.47
1:B:507:THR:O	1:B:511:ILE:HG13	2.14	0.47
1:A:502:ALA:HA	3:A:5371:HOH:O	2.15	0.47
1:A:458:ARG:HD3	3:A:5267:HOH:O	2.15	0.47
1:B:76:SER:C	1:B:78:GLY:N	2.73	0.47
1:B:300:TYR:O	1:B:304:VAL:HG23	2.15	0.47
1:A:482:MET:HE2	1:A:482:MET:HA	1.96	0.47
1:A:587:PHE:CZ	1:A:607:LEU:HD21	2.49	0.47
1:B:129:PHE:HD2	3:B:6225:HOH:O	1.98	0.47
1:A:437:LEU:HG	1:A:551:LEU:HD13	1.96	0.46
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.96	0.46
1:B:173:TYR:CZ	1:B:350:PRO:HA	2.50	0.46
1:A:207:HIS:O	1:A:208:ASN:HB2	2.15	0.46
1:B:89:ARG:HD2	3:B:6356:HOH:O	2.14	0.46
1:B:123:ILE:HD11	1:B:305:ALA:HB2	1.98	0.46
1:A:537:ILE:CG2	1:A:538:PHE:N	2.79	0.46
1:A:609:LYS:NZ	1:A:613:ASP:OD1	2.48	0.46
1:B:83:LEU:HD13	1:B:527:ALA:HB2	1.97	0.46
1:B:88:GLU:O	1:B:92:LYS:HG3	2.15	0.46
1:A:218:HIS:C	1:A:220:ASP:N	2.70	0.46
1:A:285:THR:HB	1:A:328:GLN:HG2	1.97	0.46
1:A:431:ALA:HA	1:A:503:HIS:ND1	2.30	0.46
1:A:442:TYR:OH	1:A:480:LYS:HG2	2.16	0.46
1:B:308:MET:CE	1:B:330:ILE:HG21	2.45	0.46
1:B:461:HIS:O	1:B:462:LEU:HB2	2.14	0.46
1:A:90:ARG:HG2	1:A:94:MET:SD	2.55	0.46
1:A:160:VAL:HG13	3:A:5488:HOH:O	2.15	0.46
1:B:98:LEU:O	1:B:99:SER:C	2.59	0.46
1:B:563:VAL:HB	1:B:586:ASN:HB3	1.97	0.46
1:A:123:ILE:HD11	1:A:305:ALA:CA	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:O	1:B:116:ILE:HB	2.14	0.46
1:B:118:SER:O	1:B:120:PRO:HD3	2.16	0.46
1:B:165:GLY:C	1:B:166:GLN:HG3	2.40	0.46
1:B:285:THR:OG1	1:B:325:LYS:HG2	2.16	0.46
1:A:166:GLN:N	1:A:166:GLN:CD	2.74	0.46
1:A:520:LEU:HD22	1:A:520:LEU:HA	1.67	0.46
1:B:54:LEU:O	1:B:55:GLN:C	2.58	0.46
1:B:203:ILE:HA	1:B:282:SER:HB3	1.98	0.46
1:B:210:GLN:HA	3:B:6300:HOH:O	2.14	0.46
1:A:98:LEU:HD21	1:A:518:ARG:HB3	1.98	0.46
1:A:133:GLN:HE22	1:A:137:ARG:HG3	1.81	0.46
1:A:466:ASP:HA	1:A:518:ARG:CZ	2.46	0.46
1:B:207:HIS:HD2	1:B:240:SER:O	1.98	0.46
1:B:343:HIS:CE1	3:B:6252:HOH:O	2.68	0.46
1:A:163:LEU:HD22	1:A:168:LEU:HD21	1.98	0.45
1:A:354:LEU:HD23	1:A:354:LEU:C	2.41	0.45
1:B:31:HIS:CE1	1:B:167:PRO:HB3	2.51	0.45
1:B:457:LEU:HA	3:B:6375:HOH:O	2.16	0.45
1:B:457:LEU:HG	1:B:466:ASP:HB2	1.98	0.45
1:A:90:ARG:O	1:A:94:MET:HB2	2.15	0.45
1:A:283:ILE:O	1:A:284:PHE:HB3	2.16	0.45
1:A:287:CYS:HB3	1:A:320:ASN:ND2	2.32	0.45
1:A:347:GLU:HB3	2:A:5170:COA:H32	1.98	0.45
1:A:511:ILE:HG22	1:A:511:ILE:O	2.16	0.45
1:B:85:LYS:O	1:B:89:ARG:HG3	2.17	0.45
1:B:244:ASN:O	1:B:245:LYS:HD3	2.16	0.45
1:B:420:ASP:HB3	1:B:582:GLU:O	2.16	0.45
1:B:489:GLU:HG2	1:B:617:LEU:HD11	1.98	0.45
1:B:593:ASN:C	1:B:595:CYS:N	2.74	0.45
1:B:225:THR:OG1	1:B:228:GLN:NE2	2.49	0.45
1:B:407:LEU:CD2	1:B:409:ILE:HD11	2.46	0.45
1:A:238:ASN:HA	3:A:5349:HOH:O	2.16	0.45
1:A:377:MET:SD	1:A:378:PRO:HD2	2.55	0.45
1:B:348:GLY:N	1:B:349:PRO:CD	2.79	0.45
1:A:425:GLU:O	1:A:427:LEU:HG	2.16	0.45
1:A:581:MET:HE3	1:A:584:HIS:CE1	2.51	0.45
1:B:124:LEU:HG	1:B:338:GLY:HA2	1.98	0.45
1:B:228:GLN:HE21	1:B:228:GLN:HB2	1.48	0.45
1:B:568:PRO:HD2	1:B:592:TYR:CE2	2.51	0.45
1:A:230:PHE:HB3	3:A:5205:HOH:O	2.16	0.45
1:B:41:PRO:HA	1:B:42:PRO:HD3	1.87	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HA	1:A:228:GLN:NE2	2.31	0.45
1:A:404:ILE:C	1:A:406:ASP:N	2.74	0.45
1:B:472:SER:HA	3:B:6350:HOH:O	2.16	0.45
1:B:577:CYS:SG	1:B:578:TYR:N	2.89	0.45
1:A:35:LEU:HD21	1:A:167:PRO:HB2	1.99	0.45
1:A:118:SER:O	1:A:120:PRO:HD3	2.17	0.45
1:A:475:SER:O	1:A:479:VAL:HG13	2.17	0.45
1:A:513:GLY:HA2	3:A:5254:HOH:O	2.16	0.45
1:B:44:GLN:HG2	1:B:74:GLN:OE1	2.17	0.45
1:B:429:PRO:O	1:B:433:ILE:HG13	2.17	0.45
1:A:168:LEU:HD22	1:A:458:ARG:CB	2.47	0.44
1:A:225:THR:N	1:A:228:GLN:NE2	2.61	0.44
1:A:415:HIS:CD2	1:A:416:HIS:N	2.85	0.44
1:B:32:GLN:NE2	1:B:35:LEU:HD12	2.32	0.44
1:B:132:LEU:H	1:B:132:LEU:CD2	2.16	0.44
1:B:321:ARG:NE	1:B:330:ILE:HD11	2.32	0.44
1:B:382:ARG:HG3	1:B:382:ARG:HH11	1.82	0.44
1:B:509:ARG:CB	1:B:514:GLU:HB2	2.47	0.44
1:B:459:MET:HE3	1:B:511:ILE:CG2	2.47	0.44
1:A:176:ILE:HA	1:A:326:THR:HG21	2.00	0.44
1:A:442:TYR:C	1:A:444:ILE:H	2.25	0.44
1:A:444:ILE:HD12	1:A:603:MET:HE3	1.99	0.44
1:A:555:GLN:OE1	1:A:557:PRO:HG3	2.17	0.44
1:A:612:LEU:CD2	1:A:615:ARG:HH21	2.30	0.44
1:B:98:LEU:HD22	1:B:518:ARG:HB3	2.00	0.44
1:B:155:ASN:O	1:B:156:GLU:HB2	2.17	0.44
1:B:229:ILE:HG22	1:B:233:LEU:HD11	1.99	0.44
1:A:115:VAL:HA	3:A:5179:HOH:O	2.18	0.44
1:A:177:LEU:HB2	3:A:5183:HOH:O	2.18	0.44
1:A:207:HIS:CD2	1:A:208:ASN:HD22	2.36	0.44
1:B:385:ILE:HG22	1:B:386:THR:N	2.32	0.44
1:A:70:VAL:O	1:A:74:GLN:HG2	2.17	0.44
1:A:77:GLY:HA2	1:A:81:GLU:OE1	2.17	0.44
1:A:112:GLN:HE21	1:A:113:PRO:HD3	1.83	0.44
1:A:249:GLY:C	1:A:251:LEU:H	2.25	0.44
1:A:496:LEU:HD21	1:A:614:MET:HE2	2.00	0.44
1:A:543:TYR:HB3	3:A:5454:HOH:O	2.17	0.44
1:A:558:ALA:C	1:A:560:THR:N	2.75	0.44
1:B:84:GLN:HA	1:B:84:GLN:HE21	1.82	0.44
1:B:307:GLN:O	1:B:311:GLY:HA2	2.18	0.44
1:B:349:PRO:HB2	1:B:350:PRO:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:HA	1:B:506:TYR:CE2	2.53	0.44
1:B:472:SER:HB3	3:B:6233:HOH:O	2.17	0.44
1:A:37:ARG:HG3	1:A:95:GLU:O	2.18	0.44
1:A:419:LYS:HB3	1:A:423:LYS:HE2	2.00	0.44
1:A:507:THR:O	1:A:511:ILE:HG13	2.18	0.44
1:B:31:HIS:HE1	1:B:167:PRO:HB3	1.83	0.44
1:B:72:GLU:O	1:B:72:GLU:HG3	2.17	0.44
1:B:90:ARG:HA	1:B:93:LYS:HE2	2.00	0.44
1:A:312:GLY:O	1:A:316:PHE:HD1	2.01	0.44
1:A:411:MET:CE	1:A:563:VAL:HG11	2.48	0.44
1:B:400:LEU:HG	1:B:404:ILE:HD11	2.00	0.44
1:B:467:THR:CG2	1:B:468:ILE:N	2.80	0.44
1:A:312:GLY:O	1:A:316:PHE:HB2	2.17	0.43
1:A:461:HIS:CE1	1:A:462:LEU:HG	2.53	0.43
1:B:478:PHE:CE1	1:B:482:MET:HE2	2.53	0.43
1:A:505:ALA:O	1:A:509:ARG:HG3	2.18	0.43
1:B:143:ILE:HB	1:B:229:ILE:HD13	2.00	0.43
1:A:405:GLN:HE21	1:A:405:GLN:HB2	1.67	0.43
1:B:139:ALA:C	3:B:6342:HOH:O	2.61	0.43
1:B:369:ARG:O	1:B:370:SER:HB2	2.17	0.43
1:A:458:ARG:HD3	3:A:5182:HOH:O	2.18	0.43
1:B:42:PRO:O	1:B:45:GLN:HB3	2.18	0.43
1:A:104:LYS:HE2	1:A:109:GLN:OE1	2.18	0.43
1:A:224:LEU:HA	1:A:228:GLN:HE22	1.83	0.43
1:B:119:SER:HB3	1:B:341:TYR:O	2.18	0.43
1:B:294:ARG:CZ	1:B:294:ARG:HA	2.48	0.43
1:B:321:ARG:HE	1:B:330:ILE:HD11	1.83	0.43
1:A:115:VAL:O	1:A:117:TYR:N	2.49	0.43
1:A:142:LEU:HD23	1:A:142:LEU:C	2.44	0.43
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.54	0.43
1:B:416:HIS:O	1:B:417:PHE:HB3	2.17	0.43
1:B:507:THR:CG2	2:B:6170:COA:H133	2.49	0.43
1:B:593:ASN:C	1:B:595:CYS:H	2.25	0.43
1:A:266:LEU:HD12	1:A:272:ASN:HD22	1.83	0.43
1:A:497:ARG:NH1	1:A:623:ARG:HB2	2.34	0.43
1:B:129:PHE:N	3:B:6225:HOH:O	2.51	0.43
1:B:178:SER:H	1:B:283:ILE:HA	1.83	0.43
1:B:431:ALA:HB1	1:B:500:VAL:HG13	2.00	0.43
1:B:569:VAL:HG23	1:B:570:VAL:H	1.84	0.43
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.83	0.43
1:A:224:LEU:HB3	1:A:229:ILE:CG1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ASN:HD21	1:B:245:LYS:HZ1	1.67	0.43
1:B:308:MET:O	3:B:6171:HOH:O	2.21	0.43
1:B:356:ASP:OD2	1:B:559:LYS:HB2	2.18	0.43
1:B:467:THR:HG22	1:B:468:ILE:N	2.33	0.43
1:A:429:PRO:O	1:A:433:ILE:HG13	2.18	0.43
1:A:541:THR:C	1:A:543:TYR:N	2.76	0.43
1:A:348:GLY:O	1:A:349:PRO:C	2.61	0.42
1:B:108:LEU:HD13	1:B:188:ASP:O	2.18	0.42
1:B:152:MET:HE3	1:B:158:LEU:CD1	2.49	0.42
1:A:452:TYR:HB2	1:A:549:PHE:CD1	2.54	0.42
1:A:456:SER:HA	1:A:465:THR:HG22	2.01	0.42
1:B:464:ARG:HD2	1:B:464:ARG:HA	1.84	0.42
1:A:133:GLN:O	1:A:137:ARG:HG2	2.18	0.42
1:A:224:LEU:HG	1:A:228:GLN:CB	2.48	0.42
1:A:254:ASN:CG	1:A:255:HIS:H	2.27	0.42
1:A:300:TYR:O	1:A:303:HIS:N	2.47	0.42
1:B:410:MET:HB3	1:B:600:ALA:HB1	2.01	0.42
1:A:554:SER:CB	2:A:5170:COA:H22	2.48	0.42
1:B:49:TYR:CE2	1:B:509:ARG:NE	2.87	0.42
1:B:184:GLY:HA3	1:B:187:GLN:O	2.19	0.42
1:B:349:PRO:HA	3:B:6319:HOH:O	2.18	0.42
1:A:64:ALA:O	1:A:67:LYS:HB3	2.20	0.42
1:A:90:ARG:HG2	1:A:90:ARG:O	2.19	0.42
1:A:196:SER:O	1:A:199:PRO:HD3	2.20	0.42
1:B:131:ASP:OD2	1:B:133:GLN:HG2	2.19	0.42
1:B:172:GLN:HB3	1:B:346:ALA:HB2	2.02	0.42
1:B:462:LEU:O	3:B:6190:HOH:O	2.22	0.42
1:B:496:LEU:HD22	1:B:618:LEU:HD11	2.00	0.42
1:A:548:HIS:HB3	3:A:5477:HOH:O	2.20	0.42
1:B:104:LYS:HE2	1:B:104:LYS:HB3	1.90	0.42
1:B:354:LEU:O	1:B:354:LEU:HD23	2.19	0.42
1:A:619:GLN:O	1:B:186:LYS:HD3	2.18	0.42
1:B:496:LEU:O	1:B:500:VAL:HG23	2.20	0.42
1:B:54:LEU:HD22	1:B:58:VAL:HG11	2.02	0.42
1:B:252:THR:OG1	1:B:323:PHE:HD1	2.03	0.42
1:A:183:PRO:CG	1:A:259:TRP:CD1	3.03	0.42
1:A:265:ASN:ND2	1:A:388:GLU:OE1	2.52	0.42
1:A:414:PHE:CE1	1:A:416:HIS:CD2	2.92	0.42
1:B:75:THR:OG1	1:B:76:SER:N	2.52	0.42
1:B:263:TYR:O	1:B:267:ILE:HG12	2.20	0.42
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HG	1:A:228:GLN:NE2	2.35	0.42
1:A:407:LEU:HG	1:A:409:ILE:HD11	2.02	0.42
1:A:489:GLU:HB3	1:A:621:HIS:NE2	2.35	0.42
1:A:566:PHE:CZ	1:A:577:CYS:HB2	2.55	0.42
1:B:55:GLN:HB3	1:B:56:PRO:HD3	2.02	0.42
1:B:79:VAL:O	1:B:83:LEU:HG	2.20	0.42
1:B:90:ARG:NH2	3:B:6210:HOH:O	2.52	0.42
1:B:97:TRP:O	3:B:6178:HOH:O	2.22	0.42
1:A:109:GLN:O	1:A:111:ARG:HG2	2.20	0.41
1:B:476:LEU:O	1:B:480:LYS:HG3	2.20	0.41
1:A:457:LEU:HD12	1:A:460:PHE:CD1	2.54	0.41
1:B:55:GLN:NE2	3:B:6330:HOH:O	2.52	0.41
1:A:430:ASP:HB2	1:A:555:GLN:HE22	1.84	0.41
1:A:452:TYR:CD1	1:A:467:THR:HG23	2.55	0.41
1:A:126:LYS:NZ	1:A:334:ASP:O	2.53	0.41
1:B:445:TYR:OH	1:B:597:GLU:O	2.22	0.41
1:B:565:PHE:HB3	1:B:588:SER:CB	2.51	0.41
1:A:466:ASP:HA	1:A:518:ARG:NH1	2.35	0.41
1:A:417:PHE:O	1:A:584:HIS:HA	2.21	0.41
1:A:301:ARG:HG3	1:A:411:MET:HG3	2.01	0.41
1:A:432:PHE:C	1:A:432:PHE:CD1	2.98	0.41
1:A:541:THR:C	1:A:543:TYR:H	2.28	0.41
1:B:574:TYR:OH	1:B:598:THR:HA	2.20	0.41
1:A:94:MET:HB3	3:A:5362:HOH:O	2.21	0.41
1:A:183:PRO:HG3	1:A:259:TRP:CD1	2.55	0.41
1:A:230:PHE:O	1:A:234:GLU:N	2.54	0.41
1:B:484:ASP:C	1:B:486:THR:H	2.27	0.41
1:A:132:LEU:N	1:A:132:LEU:HD22	2.35	0.41
1:A:322:TRP:H	1:A:328:GLN:HE22	1.69	0.41
1:B:47:LEU:CD1	1:B:74:GLN:HB3	2.46	0.41
1:B:53:ALA:O	1:B:56:PRO:HD2	2.21	0.41
1:B:90:ARG:NE	1:B:94:MET:HE1	2.36	0.41
1:B:149:PHE:HB2	1:B:357:HIS:ND1	2.36	0.41
1:B:295:VAL:HG11	1:B:303:HIS:NE2	2.35	0.41
1:B:456:SER:HB2	2:B:6170:COA:C7P	2.50	0.41
1:A:115:VAL:O	1:A:116:ILE:HB	2.21	0.41
1:A:132:LEU:HD12	1:A:237:TRP:CH2	2.55	0.41
1:A:487:VAL:HA	1:A:488:PRO:HD3	1.91	0.41
1:A:497:ARG:NH2	3:A:5265:HOH:O	2.53	0.41
1:A:518:ARG:HD3	1:A:518:ARG:HA	1.90	0.41
1:B:94:MET:HG2	3:B:6207:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:C	1:A:91:ALA:H	2.29	0.40
1:A:152:MET:CB	1:A:158:LEU:HD12	2.48	0.40
1:A:320:ASN:O	1:A:321:ARG:HD3	2.21	0.40
1:A:497:ARG:CZ	1:A:623:ARG:HB2	2.50	0.40
1:B:90:ARG:HE	1:B:94:MET:HE1	1.86	0.40
1:B:108:LEU:HD22	1:B:188:ASP:O	2.21	0.40
1:A:214:LEU:HD22	1:A:236:ILE:HD12	2.04	0.40
1:B:104:LYS:HD3	3:B:6362:HOH:O	2.21	0.40
1:B:252:THR:HG22	1:B:259:TRP:CZ2	2.57	0.40
1:B:480:LYS:O	1:B:484:ASP:HB2	2.20	0.40
1:B:491:GLN:O	1:B:494:GLU:HB2	2.21	0.40
1:A:59:SER:HB3	1:A:62:GLU:CG	2.51	0.40
1:A:119:SER:HA	1:A:120:PRO:HD3	1.85	0.40
1:A:129:PHE:CE1	1:A:335:GLY:HA2	2.56	0.40
1:A:236:ILE:HG13	1:A:378:PRO:HG2	2.04	0.40
1:A:427:LEU:HB3	1:A:500:VAL:HG11	2.04	0.40
1:B:44:GLN:HG2	1:B:74:GLN:CD	2.46	0.40
1:B:229:ILE:HG22	1:B:233:LEU:CD1	2.51	0.40
1:A:322:TRP:N	1:A:328:GLN:HE22	2.20	0.40
1:B:31:HIS:CE1	1:B:160:VAL:HG11	2.56	0.40
1:B:176:ILE:HG13	1:B:177:LEU:HG	2.03	0.40
1:A:54:LEU:O	1:A:55:GLN:C	2.63	0.40
1:A:480:LYS:O	1:A:484:ASP:HB2	2.21	0.40
1:B:451:THR:HG23	1:B:551:LEU:CB	2.45	0.40
1:B:512:ARG:HH11	1:B:512:ARG:CG	2.35	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	594/596 (100%)	501 (84%)	81 (14%)	12 (2%)	6 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	594/596 (100%)	532 (90%)	52 (9%)	10 (2%)	7	7
All	All	1188/1192 (100%)	1033 (87%)	133 (11%)	22 (2%)	6	5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	SER
1	B	515	ALA
1	B	485	SER
1	B	622	PRO
1	A	172	GLN
1	A	219	SER
1	A	244	ASN
1	A	284	PHE
1	A	371	PRO
1	B	196	SER
1	B	345	ALA
1	B	368	VAL
1	B	600	ALA
1	A	116	ILE
1	A	296	SER
1	B	367	LEU
1	A	76	SER
1	B	139	ALA
1	A	340	VAL
1	A	349	PRO
1	A	567	GLY
1	A	365	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/524 (100%)	492 (94%)	32 (6%)	17	24
1	B	524/524 (100%)	501 (96%)	23 (4%)	25	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1048/1048 (100%)	993 (95%)	55 (5%)	21	31

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	89	ARG
1	A	98	LEU
1	A	112	GLN
1	A	133	GLN
1	A	141	LYS
1	A	158	LEU
1	A	166	GLN
1	A	191	VAL
1	A	199	PRO
1	A	204	THR
1	A	206	VAL
1	A	210	GLN
1	A	224	LEU
1	A	275	SER
1	A	277	ASN
1	A	303	HIS
1	A	330	ILE
1	A	340	VAL
1	A	342	GLU
1	A	354	LEU
1	A	390	LYS
1	A	409	ILE
1	A	454	SER
1	A	459	MET
1	A	482	MET
1	A	498	LYS
1	A	504	ARG
1	A	514	GLU
1	A	517	ASP
1	A	520	LEU
1	A	603	MET
1	B	132	LEU
1	B	144	GLU
1	B	160	VAL
1	B	163	LEU
1	B	204	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	206	VAL
1	B	228	GLN
1	B	242	GLN
1	B	270	LYS
1	B	307	GLN
1	B	340	VAL
1	B	347	GLU
1	B	354	LEU
1	B	360	GLU
1	B	379	LYS
1	B	402	ILE
1	B	456	SER
1	B	470	SER
1	B	486	THR
1	B	559	LYS
1	B	581	MET
1	B	619	GLN
1	B	625	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	45	GLN
1	A	55	GLN
1	A	65	HIS
1	A	84	GLN
1	A	109	GLN
1	A	112	GLN
1	A	133	GLN
1	A	135	GLN
1	A	155	ASN
1	A	192	ASN
1	A	208	ASN
1	A	228	GLN
1	A	232	GLN
1	A	238	ASN
1	A	255	HIS
1	A	265	ASN
1	A	277	ASN
1	A	310	HIS
1	A	320	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	GLN
1	A	357	HIS
1	A	399	ASN
1	A	405	GLN
1	A	416	HIS
1	A	461	HIS
1	A	501	GLN
1	A	548	HIS
1	A	550	ASN
1	A	586	ASN
1	A	619	GLN
1	B	31	HIS
1	B	84	GLN
1	B	109	GLN
1	B	112	GLN
1	B	135	GLN
1	B	155	ASN
1	B	171	ASN
1	B	187	GLN
1	B	192	ASN
1	B	207	HIS
1	B	218	HIS
1	B	228	GLN
1	B	255	HIS
1	B	328	GLN
1	B	490	GLN
1	B	526	GLN
1	B	550	ASN
1	B	586	ASN
1	B	619	GLN
1	B	620	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	COA	B	6170	-	47,50,50	1.55	6 (12%)	69,75,75	1.52	10 (14%)
2	COA	A	5170	-	47,50,50	1.40	6 (12%)	69,75,75	1.53	10 (14%)

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
2	COA	B	6170	-	-	11/48/64/64	0/3/3/3
2	COA	A	5170	-	-	4/48/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6170	COA	P2A-O3A	5.06	1.65	1.59
2	B	6170	COA	P1A-O3A	4.75	1.64	1.59
2	B	6170	COA	P3B-O7A	3.83	1.62	1.50
2	A	5170	COA	P3B-O7A	3.74	1.62	1.50
2	A	5170	COA	P1A-O3A	3.63	1.63	1.59
2	A	5170	COA	C5A-N7A	-3.25	1.33	1.39
2	A	5170	COA	P2A-O3A	3.18	1.62	1.59
2	B	6170	COA	C5A-N7A	-3.08	1.33	1.39
2	B	6170	COA	P3B-O3B	2.58	1.64	1.59
2	B	6170	COA	C4A-N9A	-2.23	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5170	COA	O4B-C1B	2.14	1.46	1.42
2	A	5170	COA	C4A-N9A	-2.12	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6170	COA	N3A-C2A-N1A	-5.31	120.55	128.58
2	A	5170	COA	N3A-C2A-N1A	-5.30	120.56	128.58
2	A	5170	COA	C5A-C4A-N3A	-4.94	119.91	126.72
2	B	6170	COA	C5A-C4A-N3A	-4.91	119.95	126.72
2	A	5170	COA	C2A-N3A-C4A	3.73	120.95	111.83
2	A	5170	COA	O4B-C1B-N9A	3.73	115.25	108.09
2	B	6170	COA	C2A-N3A-C4A	3.68	120.83	111.83
2	B	6170	COA	N9A-C8A-N7A	-3.45	109.04	113.94
2	B	6170	COA	N3A-C4A-N9A	3.29	132.76	127.17
2	B	6170	COA	O4B-C1B-N9A	3.23	114.30	108.09
2	A	5170	COA	N9A-C8A-N7A	-3.20	109.40	113.94
2	A	5170	COA	N3A-C4A-N9A	3.10	132.44	127.17
2	A	5170	COA	O9A-P3B-O8A	3.09	119.39	107.80
2	B	6170	COA	O9A-P3B-O8A	3.03	119.17	107.80
2	B	6170	COA	C5A-N7A-C8A	2.70	107.70	103.45
2	A	5170	COA	C5A-N7A-C8A	2.67	107.65	103.45
2	A	5170	COA	C4A-C5A-N7A	-2.46	107.77	110.58
2	A	5170	COA	C5B-C4B-C3B	-2.43	106.28	114.38
2	B	6170	COA	C4A-C5A-N7A	-2.40	107.83	110.58
2	B	6170	COA	C4A-N9A-C8A	2.29	108.14	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5170	COA	C5B-O5B-P1A-O2A
2	B	6170	COA	C5B-O5B-P1A-O2A
2	B	6170	COA	CCP-O6A-P2A-O3A
2	B	6170	COA	CCP-O6A-P2A-O4A
2	B	6170	COA	CCP-O6A-P2A-O5A
2	B	6170	COA	O9P-C9P-CAP-OAP
2	B	6170	COA	O9P-C9P-CAP-CBP
2	B	6170	COA	N8P-C9P-CAP-CBP
2	B	6170	COA	N8P-C9P-CAP-OAP
2	A	5170	COA	C5B-O5B-P1A-O1A
2	A	5170	COA	C5B-O5B-P1A-O3A

Continued on next page...

Continued from previous page...

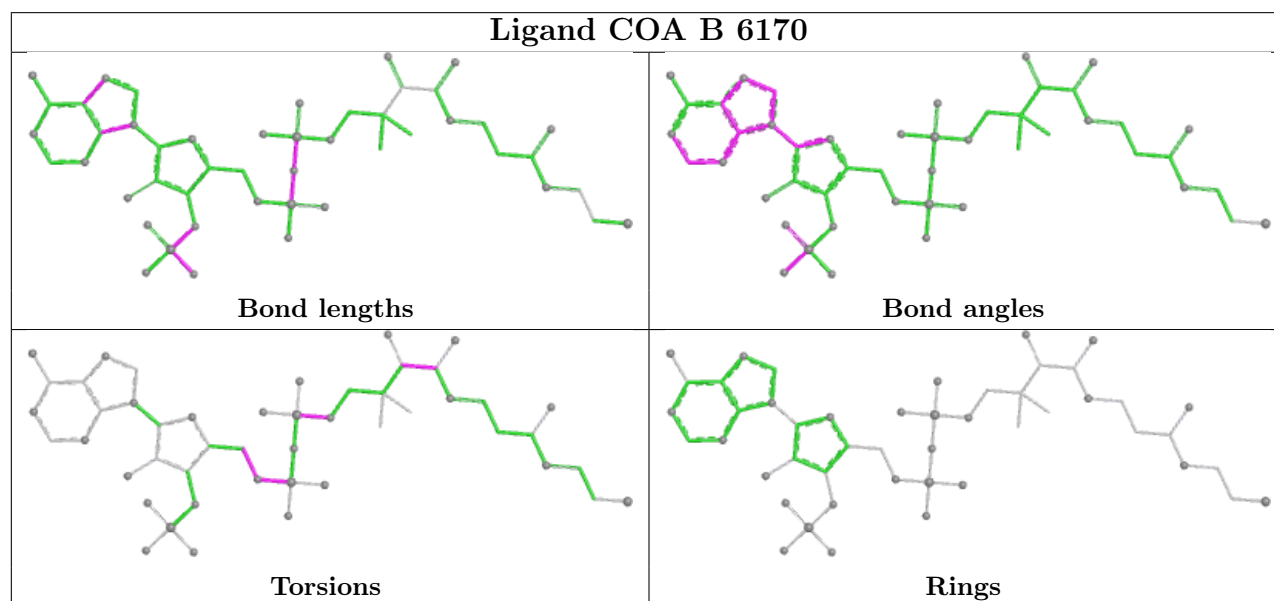
Mol	Chain	Res	Type	Atoms
2	B	6170	COA	C5B-O5B-P1A-O1A
2	B	6170	COA	C5B-O5B-P1A-O3A
2	B	6170	COA	C4B-C5B-O5B-P1A
2	A	5170	COA	N8P-C9P-CAP-OAP

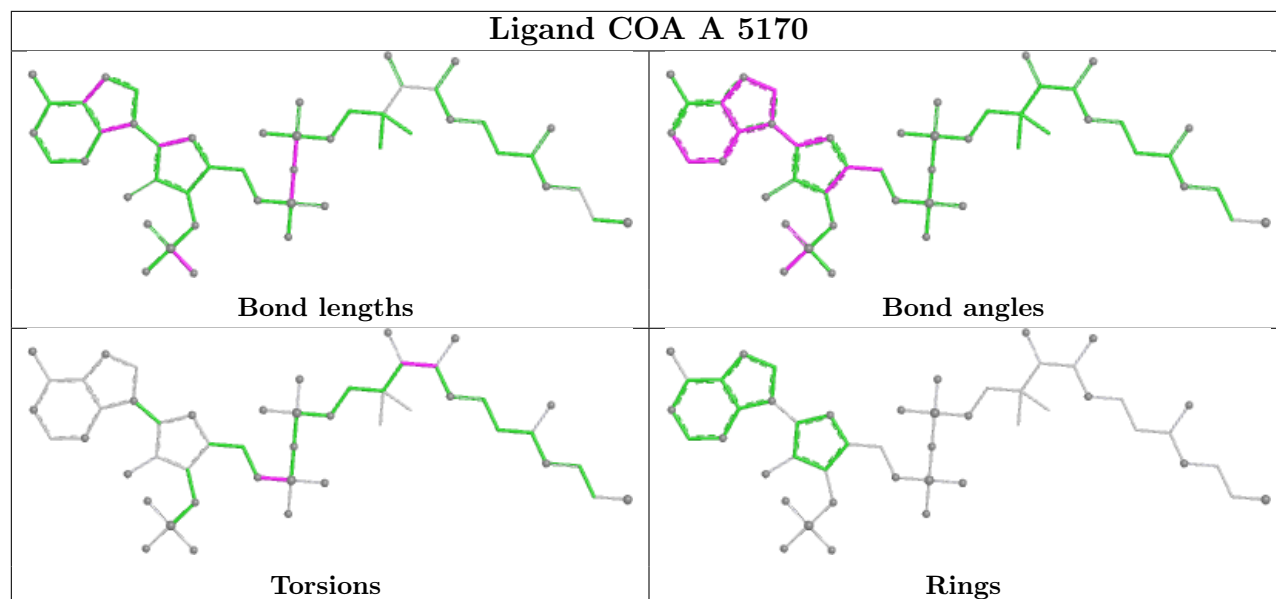
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6170	COA	7	0
2	A	5170	COA	5	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 than 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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/596 (100%)	-1.13	0 100 100	13, 47, 89, 134	0
1	B	596/596 (100%)	-1.19	0 100 100	14, 42, 72, 99	0
All	All	1192/1192 (100%)	-1.16	0 100 100	13, 44, 85, 134	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

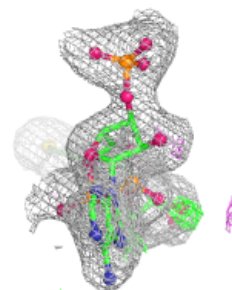
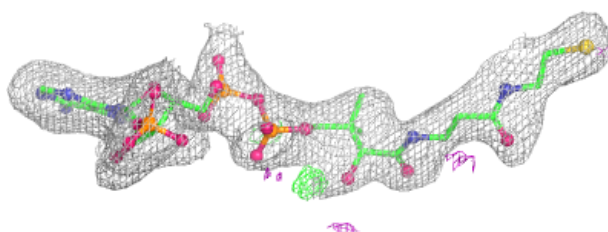
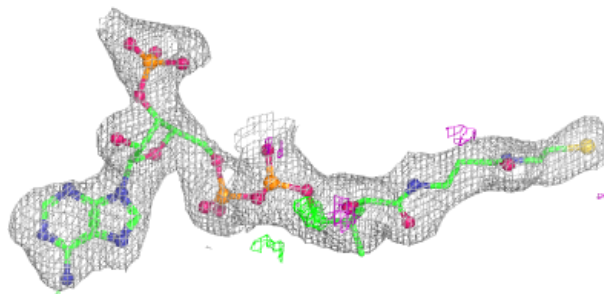
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	A	5170	48/48	0.99	0.04	39,54,60,62	0
2	COA	B	6170	48/48	0.99	0.04	36,53,64,65	0

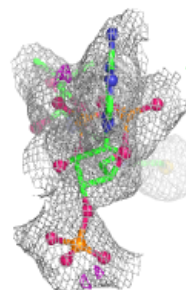
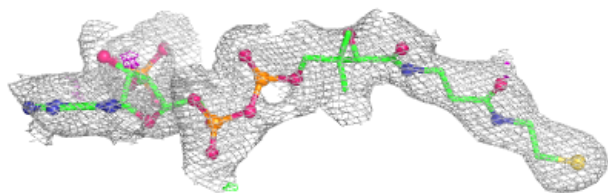
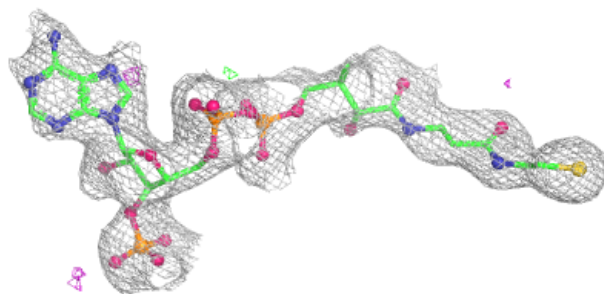
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 5170:

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

**Electron density around COA B 6170:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.