



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID : 1YA4
Title : Crystal Structure of Human Liver Carboxylesterase 1 in complex with tamoxifen
Authors : Fleming, C.D.; Bencharit, S.; Edwards, C.C.; Hyatt, J.L.; Morton, C.L.; Howard-Williams, E.L.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2004-12-17
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

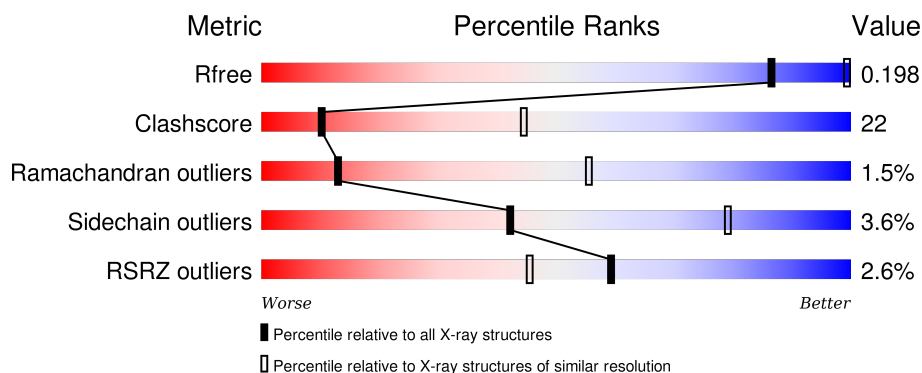
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	532	<div> <div>4%</div> <div>60%</div> <div>38%</div> <div>.</div> </div>
1	B	532	<div> <div>3%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
1	C	532	<div> <div>%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1179	X	-	-	X
4	SO4	A	1181	-	-	-	X
4	SO4	B	1282	-	-	-	X
4	SO4	C	1381	-	-	-	X
4	SO4	C	1382	-	-	-	X
5	CTX	A	11	-	-	X	X
5	CTX	B	1283	-	-	-	X
5	CTX	B	2	-	-	-	X
5	CTX	C	1383	-	-	X	X
5	CTX	C	3	-	-	-	X

2 Entry composition [i](#)

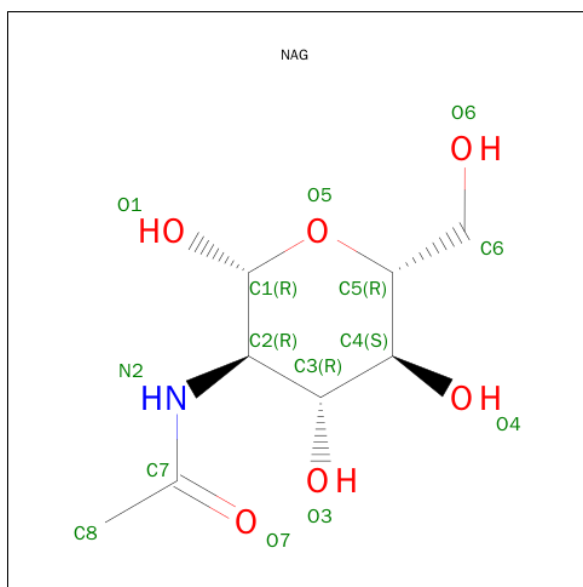
There are 6 unique types of molecules in this entry. The entry contains 12878 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CES1 protein.

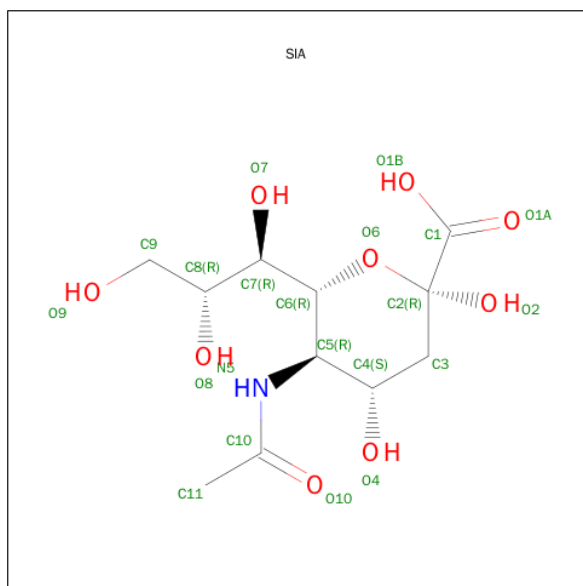
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	B	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



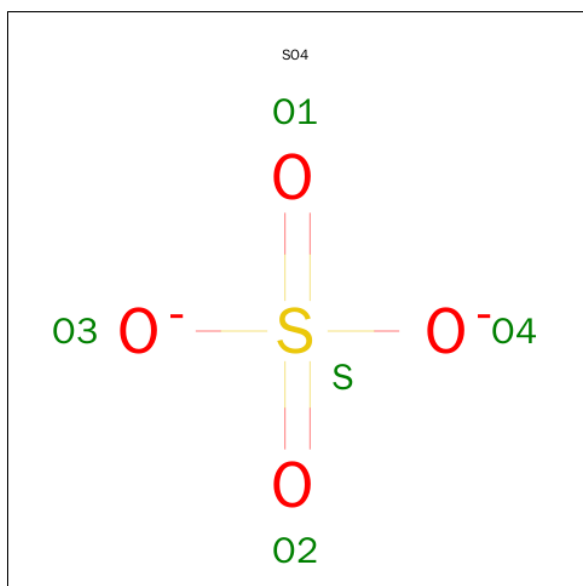
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



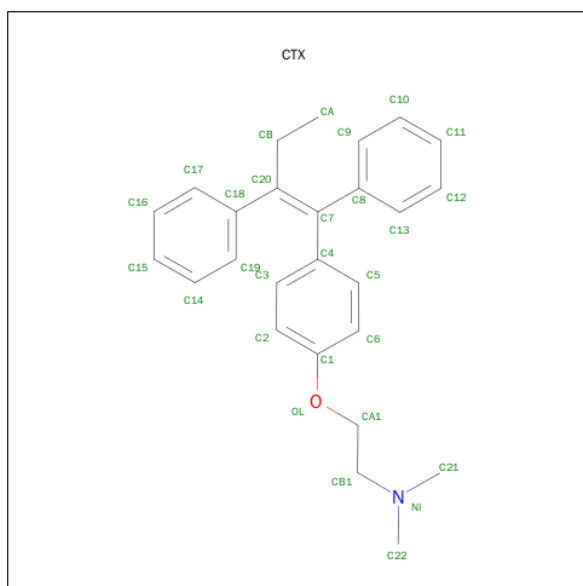
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is (Z)-2-[4-(1,2)-DIPHENYL-1-BUTENYL]-PHENOXY]-N,N-DIMETHYLETHANAMINE (three-letter code: CTX) (formula: C₂₆H₂₉NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 28 26 1 1	0	0
5	B	1	Total C N O 28 26 1 1	0	0
5	C	1	Total C N O 28 26 1 1	0	0
5	A	1	Total C N O 28 26 1 1	0	0
5	B	1	Total C N O 28 26 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			28	26	1	1		

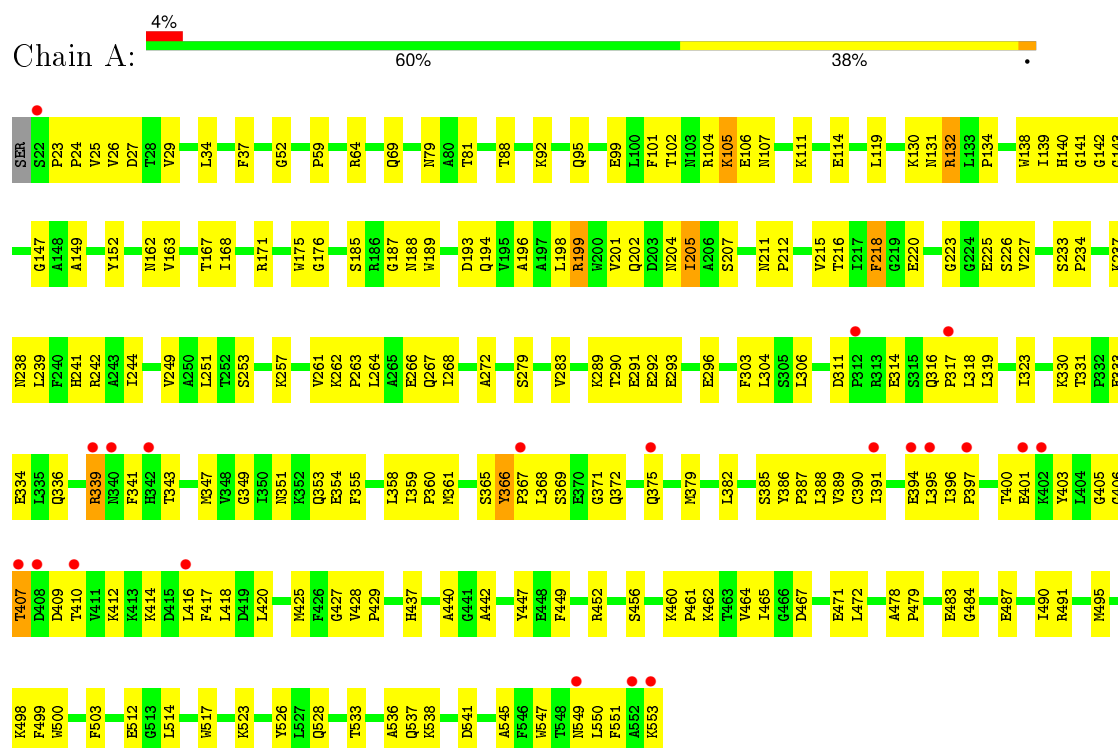
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	58	Total	O	0	0
			58	58		
6	C	63	Total	O	0	0
			63	63		

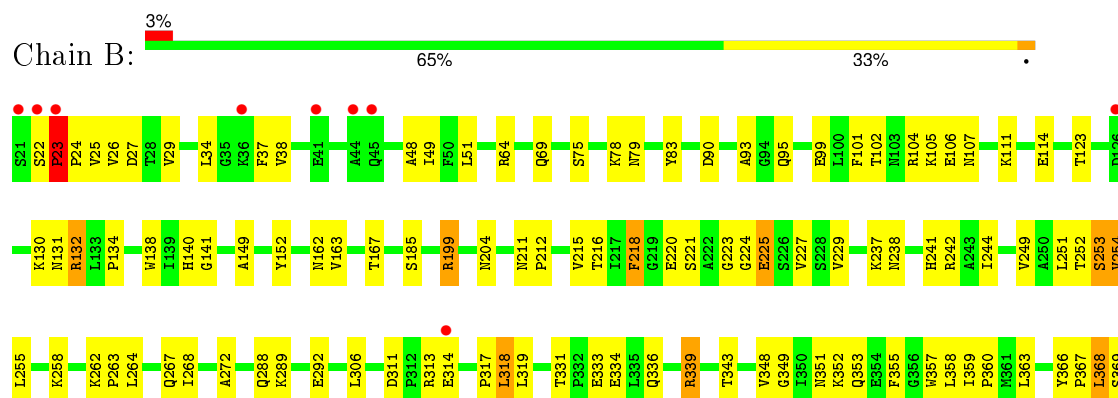
3 Residue-property plots

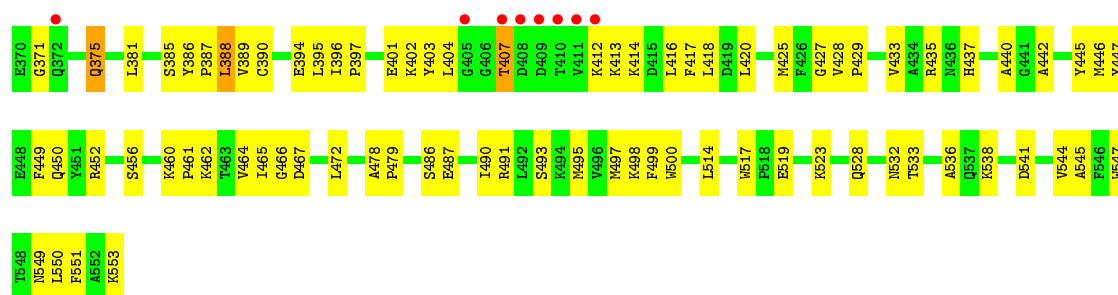
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: CES1 protein

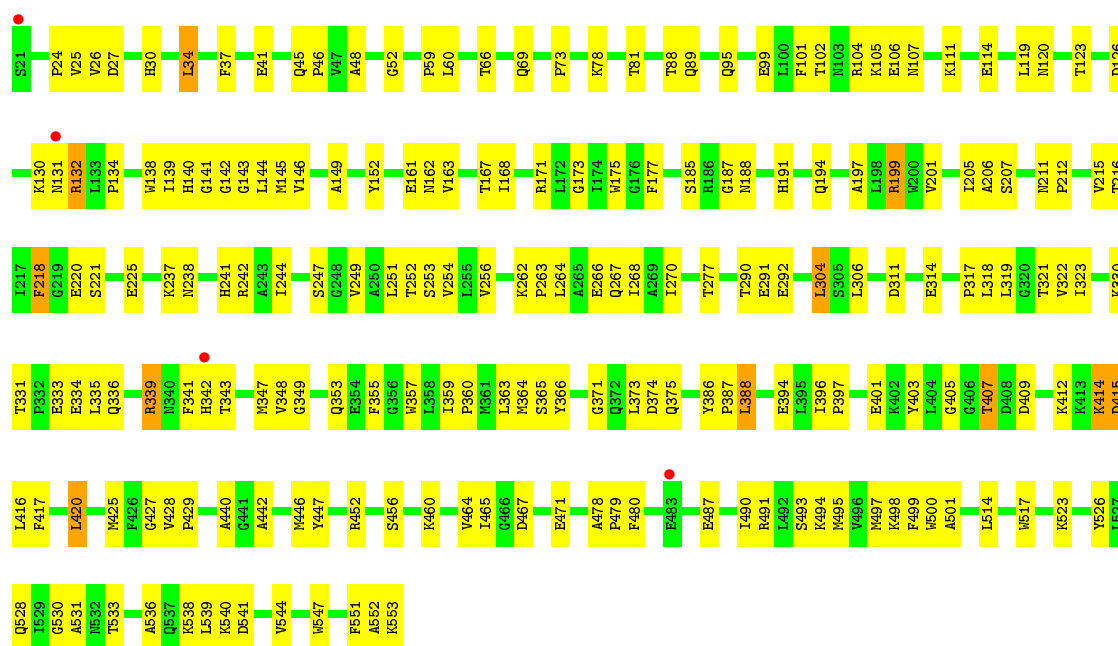


• Molecule 1: CES1 protein





• Molecule 1: CES1 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.37Å 179.95Å 201.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 3.20 48.53 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.53-3.20) 99.1 (48.53-2.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.252 0.202 , 0.198	Depositor DCC
R_{free} test set	1683 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 44285 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12878	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, CTX, NAG, SO4

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	0.39	0/4230	0.62	0/5746
1	B	0.43	0/4236	0.64	1/5754 (0.0%)
1	C	0.39	0/4236	0.63	1/5754 (0.0%)
All	All	0.40	0/12702	0.63	2/17254 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	23	PRO	N-CA-C	5.32	125.92	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4126	188	0
1	B	4130	0	4131	169	0
1	C	4130	0	4131	181	0
2	A	14	0	13	4	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	18	6	0
3	B	21	0	18	5	0
3	C	21	0	18	3	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	1	0
5	A	56	0	58	12	0
5	B	56	0	58	10	0
5	C	56	0	58	18	0
6	A	70	0	0	19	0
6	B	58	0	0	10	0
6	C	63	0	0	11	0
All	All	12878	0	12655	551	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 22.

All (551) 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:22:SER:CB	1:B:23:PRO:HD2	1.78	1.14
1:B:22:SER:HB3	1:B:23:PRO:CD	1.79	1.12
1:A:130:LYS:HE3	1:A:132:ARG:HH11	1.18	1.08
1:C:199:ARG:HB3	1:C:199:ARG:HH11	1.18	1.04
1:B:199:ARG:HB3	1:B:199:ARG:HH11	1.24	1.03
1:A:242:ARG:HH11	1:A:242:ARG:HG2	1.28	0.98
1:C:215:VAL:H	1:C:241:HIS:HD2	1.04	0.97
1:C:134:PRO:HG2	1:C:163:VAL:HG12	1.45	0.95
1:A:134:PRO:HG2	1:A:163:VAL:HG12	1.47	0.95
1:B:22:SER:HB3	1:B:23:PRO:HD2	0.96	0.95
1:A:216:THR:HG23	1:A:242:ARG:HB2	1.48	0.94
1:A:199:ARG:HB3	1:A:199:ARG:HH11	1.33	0.93
1:B:134:PRO:HG2	1:B:163:VAL:HG12	1.50	0.93
1:A:130:LYS:HE3	1:A:132:ARG:NH1	1.83	0.92
1:B:242:ARG:HH11	1:B:242:ARG:HG2	1.34	0.90
1:C:215:VAL:H	1:C:241:HIS:CD2	1.90	0.89
1:C:242:ARG:HH11	1:C:242:ARG:HG2	1.39	0.88
1:B:216:THR:HG23	1:B:242:ARG:HB2	1.57	0.87
1:A:215:VAL:H	1:A:241:HIS:HD2	1.22	0.87
1:C:237:LYS:HG2	1:C:238:ASN:ND2	1.89	0.86
1:B:105:LYS:HG3	1:B:106:GLU:H	1.40	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:SER:HB3	1:A:460:LYS:HD3	1.60	0.84
1:A:105:LYS:HG3	1:A:106:GLU:H	1.42	0.84
1:A:237:LYS:HG2	1:A:238:ASN:ND2	1.93	0.84
1:B:339:ARG:HG2	1:B:440:ALA:HA	1.60	0.83
1:B:487:GLU:HA	1:B:490:ILE:HD12	1.59	0.83
1:C:216:THR:HG23	1:C:242:ARG:HB2	1.59	0.83
1:C:99:GLU:HG2	1:C:107:ASN:OD1	1.80	0.82
1:B:237:LYS:HE3	6:B:4124:HOH:O	1.81	0.79
1:C:464:VAL:HA	6:C:4119:HOH:O	1.82	0.79
1:C:215:VAL:N	1:C:241:HIS:HD2	1.80	0.78
1:B:99:GLU:HG2	1:B:107:ASN:OD1	1.84	0.78
1:A:339:ARG:HG2	1:A:440:ALA:HA	1.65	0.78
1:C:105:LYS:HG3	1:C:106:GLU:H	1.46	0.78
1:A:418:LEU:HD11	5:A:11:CTX:HA1	1.66	0.78
1:B:237:LYS:HG2	1:B:238:ASN:ND2	1.99	0.77
1:B:461:PRO:HG2	1:B:464:VAL:HG23	1.66	0.77
1:B:388:LEU:HD21	5:B:2:CTX:H14	1.66	0.77
3:A:1180:SIA:H8	6:A:4003:HOH:O	1.85	0.76
1:A:138:TRP:CH2	1:A:220:GLU:HB2	2.21	0.75
1:B:223:GLY:O	1:B:227:VAL:HG23	1.87	0.75
1:A:359:ILE:HB	1:A:360:PRO:HD3	1.69	0.75
1:C:268:ILE:HD11	1:C:319:LEU:HD21	1.69	0.75
1:C:114:GLU:HG3	1:C:291:GLU:OE1	1.85	0.75
1:A:220:GLU:HG3	1:A:472:LEU:HD21	1.66	0.75
1:A:487:GLU:HA	1:A:490:ILE:HD12	1.69	0.74
1:A:355:PHE:CE1	1:A:360:PRO:HG3	2.23	0.73
1:C:41:GLU:HA	6:C:4069:HOH:O	1.87	0.73
1:C:339:ARG:HG2	1:C:440:ALA:HA	1.70	0.73
1:B:343:THR:HA	6:B:4032:HOH:O	1.88	0.73
1:B:138:TRP:HH2	1:B:220:GLU:HB2	1.52	0.73
1:A:215:VAL:H	1:A:241:HIS:CD2	2.07	0.73
1:A:138:TRP:HH2	1:A:220:GLU:HB2	1.52	0.72
1:B:403:TYR:O	1:B:416:LEU:HD13	1.90	0.72
1:B:215:VAL:H	1:B:241:HIS:HD2	1.36	0.71
1:A:223:GLY:O	1:A:227:VAL:HG23	1.91	0.71
1:B:24:PRO:HG3	1:B:37:PHE:CE1	2.25	0.70
1:A:487:GLU:OE2	1:A:491:ARG:NH1	2.24	0.70
1:A:388:LEU:HD21	5:A:1:CTX:H14	1.73	0.70
1:C:199:ARG:HB3	1:C:199:ARG:NH1	2.01	0.70
3:C:1380:SIA:H8	6:C:4030:HOH:O	1.92	0.69
1:C:357:TRP:O	1:C:360:PRO:HD2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LYS:HB3	1:B:541:ASP:HB2	1.75	0.69
1:B:528:GLN:HE21	1:B:536:ALA:HB2	1.58	0.69
1:A:193:ASP:O	1:A:196:ALA:HB3	1.93	0.69
1:C:538:LYS:HB3	1:C:541:ASP:HB2	1.73	0.69
1:A:339:ARG:CG	1:A:440:ALA:HA	2.23	0.69
1:C:48:ALA:HB3	1:C:123:THR:HG23	1.74	0.69
1:B:199:ARG:NH1	1:B:199:ARG:HB3	2.04	0.68
1:C:414:LYS:CE	5:C:1383:CTX:HA1	2.23	0.68
1:B:353:GLN:NE2	1:B:465:ILE:H	1.90	0.68
1:A:353:GLN:NE2	1:A:465:ILE:H	1.92	0.68
1:B:140:HIS:HD2	1:B:141:GLY:O	1.77	0.68
1:A:262:LYS:HB3	1:A:263:PRO:HD3	1.74	0.68
1:B:368:LEU:O	5:B:1283:CTX:H9	1.93	0.68
1:A:368:LEU:HB2	5:A:11:CTX:H9	1.76	0.67
1:A:215:VAL:N	1:A:241:HIS:HD2	1.92	0.67
1:B:343:THR:HB	1:B:442:ALA:HB2	1.75	0.67
1:A:437:HIS:HE1	6:A:4044:HOH:O	1.76	0.67
1:B:25:VAL:HG22	1:B:34:LEU:HD23	1.75	0.67
1:C:343:THR:HB	1:C:442:ALA:HB2	1.77	0.67
1:A:199:ARG:CB	1:A:199:ARG:HH11	2.08	0.66
1:B:339:ARG:CG	1:B:440:ALA:HA	2.25	0.66
1:A:553:LYS:NZ	1:A:553:LYS:HB3	2.10	0.66
1:A:538:LYS:HB3	1:A:541:ASP:HB2	1.77	0.66
1:B:105:LYS:HG3	1:B:106:GLU:N	2.11	0.66
1:B:428:VAL:HB	1:B:429:PRO:HD3	1.78	0.66
1:A:386:TYR:N	1:A:387:PRO:HD2	2.11	0.66
1:C:199:ARG:CB	1:C:199:ARG:HH11	2.02	0.65
1:C:25:VAL:HG22	1:C:34:LEU:HD23	1.78	0.65
1:C:339:ARG:CG	1:C:440:ALA:HA	2.27	0.65
1:C:495:MET:HE3	1:C:533:THR:HG21	1.77	0.65
1:A:79:ASN:HB2	3:A:1180:SIA:O1B	1.97	0.65
1:C:89:GLN:HB2	1:C:146:VAL:HG12	1.78	0.65
1:A:349:GLY:HA3	1:A:447:TYR:CE1	2.32	0.65
1:A:257:LYS:HE2	1:A:316:GLN:OE1	1.96	0.65
1:B:22:SER:CB	1:B:23:PRO:CD	2.52	0.65
1:C:242:ARG:NH1	1:C:242:ARG:HG2	2.04	0.65
1:A:143:GLY:O	1:A:318:LEU:HD22	1.96	0.64
1:B:333:GLU:HA	1:B:336:GLN:HE21	1.63	0.64
2:A:1179:NAG:H3	2:A:1179:NAG:H83	1.79	0.64
1:B:456:SER:HB3	1:B:460:LYS:HD3	1.79	0.64
6:A:4148:HOH:O	1:B:288:GLN:HG3	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:GLU:HG3	6:A:4046:HOH:O	1.96	0.64
1:B:396:ILE:HB	1:B:397:PRO:HD3	1.79	0.64
1:C:452:ARG:HB2	1:C:465:ILE:HG12	1.79	0.64
1:B:138:TRP:CH2	1:B:220:GLU:HB2	2.32	0.64
1:C:487:GLU:OE2	1:C:491:ARG:NH1	2.31	0.63
1:C:396:ILE:HB	1:C:397:PRO:HD3	1.78	0.63
1:B:357:TRP:O	1:B:360:PRO:HD2	1.98	0.63
1:C:131:ASN:C	1:C:132:ARG:HD2	2.18	0.63
1:A:461:PRO:HG2	1:A:464:VAL:CG2	2.28	0.63
1:A:461:PRO:HG2	1:A:464:VAL:HG23	1.79	0.63
1:B:461:PRO:HG2	1:B:464:VAL:CG2	2.29	0.63
1:A:261:VAL:HG22	6:A:4101:HOH:O	1.99	0.63
1:A:333:GLU:HA	1:A:336:GLN:HE21	1.63	0.63
1:C:317:PRO:HG2	1:C:387:PRO:HB2	1.81	0.63
1:B:131:ASN:C	1:B:132:ARG:HD2	2.19	0.63
1:A:220:GLU:HB3	6:A:4034:HOH:O	1.99	0.63
1:C:266:GLU:O	1:C:270:ILE:HG13	1.99	0.63
1:A:403:TYR:CG	1:A:420:LEU:HD23	2.34	0.62
1:A:24:PRO:HG3	1:A:37:PHE:CE1	2.35	0.62
1:A:396:ILE:HB	1:A:397:PRO:HD3	1.82	0.62
1:C:373:LEU:HB2	1:C:414:LYS:HB2	1.82	0.62
1:B:495:MET:HE3	1:B:533:THR:HG21	1.80	0.62
1:C:394:GLU:O	1:C:397:PRO:HD2	2.00	0.62
1:C:360:PRO:HB2	5:C:1383:CTX:H11	1.81	0.62
1:A:311:ASP:HB3	1:A:314:GLU:HG3	1.82	0.62
1:A:403:TYR:O	1:A:416:LEU:HD13	2.00	0.61
1:B:355:PHE:CE1	1:B:360:PRO:HG3	2.35	0.61
1:A:241:HIS:O	1:A:242:ARG:HG2	2.01	0.61
1:C:388:LEU:HD21	5:C:3:CTX:H14	1.83	0.61
1:A:394:GLU:O	1:A:397:PRO:HD2	2.01	0.61
1:C:428:VAL:HB	1:C:429:PRO:HD3	1.82	0.61
1:C:95:GLN:HG2	6:C:4036:HOH:O	2.00	0.61
1:B:386:TYR:N	1:B:387:PRO:HD2	2.16	0.61
1:A:395:LEU:HB3	1:A:550:LEU:HD11	1.82	0.60
1:C:24:PRO:HG3	1:C:37:PHE:CE1	2.36	0.60
1:B:241:HIS:O	1:B:242:ARG:HG2	2.01	0.60
1:B:105:LYS:CG	1:B:106:GLU:H	2.11	0.60
1:B:130:LYS:HE3	1:B:132:ARG:HD3	1.83	0.60
1:C:132:ARG:HB3	1:C:211:ASN:HB2	1.82	0.60
1:C:386:TYR:N	1:C:387:PRO:HD2	2.16	0.60
1:C:105:LYS:HG3	1:C:106:GLU:N	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ALA:HB3	1:C:123:THR:CG2	2.30	0.60
1:C:353:GLN:NE2	1:C:465:ILE:H	1.99	0.60
1:C:143:GLY:O	1:C:144:LEU:HB2	2.01	0.60
1:B:215:VAL:H	1:B:241:HIS:CD2	2.18	0.59
1:A:237:LYS:HG2	1:A:238:ASN:HD22	1.66	0.59
1:B:95:GLN:O	1:B:99:GLU:HG3	2.03	0.59
1:B:215:VAL:N	1:B:241:HIS:HD2	2.01	0.59
1:B:242:ARG:NH1	1:B:242:ARG:HG2	2.07	0.59
1:A:244:ILE:HG12	1:A:347:MET:HB3	1.85	0.59
1:A:242:ARG:NH1	1:A:242:ARG:HG2	2.04	0.59
1:C:355:PHE:CD1	1:C:360:PRO:HG3	2.38	0.58
1:B:78:LYS:HG3	3:B:1280:SIA:O1B	2.04	0.58
1:A:369:SER:HB3	6:A:4102:HOH:O	2.03	0.58
1:C:140:HIS:HD2	1:C:141:GLY:O	1.87	0.58
1:A:333:GLU:H	1:A:333:GLU:CD	2.08	0.58
1:C:292:GLU:OE1	1:C:292:GLU:N	2.35	0.58
1:A:414:LYS:HD2	5:A:11:CTX:HA3	1.85	0.57
1:B:437:HIS:HE1	6:B:4032:HOH:O	1.85	0.57
1:C:221:SER:HA	1:C:247:SER:O	2.03	0.57
1:A:456:SER:CB	1:A:460:LYS:HD3	2.31	0.57
1:A:272:ALA:O	1:A:289:LYS:HE3	2.03	0.57
1:B:311:ASP:OD1	1:B:313:ARG:HB2	2.05	0.57
1:B:90:ASP:HB3	1:B:93:ALA:HB3	1.85	0.57
2:A:1179:NAG:C1	6:A:4052:HOH:O	2.52	0.57
1:A:131:ASN:C	1:A:132:ARG:HD2	2.25	0.57
1:A:341:PHE:HA	6:A:4165:HOH:O	2.04	0.56
1:A:237:LYS:O	1:A:238:ASN:HB2	2.05	0.56
1:A:149:ALA:HB1	1:A:167:THR:HB	1.86	0.56
1:B:348:VAL:O	1:B:446:MET:HA	2.05	0.56
1:C:403:TYR:O	1:C:416:LEU:HD13	2.05	0.56
1:B:132:ARG:N	1:B:132:ARG:HD2	2.21	0.56
1:A:81:THR:HA	6:A:4117:HOH:O	2.05	0.56
1:C:311:ASP:HB3	1:C:314:GLU:HG3	1.88	0.56
1:A:343:THR:HA	6:A:4044:HOH:O	2.06	0.56
1:A:292:GLU:N	1:A:292:GLU:OE1	2.35	0.56
1:C:251:LEU:HD11	1:C:336:GLN:HE22	1.71	0.56
1:B:367:PRO:HG3	1:B:381:LEU:HD21	1.88	0.55
1:B:272:ALA:O	1:B:289:LYS:HE3	2.06	0.55
1:A:551:PHE:C	1:A:553:LYS:H	2.09	0.55
1:C:491:ARG:HH11	1:C:491:ARG:HG3	1.70	0.55
1:A:249:VAL:HG23	1:A:251:LEU:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HE3	1:B:132:ARG:NH1	2.22	0.55
1:B:262:LYS:HB3	1:B:263:PRO:HD3	1.89	0.55
1:A:528:GLN:HE21	1:A:536:ALA:HB2	1.70	0.55
1:A:343:THR:HB	1:A:442:ALA:HB2	1.87	0.55
1:A:140:HIS:HD2	1:A:141:GLY:O	1.90	0.55
1:A:105:LYS:HG3	1:A:106:GLU:N	2.18	0.55
1:C:317:PRO:CG	1:C:387:PRO:HB2	2.37	0.55
1:B:311:ASP:HB3	1:B:314:GLU:HG3	1.88	0.55
1:A:339:ARG:N	1:A:339:ARG:HD2	2.22	0.55
1:C:339:ARG:N	1:C:339:ARG:HD2	2.22	0.55
1:A:306:LEU:HD22	1:A:366:TYR:CE1	2.42	0.55
1:A:105:LYS:CG	1:A:106:GLU:H	2.14	0.54
1:C:106:GLU:HG3	1:C:106:GLU:O	2.08	0.54
1:A:361:MET:HB2	5:A:11:CTX:H12	1.88	0.54
1:B:417:PHE:O	1:B:420:LEU:HB3	2.08	0.54
1:B:428:VAL:HG13	1:B:544:VAL:HA	1.88	0.54
1:B:339:ARG:HD2	1:B:339:ARG:N	2.22	0.54
1:A:401:GLU:OE2	1:A:405:GLY:HA3	2.06	0.54
1:A:385:SER:C	1:A:387:PRO:HD2	2.28	0.54
1:C:401:GLU:OE2	1:C:405:GLY:HA3	2.07	0.54
2:A:1179:NAG:H83	2:A:1179:NAG:C3	2.37	0.54
1:C:417:PHE:O	1:C:420:LEU:HB3	2.08	0.54
1:C:119:LEU:HD12	1:C:119:LEU:C	2.27	0.54
1:C:78:LYS:HG3	3:C:1380:SIA:O1B	2.07	0.53
1:C:130:LYS:HE3	1:C:132:ARG:HD3	1.89	0.53
1:B:75:SER:HB2	6:B:4081:HOH:O	2.08	0.53
1:C:414:LYS:HE2	1:C:415:ASP:HA	1.90	0.53
1:A:545:ALA:O	1:A:549:ASN:ND2	2.42	0.53
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.73	0.53
1:B:420:LEU:HD22	1:B:547:TRP:HZ2	1.74	0.53
1:B:102:THR:OG1	1:B:104:ARG:HG2	2.09	0.53
1:A:478:ALA:N	1:A:479:PRO:CD	2.72	0.53
1:C:59:PRO:HG3	1:C:171:ARG:HD3	1.89	0.53
1:C:456:SER:HB3	1:C:460:LYS:HD3	1.91	0.53
1:B:221:SER:O	1:B:224:GLY:N	2.42	0.53
1:C:262:LYS:HB3	1:C:263:PRO:HD3	1.91	0.53
1:A:495:MET:HE3	1:A:533:THR:HG21	1.90	0.53
1:B:447:TYR:CD2	1:B:447:TYR:C	2.83	0.52
1:C:105:LYS:CG	1:C:106:GLU:H	2.19	0.52
1:C:355:PHE:CE1	1:C:360:PRO:HG3	2.43	0.52
1:A:371:GLY:HA2	5:A:11:CTX:H17	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:OG1	1:C:104:ARG:HG2	2.09	0.52
1:C:333:GLU:HA	1:C:336:GLN:HE21	1.74	0.52
1:C:304:LEU:HB3	5:C:3:CTX:HA12	1.92	0.52
1:C:304:LEU:O	5:C:3:CTX:HA12	2.10	0.52
1:B:292:GLU:OE1	1:B:292:GLU:N	2.39	0.52
1:B:101:PHE:CZ	5:B:2:CTX:H11	2.44	0.52
1:C:349:GLY:HA3	1:C:447:TYR:CE1	2.45	0.52
1:B:258:LYS:HE2	6:B:4055:HOH:O	2.09	0.52
1:B:105:LYS:HE2	6:B:4152:HOH:O	2.09	0.52
1:B:317:PRO:HB2	5:B:2:CTX:H15	1.91	0.52
1:B:25:VAL:HG22	1:B:34:LEU:CD2	2.40	0.51
1:C:333:GLU:CD	1:C:333:GLU:H	2.13	0.51
1:C:386:TYR:HA	6:C:4150:HOH:O	2.10	0.51
1:A:452:ARG:CZ	1:A:462:LYS:HG2	2.41	0.51
1:C:414:LYS:NZ	5:C:1383:CTX:HA1	2.26	0.51
1:B:359:ILE:HB	1:B:360:PRO:HD3	1.91	0.51
1:C:197:ALA:O	1:C:201:VAL:HG23	2.11	0.51
1:B:403:TYR:CG	1:B:420:LEU:HD23	2.45	0.51
1:B:130:LYS:CE	1:B:132:ARG:HD3	2.41	0.51
1:B:79:ASN:O	3:B:1280:SIA:O2	2.27	0.51
1:B:331:THR:OG1	1:B:334:GLU:HG3	2.10	0.51
1:C:447:TYR:HB3	1:C:517:TRP:CZ2	2.45	0.51
1:A:279:SER:O	1:A:283:VAL:HG23	2.11	0.51
1:B:358:LEU:O	1:B:363:LEU:HG	2.11	0.51
1:B:29:VAL:HG23	1:B:204:ASN:OD1	2.11	0.51
1:A:99:GLU:HG2	1:A:107:ASN:OD1	2.10	0.51
1:A:339:ARG:H	1:A:339:ARG:HD2	1.74	0.51
1:B:123:THR:O	1:B:123:THR:HG23	2.11	0.51
1:B:149:ALA:HB1	1:B:167:THR:HB	1.92	0.51
1:A:242:ARG:NH1	1:A:242:ARG:CG	2.72	0.51
1:C:119:LEU:HD12	1:C:119:LEU:O	2.10	0.51
1:C:241:HIS:O	1:C:242:ARG:HG2	2.11	0.50
1:C:237:LYS:HG2	1:C:238:ASN:HD22	1.71	0.50
1:B:368:LEU:O	5:B:1283:CTX:H5	2.11	0.50
1:C:132:ARG:HD2	1:C:132:ARG:N	2.26	0.50
1:C:526:TYR:CD2	1:C:539:LEU:HB2	2.46	0.50
1:C:409:ASP:OD2	1:C:412:LYS:HE3	2.10	0.50
1:B:447:TYR:HB3	1:B:517:TRP:CZ2	2.46	0.50
1:A:114:GLU:HG3	1:A:291:GLU:OE1	2.12	0.50
1:C:487:GLU:HA	1:C:490:ILE:HD12	1.93	0.50
1:C:30:HIS:HB3	1:C:73:PRO:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD11	5:B:1283:CTX:HA1	1.93	0.50
1:B:355:PHE:CD1	1:B:360:PRO:HG3	2.46	0.50
1:B:487:GLU:OE2	1:B:491:ARG:NH1	2.45	0.50
1:B:366:TYR:HH	1:B:385:SER:HG	1.60	0.50
1:C:237:LYS:NZ	6:C:4170:HOH:O	2.44	0.50
1:A:303:PHE:CD2	1:A:318:LEU:HA	2.46	0.50
1:B:130:LYS:HE3	1:B:132:ARG:HH11	1.77	0.50
1:C:138:TRP:HH2	1:C:220:GLU:HB2	1.77	0.50
1:B:249:VAL:HG23	1:B:251:LEU:H	1.77	0.49
1:A:218:PHE:HB3	1:A:244:ILE:HB	1.93	0.49
1:C:498:LYS:HB3	1:C:514:LEU:HD11	1.92	0.49
1:A:25:VAL:HG22	1:A:34:LEU:HD23	1.94	0.49
1:C:339:ARG:HD2	1:C:339:ARG:H	1.78	0.49
1:C:52:GLY:HA3	3:C:1380:SIA:O9	2.12	0.49
1:A:194:GLN:OE1	1:A:226:SER:HB3	2.12	0.49
1:B:225:GLU:O	1:B:229:VAL:HG23	2.12	0.49
1:C:130:LYS:HE3	1:C:132:ARG:NH1	2.28	0.49
1:B:99:GLU:O	1:B:102:THR:HG22	2.13	0.49
1:B:491:ARG:HH11	1:B:491:ARG:HG3	1.76	0.49
1:B:101:PHE:CE1	1:B:358:LEU:HD21	2.47	0.49
1:C:237:LYS:O	1:C:238:ASN:HB2	2.13	0.49
1:A:304:LEU:HB2	5:A:1:CTX:H212	1.95	0.49
1:C:353:GLN:HE22	1:C:465:ILE:H	1.59	0.49
1:C:132:ARG:O	1:C:211:ASN:HB2	2.13	0.49
1:B:495:MET:CE	1:B:533:THR:HG21	2.43	0.49
1:A:369:SER:HA	5:A:11:CTX:H6	1.95	0.49
1:C:371:GLY:HA2	5:C:1383:CTX:HA3	1.95	0.49
1:A:379:MET:HG3	1:A:400:THR:HG21	1.94	0.49
1:A:355:PHE:CE2	1:A:425:MET:HE1	2.48	0.48
1:B:306:LEU:HD22	1:B:366:TYR:CE1	2.48	0.48
1:C:120:ASN:HB2	1:C:167:THR:OG1	2.13	0.48
1:B:339:ARG:H	1:B:339:ARG:HD2	1.77	0.48
1:A:551:PHE:C	1:A:553:LYS:N	2.66	0.48
1:A:102:THR:OG1	1:A:104:ARG:HG2	2.12	0.48
1:C:526:TYR:CE2	1:C:539:LEU:HB2	2.48	0.48
1:B:254:VAL:O	1:B:318:LEU:HD11	2.13	0.48
1:C:101:PHE:CZ	5:C:3:CTX:H11	2.49	0.48
1:B:394:GLU:O	1:B:397:PRO:HD2	2.13	0.48
1:A:233:SER:HA	1:A:234:PRO:HD3	1.75	0.48
1:A:176:GLY:HA2	1:A:189:TRP:HB2	1.96	0.48
1:C:218:PHE:HB3	1:C:244:ILE:HB	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:PHE:CD1	1:A:360:PRO:HG3	2.48	0.48
1:A:553:LYS:HZ3	1:A:553:LYS:HB3	1.78	0.48
1:A:26:VAL:CG1	1:A:207:SER:HB3	2.44	0.48
1:C:126:ASP:HA	6:C:4050:HOH:O	2.13	0.48
1:A:251:LEU:HD11	1:A:336:GLN:HE22	1.79	0.48
1:B:101:PHE:HE1	1:B:358:LEU:HD21	1.79	0.47
1:A:361:MET:C	1:A:361:MET:SD	2.93	0.47
1:C:317:PRO:HB3	5:C:3:CTX:H15	1.95	0.47
1:A:64:ARG:NH2	1:A:114:GLU:OE2	2.47	0.47
1:C:26:VAL:HG12	1:C:27:ASP:N	2.29	0.47
1:C:318:LEU:C	1:C:318:LEU:HD12	2.34	0.47
1:C:206:ALA:HB2	6:C:4126:HOH:O	2.14	0.47
1:A:52:GLY:HA3	3:A:1180:SIA:C9	2.45	0.47
1:C:414:LYS:HZ2	5:C:1383:CTX:HA1	1.79	0.47
1:C:538:LYS:HB3	1:C:541:ASP:CB	2.44	0.47
1:C:420:LEU:HD22	1:C:547:TRP:HZ2	1.80	0.47
1:C:414:LYS:HD2	5:C:1383:CTX:HA1	1.96	0.47
1:A:349:GLY:HA3	1:A:447:TYR:CD1	2.50	0.47
1:A:26:VAL:HG13	1:A:207:SER:HB3	1.97	0.47
1:A:268:ILE:HD11	1:A:319:LEU:HD21	1.96	0.47
1:C:88:THR:CG2	1:C:175:TRP:CH2	2.97	0.47
1:C:363:LEU:O	5:C:3:CTX:HA11	2.14	0.47
1:C:88:THR:HG21	1:C:175:TRP:CH2	2.50	0.47
1:C:478:ALA:N	1:C:479:PRO:CD	2.78	0.47
1:A:52:GLY:O	3:A:1180:SIA:H91	2.15	0.47
1:B:538:LYS:HB3	1:B:541:ASP:CB	2.45	0.47
1:A:92:LYS:NZ	6:A:4068:HOH:O	2.48	0.47
1:B:48:ALA:HB3	1:B:123:THR:CG2	2.45	0.47
1:B:388:LEU:CD2	5:B:2:CTX:H14	2.40	0.46
1:C:388:LEU:HD23	1:C:425:MET:SD	2.55	0.46
3:B:1280:SIA:H92	6:B:4060:HOH:O	2.15	0.46
1:B:528:GLN:NE2	1:B:536:ALA:HB2	2.28	0.46
1:C:331:THR:OG1	1:C:334:GLU:HG3	2.14	0.46
1:B:352:LYS:HB2	1:B:450:GLN:HB3	1.97	0.46
1:B:545:ALA:O	1:B:549:ASN:ND2	2.47	0.46
1:B:498:LYS:HB3	1:B:514:LEU:HD11	1.96	0.46
1:B:251:LEU:HD11	1:B:336:GLN:HE22	1.80	0.46
1:A:417:PHE:O	1:A:420:LEU:HB3	2.15	0.46
1:A:140:HIS:HE1	6:A:4005:HOH:O	1.97	0.46
1:C:139:ILE:HG12	1:C:168:ILE:HD11	1.98	0.46
1:B:237:LYS:O	1:B:238:ASN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PRO:O	1:B:369:SER:N	2.47	0.46
1:A:88:THR:HG21	1:A:175:TRP:CH2	2.50	0.46
1:C:330:LYS:HG3	1:C:335:LEU:HG	1.98	0.46
1:C:493:SER:O	1:C:497:MET:HG3	2.15	0.46
1:A:106:GLU:O	1:A:106:GLU:HG3	2.15	0.46
1:A:447:TYR:HB3	1:A:517:TRP:CZ2	2.51	0.46
1:C:480:PHE:HZ	1:C:494:LYS:HG3	1.80	0.46
1:C:95:GLN:O	1:C:99:GLU:HG3	2.16	0.46
1:C:428:VAL:HG13	1:C:544:VAL:HG13	1.98	0.46
1:C:552:ALA:O	1:C:553:LYS:HB3	2.16	0.46
1:A:495:MET:CE	1:A:533:THR:HG21	2.45	0.46
1:B:220:GLU:HG3	1:B:472:LEU:HD21	1.98	0.45
1:A:29:VAL:HG23	1:A:204:ASN:OD1	2.16	0.45
1:B:23:PRO:HA	1:B:24:PRO:HD3	1.79	0.45
1:B:355:PHE:CE2	1:B:425:MET:HE2	2.50	0.45
1:B:395:LEU:HB3	1:B:550:LEU:HD11	1.97	0.45
1:B:38:VAL:HG21	1:B:49:ILE:HD12	1.98	0.45
1:C:414:LYS:HD2	5:C:1383:CTX:CA	2.46	0.45
1:C:218:PHE:CB	1:C:244:ILE:HB	2.47	0.45
1:C:341:PHE:HD1	1:C:342:HIS:N	2.14	0.45
1:A:437:HIS:O	1:A:440:ALA:HB3	2.16	0.45
1:B:132:ARG:HB3	1:B:211:ASN:HB2	1.98	0.45
1:A:26:VAL:HG13	1:A:207:SER:O	2.16	0.45
1:C:145:MET:SD	1:C:173:GLY:HA2	2.56	0.45
1:C:447:TYR:C	1:C:447:TYR:CD2	2.90	0.45
1:A:187:GLY:O	1:A:188:ASN:HB2	2.16	0.45
1:B:26:VAL:HG12	1:B:27:ASP:N	2.32	0.45
1:C:290:THR:HA	4:C:1381:SO4:O4	2.17	0.45
1:B:414:LYS:HD2	5:B:1283:CTX:HA3	1.99	0.45
1:B:407:THR:CB	1:B:412:LYS:HD2	2.46	0.45
1:C:244:ILE:HG12	1:C:347:MET:HB3	1.99	0.45
1:A:241:HIS:C	1:A:242:ARG:CG	2.85	0.45
1:A:388:LEU:HD21	5:A:1:CTX:C14	2.46	0.45
1:C:414:LYS:CD	5:C:1383:CTX:HA1	2.47	0.45
1:A:101:PHE:CE1	1:A:358:LEU:HD21	2.52	0.45
1:A:201:VAL:HG13	1:A:205:ILE:HB	1.98	0.45
1:B:253:SER:O	1:B:255:LEU:N	2.50	0.44
1:B:106:GLU:O	1:B:106:GLU:HG3	2.16	0.44
5:A:11:CTX:H223	5:A:11:CTX:HA12	1.87	0.44
1:A:447:TYR:C	1:A:447:TYR:CD2	2.90	0.44
1:A:152:TYR:N	1:A:152:TYR:CD1	2.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:HB3	1:A:412:LYS:HD2	2.00	0.44
1:A:147:GLY:HA2	6:A:4182:HOH:O	2.17	0.44
1:A:366:TYR:HA	1:A:367:PRO:HD3	1.69	0.44
1:C:414:LYS:HE2	1:C:415:ASP:CA	2.47	0.44
1:B:435:ARG:NH1	1:B:544:VAL:HG11	2.33	0.44
1:A:290:THR:O	1:A:293:GLU:HB2	2.18	0.44
1:A:139:ILE:HG12	1:A:168:ILE:HD11	1.99	0.44
1:C:388:LEU:CD2	5:C:3:CTX:H14	2.46	0.44
1:A:267:GLN:HE21	1:A:267:GLN:HB3	1.60	0.44
1:B:339:ARG:CD	1:B:339:ARG:H	2.31	0.44
1:A:371:GLY:C	1:A:414:LYS:HD3	2.38	0.44
1:C:414:LYS:HE3	5:C:1383:CTX:HA1	1.96	0.44
1:B:429:PRO:O	1:B:433:VAL:HG23	2.18	0.44
1:B:551:PHE:C	1:B:553:LYS:H	2.19	0.44
1:A:483:GLU:HG3	1:A:484:GLY:N	2.33	0.44
3:B:1280:SIA:C7	3:B:1280:SIA:O2	2.65	0.44
1:A:526:TYR:HE2	1:A:537:GLN:O	2.00	0.44
1:C:321:THR:HG22	1:C:322:VAL:N	2.32	0.44
1:B:242:ARG:NH1	1:B:242:ARG:CG	2.75	0.44
1:B:368:LEU:HD21	1:B:381:LEU:HD11	2.00	0.44
1:A:95:GLN:O	1:A:99:GLU:HG3	2.16	0.44
1:B:64:ARG:NH2	1:B:114:GLU:OE2	2.51	0.44
1:B:351:ASN:HB3	1:B:466:GLY:O	2.18	0.44
1:C:26:VAL:CG1	1:C:207:SER:HB3	2.48	0.43
1:A:198:LEU:HB3	1:A:239:LEU:HB3	2.00	0.43
1:C:528:GLN:HE21	1:C:536:ALA:HB2	1.83	0.43
1:A:428:VAL:HB	1:A:429:PRO:HD3	2.00	0.43
1:A:132:ARG:HD2	1:A:132:ARG:N	2.33	0.43
1:A:372:GLN:HB2	1:A:410:THR:OG1	2.19	0.43
1:C:355:PHE:O	1:C:360:PRO:HG2	2.19	0.43
1:A:386:TYR:N	1:A:387:PRO:CD	2.80	0.43
1:A:331:THR:OG1	1:A:334:GLU:HG3	2.18	0.43
1:A:220:GLU:HG3	1:A:472:LEU:CD2	2.45	0.43
1:C:144:LEU:HD22	1:C:177:PHE:CZ	2.54	0.43
1:C:420:LEU:O	1:C:420:LEU:HD13	2.19	0.43
1:C:409:ASP:HB3	1:C:412:LYS:HD2	2.01	0.43
1:C:149:ALA:HB1	1:C:167:THR:HB	2.01	0.43
1:C:161:GLU:HB3	1:C:501:ALA:CB	2.49	0.43
1:C:221:SER:HB3	6:C:4193:HOH:O	2.18	0.43
1:B:349:GLY:HA3	1:B:447:TYR:CE1	2.54	0.43
5:B:2:CTX:HA2	6:B:4017:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:CD1	1:A:218:PHE:N	2.87	0.43
1:A:498:LYS:HB3	1:A:514:LEU:HD11	2.01	0.43
1:B:241:HIS:C	1:B:242:ARG:CG	2.87	0.43
1:C:323:ILE:HG21	1:C:330:LYS:HA	2.01	0.43
1:A:428:VAL:N	1:A:429:PRO:CD	2.82	0.43
1:C:348:VAL:O	1:C:446:MET:HA	2.19	0.43
1:B:105:LYS:CG	1:B:106:GLU:N	2.75	0.43
1:A:339:ARG:H	1:A:339:ARG:CD	2.31	0.43
1:C:306:LEU:HD22	1:C:366:TYR:CE1	2.54	0.43
1:C:374:ASP:O	1:C:375:GLN:C	2.58	0.43
5:C:1383:CTX:H212	6:C:4057:HOH:O	2.19	0.42
1:C:540:LYS:O	1:C:544:VAL:HG23	2.19	0.42
1:C:187:GLY:O	1:C:188:ASN:HB2	2.19	0.42
1:B:331:THR:HB	1:B:333:GLU:OE1	2.18	0.42
1:A:420:LEU:HD22	1:A:547:TRP:HZ2	1.83	0.42
1:C:551:PHE:C	1:C:553:LYS:H	2.22	0.42
1:C:45:GLN:NE2	1:C:46:PRO:HD2	2.34	0.42
1:A:372:GLN:HA	1:A:414:LYS:HB2	2.01	0.42
1:B:371:GLY:HA2	5:B:1283:CTX:H17	2.01	0.42
1:B:34:LEU:HD13	1:B:34:LEU:C	2.40	0.42
1:C:211:ASN:HA	1:C:212:PRO:HD2	1.91	0.42
1:C:26:VAL:HG13	1:C:207:SER:HB3	2.00	0.42
1:B:24:PRO:HG3	1:B:37:PHE:CD1	2.54	0.42
1:A:414:LYS:CE	5:A:11:CTX:HA3	2.49	0.42
1:B:389:VAL:O	1:B:390:CYS:HB2	2.19	0.42
1:C:267:GLN:HE21	1:C:267:GLN:HB3	1.55	0.42
1:C:60:LEU:CD2	1:C:114:GLU:HB2	2.50	0.42
1:A:292:GLU:O	1:A:296:GLU:HB2	2.20	0.42
1:C:138:TRP:CH2	1:C:220:GLU:HB2	2.54	0.42
1:C:364:MET:O	1:C:365:SER:HB2	2.20	0.42
1:A:202:GLN:HG2	6:A:4166:HOH:O	2.19	0.42
1:A:119:LEU:HD12	1:A:119:LEU:O	2.20	0.42
1:B:51:LEU:HD13	1:B:83:TYR:CE1	2.54	0.42
1:B:134:PRO:CG	1:B:163:VAL:HG12	2.37	0.42
1:A:407:THR:CB	1:A:412:LYS:HD2	2.49	0.42
1:B:268:ILE:HD11	1:B:319:LEU:HD21	2.00	0.42
1:B:486:SER:O	1:B:490:ILE:HG13	2.20	0.42
3:A:1180:SIA:C8	6:A:4003:HOH:O	2.55	0.42
1:C:353:GLN:O	1:C:467:ASP:HA	2.20	0.42
1:B:407:THR:OG1	1:B:412:LYS:HD2	2.19	0.42
1:C:256:VAL:HG22	1:C:321:THR:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:SER:N	6:A:4053:HOH:O	2.52	0.42
1:B:140:HIS:HB2	1:B:152:TYR:HE1	1.85	0.42
1:A:88:THR:CG2	1:A:175:TRP:CH2	3.03	0.42
1:C:205:ILE:HA	1:C:205:ILE:HD12	1.78	0.42
1:B:267:GLN:HE21	1:B:267:GLN:HB3	1.64	0.42
1:C:355:PHE:CE2	1:C:425:MET:HE1	2.54	0.42
1:B:404:LEU:HB3	1:B:413:LYS:HZ2	1.85	0.42
1:A:237:LYS:HE2	1:A:238:ASN:HD21	1.85	0.42
1:A:414:LYS:CD	5:A:11:CTX:HA3	2.48	0.42
1:C:349:GLY:HA3	1:C:447:TYR:CD1	2.55	0.42
1:B:252:THR:HG22	1:B:254:VAL:HG12	2.02	0.42
1:A:119:LEU:HD12	1:A:119:LEU:C	2.41	0.42
1:B:445:TYR:CE1	1:B:519:GLU:HA	2.54	0.42
1:A:317:PRO:HG2	1:A:318:LEU:H	1.85	0.41
1:A:26:VAL:HG12	1:A:27:ASP:N	2.35	0.41
1:A:353:GLN:O	1:A:467:ASP:HA	2.19	0.41
1:A:34:LEU:C	1:A:34:LEU:HD13	2.41	0.41
1:A:101:PHE:HE1	1:A:358:LEU:CD2	2.32	0.41
1:B:401:GLU:O	1:B:403:TYR:N	2.53	0.41
1:B:420:LEU:C	1:B:420:LEU:HD13	2.40	0.41
1:B:493:SER:O	1:B:497:MET:HG3	2.19	0.41
1:C:359:ILE:HB	1:C:360:PRO:HD3	2.01	0.41
1:C:262:LYS:N	1:C:263:PRO:CD	2.83	0.41
1:C:420:LEU:C	1:C:420:LEU:HD13	2.41	0.41
1:B:358:LEU:HB2	1:B:467:ASP:OD2	2.20	0.41
1:B:140:HIS:HB2	1:B:152:TYR:CE1	2.55	0.41
1:B:333:GLU:O	1:B:336:GLN:HG2	2.20	0.41
1:C:409:ASP:CG	1:C:412:LYS:HG3	2.41	0.41
1:A:242:ARG:HD3	1:A:503:PHE:O	2.20	0.41
1:C:357:TRP:HA	5:C:1383:CTX:H12	2.01	0.41
1:A:420:LEU:C	1:A:420:LEU:HD13	2.41	0.41
1:B:375:GLN:OE1	1:B:413:LYS:NZ	2.53	0.41
1:C:252:THR:HG22	1:C:254:VAL:HG12	2.03	0.41
1:A:59:PRO:HG3	1:A:171:ARG:HD3	2.02	0.41
1:B:218:PHE:CD1	1:B:218:PHE:N	2.89	0.41
1:A:105:LYS:CG	1:A:106:GLU:N	2.81	0.41
1:C:339:ARG:H	1:C:339:ARG:CD	2.33	0.41
2:A:1179:NAG:H3	2:A:1179:NAG:C8	2.49	0.41
1:A:407:THR:OG1	1:A:412:LYS:HD2	2.20	0.41
1:B:351:ASN:ND2	1:B:449:PHE:HB3	2.36	0.41
1:A:354:GLU:HG2	6:A:4031:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HD11	1:A:391:ILE:HD12	2.01	0.41
1:A:132:ARG:HB3	1:A:211:ASN:HB2	2.03	0.41
1:B:218:PHE:HB3	1:B:244:ILE:HB	2.03	0.41
1:C:530:GLY:O	1:C:531:ALA:C	2.59	0.41
1:A:130:LYS:CE	1:A:132:ARG:HD3	2.51	0.41
1:A:460:LYS:HA	1:A:461:PRO:HD2	1.95	0.41
1:B:104:ARG:HD3	1:B:104:ARG:HH11	1.77	0.41
1:C:130:LYS:HE3	1:C:132:ARG:HH11	1.86	0.41
1:B:211:ASN:HA	1:B:212:PRO:HD2	1.89	0.41
1:B:386:TYR:O	1:B:390:CYS:N	2.51	0.41
1:C:407:THR:HG21	1:C:412:LYS:NZ	2.35	0.41
1:A:101:PHE:HE1	1:A:358:LEU:HD21	1.86	0.41
1:A:351:ASN:ND2	1:A:449:PHE:HB3	2.36	0.41
1:B:355:PHE:N	6:B:4058:HOH:O	2.48	0.41
1:A:331:THR:HB	1:A:333:GLU:OE1	2.21	0.41
3:B:1280:SIA:H113	1:C:262:LYS:HZ1	1.86	0.41
1:A:406:GLY:O	1:A:407:THR:C	2.59	0.41
1:B:420:LEU:O	1:B:420:LEU:HD13	2.21	0.40
1:C:130:LYS:CE	1:C:132:ARG:HD3	2.51	0.40
1:C:218:PHE:HA	1:C:244:ILE:O	2.21	0.40
1:C:152:TYR:N	1:C:152:TYR:CD1	2.88	0.40
1:A:211:ASN:HA	1:A:212:PRO:HD2	1.91	0.40
3:A:1180:SIA:C10	6:A:4143:HOH:O	2.68	0.40
1:B:38:VAL:CG2	1:B:49:ILE:HD12	2.50	0.40
1:B:452:ARG:NE	1:B:462:LYS:HA	2.37	0.40
1:A:323:ILE:HG21	1:A:330:LYS:HA	2.04	0.40
1:C:191:HIS:O	1:C:194:GLN:HB2	2.21	0.40
1:A:389:VAL:O	1:A:390:CYS:HB2	2.20	0.40
1:C:81:THR:HB	6:C:4183:HOH:O	2.21	0.40
1:A:262:LYS:HG3	1:A:266:GLU:OE2	2.22	0.40
1:C:396:ILE:N	1:C:397:PRO:CD	2.85	0.40
1:A:218:PHE:CB	1:A:244:ILE:HB	2.52	0.40
1:C:249:VAL:HG23	1:C:251:LEU:H	1.86	0.40
1:A:199:ARG:NH1	1:A:199:ARG:CB	2.83	0.40
1:C:428:VAL:HG13	1:C:544:VAL:HA	2.03	0.40
1:A:409:ASP:HB3	1:A:412:LYS:CG	2.51	0.40
1:B:64:ARG:NH2	6:B:4172:HOH:O	2.55	0.40
1:B:478:ALA:N	1:B:479:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	529/532 (99%)	477 (90%)	43 (8%)	9 (2%)	11	52
1	B	530/532 (100%)	472 (89%)	49 (9%)	9 (2%)	11	52
1	C	530/532 (100%)	477 (90%)	47 (9%)	6 (1%)	17	62
All	All	1589/1596 (100%)	1426 (90%)	139 (9%)	24 (2%)	13	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	PRO
1	B	185	SER
1	C	253	SER
1	C	304	LEU
1	B	254	VAL
1	B	375	GLN
1	B	427	GLY
1	C	185	SER
1	C	407	THR
1	C	427	GLY
1	A	375	GLN
1	B	253	SER
1	B	368	LEU
1	B	407	THR
1	A	365	SER
1	A	407	THR
1	A	105	LYS
1	A	185	SER
1	B	402	LYS
1	A	23	PRO
1	A	427	GLY
1	A	142	GLY
1	A	205	ILE
1	C	142	GLY

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	447/448 (100%)	433 (97%)	14 (3%)	47	82
1	B	448/448 (100%)	433 (97%)	15 (3%)	45	81
1	C	448/448 (100%)	429 (96%)	19 (4%)	36	75
All	All	1343/1344 (100%)	1295 (96%)	48 (4%)	42	79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	111	LYS
1	A	132	ARG
1	A	162	ASN
1	A	199	ARG
1	A	218	PHE
1	A	225	GLU
1	A	264	LEU
1	A	339	ARG
1	A	366	TYR
1	A	471	GLU
1	A	499	PHE
1	A	500	TRP
1	A	523	LYS
1	B	69	GLN
1	B	111	LYS
1	B	132	ARG
1	B	162	ASN
1	B	199	ARG
1	B	218	PHE
1	B	225	GLU
1	B	264	LEU
1	B	318	LEU
1	B	339	ARG
1	B	388	LEU
1	B	499	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	500	TRP
1	B	523	LYS
1	B	532	ASN
1	C	66	THR
1	C	69	GLN
1	C	111	LYS
1	C	132	ARG
1	C	162	ASN
1	C	199	ARG
1	C	218	PHE
1	C	225	GLU
1	C	264	LEU
1	C	277	THR
1	C	339	ARG
1	C	388	LEU
1	C	414	LYS
1	C	415	ASP
1	C	420	LEU
1	C	471	GLU
1	C	499	PHE
1	C	500	TRP
1	C	523	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	140	HIS
1	A	184	HIS
1	A	238	ASN
1	A	241	HIS
1	A	267	GLN
1	A	336	GLN
1	A	351	ASN
1	A	353	GLN
1	A	372	GLN
1	A	436	ASN
1	A	528	GLN
1	A	537	GLN
1	A	549	ASN
1	B	140	HIS
1	B	160	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	238	ASN
1	B	241	HIS
1	B	267	GLN
1	B	336	GLN
1	B	351	ASN
1	B	353	GLN
1	B	372	GLN
1	B	436	ASN
1	B	528	GLN
1	B	537	GLN
1	B	549	ASN
1	C	45	GLN
1	C	140	HIS
1	C	160	HIS
1	C	184	HIS
1	C	238	ASN
1	C	241	HIS
1	C	267	GLN
1	C	336	GLN
1	C	351	ASN
1	C	353	GLN
1	C	372	GLN
1	C	436	ASN
1	C	528	GLN
1	C	537	GLN
1	C	549	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

18 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
5	CTX	A	1	-	30,30,30	2.81	17 (56%)	39,39,39	1.40	4 (10%)
5	CTX	A	11	-	30,30,30	2.69	16 (53%)	39,39,39	1.32	5 (12%)
2	NAG	A	1179	1	14,14,15	0.95	1 (7%)	15,19,21	0.87	0
3	SIA	A	1180	-	17,21,21	0.95	1 (5%)	19,31,31	0.94	1 (5%)
4	SO4	A	1181	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	A	1182	-	4,4,4	0.28	0	6,6,6	0.21	0
2	NAG	B	1279	1	14,14,15	0.56	0	15,19,21	0.95	1 (6%)
3	SIA	B	1280	-	17,21,21	0.92	1 (5%)	19,31,31	0.92	1 (5%)
4	SO4	B	1281	-	4,4,4	0.23	0	6,6,6	0.14	0
4	SO4	B	1282	-	4,4,4	0.21	0	6,6,6	0.11	0
5	CTX	B	1283	-	30,30,30	2.79	15 (50%)	39,39,39	1.15	5 (12%)
5	CTX	B	2	-	30,30,30	2.84	13 (43%)	39,39,39	1.35	5 (12%)
2	NAG	C	1379	1	14,14,15	0.57	0	15,19,21	0.64	0
3	SIA	C	1380	-	17,21,21	1.00	1 (5%)	19,31,31	1.54	1 (5%)
4	SO4	C	1381	-	4,4,4	0.25	0	6,6,6	0.14	0
4	SO4	C	1382	-	4,4,4	0.27	0	6,6,6	0.15	0
5	CTX	C	1383	-	30,30,30	2.58	15 (50%)	39,39,39	1.13	4 (10%)
5	CTX	C	3	-	30,30,30	2.72	13 (43%)	39,39,39	1.55	7 (17%)

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
5	CTX	A	1	-	-	0/24/24/24	0/3/3/3
5	CTX	A	11	-	-	0/24/24/24	0/3/3/3
2	NAG	A	1179	1	1/1/5/7	1/6/23/26	0/1/1/1
3	SIA	A	1180	-	-	0/14/38/38	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1181	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1182	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1279	1	-	0/6/23/26	0/1/1/1
3	SIA	B	1280	-	-	0/14/38/38	0/1/1/1
4	SO4	B	1281	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1282	-	-	0/0/0/0	0/0/0/0
5	CTX	B	1283	-	-	0/24/24/24	0/3/3/3
5	CTX	B	2	-	-	0/24/24/24	0/3/3/3
2	NAG	C	1379	1	-	0/6/23/26	0/1/1/1
3	SIA	C	1380	-	-	1/14/38/38	0/1/1/1
4	SO4	C	1381	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1382	-	-	0/0/0/0	0/0/0/0
5	CTX	C	1383	-	-	0/24/24/24	0/3/3/3
5	CTX	C	3	-	-	0/24/24/24	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	11	CTX	C17-C18	2.00	1.42	1.39
5	A	11	CTX	C10-C9	2.03	1.43	1.38
5	C	1383	CTX	C12-C11	2.03	1.43	1.38
5	A	1	CTX	C10-C9	2.07	1.43	1.38
5	A	11	CTX	C16-C17	2.09	1.43	1.38
5	A	1	CTX	C12-C11	2.11	1.43	1.38
5	B	1283	CTX	C16-C17	2.11	1.43	1.38
5	B	1283	CTX	C14-C19	2.14	1.43	1.38
5	B	1283	CTX	C6-C5	2.14	1.42	1.38
5	C	3	CTX	C12-C11	2.15	1.43	1.38
5	A	11	CTX	C12-C11	2.15	1.43	1.38
3	B	1280	SIA	C7-C6	2.15	1.55	1.52
5	A	11	CTX	C6-C5	2.18	1.42	1.38
5	A	1	CTX	C8-C7	2.20	1.53	1.49
5	C	1383	CTX	C5-C4	2.21	1.43	1.39
5	B	2	CTX	C12-C11	2.23	1.43	1.38
5	A	1	CTX	CB-C20	2.23	1.57	1.52
5	C	1383	CTX	C16-C17	2.26	1.43	1.38
5	C	1383	CTX	C8-C7	2.27	1.53	1.49
5	A	1	CTX	C19-C18	2.28	1.43	1.39
5	A	1	CTX	CB1-NI	2.29	1.55	1.46
5	B	2	CTX	C17-C18	2.41	1.43	1.39
5	B	2	CTX	C19-C18	2.44	1.43	1.39
5	B	1283	CTX	CB1-NI	2.46	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	11	CTX	C5-C4	2.49	1.43	1.39
5	C	1383	CTX	CB1-NI	2.53	1.56	1.46
5	B	1283	CTX	C17-C18	2.58	1.43	1.39
3	A	1180	SIA	O6-C2	2.62	1.45	1.42
5	C	3	CTX	C17-C18	2.62	1.43	1.39
5	C	1383	CTX	C19-C18	2.69	1.43	1.39
5	C	3	CTX	C19-C18	2.71	1.43	1.39
3	C	1380	SIA	O6-C2	2.75	1.45	1.42
5	A	1	CTX	C17-C18	2.75	1.44	1.39
5	A	11	CTX	C19-C18	2.78	1.44	1.39
5	B	2	CTX	C6-C5	2.79	1.43	1.38
5	C	3	CTX	C6-C5	2.80	1.43	1.38
5	A	11	CTX	C18-C20	2.83	1.55	1.49
2	A	1179	NAG	C1-C2	2.84	1.56	1.52
5	A	1	CTX	C6-C5	2.89	1.44	1.38
5	A	1	CTX	C18-C20	2.89	1.55	1.49
5	B	1283	CTX	C19-C18	2.90	1.44	1.39
5	B	1283	CTX	C5-C4	2.93	1.44	1.39
5	A	11	CTX	CB1-NI	3.04	1.58	1.46
5	C	3	CTX	C18-C20	3.05	1.55	1.49
5	C	1383	CTX	C17-C18	3.06	1.44	1.39
5	B	2	CTX	C18-C20	3.17	1.55	1.49
5	A	1	CTX	C5-C4	3.17	1.44	1.39
5	B	1283	CTX	C6-C1	3.26	1.45	1.38
5	B	2	CTX	C5-C4	3.29	1.44	1.39
5	A	11	CTX	C13-C8	3.34	1.45	1.39
5	C	1383	CTX	C18-C20	3.40	1.56	1.49
5	C	3	CTX	C13-C8	3.41	1.45	1.39
5	C	3	CTX	C9-C8	3.53	1.45	1.39
5	B	1283	CTX	C13-C8	3.53	1.45	1.39
5	C	1383	CTX	C6-C1	3.54	1.45	1.38
5	C	3	CTX	C5-C4	3.54	1.45	1.39
5	B	2	CTX	C6-C1	3.55	1.45	1.38
5	C	3	CTX	C6-C1	3.55	1.45	1.38
5	C	1383	CTX	C3-C4	3.58	1.45	1.39
5	A	1	CTX	C6-C1	3.58	1.45	1.38
5	C	3	CTX	C2-C1	3.60	1.45	1.38
5	B	1283	CTX	C9-C8	3.64	1.45	1.39
5	C	1383	CTX	C9-C8	3.64	1.45	1.39
5	A	11	CTX	C6-C1	3.67	1.46	1.38
5	A	11	CTX	C3-C4	3.68	1.45	1.39
5	A	1	CTX	C13-C8	3.69	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1283	CTX	C18-C20	3.75	1.57	1.49
5	A	1	CTX	C9-C8	3.76	1.45	1.39
5	B	2	CTX	C2-C1	3.83	1.46	1.38
5	C	3	CTX	C3-C4	3.84	1.45	1.39
5	B	1283	CTX	C3-C4	3.85	1.45	1.39
5	A	1	CTX	C2-C1	3.87	1.46	1.38
5	C	1383	CTX	C2-C1	3.89	1.46	1.38
5	B	2	CTX	C13-C8	3.93	1.46	1.39
5	A	11	CTX	C9-C8	3.94	1.46	1.39
5	A	1	CTX	C3-C4	4.00	1.46	1.39
5	B	2	CTX	C9-C8	4.09	1.46	1.39
5	C	1383	CTX	C13-C8	4.14	1.46	1.39
5	A	11	CTX	C2-C1	4.22	1.47	1.38
5	B	1283	CTX	C2-C1	4.27	1.47	1.38
5	B	2	CTX	C3-C4	4.43	1.46	1.39
5	C	1383	CTX	C7-C20	4.84	1.48	1.34
5	C	1383	CTX	C4-C7	4.98	1.57	1.49
5	A	11	CTX	C7-C20	5.13	1.49	1.34
5	B	1283	CTX	C7-C20	5.54	1.50	1.34
5	B	2	CTX	C7-C20	5.55	1.50	1.34
5	A	1	CTX	C7-C20	5.55	1.50	1.34
5	C	3	CTX	C7-C20	5.85	1.51	1.34
5	A	11	CTX	C4-C7	5.87	1.59	1.49
5	B	1283	CTX	C4-C7	6.46	1.60	1.49
5	C	3	CTX	C4-C7	6.71	1.60	1.49
5	B	2	CTX	C4-C7	6.88	1.60	1.49
5	A	1	CTX	C4-C7	6.93	1.61	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1380	SIA	C7-C6-C5	-5.26	106.36	114.32
5	C	3	CTX	C8-C7-C4	-3.53	108.44	115.69
5	C	3	CTX	CA1-CB1-NI	-3.51	104.98	114.66
5	A	1	CTX	C8-C7-C4	-3.31	108.89	115.69
5	B	2	CTX	C8-C7-C4	-3.06	109.41	115.69
5	A	11	CTX	C8-C7-C4	-3.00	109.53	115.69
2	B	1279	NAG	C2-N2-C7	-2.92	119.29	123.04
5	B	1283	CTX	C18-C20-C7	-2.62	119.02	122.40
5	B	2	CTX	CA1-CB1-NI	-2.33	108.25	114.66
5	C	1383	CTX	CA1-CB1-NI	-2.15	108.72	114.66
5	B	1283	CTX	CA1-CB1-NI	-2.09	108.89	114.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1180	SIA	C7-C6-C5	-2.09	111.15	114.32
5	C	3	CTX	CB-C20-C18	-2.01	111.46	114.39
5	C	1383	CTX	C18-C20-C7	-2.00	119.81	122.40
5	B	1283	CTX	OL-CA1-CB1	2.11	112.53	107.67
5	B	2	CTX	CB-C20-C7	2.32	126.11	123.47
3	B	1280	SIA	O6-C6-C7	2.41	110.90	107.26
5	C	3	CTX	CA1-OL-C1	2.53	124.14	117.91
5	C	3	CTX	CB-C20-C7	2.66	126.49	123.47
5	C	3	CTX	OL-CA1-CB1	2.80	114.12	107.67
5	A	11	CTX	OL-CA1-CB1	2.88	114.32	107.67
5	B	2	CTX	CA1-OL-C1	2.89	125.02	117.91
5	A	11	CTX	CA1-OL-C1	3.00	125.30	117.91
5	B	1283	CTX	CA1-OL-C1	3.08	125.49	117.91
5	A	1	CTX	CA1-OL-C1	3.17	125.71	117.91
5	A	11	CTX	CB-C20-C7	3.25	127.17	123.47
5	C	1383	CTX	CB-C20-C7	3.33	127.25	123.47
5	A	1	CTX	CB-C20-C7	3.43	127.38	123.47
5	C	1383	CTX	CA1-OL-C1	3.63	126.84	117.91
5	B	1283	CTX	CB-C20-C7	4.22	128.27	123.47
5	A	11	CTX	C4-C7-C20	4.25	128.53	122.84
5	A	1	CTX	C4-C7-C20	4.80	129.27	122.84
5	B	2	CTX	C4-C7-C20	5.19	129.79	122.84
5	C	3	CTX	C4-C7-C20	5.77	130.57	122.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1179	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1380	SIA	O10-C10-N5-C5
2	A	1179	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	CTX	3	0
5	A	11	CTX	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1179	NAG	4	0
3	A	1180	SIA	6	0
3	B	1280	SIA	5	0
5	B	1283	CTX	5	0
5	B	2	CTX	5	0
3	C	1380	SIA	3	0
4	C	1381	SO4	1	0
5	C	1383	CTX	11	0
5	C	3	CTX	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	531/532 (99%)	-0.08	21 (3%)	42 27	11, 33, 69, 91	0
1	B	532/532 (100%)	-0.06	17 (3%)	51 36	11, 35, 69, 89	0
1	C	532/532 (100%)	-0.18	4 (0%)	87 80	13, 33, 66, 89	0
All	All	1595/1596 (99%)	-0.11	42 (2%)	59 45	11, 34, 68, 91	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	SER	6.4
1	A	340	ASN	6.3
1	C	342	HIS	3.6
1	A	549	ASN	3.5
1	A	407	THR	3.4
1	A	312	PRO	3.4
1	B	41	GLU	3.3
1	B	407	THR	3.3
1	C	483	GLU	3.2
1	C	21	SER	3.2
1	A	553	LYS	3.1
1	B	23	PRO	2.8
1	A	339	ARG	2.8
1	A	367	PRO	2.8
1	B	410	THR	2.7
1	A	22	SER	2.6
1	B	408	ASP	2.6
1	A	552	ALA	2.6
1	A	402	LYS	2.5
1	B	411	VAL	2.5
1	B	44	ALA	2.5
1	B	45	GLN	2.5
1	B	372	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	22	SER	2.4
1	A	375	GLN	2.4
1	A	317	PRO	2.4
1	B	314	GLU	2.3
1	A	395	LEU	2.3
1	B	36	LYS	2.3
1	A	410	THR	2.3
1	B	405	GLY	2.2
1	A	401	GLU	2.2
1	A	391	ILE	2.2
1	A	397	PRO	2.2
1	B	409	ASP	2.2
1	B	412	LYS	2.2
1	C	131	ASN	2.2
1	A	408	ASP	2.1
1	A	394	GLU	2.1
1	B	126	ASP	2.1
1	A	342	HIS	2.0
1	A	416	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	CTX	C	1383	28/28	0.61	0.49	8.32	75,79,87,87	0
2	NAG	A	1179	14/15	0.74	0.41	4.11	64,67,69,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	C	1381	5/5	0.89	0.29	2.98	92,92,92,92	0
4	SO4	B	1282	5/5	0.78	0.33	2.72	106,107,107,107	0
5	CTX	B	2	28/28	0.88	0.27	2.61	38,44,54,54	0
5	CTX	C	3	28/28	0.90	0.26	2.55	31,35,41,42	0
4	SO4	A	1181	5/5	0.83	0.22	2.47	78,79,80,80	0
4	SO4	C	1382	5/5	0.91	0.21	2.47	75,75,76,76	0
5	CTX	A	11	28/28	0.61	0.50	2.43	67,70,80,81	0
5	CTX	B	1283	28/28	0.59	0.50	2.38	82,85,90,90	0
4	SO4	A	1182	5/5	0.88	0.28	1.86	78,79,79,79	0
5	CTX	A	1	28/28	0.89	0.31	1.59	44,47,52,53	0
3	SIA	A	1180	21/21	0.82	0.33	1.16	48,62,67,68	0
3	SIA	C	1380	21/21	0.87	0.23	1.13	17,33,42,43	0
3	SIA	B	1280	21/21	0.81	0.27	1.05	35,48,55,56	0
4	SO4	B	1281	5/5	0.95	0.17	0.14	63,63,64,64	0
2	NAG	C	1379	14/15	0.81	0.31	-	51,53,57,58	0
2	NAG	B	1279	14/15	0.80	0.47	-	55,56,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.