



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:17 PM GMT

PDB ID : 1A0H  
Title : THE X-RAY CRYSTAL STRUCTURE OF PPACK-MEIZOTHROMBIN  
DESF1: KRINGLE/THROMBIN AND CARBOHYDRATE/KRINGLE/TH  
ROMBIN INTERACTIONS AND LOCATION OF THE LINKER CHAIN  
Authors : Martin, P.D.; Malkowski, M.G.; Box, J.; Esmon, C.T.; Edwards, B.F.P.  
Deposited on : 1997-11-30  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

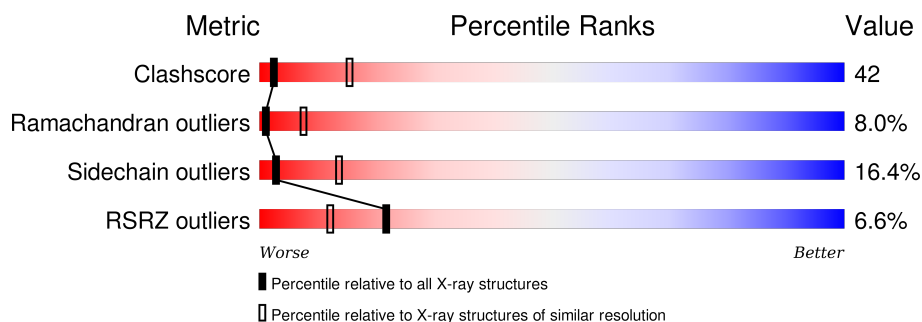
# 1 Overall quality at a glance

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))
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	<div> <div>15%</div> <div>43%</div> <div>43%</div> <div>11%</div> <div>.</div> </div>
1	D	159	<div> <div>17%</div> <div>35%</div> <div>49%</div> <div>13%</div> <div>.</div> </div>
2	B	259	<div> <div>%</div> <div>36%</div> <div>53%</div> <div>10%</div> <div>.</div> </div>
2	E	259	<div> <div>%</div> <div>29%</div> <div>56%</div> <div>12%</div> <div>.</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6901 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 MEIZOTHROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1255	773	213	262	7			
1	D	159	Total	C	N	O	S	0	0	0
			1255	773	213	262	7			

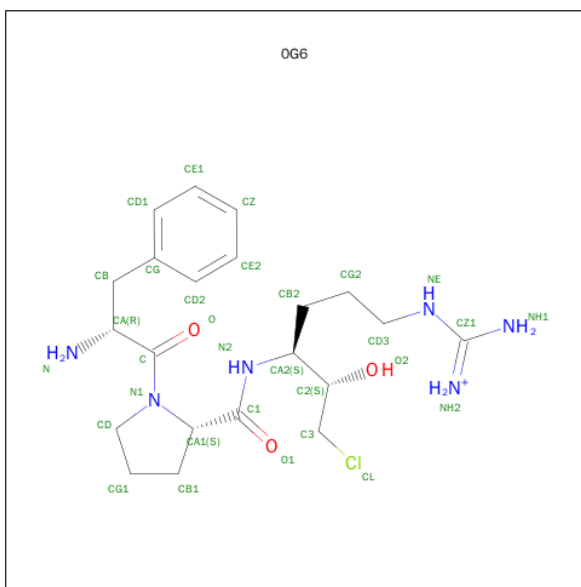
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	HIS	SER	CONFLICT	UNP P00735
D	187	HIS	SER	CONFLICT	UNP P00735

- Molecule 2 is a protein called MEIZOTHROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			
2	E	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 3 is D-PHENYLALANYL-N-[(2S,3S)-6-{[AMINO(IMINIO)METHYL]AMINO}-1-CHLORO-2-HYDROXYHEXAN-3-YL]-L-PROLINAMIDE (three-letter code: 0G6) (formula: C<sub>21</sub>H<sub>34</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			30	21	6	3		
3	E	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

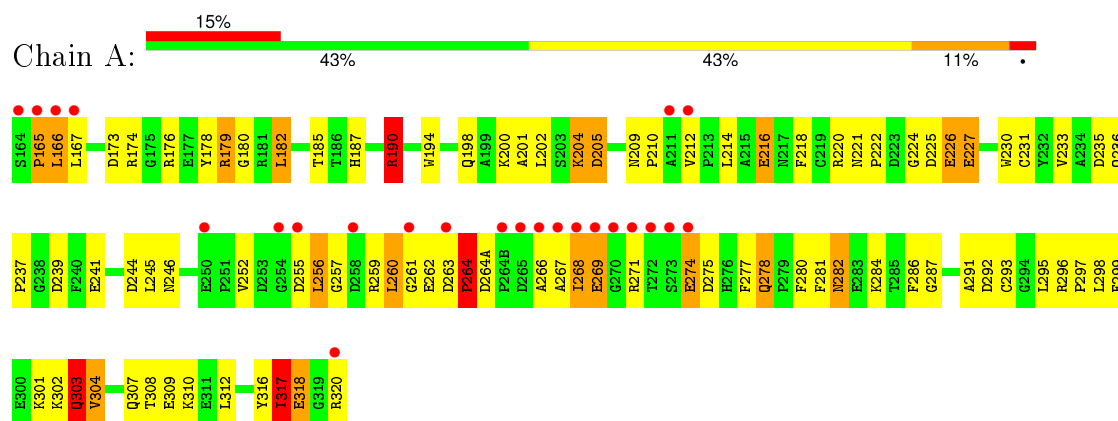
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	23	Total	O	0	0
			23	23		
5	D	16	Total	O	0	0
			16	16		
5	E	23	Total	O	0	0
			23	23		

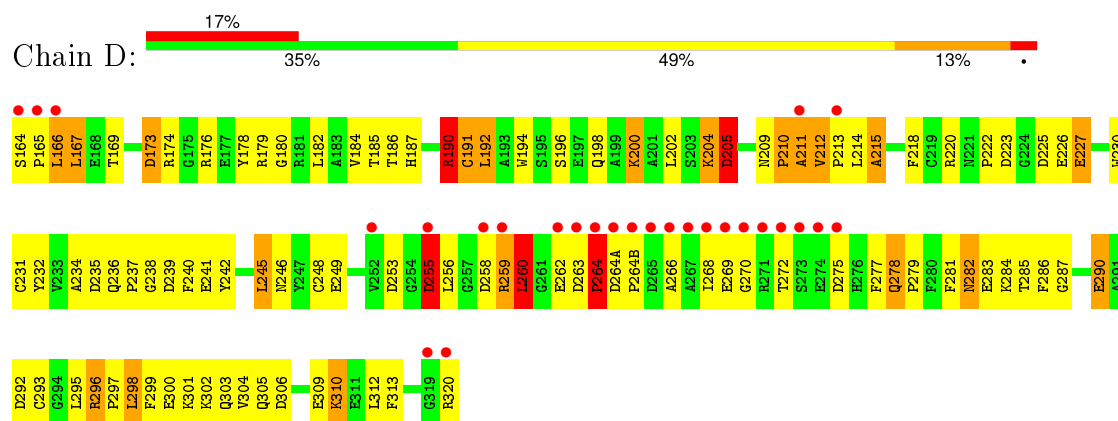
### 3 Residue-property plots

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.

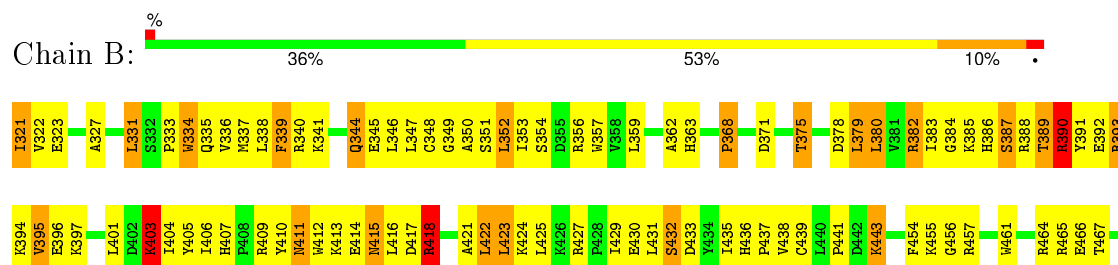
#### • Molecule 1: MEIZOTHROMBIN

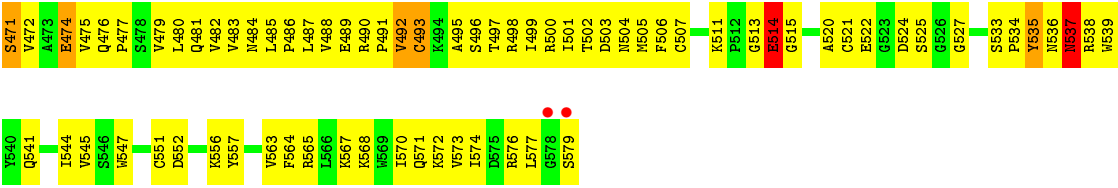


#### • Molecule 1: MEIZOTHROMBIN

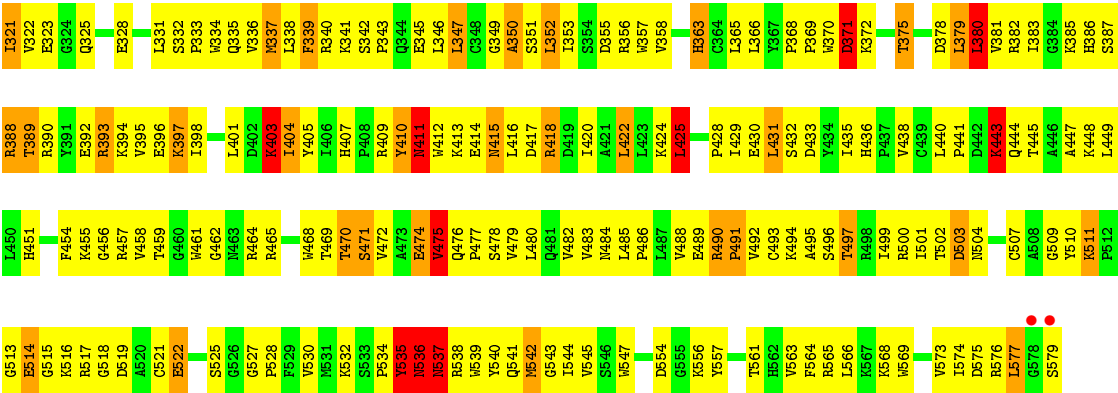


#### • Molecule 2: MEIZOTHROMBIN





● Molecule 2: MEIZOTHROMBIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.15Å 186.15Å 120.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.20 42.27 – 3.14	Depositor EDS
% Data completeness (in resolution range)	84.0 (7.00-3.20) 84.6 (42.27-3.14)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 3.12Å)	Xtriage
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.205 , 0.242 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 110.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 31648 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	6901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0G6, NAG

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	0.79	2/1285 (0.2%)	0.93	4/1739 (0.2%)
1	D	0.64	0/1285	0.89	3/1739 (0.2%)
2	B	0.69	0/2148	0.97	3/2905 (0.1%)
2	E	0.71	0/2148	0.98	4/2905 (0.1%)
All	All	0.71	2/6866 (0.0%)	0.95	14/9288 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ILE	CA-CB	15.76	1.91	1.54
1	A	317	ILE	CA-C	6.62	1.70	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LEU	CB-CG-CD2	-9.49	94.87	111.00
1	A	182	LEU	CB-CG-CD1	8.51	125.47	111.00
1	D	182	LEU	CB-CG-CD1	-7.02	99.07	111.00
2	E	535	TYR	N-CA-C	-6.13	94.44	111.00
2	B	395	VAL	N-CA-C	5.83	126.74	111.00
1	A	231	CYS	CB-CA-C	-5.59	99.22	110.40
2	E	380	LEU	CA-CB-CG	5.53	128.01	115.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	GLU	N-CA-C	5.47	125.77	111.00
2	E	403	LYS	N-CA-C	5.43	125.65	111.00
1	A	317	ILE	CG1-CB-CG2	5.25	122.95	111.40
1	D	264	PRO	N-CA-C	5.16	125.51	112.10
2	E	425	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	232	TYR	N-CA-C	-5.07	97.31	111.00
2	B	403	LYS	N-CA-C	5.05	124.62	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	540	TYR	Sidechain

## 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	1255	0	1127	88	0
1	D	1255	0	1127	119	0
2	B	2094	0	2095	194	0
2	E	2094	0	2095	229	0
3	B	30	0	31	3	0
3	E	30	0	31	4	0
4	B	28	0	25	0	0
4	E	28	0	25	2	0
5	A	25	0	0	2	0
5	B	23	0	0	3	1
5	D	16	0	0	3	0
5	E	23	0	0	0	1
All	All	6901	0	6556	564	1

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 42.

All (564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:CB	1:A:317:ILE:CA	1.91	1.48
1:D:192:LEU:HA	5:D:62:HOH:O	1.59	1.02
1:D:165:PRO:HG2	1:D:166:LEU:HD13	1.43	1.01
2:B:397:LYS:HB3	2:B:429:ILE:HD11	1.45	0.98
1:A:227:GLU:HG3	2:B:500:ARG:HH11	1.24	0.98
2:B:382:ARG:NH1	2:B:385:LYS:HD2	1.79	0.96
2:E:397:LYS:HB3	2:E:429:ILE:HD11	1.51	0.93
2:B:322:VAL:HG11	2:B:552:ASP:HB2	1.51	0.92
1:D:306:ASP:HB3	1:D:309:GLU:HB2	1.48	0.91
1:D:202:LEU:HD21	1:D:235:ASP:O	1.68	0.90
2:E:338:LEU:HD21	2:E:379:LEU:HD23	1.53	0.89
1:A:182:LEU:HD11	2:E:369:PRO:O	1.73	0.88
1:D:227:GLU:HG3	2:E:500:ARG:HH11	1.37	0.88
1:A:227:GLU:HG3	2:B:500:ARG:NH1	1.91	0.86
2:E:403:LYS:HG3	2:E:405:TYR:CZ	2.10	0.85
2:B:483:VAL:HG13	2:B:485:LEU:HD13	1.57	0.85
1:D:194:TRP:HB3	1:D:214:LEU:HD13	1.59	0.84
2:E:365:LEU:HD13	2:E:404:ILE:HG23	1.59	0.83
2:E:416:LEU:HD11	3:E:1:OG6:HB21	1.60	0.83
2:B:388:ARG:HB3	2:B:461:TRP:CD1	2.15	0.82
5:B:64:HOH:O	1:D:166:LEU:HG	1.79	0.82
1:D:286:PHE:HD1	2:E:574:ILE:HD13	1.42	0.82
1:D:227:GLU:HG3	2:E:500:ARG:NH1	1.94	0.81
1:D:299:PHE:HA	1:D:304:VAL:CG1	2.10	0.81
2:B:443:LYS:HD2	2:B:443:LYS:H	1.45	0.81
2:B:488:VAL:HG11	2:B:557:TYR:CE2	2.15	0.81
2:E:536:ASN:ND2	2:E:538:ARG:HG3	1.95	0.81
2:E:490:ARG:HH21	2:E:494:LYS:HD2	1.47	0.80
2:B:382:ARG:HH12	2:B:385:LYS:HD2	1.48	0.78
1:D:302:LYS:O	1:D:302:LYS:HG2	1.84	0.77
2:E:322:VAL:HG22	2:E:464:ARG:O	1.85	0.77
2:E:445:THR:HA	2:E:448:LYS:HD2	1.67	0.76
2:B:417:ASP:O	2:B:418:ARG:HB2	1.86	0.76
1:D:204:LYS:O	1:D:205:ASP:HB2	1.85	0.76
2:B:479:VAL:HG23	2:B:480:LEU:O	1.86	0.75
1:A:179:ARG:HE	1:A:212:VAL:HG12	1.51	0.75
2:E:415:ASN:HD22	2:E:415:ASN:H	1.34	0.75
2:E:544:ILE:HB	2:E:561:THR:HB	1.68	0.75
2:B:464:ARG:HG2	2:B:477:PRO:HG3	1.69	0.75
2:E:447:ALA:O	2:E:451:HIS:HE1	1.70	0.74
2:E:357:TRP:CZ3	2:E:424:LYS:HB2	2.22	0.74
2:E:403:LYS:HD3	2:E:424:LYS:HD3	1.69	0.74

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:HG3	1:A:212:VAL:HB	1.69	0.74
2:E:385:LYS:HZ2	2:E:385:LYS:HB3	1.51	0.74
1:A:227:GLU:HG3	2:B:500:ARG:HD2	1.69	0.74
1:A:260:LEU:HG	1:A:261:GLY:H	1.52	0.73
1:D:313:PHE:HZ	2:E:532:LYS:HE3	1.50	0.73
2:B:504:ASN:HB3	2:B:565:ARG:HD2	1.68	0.73
1:A:302:LYS:O	1:A:304:VAL:HG12	1.89	0.72
2:B:397:LYS:HD2	2:B:429:ILE:HD11	1.71	0.72
2:E:346:LEU:HD23	2:E:347:LEU:N	2.04	0.72
2:E:385:LYS:HB3	2:E:385:LYS:NZ	2.05	0.72
2:B:344:GLN:HE21	2:B:344:GLN:HA	1.54	0.72
1:D:166:LEU:HD13	1:D:166:LEU:H	1.53	0.72
2:B:352:LEU:HD22	2:B:354:SER:O	1.89	0.72
1:A:166:LEU:HD22	1:A:166:LEU:H	1.53	0.72
2:E:388:ARG:HB3	2:E:461:TRP:CD1	2.25	0.71
2:B:464:ARG:NH1	2:B:477:PRO:HA	2.06	0.70
2:E:451:HIS:HB2	2:E:454:PHE:CE2	2.26	0.70
1:A:167:LEU:HB3	5:A:31:HOH:O	1.91	0.70
1:D:190:ARG:HD2	1:D:190:ARG:H	1.56	0.70
2:E:403:LYS:HE3	2:E:405:TYR:OH	1.92	0.70
1:D:194:TRP:CZ3	1:D:222:PRO:HG3	2.27	0.70
2:E:397:LYS:CB	2:E:429:ILE:HD11	2.22	0.70
2:B:339:PHE:HB2	2:B:345:GLU:O	1.91	0.69
1:D:286:PHE:CD1	2:E:574:ILE:HD13	2.25	0.69
1:D:200:LYS:HA	1:D:200:LYS:HE3	1.74	0.69
1:A:190:ARG:HD2	1:A:190:ARG:H	1.57	0.69
2:E:530:VAL:HG12	2:E:541:GLN:HA	1.75	0.69
1:D:299:PHE:HA	1:D:304:VAL:HG12	1.74	0.68
2:E:528:PRO:HB3	2:E:541:GLN:NE2	2.06	0.68
2:B:443:LYS:HD2	2:B:443:LYS:N	2.08	0.68
3:B:1:0G6:HD3	3:B:1:0G6:CD1	2.24	0.68
1:A:281:PHE:HB3	1:A:286:PHE:HB2	1.76	0.68
1:D:312:LEU:HD13	2:E:484:ASN:OD1	1.93	0.67
1:D:215:ALA:HB3	1:D:220:ARG:NH2	2.09	0.67
2:E:469:THR:OG1	2:E:470:THR:HG22	1.94	0.67
1:D:185:THR:HG21	1:D:241:GLU:HB2	1.75	0.67
1:A:264(A):ASP:HB2	1:A:266:ALA:O	1.95	0.67
2:E:489:GLU:O	2:E:492:VAL:HG12	1.95	0.67
2:E:527:GLY:O	2:E:545:VAL:HG23	1.95	0.66
2:E:420:ILE:HG21	2:E:566:LEU:HD13	1.77	0.66
2:B:357:TRP:CH2	2:B:424:LYS:HD2	2.30	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:397:LYS:HE2	2:E:429:ILE:HG12	1.78	0.66
2:B:344:GLN:NE2	2:B:344:GLN:HA	2.11	0.66
1:D:310:LYS:NZ	1:D:310:LYS:HB2	2.11	0.66
2:E:569:TRP:O	2:E:573:VAL:HG23	1.96	0.65
1:D:194:TRP:CH2	1:D:222:PRO:HG3	2.30	0.65
2:B:350:ALA:HB1	2:B:359:LEU:O	1.97	0.65
2:E:321:ILE:HD11	2:E:458:VAL:HG22	1.79	0.65
2:B:480:LEU:HD12	2:B:481:GLN:H	1.62	0.65
2:B:415:ASN:HD21	2:B:500:ARG:NH2	1.95	0.65
1:A:179:ARG:NE	1:A:212:VAL:HG12	2.11	0.65
1:A:178:TYR:CZ	1:A:180:GLY:HA3	2.32	0.65
2:B:385:LYS:HG2	2:B:396:GLU:HG2	1.79	0.64
2:E:411:ASN:HB2	2:E:417:ASP:HB3	1.79	0.64
1:A:286:PHE:HD1	2:B:574:ILE:HD13	1.61	0.64
1:D:253:ASP:HB3	2:E:490:ARG:NE	2.11	0.64
1:A:236:GLN:HB3	1:A:237:PRO:HD2	1.79	0.64
2:B:359:LEU:HD12	2:B:422:LEU:HD13	1.80	0.64
2:B:464:ARG:CZ	2:B:477:PRO:HA	2.28	0.64
2:E:410:TYR:CZ	2:E:412:TRP:HB3	2.33	0.64
2:B:500:ARG:HD3	5:B:47:HOH:O	1.97	0.63
2:B:390:ARG:HG3	2:B:390:ARG:O	1.97	0.63
2:E:403:LYS:HB2	2:E:424:LYS:HB3	1.80	0.63
2:E:355:ASP:OD2	2:E:428:PRO:HB3	1.97	0.63
1:A:264:PRO:HG2	2:B:567:LYS:HG2	1.81	0.63
1:D:259:ARG:CZ	1:D:259:ARG:HA	2.28	0.63
2:E:370:TRP:O	2:E:371:ASP:HB2	1.99	0.63
1:D:309:GLU:OE2	2:E:532:LYS:HE2	1.99	0.63
2:B:502:THR:HG22	2:B:503:ASP:N	2.13	0.62
2:E:525:SER:HA	2:E:545:VAL:HB	1.82	0.62
1:D:198:GLN:CD	1:D:198:GLN:H	2.03	0.62
1:D:279:PRO:HA	1:D:290:GLU:OE2	2.00	0.62
2:B:497:THR:OG1	2:B:499:ILE:HG13	1.99	0.62
1:A:318:GLU:HG3	1:A:320:ARG:H	1.64	0.62
1:D:179:ARG:HG3	1:D:220:ARG:HH12	1.65	0.62
2:E:352:LEU:HD23	2:E:358:VAL:HG22	1.82	0.62
2:E:357:TRP:CE2	2:E:574:ILE:HG12	2.35	0.61
2:E:415:ASN:ND2	2:E:500:ARG:HH21	1.98	0.61
1:A:317:ILE:CB	1:A:317:ILE:N	2.62	0.61
2:E:403:LYS:HA	2:E:403:LYS:NZ	2.14	0.61
2:B:443:LYS:CD	2:B:443:LYS:H	2.11	0.61
2:B:416:LEU:HD12	2:B:547:TRP:HB3	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:HG2	1:A:275:ASP:N	2.15	0.61
2:E:321:ILE:N	2:E:462:GLY:O	2.33	0.61
2:E:492:VAL:O	2:E:495:ALA:HB3	2.00	0.61
1:D:302:LYS:HD3	1:D:304:VAL:HG11	1.83	0.61
1:D:263:ASP:CB	1:D:264:PRO:HD2	2.29	0.61
2:E:387:SER:HA	2:E:479:VAL:HA	1.81	0.61
2:E:397:LYS:HB3	2:E:429:ILE:CD1	2.27	0.61
2:E:457:ARG:HD2	2:E:482:VAL:CG2	2.31	0.61
1:A:178:TYR:O	1:A:212:VAL:HG21	2.01	0.60
2:E:379:LEU:HD12	2:E:379:LEU:N	2.16	0.60
2:B:466:GLU:HB2	2:B:551:CYS:HB2	1.84	0.60
1:A:259:ARG:HB2	2:B:565:ARG:HH22	1.67	0.60
2:E:411:ASN:OD1	2:E:414:GLU:HG2	2.02	0.60
2:E:407:HIS:HD2	2:E:409:ARG:H	1.49	0.60
5:A:6:HOH:O	2:B:568:LYS:HD3	2.02	0.60
2:B:363:HIS:CE1	2:B:525:SER:OG	2.54	0.60
2:B:431:LEU:HD12	2:B:435:ILE:O	2.02	0.60
2:B:394:LYS:HG3	2:B:395:VAL:HG23	1.84	0.59
2:E:415:ASN:HD21	2:E:500:ARG:HH21	1.48	0.59
1:D:263:ASP:HA	2:E:568:LYS:NZ	2.17	0.59
2:B:472:VAL:HG11	1:D:166:LEU:HA	1.83	0.59
2:E:356:ARG:O	2:E:425:LEU:HD22	2.01	0.59
2:E:441:PRO:HG3	2:E:542:MET:SD	2.43	0.59
1:D:282:ASN:HD21	1:D:284:LYS:HB3	1.66	0.59
1:D:194:TRP:CD2	1:D:214:LEU:HD22	2.37	0.59
2:B:409:ARG:CZ	2:B:418:ARG:HH22	2.16	0.59
2:B:340:ARG:HB3	2:B:347:LEU:HD11	1.84	0.59
2:E:331:LEU:O	2:E:331:LEU:HD23	2.03	0.59
2:E:379:LEU:HD12	2:E:379:LEU:H	1.68	0.59
2:B:490:ARG:O	2:B:493:CYS:HB2	2.02	0.59
2:E:485:LEU:HD12	2:E:509:GLY:HA2	1.84	0.58
2:B:441:PRO:HD3	2:B:541:GLN:O	2.03	0.58
2:E:518:GLY:O	2:E:519:ASP:HB2	2.03	0.58
2:B:341:LYS:HB3	2:B:380:LEU:HD22	1.84	0.58
2:B:438:VAL:HG22	2:B:439:CYS:H	1.68	0.58
2:E:385:LYS:HE2	2:E:392:GLU:HG3	1.84	0.58
1:D:297:PRO:HB2	1:D:298:LEU:HD12	1.84	0.58
2:E:456:GLY:O	2:E:484:ASN:HA	2.04	0.58
2:E:489:GLU:CD	2:E:489:GLU:H	2.07	0.58
2:E:488:VAL:CG2	2:E:507:CYS:SG	2.91	0.58
1:D:313:PHE:CZ	2:E:532:LYS:HE3	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:TRP:O	2:B:351:SER:HA	2.03	0.58
1:D:264(A):ASP:HB2	1:D:266:ALA:O	2.04	0.58
1:A:174:ARG:HG2	1:A:226:GLU:O	2.04	0.58
2:B:488:VAL:HG11	2:B:557:TYR:CD2	2.38	0.57
2:E:322:VAL:HG12	2:E:323:GLU:HG2	1.84	0.57
1:A:267:ALA:O	1:A:268:ILE:HB	2.04	0.57
2:E:497:THR:OG1	2:E:499:ILE:HD12	2.04	0.57
1:D:281:PHE:HB3	1:D:286:PHE:CG	2.40	0.57
2:B:387:SER:C	2:B:389:THR:H	2.08	0.57
2:B:375:THR:O	2:B:378:ASP:HB2	2.04	0.57
2:B:431:LEU:HD11	2:B:437:PRO:HD3	1.87	0.57
2:E:414:GLU:HG3	2:E:415:ASN:H	1.69	0.57
2:B:487:LEU:HD21	2:B:506:PHE:CD1	2.40	0.57
2:E:342:SER:HA	2:E:343:PRO:C	2.24	0.57
2:B:339:PHE:HB2	2:B:346:LEU:HA	1.87	0.56
1:D:187:HIS:HB2	1:D:241:GLU:OE1	2.04	0.56
1:D:282:ASN:O	1:D:283:GLU:HB2	2.05	0.56
1:A:287:GLY:HA2	2:B:356:ARG:NH1	2.19	0.56
2:E:501:ILE:O	2:E:501:ILE:HG13	2.06	0.56
1:A:252:VAL:HB	1:A:259:ARG:HH21	1.70	0.56
2:E:445:THR:HA	2:E:448:LYS:CD	2.33	0.56
1:D:298:LEU:N	1:D:298:LEU:HD12	2.21	0.56
2:B:382:ARG:HG2	2:B:382:ARG:HH11	1.71	0.56
2:E:459:THR:HB	2:E:480:LEU:HD11	1.88	0.56
2:B:344:GLN:HE21	2:B:344:GLN:CA	2.18	0.55
1:D:185:THR:CG2	1:D:241:GLU:HB2	2.36	0.55
1:A:198:GLN:O	1:A:202:LEU:HD23	2.06	0.55
2:B:504:ASN:CB	2:B:565:ARG:HD2	2.33	0.55
2:B:457:ARG:HD2	2:B:482:VAL:CG2	2.35	0.55
2:B:527:GLY:O	2:B:545:VAL:HG23	2.06	0.55
2:B:411:ASN:OD1	2:B:414:GLU:HG2	2.06	0.55
2:B:415:ASN:H	2:B:415:ASN:HD22	1.52	0.55
2:B:502:THR:HG22	2:B:503:ASP:H	1.70	0.55
2:B:465:ARG:H	2:B:475:VAL:CG2	2.19	0.55
2:E:368:PRO:HD2	2:E:369:PRO:HD2	1.88	0.55
2:B:415:ASN:HD21	2:B:500:ARG:HH21	1.53	0.55
1:D:299:PHE:HA	1:D:304:VAL:HG13	1.84	0.55
2:B:421:ALA:O	2:B:422:LEU:HB2	2.07	0.55
2:B:465:ARG:H	2:B:475:VAL:HG23	1.72	0.55
2:E:397:LYS:NZ	2:E:430:GLU:HB3	2.22	0.55
2:B:471:SER:O	2:B:474:GLU:HG2	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:SER:HB3	1:D:167:LEU:HB2	1.89	0.55
2:E:574:ILE:HG22	2:E:575:ASP:N	2.20	0.55
2:E:368:PRO:HD2	2:E:412:TRP:CE3	2.42	0.55
2:B:341:LYS:HE2	2:B:380:LEU:HD22	1.89	0.54
2:E:471:SER:O	2:E:474:GLU:HG2	2.07	0.54
2:B:390:ARG:NH1	2:B:392:GLU:HG2	2.23	0.54
2:E:502:THR:HG22	2:E:503:ASP:N	2.22	0.54
2:E:510:TYR:CE2	2:E:516:LYS:HB2	2.42	0.54
2:B:357:TRP:CZ3	2:B:424:LYS:HB2	2.43	0.54
1:D:282:ASN:ND2	1:D:284:LYS:HB3	2.22	0.54
1:D:279:PRO:HA	1:D:290:GLU:CD	2.27	0.54
2:B:384:GLY:O	2:B:395:VAL:HG12	2.08	0.54
2:B:382:ARG:HH11	2:B:385:LYS:HD2	1.68	0.54
2:B:387:SER:HB2	2:B:389:THR:O	2.08	0.54
1:D:230:TRP:HB3	1:D:242:TYR:HA	1.89	0.54
1:A:286:PHE:CD1	2:B:574:ILE:HD13	2.43	0.54
1:A:263:ASP:CB	1:A:264:PRO:HD2	2.37	0.54
2:B:327:ALA:O	2:B:386:HIS:HE1	1.90	0.54
2:B:415:ASN:ND2	2:B:500:ARG:HH21	2.06	0.54
2:B:323:GLU:HG2	5:B:60:HOH:O	2.07	0.54
2:E:322:VAL:HG23	2:E:521:CYS:HB2	1.90	0.54
2:B:427:ARG:HH11	2:B:427:ARG:HG2	1.73	0.54
2:B:391:TYR:CE2	2:B:393:ARG:HA	2.43	0.54
2:E:414:GLU:HG3	2:E:415:ASN:N	2.22	0.54
1:D:196:SER:O	1:D:200:LYS:HB2	2.08	0.54
2:B:477:PRO:HB3	2:B:481:GLN:HG3	1.90	0.53
2:B:405:TYR:CD2	2:B:573:VAL:HG11	2.43	0.53
1:A:281:PHE:HB3	1:A:286:PHE:CB	2.38	0.53
1:D:215:ALA:HB3	1:D:220:ARG:CZ	2.37	0.53
2:E:340:ARG:NH1	2:E:343:PRO:HD2	2.24	0.53
1:D:230:TRP:NE1	2:E:409:ARG:NH1	2.56	0.53
2:E:490:ARG:HB3	2:E:491:PRO:HD3	1.89	0.53
1:A:221:ASN:OD1	1:A:225:ASP:N	2.40	0.53
1:D:260:LEU:HD23	1:D:260:LEU:H	1.72	0.53
2:E:444:GLN:O	2:E:448:LYS:HG3	2.08	0.53
1:D:296:ARG:HG3	1:D:300:GLU:OE1	2.07	0.53
1:A:286:PHE:CE2	2:B:354:SER:HB3	2.44	0.53
1:D:255:ASP:N	1:D:258:ASP:HB2	2.23	0.53
1:A:204:LYS:HG2	2:B:576:ARG:NH2	2.24	0.53
2:E:405:TYR:HB2	2:E:422:LEU:HB3	1.89	0.52
2:E:510:TYR:CD2	2:E:516:LYS:HB2	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ARG:HB3	1:D:320:ARG:CZ	2.38	0.52
2:E:351:SER:O	2:E:358:VAL:HG13	2.09	0.52
2:B:534:PRO:HG2	2:B:535:TYR:CD1	2.44	0.52
2:E:375:THR:O	2:E:378:ASP:HB2	2.09	0.52
1:A:259:ARG:HB2	2:B:565:ARG:NH2	2.24	0.52
2:E:431:LEU:HD13	2:E:435:ILE:O	2.09	0.52
2:E:339:PHE:HB2	2:E:345:GLU:O	2.10	0.52
1:D:165:PRO:HG2	1:D:166:LEU:CD1	2.29	0.52
1:D:223:ASP:OD2	1:D:225:ASP:HB2	2.09	0.52
1:A:165:PRO:HD2	1:A:166:LEU:HD22	1.92	0.52
2:B:362:ALA:HA	2:B:421:ALA:HB2	1.90	0.52
5:D:61:HOH:O	2:E:436:HIS:HE1	1.92	0.52
2:B:415:ASN:N	2:B:415:ASN:HD22	2.07	0.52
1:D:234:ALA:HB3	1:D:239:ASP:HB3	1.93	0.51
1:A:227:GLU:HG3	2:B:500:ARG:CD	2.40	0.51
2:E:403:LYS:HG3	2:E:405:TYR:CE1	2.43	0.51
1:A:260:LEU:HG	1:A:261:GLY:N	2.23	0.51
2:E:368:PRO:CD	2:E:369:PRO:HD2	2.41	0.51
1:D:230:TRP:CH2	2:E:409:ARG:HD2	2.46	0.51
1:A:259:ARG:HD2	2:B:503:ASP:OD1	2.11	0.51
2:B:397:LYS:HD2	2:B:429:ILE:CD1	2.38	0.51
2:B:488:VAL:HG11	2:B:557:TYR:HE2	1.69	0.51
2:E:333:PRO:HB2	2:E:436:HIS:H	1.76	0.51
2:E:415:ASN:N	2:E:415:ASN:HD22	2.00	0.51
2:E:403:LYS:HB2	2:E:424:LYS:CB	2.40	0.51
2:B:357:TRP:HE3	2:B:423:LEU:O	1.94	0.51
1:D:226:GLU:HG3	5:D:74:HOH:O	2.09	0.51
2:E:534:PRO:HG2	2:E:535:TYR:CE1	2.45	0.51
1:D:263:ASP:HA	2:E:568:LYS:HZ2	1.76	0.51
2:B:490:ARG:HA	2:B:493:CYS:HB2	1.93	0.51
2:B:334:TRP:CG	2:B:438:VAL:HB	2.45	0.51
2:E:368:PRO:N	2:E:369:PRO:HD2	2.26	0.51
2:B:483:VAL:CG1	2:B:485:LEU:HD13	2.37	0.51
2:B:340:ARG:HA	2:B:379:LEU:HB3	1.92	0.51
2:E:488:VAL:HG11	2:E:557:TYR:CD2	2.46	0.51
1:A:198:GLN:OE1	1:A:198:GLN:N	2.44	0.51
2:E:443:LYS:H	2:E:443:LYS:HD2	1.76	0.51
2:B:382:ARG:HG2	2:B:382:ARG:NH1	2.24	0.50
1:A:230:TRP:CH2	2:B:409:ARG:HD2	2.46	0.50
1:A:166:LEU:N	1:A:166:LEU:HD22	2.23	0.50
2:B:466:GLU:HG2	2:B:466:GLU:O	2.10	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:CYS:HB3	2:B:525:SER:O	2.11	0.50
2:B:414:GLU:HG3	2:B:415:ASN:ND2	2.26	0.50
2:E:379:LEU:N	2:E:379:LEU:CD1	2.74	0.50
1:D:173:ASP:HB3	1:D:176:ARG:HB2	1.93	0.50
2:E:457:ARG:HD2	2:E:482:VAL:HG21	1.91	0.50
2:E:535:TYR:O	2:E:537:ASN:N	2.44	0.50
2:B:409:ARG:NH1	2:B:418:ARG:NH2	2.60	0.50
1:D:218:PHE:O	1:D:220:ARG:HG2	2.12	0.50
1:A:187:HIS:HB2	1:A:241:GLU:OE1	2.12	0.50
1:D:281:PHE:HB3	1:D:286:PHE:CB	2.42	0.50
2:E:407:HIS:CD2	2:E:409:ARG:H	2.29	0.50
2:E:385:LYS:HG2	2:E:396:GLU:HB3	1.93	0.50
1:D:310:LYS:HZ2	1:D:310:LYS:HB2	1.77	0.50
1:A:187:HIS:HE1	2:B:413:LYS:HD3	1.76	0.50
1:A:292:ASP:HA	2:B:538:ARG:HH12	1.76	0.50
1:A:218:PHE:HB2	1:A:220:ARG:NH1	2.27	0.50
1:A:214:LEU:HD21	1:A:222:PRO:HB3	1.94	0.50
2:E:544:ILE:HG13	2:E:563:VAL:HG22	1.93	0.50
1:D:264:PRO:HD3	2:E:568:LYS:HG3	1.93	0.50
1:A:202:LEU:HD21	1:A:235:ASP:O	2.12	0.50
1:A:298:LEU:HD11	2:B:433:ASP:HB3	1.93	0.50
2:E:394:LYS:HG3	2:E:395:VAL:HG23	1.94	0.49
2:B:427:ARG:HG2	2:B:427:ARG:NH1	2.27	0.49
2:E:532:LYS:HD2	2:E:539:TRP:CZ2	2.48	0.49
2:E:403:LYS:HA	2:E:403:LYS:HZ3	1.77	0.49
1:D:218:PHE:HB2	1:D:220:ARG:HH21	1.76	0.49
2:E:416:LEU:HD11	3:E:1:OG6:CB1	2.38	0.49
1:D:230:TRP:CZ2	2:E:409:ARG:HD2	2.48	0.49
2:E:385:LYS:NZ	2:E:386:HIS:H	2.11	0.49
1:D:263:ASP:HB3	1:D:264:PRO:HD2	1.93	0.49
2:E:465:ARG:HH22	2:E:468:TRP:HA	1.76	0.49
2:E:415:ASN:HD21	2:E:500:ARG:NH2	2.11	0.49
2:E:475:VAL:HG13	2:E:475:VAL:O	2.11	0.49
1:A:277:PHE:O	1:A:278:GLN:HB3	2.13	0.49
2:B:544:ILE:HD11	2:B:563:VAL:CG2	2.43	0.49
2:B:322:VAL:HA	2:B:464:ARG:O	2.13	0.49
1:D:286:PHE:CE1	2:E:353:ILE:HD12	2.48	0.49
2:E:544:ILE:HG13	2:E:563:VAL:CG2	2.42	0.49
1:D:210:PRO:O	1:D:211:ALA:HB3	2.12	0.49
1:D:223:ASP:OD2	2:E:409:ARG:NH1	2.46	0.48
2:B:438:VAL:HG22	2:B:439:CYS:N	2.27	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:443:LYS:HD2	2:E:443:LYS:N	2.28	0.48
1:A:284:LYS:HG2	2:B:579:SER:HB2	1.95	0.48
2:B:397:LYS:CB	2:B:429:ILE:HD11	2.32	0.48
2:E:337:MET:HE2	2:E:461:TRP:CZ2	2.49	0.48
2:E:557:TYR:CD1	2:E:557:TYR:N	2.81	0.48
2:E:493:CYS:O	2:E:496:SER:HB3	2.14	0.48
2:B:321:ILE:HD12	2:B:524:ASP:OD2	2.13	0.48
1:A:316:TYR:HD1	2:B:454:PHE:CD2	2.31	0.48
2:E:397:LYS:HZ1	2:E:430:GLU:HB3	1.78	0.48
2:B:389:THR:O	2:B:390:ARG:HB3	2.13	0.48
1:D:309:GLU:CD	2:E:532:LYS:HE2	2.34	0.48
1:A:178:TYR:OH	1:A:180:GLY:HA3	2.13	0.48
2:E:336:VAL:HB	2:E:350:ALA:HB3	1.96	0.48
1:D:277:PHE:CZ	1:D:293:CYS:SG	3.07	0.48
1:D:227:GLU:HG3	2:E:500:ARG:HD2	1.96	0.47
2:B:339:PHE:CB	2:B:346:LEU:HA	2.43	0.47
1:D:264(A):ASP:HB2	1:D:264(B):PRO:HD2	1.96	0.47
2:E:383:ILE:HG22	2:E:435:ILE:HG12	1.96	0.47
1:A:200:LYS:HD2	1:A:200:LYS:HA	1.67	0.47
2:E:444:GLN:OE1	2:E:448:LYS:HE3	2.14	0.47
1:D:259:ARG:HA	1:D:259:ARG:NE	2.29	0.47
1:A:298:LEU:N	1:A:298:LEU:HD12	2.29	0.47
2:B:388:ARG:HB3	2:B:461:TRP:CG	2.49	0.47
2:E:333:PRO:HB2	2:E:436:HIS:N	2.29	0.47
2:E:482:VAL:CG2	2:E:483:VAL:N	2.77	0.47
1:D:190:ARG:O	1:D:191:CYS:HB2	2.14	0.47
2:B:349:GLY:O	2:B:350:ALA:HB2	2.14	0.47
1:D:302:LYS:HD3	1:D:304:VAL:CG1	2.44	0.47
2:E:353:ILE:HG21	2:E:440:LEU:HD11	1.97	0.47
2:E:490:ARG:O	2:E:493:CYS:HB2	2.15	0.47
2:E:414:GLU:HG3	2:E:415:ASN:ND2	2.30	0.47
2:E:418:ARG:O	2:E:420:ILE:N	2.46	0.47
1:A:201:ALA:O	1:A:204:LYS:HB3	2.14	0.47
1:D:277:PHE:O	1:D:278:GLN:CB	2.62	0.47
2:B:331:LEU:O	2:B:333:PRO:HD3	2.14	0.47
2:E:521:CYS:SG	2:E:522:GLU:N	2.88	0.47
2:E:511:LYS:HG3	2:E:557:TYR:OH	2.15	0.47
2:B:415:ASN:O	2:B:505:MET:HE1	2.15	0.47
2:B:387:SER:HA	2:B:479:VAL:HA	1.96	0.47
1:D:230:TRP:CE2	2:E:409:ARG:NH1	2.82	0.47
1:D:184:VAL:HG12	1:D:185:THR:H	1.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:N	1:D:260:LEU:HD23	2.29	0.47
1:A:303:GLN:HA	1:A:303:GLN:HE21	1.80	0.47
2:E:457:ARG:HG2	2:E:484:ASN:CG	2.36	0.47
2:B:412:TRP:CZ3	2:B:413:LYS:HG2	2.49	0.47
2:B:511:LYS:HA	2:B:557:TYR:OH	2.16	0.46
2:B:368:PRO:HG2	2:B:412:TRP:CE2	2.50	0.46
2:E:387:SER:C	2:E:389:THR:H	2.18	0.46
2:B:363:HIS:HE1	2:B:525:SER:OG	1.99	0.46
1:A:187:HIS:CE1	2:B:413:LYS:HD3	2.51	0.46
2:B:511:LYS:HB2	2:B:514:GLU:OE2	2.16	0.46
2:B:455:LYS:HA	2:B:486:PRO:HA	1.98	0.46
1:A:182:LEU:CD1	2:E:369:PRO:O	2.55	0.46
2:B:401:LEU:CD1	2:B:423:LEU:HG	2.45	0.46
2:E:488:VAL:HG22	2:E:507:CYS:SG	2.54	0.46
2:B:385:LYS:HE2	2:B:385:LYS:HB3	1.74	0.46
1:A:286:PHE:CE1	2:B:353:ILE:HD12	2.50	0.46
2:B:443:LYS:HA	2:B:564:PHE:CE1	2.50	0.46
2:B:533:SER:O	2:B:537:ASN:HA	2.15	0.46
2:E:338:LEU:O	2:E:347:LEU:HB2	2.15	0.46
1:A:277:PHE:CZ	1:A:293:CYS:SG	3.08	0.46
2:B:352:LEU:HG	2:B:383:ILE:HD13	1.99	0.45
2:B:498:ARG:NH2	2:E:494:LYS:HE3	2.31	0.45
2:E:447:ALA:O	2:E:451:HIS:CE1	2.60	0.45
2:B:341:LYS:HB3	2:B:341:LYS:HE2	1.64	0.45
1:D:296:ARG:NH1	2:E:331:LEU:HD23	2.32	0.45
2:B:513:GLY:O	2:B:515:GLY:N	2.49	0.45
2:B:488:VAL:CG2	2:B:507:CYS:SG	3.05	0.45
2:E:469:THR:OG1	2:E:470:THR:N	2.49	0.45
1:D:264:PRO:HD3	2:E:568:LYS:CG	2.45	0.45
1:D:282:ASN:O	1:D:283:GLU:CB	2.64	0.45
2:E:334:TRP:CG	2:E:438:VAL:HB	2.51	0.45
2:E:321:ILE:CD1	2:E:458:VAL:HG22	2.46	0.45
1:A:312:LEU:HD11	2:B:456:GLY:CA	2.46	0.45
2:B:436:HIS:CD2	2:B:437:PRO:HD2	2.52	0.45
1:A:176:ARG:NH1	1:A:224:GLY:O	2.49	0.45
2:E:349:GLY:O	2:E:350:ALA:HB2	2.16	0.45
1:D:238:GLY:O	2:E:413:LYS:HE3	2.17	0.45
1:D:178:TYR:CE1	1:D:245:LEU:HD21	2.51	0.45
1:A:263:ASP:HB3	1:A:264:PRO:HD2	1.97	0.45
2:B:455:LYS:HG2	2:B:486:PRO:HB3	1.99	0.45
2:B:397:LYS:NZ	2:B:430:GLU:HB3	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:PHE:HD1	2:E:574:ILE:CD1	2.21	0.45
2:E:337:MET:HB3	2:E:382:ARG:HB2	1.99	0.45
2:E:458:VAL:CG1	2:E:483:VAL:HG13	2.47	0.44
1:A:282:ASN:HD21	1:A:284:LYS:HB3	1.80	0.44
2:E:366:LEU:HD12	2:E:372:LYS:O	2.17	0.44
2:E:511:LYS:HD3	2:E:514:GLU:OE2	2.17	0.44
2:E:333:PRO:HG2	2:E:334:TRP:CE3	2.52	0.44
2:E:577:LEU:HD22	2:E:577:LEU:HA	1.83	0.44
2:E:331:LEU:HD21	2:E:457:ARG:NH2	2.32	0.44
2:B:456:GLY:N	2:B:485:LEU:O	2.49	0.44
2:E:379:LEU:CD1	2:E:379:LEU:H	2.29	0.44
1:D:296:ARG:NH2	1:D:306:ASP:HB2	2.33	0.44
1:D:253:ASP:HB3	2:E:490:ARG:HE	1.79	0.44
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.60	0.44
2:B:396:GLU:O	2:B:397:LYS:HG2	2.17	0.44
2:E:385:LYS:HZ3	2:E:386:HIS:H	1.66	0.44
1:D:264:PRO:HG3	2:E:568:LYS:HA	2.00	0.44
2:E:536:ASN:ND2	2:E:538:ARG:CG	2.76	0.44
1:D:178:TYR:CZ	1:D:180:GLY:HA3	2.53	0.44
2:E:366:LEU:HD11	4:E:584:NAG:H82	2.00	0.44
2:E:385:LYS:CB	2:E:385:LYS:NZ	2.74	0.44
2:B:490:ARG:N	2:B:491:PRO:CD	2.81	0.44
1:A:218:PHE:HB2	1:A:220:ARG:HH12	1.83	0.44
2:E:458:VAL:HG13	2:E:483:VAL:HG13	2.00	0.44
2:E:414:GLU:HG3	2:E:415:ASN:HD22	1.83	0.44
1:D:253:ASP:HB3	2:E:490:ARG:CZ	2.48	0.44
2:B:409:ARG:NH1	2:B:418:ARG:HH22	2.16	0.44
1:A:281:PHE:HB3	1:A:286:PHE:CG	2.52	0.44
2:B:489:GLU:HB2	2:B:492:VAL:HG12	2.00	0.44
2:E:556:LYS:C	2:E:557:TYR:CD1	2.91	0.44
1:D:292:ASP:HB2	1:D:301:LYS:HZ1	1.83	0.44
1:A:178:TYR:CG	1:A:245:LEU:HD21	2.52	0.43
1:D:287:GLY:HA2	2:E:356:ARG:NH1	2.33	0.43
2:E:410:TYR:CE2	2:E:412:TRP:HB3	2.52	0.43
2:E:420:ILE:HG13	2:E:544:ILE:CD1	2.48	0.43
2:E:528:PRO:CB	2:E:541:GLN:NE2	2.79	0.43
2:B:489:GLU:H	2:B:489:GLU:CD	2.21	0.43
1:A:299:PHE:O	1:A:303:GLN:N	2.52	0.43
2:B:397:LYS:HZ3	2:B:430:GLU:H	1.67	0.43
1:D:286:PHE:CD1	2:E:574:ILE:CD1	3.00	0.43
2:B:511:LYS:HD2	2:B:557:TYR:OH	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LYS:HD2	2:E:576:ARG:NH2	2.32	0.43
2:E:409:ARG:O	2:E:418:ARG:NH1	2.51	0.43
1:D:231:CYS:O	1:D:240:PHE:HB2	2.18	0.43
1:D:295:LEU:HD12	2:E:538:ARG:HH21	1.83	0.43
2:B:394:LYS:NZ	2:B:395:VAL:HA	2.33	0.43
1:A:312:LEU:HD11	2:B:456:GLY:HA2	2.00	0.43
2:E:420:ILE:HG13	2:E:544:ILE:HD12	2.00	0.43
2:B:363:HIS:CE1	2:B:525:SER:CB	3.02	0.43
2:B:388:ARG:O	2:B:389:THR:HG23	2.18	0.43
2:B:387:SER:OG	2:B:390:ARG:HG2	2.19	0.43
2:B:443:LYS:HA	2:B:564:PHE:CZ	2.54	0.43
1:D:245:LEU:O	1:D:246:ASN:HB3	2.19	0.43
2:E:476:GLN:HA	2:E:477:PRO:HD3	1.89	0.43
1:D:296:ARG:HD2	1:D:299:PHE:CD1	2.54	0.43
2:E:381:VAL:O	2:E:398:ILE:HA	2.18	0.43
2:E:321:ILE:HG12	2:E:483:VAL:HG12	2.01	0.43
1:A:312:LEU:HD13	2:B:484:ASN:OD1	2.18	0.43
2:E:335:GLN:HG3	2:E:461:TRP:CH2	2.53	0.43
2:B:502:THR:CG2	2:B:503:ASP:N	2.81	0.43
2:B:339:PHE:HD1	2:B:339:PHE:O	2.02	0.43
2:B:567:LYS:HA	2:B:570:ILE:HD12	2.00	0.43
2:B:457:ARG:NH2	2:B:539:TRP:CH2	2.87	0.43
1:A:218:PHE:CD1	1:A:218:PHE:N	2.84	0.43
2:E:325:GLN:HG2	2:E:325:GLN:H	1.70	0.43
2:E:369:PRO:HD3	2:E:412:TRP:CZ3	2.54	0.43
1:D:264:PRO:HD3	2:E:568:LYS:HE3	2.00	0.43
2:B:322:VAL:CG2	2:B:464:ARG:O	2.66	0.42
2:B:340:ARG:HD3	2:B:345:GLU:OE1	2.19	0.42
2:E:387:SER:CB	2:E:479:VAL:HG12	2.49	0.42
2:B:466:GLU:HG3	2:B:551:CYS:SG	2.59	0.42
1:A:287:GLY:HA2	2:B:356:ARG:CZ	2.49	0.42
2:E:536:ASN:CG	2:E:538:ARG:HG3	2.38	0.42
2:B:475:VAL:O	2:B:475:VAL:HG22	2.18	0.42
2:B:472:VAL:HG22	2:B:472:VAL:O	2.19	0.42
1:A:233:VAL:HB	1:A:239:ASP:O	2.19	0.42
2:E:379:LEU:HD13	2:E:401:LEU:HD12	2.02	0.42
1:D:204:LYS:HD2	2:E:576:ARG:HH22	1.85	0.42
1:D:214:LEU:HA	1:D:214:LEU:HD23	1.71	0.42
2:E:528:PRO:HB2	2:E:541:GLN:HG3	2.01	0.42
2:E:568:LYS:HB2	2:E:568:LYS:HZ2	1.84	0.42
1:D:234:ALA:HB3	1:D:239:ASP:CB	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLN:OE1	4:E:584:NAG:H3	2.19	0.42
2:B:403:LYS:HD2	2:B:403:LYS:N	2.33	0.42
2:E:472:VAL:HG22	2:E:472:VAL:O	2.20	0.42
1:A:227:GLU:CG	2:B:500:ARG:NH1	2.72	0.42
2:E:503:ASP:OD1	2:E:565:ARG:NE	2.53	0.42
2:E:465:ARG:H	2:E:475:VAL:CG2	2.33	0.42
1:A:308:THR:O	1:A:309:GLU:C	2.58	0.42
2:B:387:SER:C	2:B:389:THR:N	2.73	0.42
2:B:476:GLN:HA	2:B:477:PRO:HD3	1.85	0.42
2:E:547:TRP:C	3:E:1:0G6:HD31	2.39	0.42
1:A:245:LEU:O	1:A:246:ASN:HB3	2.20	0.42
2:B:489:GLU:HB3	2:B:491:PRO:HD2	2.02	0.42
2:B:331:LEU:HD23	2:B:331:LEU:C	2.40	0.42
1:D:212:VAL:HB	1:D:213:PRO:HD2	2.01	0.42
2:E:363:HIS:CE1	3:E:1:0G6:H1	2.38	0.42
2:B:362:ALA:HB1	2:B:406:ILE:HG23	2.01	0.42
2:E:397:LYS:HE2	2:E:429:ILE:CG1	2.48	0.41
2:E:397:LYS:CG	2:E:429:ILE:HD11	2.50	0.41
2:E:543:GLY:HA2	2:E:561:THR:O	2.19	0.41
1:A:286:PHE:CZ	2:B:354:SER:HB3	2.54	0.41
1:A:293:CYS:C	2:B:439:CYS:SG	2.98	0.41
1:A:185:THR:HG21	1:A:241:GLU:HB2	2.02	0.41
1:A:236:GLN:O	1:A:239:ASP:HB2	2.20	0.41
1:A:256:LEU:HB3	1:A:257:GLY:H	1.60	0.41
1:A:295:LEU:HB2	1:A:301:LYS:HE2	2.02	0.41
2:E:337:MET:HE3	2:E:385:LYS:HD3	2.02	0.41
1:D:184:VAL:HG12	1:D:185:THR:N	2.36	0.41
1:D:260:LEU:HD12	1:D:262:GLU:OE2	2.20	0.41
2:E:341:LYS:HE3	2:E:380:LEU:HD13	2.03	0.41
2:B:416:LEU:HD11	3:B:1:0G6:HG2	2.00	0.41
2:B:321:ILE:HD12	2:B:520:ALA:HA	2.01	0.41
2:E:338:LEU:CD2	2:E:379:LEU:HD23	2.39	0.41
1:D:281:PHE:HB2	1:D:290:GLU:OE1	2.21	0.41
2:E:449:LEU:O	2:E:454:PHE:HD2	2.03	0.41
2:B:401:LEU:HD13	2:B:423:LEU:HG	2.02	0.41
2:B:357:TRP:CZ3	2:B:424:LYS:HD2	2.55	0.41
2:B:521:CYS:O	3:B:1:0G6:HG31	2.20	0.41
2:E:435:ILE:O	2:E:435:ILE:HG22	2.20	0.41
2:E:404:ILE:O	2:E:405:TYR:HD1	2.03	0.41
2:E:489:GLU:O	2:E:490:ARG:C	2.59	0.41
2:E:513:GLY:O	2:E:515:GLY:N	2.54	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:HG2	2:E:579:SER:O	2.21	0.41
1:D:236:GLN:HB3	1:D:237:PRO:HD2	2.03	0.41
2:E:403:LYS:HA	2:E:403:LYS:HZ2	1.86	0.41
2:E:405:TYR:HD2	2:E:573:VAL:HG12	1.86	0.41
2:B:321:ILE:CD1	2:B:520:ALA:HA	2.51	0.41
2:E:375:THR:O	2:E:379:LEU:HD12	2.21	0.41
2:B:407:HIS:HD2	2:B:409:ARG:H	1.69	0.41
2:E:332:SER:HA	2:E:333:PRO:HD2	1.82	0.41
1:A:298:LEU:H	1:A:298:LEU:HD12	1.86	0.41
2:B:537:ASN:HD22	2:B:537:ASN:C	2.25	0.41
2:B:496:SER:OG	2:B:556:LYS:HA	2.21	0.41
1:A:166:LEU:CD2	1:A:166:LEU:H	2.27	0.40
1:D:264(B):PRO:C	1:D:266:ALA:H	2.24	0.40
2:E:341:LYS:HZ1	2:E:380:LEU:HB3	1.85	0.40
2:B:336:VAL:HG12	2:B:337:MET:N	2.37	0.40
2:E:532:LYS:NZ	2:E:537:ASN:HB2	2.36	0.40
2:E:363:HIS:CE1	2:E:525:SER:OG	2.74	0.40
2:E:387:SER:O	2:E:389:THR:N	2.54	0.40
2:B:568:LYS:O	2:B:572:LYS:HG3	2.22	0.40
1:A:282:ASN:C	1:A:282:ASN:OD1	2.59	0.40
1:A:296:ARG:HA	1:A:297:PRO:HD3	1.81	0.40
1:D:263:ASP:HB2	2:E:564:PHE:CZ	2.55	0.40
2:E:455:LYS:HG2	2:E:486:PRO:HB3	2.03	0.40
2:B:477:PRO:HB3	2:B:481:GLN:CG	2.50	0.40
1:D:309:GLU:HG2	1:D:313:PHE:CE2	2.57	0.40
2:E:482:VAL:HG22	2:E:483:VAL:N	2.37	0.40
1:D:269:GLU:HB3	1:D:272:THR:HG21	2.03	0.40
2:B:443:LYS:CD	2:B:443:LYS:N	2.79	0.40
2:B:457:ARG:HD2	2:B:482:VAL:HG21	2.04	0.40
2:B:432:SER:OG	2:B:433:ASP:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:78:HOH:O	5:E:40:HOH:O[3_545]	0.44	1.76

## 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	157/159 (99%)	108 (69%)	30 (19%)	19 (12%)	0	2
1	D	157/159 (99%)	96 (61%)	42 (27%)	19 (12%)	0	2
2	B	257/259 (99%)	204 (79%)	40 (16%)	13 (5%)	2	20
2	E	257/259 (99%)	203 (79%)	39 (15%)	15 (6%)	2	17
All	All	828/836 (99%)	611 (74%)	151 (18%)	66 (8%)	1	7

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	205	ASP
1	A	210	PRO
1	A	255	ASP
1	A	264	PRO
2	B	331	LEU
2	B	390	ARG
2	B	393	ARG
2	B	411	ASN
2	B	514	GLU
1	D	169	THR
1	D	190	ARG
1	D	205	ASP
1	D	210	PRO
1	D	260	LEU
1	D	264	PRO
1	D	268	ILE
1	D	278	GLN
2	E	388	ARG
2	E	390	ARG
2	E	475	VAL
2	E	514	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	E	536	ASN
2	E	537	ASN
1	A	262	GLU
1	A	307	GLN
2	B	422	LEU
2	B	471	SER
2	B	537	ASN
1	D	167	LEU
1	D	215	ALA
1	D	248	CYS
1	D	270	GLY
1	D	275	ASP
1	D	290	GLU
2	E	371	ASP
2	E	411	ASN
2	E	471	SER
1	A	173	ASP
1	A	260	LEU
1	A	291	ALA
2	B	495	ALA
1	D	204	LYS
2	E	393	ARG
2	E	443	LYS
1	A	216	GLU
1	A	268	ILE
1	A	278	GLN
2	B	418	ARG
2	B	474	GLU
1	D	191	CYS
1	D	255	ASP
2	E	474	GLU
1	A	194	TRP
1	A	204	LYS
1	A	269	GLU
1	A	303	GLN
1	A	318	GLU
2	B	536	ASN
1	D	173	ASP
1	D	211	ALA
2	E	350	ALA
2	E	363	HIS
2	E	404	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	404	ILE
1	A	165	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	133/133 (100%)	113 (85%)	20 (15%)	3	17
1	D	133/133 (100%)	109 (82%)	24 (18%)	2	11
2	B	226/226 (100%)	193 (85%)	33 (15%)	4	19
2	E	226/226 (100%)	185 (82%)	41 (18%)	2	11
All	All	718/718 (100%)	600 (84%)	118 (16%)	3	13

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	179	ARG
1	A	190	ARG
1	A	205	ASP
1	A	209	ASN
1	A	216	GLU
1	A	226	GLU
1	A	227	GLU
1	A	244	ASP
1	A	256	LEU
1	A	264	PRO
1	A	269	GLU
1	A	271	ARG
1	A	274	GLU
1	A	280	PHE
1	A	282	ASN
1	A	303	GLN
1	A	304	VAL
1	A	310	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	317	ILE
2	B	321	ILE
2	B	334	TRP
2	B	335	GLN
2	B	338	LEU
2	B	339	PHE
2	B	344	GLN
2	B	352	LEU
2	B	368	PRO
2	B	371	ASP
2	B	375	THR
2	B	379	LEU
2	B	380	LEU
2	B	382	ARG
2	B	387	SER
2	B	389	THR
2	B	390	ARG
2	B	403	LYS
2	B	410	TYR
2	B	415	ASN
2	B	418	ARG
2	B	423	LEU
2	B	425	LEU
2	B	432	SER
2	B	443	LYS
2	B	467	THR
2	B	492	VAL
2	B	493	CYS
2	B	501	ILE
2	B	522	GLU
2	B	535	TYR
2	B	537	ASN
2	B	571	GLN
2	B	577	LEU
1	D	166	LEU
1	D	174	ARG
1	D	186	THR
1	D	190	ARG
1	D	192	LEU
1	D	200	LYS
1	D	205	ASP
1	D	209	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	212	VAL
1	D	227	GLU
1	D	245	LEU
1	D	249	GLU
1	D	255	ASP
1	D	256	LEU
1	D	259	ARG
1	D	260	LEU
1	D	264	PRO
1	D	282	ASN
1	D	285	THR
1	D	296	ARG
1	D	298	LEU
1	D	303	GLN
1	D	305	GLN
1	D	310	LYS
2	E	321	ILE
2	E	328	GLU
2	E	337	MET
2	E	339	PHE
2	E	347	LEU
2	E	352	LEU
2	E	371	ASP
2	E	375	THR
2	E	379	LEU
2	E	380	LEU
2	E	389	THR
2	E	393	ARG
2	E	397	LYS
2	E	403	LYS
2	E	410	TYR
2	E	411	ASN
2	E	415	ASN
2	E	418	ARG
2	E	422	LEU
2	E	425	LEU
2	E	431	LEU
2	E	432	SER
2	E	433	ASP
2	E	443	LYS
2	E	470	THR
2	E	475	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	478	SER
2	E	490	ARG
2	E	491	PRO
2	E	497	THR
2	E	503	ASP
2	E	504	ASN
2	E	511	LYS
2	E	517	ARG
2	E	522	GLU
2	E	535	TYR
2	E	536	ASN
2	E	537	ASN
2	E	542	MET
2	E	554	ASP
2	E	577	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
2	B	344	GLN
2	B	386	HIS
2	B	407	HIS
2	B	415	ASN
1	D	209	ASN
1	D	303	GLN
1	D	305	GLN
2	E	386	HIS
2	E	407	HIS
2	E	415	ASN
2	E	451	HIS
2	E	481	GLN
2	E	536	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 ⓘ

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	NAG	B	584	2,4	14,14,15	0.64	0	15,19,21	1.00	1 (6%)
4	NAG	B	585	4	14,14,15	0.47	0	15,19,21	0.93	1 (6%)
4	NAG	E	584	2,4	14,14,15	0.55	0	15,19,21	0.87	1 (6%)
4	NAG	E	585	4	14,14,15	0.44	0	15,19,21	0.81	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	584	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	585	4	-	0/6/23/26	0/1/1/1
4	NAG	E	584	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	585	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	585	NAG	C2-N2-C7	-2.58	119.73	123.04
4	B	584	NAG	C2-N2-C7	-2.55	119.77	123.04
4	E	584	NAG	C2-N2-C7	-2.31	120.07	123.04
4	E	585	NAG	C2-N2-C7	-2.22	120.19	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	584	NAG	2	0

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	0G6	B	1	2	27,31,32	0.87	0	35,41,42	0.80	0
3	0G6	E	1	2	27,31,32	0.68	1 (3%)	35,41,42	0.84	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0G6	B	1	2	-	0/29/41/43	0/2/2/2
3	0G6	E	1	2	-	0/29/41/43	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	0G6	O2-C2	-2.66	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	0G6	C1-CA1-N1	-3.29	104.21	112.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	0G6	3	0
3	E	1	0G6	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	159/159 (100%)	0.31	24 (15%) 3 2	3, 40, 99, 100	0
1	D	159/159 (100%)	0.48	27 (16%) 2 1	4, 42, 100, 100	0
2	B	259/259 (100%)	-0.56	2 (0%) 87 80	2, 11, 42, 97	0
2	E	259/259 (100%)	-0.57	2 (0%) 87 80	2, 15, 43, 92	0
All	All	836/836 (100%)	-0.20	55 (6%) 22 12	2, 19, 96, 100	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	579	SER	9.5
2	B	579	SER	9.3
1	A	270	GLY	7.4
1	A	272	THR	7.4
1	A	273	SER	6.7
1	D	319	GLY	6.6
1	D	272	THR	6.3
1	A	266	ALA	5.9
1	A	274	GLU	5.9
1	D	267	ALA	5.0
1	A	268	ILE	4.8
1	D	266	ALA	4.6
1	A	267	ALA	4.5
1	A	166	LEU	4.4
1	A	212	VAL	4.2
1	D	320	ARG	4.2
1	D	270	GLY	4.2
1	D	273	SER	3.9
1	A	269	GLU	3.7
1	D	271	ARG	3.7
1	D	263	ASP	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	578	GLY	3.5
1	A	264(B)	PRO	3.5
1	D	274	GLU	3.5
1	A	211	ALA	3.4
1	D	211	ALA	3.3
1	D	164	SER	3.3
1	D	259	ARG	3.2
1	D	264(A)	ASP	3.2
1	D	269	GLU	3.1
1	D	264	PRO	3.1
1	D	268	ILE	3.1
1	D	264(B)	PRO	3.0
2	E	578	GLY	3.0
1	D	255	ASP	2.9
1	A	261	GLY	2.9
1	D	165	PRO	2.8
1	A	320	ARG	2.7
1	A	265	ASP	2.7
1	A	263	ASP	2.7
1	A	254	GLY	2.6
1	A	255	ASP	2.6
1	D	275	ASP	2.6
1	A	271	ARG	2.6
1	A	167	LEU	2.5
1	A	165	PRO	2.5
1	D	265	ASP	2.4
1	A	164	SER	2.4
1	D	166	LEU	2.4
1	D	262	GLU	2.3
1	D	258	ASP	2.3
1	D	252	VAL	2.3
1	A	250	GLU	2.2
1	A	258	ASP	2.1
1	D	213	PRO	2.1

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

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

### 6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	584	14/15	0.92	0.22	-	43,50,64,75	0
4	NAG	E	585	14/15	0.85	0.23	-	69,74,82,83	0
4	NAG	B	585	14/15	0.88	0.23	-	68,72,82,82	0
4	NAG	E	584	14/15	0.90	0.22	-	42,49,66,72	0

### 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	0G6	B	1	30/31	0.96	0.17	0.77	2,9,19,26	0
3	0G6	E	1	30/31	0.96	0.17	0.00	2,5,18,20	0

### 6.5 Other polymers

There are no such residues in this entry.