



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2017 – 08:46 pm GMT

PDB ID : 1B7Y  
Title : PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYL  
ALANINYL-ADENYLATE  
Authors : Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassilyev, D.G.  
Deposited on : 1999-01-26  
Resolution : 2.50 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc29047
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc29047

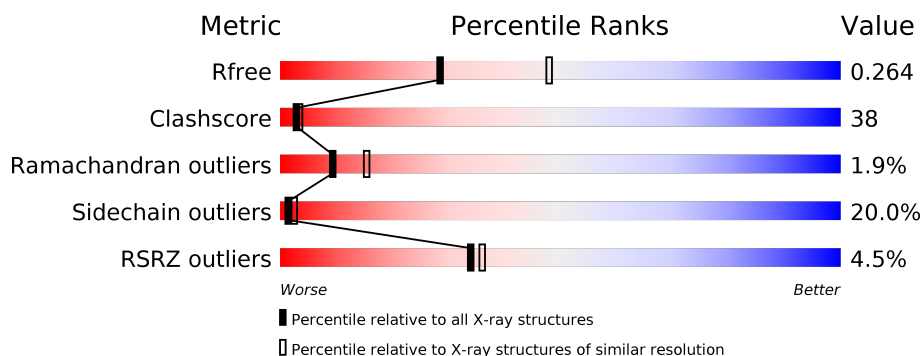
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	350	<div> <div>2%</div> <div>33%</div> <div>34%</div> <div>9%</div> <div>24%</div> </div>
2	B	785	<div> <div>5%</div> <div>43%</div> <div>43%</div> <div>12%</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
3	MG	A	1001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8439 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 PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2112	1382	359	364	7			

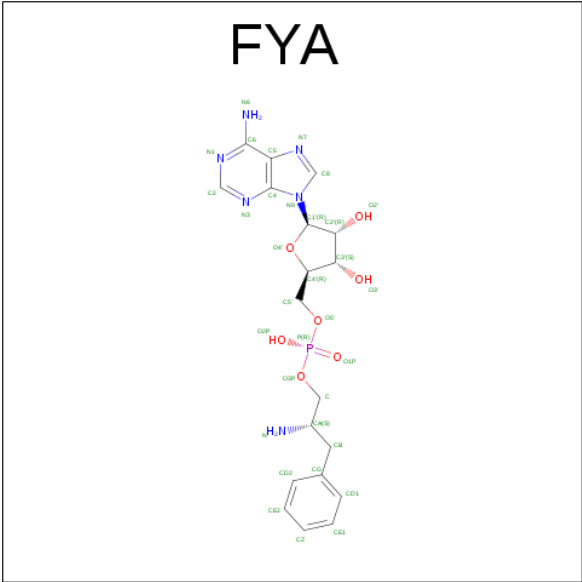
- Molecule 2 is a protein called PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	775	Total	C	N	O	S	0	0	0
			6054	3879	1078	1087	10			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (three-letter code: FYA) (formula: C<sub>19</sub>H<sub>25</sub>N<sub>6</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			33	19	6	7	1		

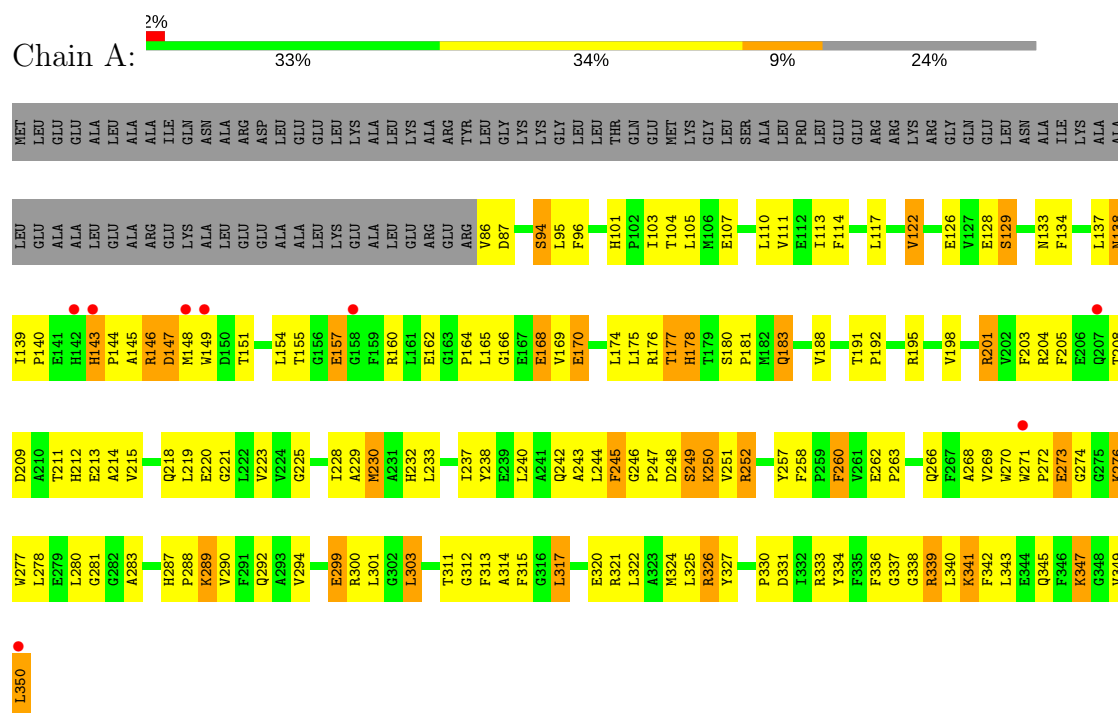
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	191	Total	O	0	0
			191	191		

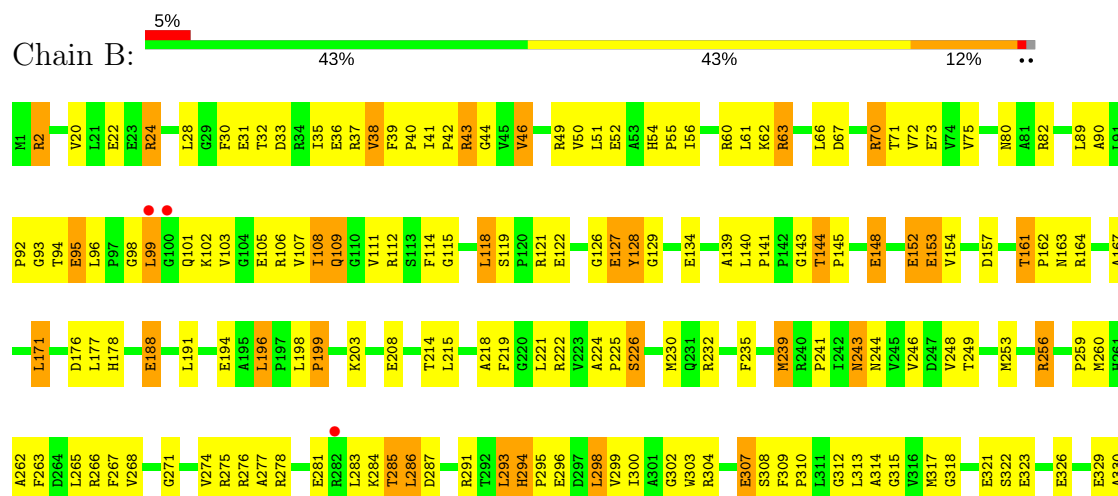
### 3 Residue-property plots

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

#### • Molecule 1: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)



#### • Molecule 2: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)



LEU	A717	G650	E581	D517	T417	I331
ARG	A713	F651	E582	F518	I427	A332
GLY	L652	T583	H584	E519	L428	C337
LEU	Y721	H656	G587	A521	K429	F338
ASP	E723	P657	L588	R522	R430	D339
THR	S724	E658	L589	R523	E438	R344
PRO		I659	F590	F524	T441	K345
		A660	G591	R525		
	L727	Q661	E592	D527	P446	E355
	F728	E662	G593	P528	P447	A356
	D729	L663	V594	P529	S448	S357
	L730	E664	G595	R530	H449	H556
	Y731	L665	L596	L531	R450	R359
	Q732	P666	P597	L532	F360	F360
	G733	P667	V598	L533	L451	E361
	P734	V668	A599	L534	D452	
	P735	H669	K600	N535	D458	V364
	L736	L670	E601	F536	L459	D365
	P737	F671	R602	L537	V460	P366
	E738	E672	L603	A538	E461	L367
	G739	L673	S604	P539	Q369	Q368
	H740	R674	L608	E540	V370	V370
	K741	L675	L609	X541	P371	
	S742	P676	K610	A542	R465	
	L743		E610	A543	I466	
	A744	K680	L613	R545	Q467	R374
	F745	P681	E614	T546	P473	
	H746	L682	A615	H547	D484	L377
	L747		L616	L548	M485	S378
	R748	Q685	F617	F549	R486	L379
	R749		A618	P550	G487	L380
	F750	S688	G621	G551		Q381
	H751	R689	L622	V553		
	P752		A623	R554		G385
	K753		F624	V555		A386
	R754	A692	Q629	L556		R387
	L755	A693	A630	K557		V388
	L756	F694	F631	E558		A389
	R757	R695	P632			E390
	D758	D696	L633	L562		L393
	E759	L697	L634	D563		E394
	E760	A698	H635	R564		S397
	V761	V699	P636	P565		P398
	E762	V700	G637	E566		K399
	E763	V701	V638	R567		P400
	A764	P702	S639	L570		A401
	V765	A703	V642	F571		E402
	S766	P704	L643	E572		A403
	R767	T705	V644	V573		I404
	V768	P706	R645	G574		E409
	A769	V707	G646	R575		
	E770	G708	E647	V576		R413
	A771	E709	V649			L414
	L772	V710				L415
	R773	E711				F515
	A774	A712				M516
	R775	L713				
	GLY	V714				
	PHE	R715				
	GLY	E716				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.50Å 174.50Å 140.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.50) 95.7 (47.41-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15112.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.230 , 0.267 0.229 , 0.264	Depositor DCC
$R_{free}$ test set	4107 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 82.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, FYA

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	0.54	0/2180	0.76	0/2957
2	B	0.53	0/6205	0.79	4/8436 (0.0%)
All	All	0.53	0/8385	0.78	4/11393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	GLY	N-CA-C	-5.83	98.54	113.10
2	B	601	GLU	CB-CA-C	-5.59	99.22	110.40
2	B	128	TYR	N-CA-C	5.35	125.44	111.00
2	B	570	LEU	CA-CB-CG	5.28	127.44	115.30

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	2112	0	2062	164	0
2	B	6054	0	6109	495	0
3	A	1	0	0	0	0
4	A	33	0	24	4	0
5	A	48	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	191	0	0	6	0
All	All	8439	0	8195	626	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 38.

All (626) 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:262:GLU:HG2	5:A:1015:HOH:O	1.45	1.16
2:B:600:LYS:HG2	2:B:601:GLU:H	1.04	1.14
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.31	1.12
2:B:285:THR:HG21	2:B:291:ARG:HE	1.20	1.02
2:B:294:HIS:CD2	2:B:296:GLU:H	1.79	1.00
1:A:213:GLU:HG3	1:A:214:ALA:H	1.28	0.99
2:B:601:GLU:O	2:B:602:ARG:HD2	1.64	0.98
2:B:600:LYS:HG2	2:B:601:GLU:N	1.78	0.96
2:B:614:GLU:HG2	2:B:624:PHE:HE1	1.29	0.95
2:B:602:ARG:HH11	2:B:602:ARG:HG2	1.28	0.95
2:B:596:LEU:HB2	2:B:599:ALA:HB3	1.46	0.95
1:A:263:PRO:HG3	2:B:461:GLU:HA	1.50	0.94
1:A:165:LEU:HD12	1:A:301:LEU:HD13	1.51	0.93
1:A:101:HIS:HB2	2:B:509:GLU:HG2	1.50	0.93
1:A:143:HIS:ND1	1:A:144:PRO:HD2	1.84	0.93
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.50	0.92
2:B:707:TYR:HE1	2:B:711:GLU:HB2	1.32	0.91
2:B:764:ALA:HA	2:B:767:ARG:HG2	1.52	0.89
2:B:602:ARG:CG	2:B:602:ARG:HH11	1.84	0.89
2:B:294:HIS:HD2	2:B:296:GLU:H	0.89	0.89
1:A:213:GLU:HG2	1:A:215:VAL:H	1.38	0.88
2:B:673:LEU:HD22	2:B:673:LEU:N	1.90	0.86
2:B:710:VAL:O	2:B:714:VAL:HG23	1.75	0.86
2:B:707:TYR:CE1	2:B:711:GLU:HB2	2.11	0.85
1:A:138:ASN:HD21	1:A:289:LYS:HE2	1.39	0.85
1:A:257:TYR:HB3	2:B:161:THR:HG21	1.59	0.85
1:A:209:ASP:O	1:A:333:ARG:HD2	1.77	0.84
2:B:278:ARG:NH2	2:B:308:SER:HB3	1.92	0.84
2:B:729:ASP:N	2:B:744:ALA:HB3	1.92	0.84
1:A:101:HIS:HD2	1:A:103:ILE:H	1.26	0.83
2:B:596:LEU:CB	2:B:599:ALA:HB3	2.09	0.83
2:B:688:SER:HB3	2:B:752:PRO:HA	1.61	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:CG	1:A:214:ALA:H	1.92	0.82
2:B:497:ARG:O	2:B:501:VAL:HG23	1.78	0.82
1:A:287:HIS:HD2	1:A:289:LYS:H	1.24	0.82
2:B:278:ARG:HH21	2:B:308:SER:HB3	1.42	0.82
2:B:563:ASP:O	2:B:565:PRO:HD3	1.78	0.82
1:A:138:ASN:ND2	1:A:289:LYS:HE2	1.96	0.81
2:B:701:VAL:HG22	2:B:702:PRO:HD2	1.62	0.81
2:B:38:VAL:O	2:B:40:PRO:HD3	1.80	0.81
2:B:70:ARG:HG3	5:B:974:HOH:O	1.79	0.81
2:B:294:HIS:HD2	2:B:296:GLU:N	1.75	0.81
1:A:311:THR:HG22	1:A:312:GLY:N	1.94	0.81
1:A:140:PRO:O	1:A:146:ARG:HB2	1.81	0.81
2:B:549:PHE:O	2:B:553:VAL:HG23	1.81	0.80
1:A:140:PRO:HD2	1:A:145:ALA:HB3	1.63	0.80
2:B:121:ARG:HD3	2:B:127:GLU:O	1.80	0.80
2:B:751:HIS:HD2	2:B:752:PRO:HD2	1.47	0.80
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.64	0.79
2:B:99:LEU:HD13	2:B:101:GLN:HB2	1.63	0.79
2:B:757:ARG:HG3	2:B:759:GLU:HB2	1.63	0.79
1:A:213:GLU:CG	1:A:214:ALA:N	2.47	0.78
2:B:161:THR:HG22	2:B:162:PRO:HD2	1.64	0.78
2:B:438:GLU:HA	2:B:438:GLU:OE1	1.84	0.78
2:B:519:GLU:HB3	2:B:523:ARG:HH12	1.47	0.77
2:B:643:LEU:HA	2:B:647:GLU:O	1.84	0.77
1:A:250:LYS:H	1:A:270:TRP:HB3	1.48	0.77
1:A:218:GLN:NE2	4:A:1002:FYA:H5'1	1.98	0.77
2:B:427:ILE:HG12	2:B:466:ILE:HG21	1.67	0.76
2:B:614:GLU:HG2	2:B:624:PHE:CE1	2.19	0.76
2:B:656:HIS:HB3	2:B:659:ILE:HD12	1.68	0.75
1:A:311:THR:HG22	1:A:312:GLY:H	1.50	0.75
1:A:160:ARG:HG2	1:A:168:GLU:OE2	1.85	0.75
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.67	0.75
2:B:730:LEU:HD12	2:B:730:LEU:C	2.07	0.74
2:B:603:LEU:C	2:B:603:LEU:HD12	2.08	0.74
2:B:243:ASN:ND2	2:B:246:VAL:H	1.86	0.74
2:B:697:LEU:HD23	2:B:698:ALA:N	2.03	0.74
2:B:751:HIS:HB3	2:B:754:ARG:O	1.87	0.74
2:B:722:LEU:HD11	2:B:724:SER:O	1.88	0.74
2:B:688:SER:CB	2:B:752:PRO:HA	2.17	0.73
2:B:194:GLU:OE2	2:B:387:ARG:HG2	1.87	0.73
2:B:770:GLU:O	2:B:774:ALA:HB2	1.88	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:ILE:HD12	2:B:446:PRO:HD3	1.70	0.73
1:A:263:PRO:HG3	2:B:461:GLU:CA	2.18	0.73
2:B:635:HIS:HB2	2:B:656:HIS:HA	1.70	0.72
2:B:700:VAL:HA	2:B:741:LYS:O	1.88	0.72
2:B:730:LEU:HB2	2:B:742:SER:O	1.89	0.72
2:B:663:LEU:O	2:B:665:LEU:N	2.23	0.72
1:A:262:GLU:OE1	2:B:458:ASP:HA	1.90	0.71
2:B:666:PRO:HB2	2:B:667:PRO:CD	2.19	0.71
2:B:38:VAL:HG22	2:B:153:GLU:O	1.89	0.71
2:B:663:LEU:C	2:B:665:LEU:H	1.94	0.71
2:B:285:THR:HG21	2:B:291:ARG:NE	2.01	0.71
1:A:349:VAL:O	1:A:350:LEU:HD22	1.91	0.71
2:B:178:HIS:O	2:B:430:ARG:NH1	2.24	0.71
2:B:95:GLU:OE2	2:B:102:LYS:HE2	1.91	0.70
2:B:243:ASN:HD21	2:B:246:VAL:H	1.38	0.70
2:B:770:GLU:CG	2:B:771:ALA:N	2.52	0.70
1:A:101:HIS:CD2	1:A:103:ILE:H	2.08	0.70
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.73	0.70
2:B:736:LEU:HB2	2:B:737:PRO:HD2	1.73	0.70
2:B:761:VAL:HG23	2:B:762:GLU:N	2.06	0.70
2:B:672:GLU:C	2:B:673:LEU:HD22	2.12	0.70
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.57	0.70
2:B:294:HIS:NE2	2:B:296:GLU:HB2	2.07	0.70
2:B:761:VAL:HG23	2:B:762:GLU:H	1.56	0.70
2:B:602:ARG:NH1	2:B:602:ARG:CG	2.49	0.70
2:B:589:LEU:HB3	2:B:609:LEU:HD12	1.73	0.70
2:B:757:ARG:HD3	2:B:759:GLU:H	1.56	0.70
2:B:303:TRP:HA	2:B:307:GLU:O	1.91	0.69
2:B:583:THR:HG22	2:B:675:LEU:HD12	1.75	0.69
2:B:728:PHE:HE1	2:B:745:PHE:C	1.96	0.69
2:B:287:ASP:H	2:B:317:MET:HE2	1.57	0.69
1:A:278:LEU:HD13	1:A:325:LEU:HD13	1.74	0.69
1:A:349:VAL:HG12	1:A:350:LEU:HD22	1.75	0.69
1:A:149:TRP:CD1	1:A:177:THR:HG23	2.27	0.69
2:B:604:SER:HA	2:B:608:LEU:HD22	1.74	0.68
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.28	0.68
1:A:209:ASP:OD2	1:A:212:HIS:HB2	1.93	0.68
2:B:673:LEU:CD2	2:B:673:LEU:N	2.57	0.68
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.29	0.68
2:B:734:PRO:HB2	2:B:735:PRO:HD3	1.76	0.68
2:B:698:ALA:HA	2:B:743:LEU:O	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:724:SER:HB2	2:B:748:ARG:HB2	1.75	0.67
1:A:155:THR:CG2	2:B:534:LEU:HD21	2.24	0.67
1:A:229:ALA:H	1:A:232:HIS:HD2	1.41	0.67
2:B:287:ASP:N	2:B:317:MET:HE2	2.09	0.67
2:B:610:LYS:O	2:B:614:GLU:HG3	1.94	0.67
1:A:349:VAL:O	1:A:350:LEU:HD13	1.94	0.67
1:A:148:MET:HE2	2:B:162:PRO:HG2	1.75	0.67
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.25	0.67
1:A:278:LEU:HD13	1:A:325:LEU:CD1	2.25	0.67
2:B:652:LEU:HD12	2:B:670:LEU:O	1.94	0.67
2:B:520:ASP:OD2	2:B:524:PHE:HE1	1.79	0.66
2:B:239:MET:HE1	2:B:355:GLU:HG3	1.77	0.66
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.77	0.66
1:A:249:SER:HB2	1:A:270:TRP:O	1.96	0.66
2:B:693:ALA:HB3	2:B:749:PHE:HB2	1.77	0.65
1:A:331:ASP:O	1:A:334:TYR:HB2	1.96	0.65
1:A:246:GLY:HA2	1:A:248:ASP:N	2.12	0.65
1:A:157:GLU:HG3	5:A:1035:HOH:O	1.96	0.65
2:B:767:ARG:N	2:B:767:ARG:HE	1.95	0.65
1:A:205:PHE:CD1	1:A:205:PHE:O	2.50	0.64
1:A:290:VAL:O	1:A:294:VAL:HG23	1.96	0.64
2:B:108:ILE:HG22	2:B:109:GLN:N	2.11	0.64
2:B:557:LYS:HZ3	2:B:663:LEU:HD12	1.63	0.64
2:B:656:HIS:NE2	2:B:658:GLU:HB2	2.12	0.64
1:A:155:THR:HG21	2:B:534:LEU:HD21	1.80	0.64
2:B:645:GLU:OE2	2:B:680:LYS:HB2	1.98	0.64
2:B:194:GLU:HB2	2:B:196:LEU:CD2	2.28	0.64
2:B:588:LEU:HD23	2:B:588:LEU:C	2.18	0.64
2:B:108:ILE:O	2:B:109:GLN:HG2	1.98	0.64
2:B:139:ALA:O	2:B:140:LEU:HD12	1.98	0.64
1:A:248:ASP:HB2	5:A:1013:HOH:O	1.98	0.63
2:B:757:ARG:HD2	2:B:759:GLU:HG2	1.81	0.63
2:B:729:ASP:H	2:B:744:ALA:HB3	1.59	0.63
2:B:194:GLU:O	2:B:390:GLU:HG2	1.98	0.63
2:B:662:GLU:HG3	2:B:662:GLU:O	1.97	0.63
2:B:215:LEU:HB2	2:B:393:LEU:HB2	1.80	0.63
2:B:635:HIS:HB2	2:B:657:PRO:CD	2.28	0.63
2:B:758:ASP:O	2:B:761:VAL:HG22	1.99	0.62
2:B:770:GLU:HG2	2:B:771:ALA:H	1.64	0.62
2:B:299:VAL:HG23	2:B:312:GLY:O	1.98	0.62
2:B:671:PHE:HD1	2:B:673:LEU:HD21	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:767:ARG:CA	2:B:767:ARG:HE	2.12	0.62
2:B:219:PHE:HE2	2:B:387:ARG:HE	1.47	0.62
2:B:553:VAL:O	2:B:556:LEU:HB3	1.99	0.62
2:B:600:LYS:CG	2:B:601:GLU:H	1.93	0.62
2:B:751:HIS:CD2	2:B:752:PRO:HD2	2.32	0.62
2:B:767:ARG:NE	2:B:767:ARG:HA	2.14	0.62
1:A:213:GLU:HG2	1:A:215:VAL:N	2.12	0.61
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.82	0.61
2:B:707:TYR:CD1	2:B:707:TYR:C	2.73	0.61
2:B:517:ASP:HB3	2:B:520:ASP:OD1	1.99	0.61
2:B:671:PHE:CD1	2:B:673:LEU:HD21	2.36	0.61
2:B:707:TYR:HD1	2:B:707:TYR:C	2.03	0.61
2:B:381:GLN:HE21	2:B:388:VAL:HG23	1.66	0.61
2:B:551:GLY:O	2:B:555:VAL:HG23	2.01	0.61
2:B:702:PRO:CB	2:B:704:PRO:HD2	2.31	0.61
1:A:137:LEU:O	1:A:139:ILE:N	2.30	0.61
1:A:311:THR:CG2	1:A:312:GLY:N	2.63	0.61
2:B:153:GLU:HG3	2:B:154:VAL:N	2.14	0.61
2:B:508:GLN:O	2:B:570:LEU:HB2	2.01	0.61
2:B:707:TYR:O	2:B:707:TYR:HD1	1.84	0.61
2:B:764:ALA:HA	2:B:767:ARG:CG	2.29	0.61
1:A:205:PHE:HE2	2:B:535:ASN:O	1.84	0.60
1:A:341:LYS:HE3	2:B:563:ASP:OD2	2.01	0.60
2:B:707:TYR:HE1	2:B:711:GLU:CB	2.10	0.60
1:A:311:THR:CG2	1:A:312:GLY:H	2.15	0.60
2:B:589:LEU:CB	2:B:609:LEU:HD12	2.31	0.60
2:B:243:ASN:HD22	2:B:243:ASN:C	2.05	0.60
2:B:757:ARG:HB3	2:B:760:GLU:OE2	2.01	0.60
2:B:762:GLU:O	2:B:765:VAL:HG12	2.02	0.60
2:B:603:LEU:HD12	2:B:603:LEU:O	2.02	0.59
2:B:635:HIS:ND1	2:B:636:PRO:O	2.35	0.59
2:B:285:THR:CG2	2:B:291:ARG:HE	2.06	0.59
2:B:512:THR:HG22	2:B:545:ARG:HH21	1.68	0.59
2:B:657:PRO:HA	2:B:660:ALA:HB3	1.85	0.59
2:B:281:GLU:HG2	2:B:310:PRO:HG3	1.84	0.59
2:B:771:ALA:HA	2:B:774:ALA:HB3	1.84	0.59
1:A:134:PHE:O	1:A:137:LEU:O	2.21	0.59
2:B:39:PHE:HB2	2:B:152:GLU:HA	1.84	0.59
2:B:629:GLN:O	2:B:639:SER:HB3	2.03	0.59
1:A:331:ASP:OD1	1:A:333:ARG:HD3	2.01	0.59
2:B:409:GLU:OE2	2:B:413:ARG:HD3	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:GLU:HB3	2:B:523:ARG:NH1	2.17	0.59
1:A:165:LEU:HD11	1:A:303:LEU:HD21	1.84	0.59
2:B:656:HIS:CD2	2:B:658:GLU:H	2.20	0.59
2:B:75:VAL:CG1	2:B:108:ILE:HG21	2.21	0.59
2:B:153:GLU:HB2	2:B:232:ARG:NH2	2.17	0.58
2:B:703:ALA:N	2:B:704:PRO:CD	2.66	0.58
2:B:710:VAL:HG11	2:B:743:LEU:CD1	2.33	0.58
1:A:341:LYS:H	1:A:341:LYS:HE2	1.68	0.58
1:A:299:GLU:HG3	1:A:300:ARG:N	2.18	0.58
2:B:119:SER:OG	2:B:122:GLU:HG3	2.04	0.58
2:B:259:PRO:HG2	2:B:360:PHE:CE2	2.38	0.58
2:B:649:VAL:HG23	2:B:674:ARG:H	1.69	0.58
2:B:161:THR:HB	2:B:163:ASN:OD1	2.03	0.58
2:B:671:PHE:HD1	2:B:673:LEU:CD2	2.15	0.58
2:B:265:LEU:HD23	2:B:268:VAL:HG21	1.86	0.58
2:B:294:HIS:CD2	2:B:296:GLU:HB2	2.39	0.58
2:B:706:PRO:O	2:B:710:VAL:HG23	2.04	0.58
2:B:99:LEU:HD22	2:B:101:GLN:NE2	2.19	0.57
2:B:108:ILE:CG2	2:B:109:GLN:N	2.67	0.57
2:B:728:PHE:HD1	2:B:728:PHE:H	1.49	0.57
1:A:148:MET:CE	2:B:162:PRO:HG2	2.34	0.57
2:B:757:ARG:CG	2:B:759:GLU:HB2	2.34	0.57
2:B:702:PRO:C	2:B:704:PRO:HD2	2.24	0.57
2:B:767:ARG:NE	2:B:767:ARG:CA	2.67	0.57
1:A:180:SER:O	1:A:183:GLN:HB2	2.05	0.57
2:B:377:LEU:HD22	2:B:388:VAL:HG13	1.87	0.57
2:B:293:LEU:HD13	2:B:293:LEU:N	2.18	0.57
2:B:635:HIS:HB2	2:B:657:PRO:HD3	1.85	0.57
2:B:657:PRO:HA	2:B:660:ALA:CB	2.35	0.57
2:B:286:LEU:HD11	2:B:323:GLU:CD	2.25	0.57
2:B:557:LYS:NZ	2:B:663:LEU:HD12	2.19	0.57
1:A:162:GLU:CG	1:A:166:GLY:HA2	2.35	0.57
1:A:126:GLU:HG3	2:B:575:ARG:HD2	1.87	0.56
2:B:707:TYR:HE2	2:B:727:LEU:HD22	1.70	0.56
2:B:38:VAL:O	2:B:40:PRO:CD	2.53	0.56
1:A:143:HIS:CG	1:A:144:PRO:HD2	2.40	0.56
1:A:252:ARG:HE	1:A:268:ALA:HB3	1.71	0.56
2:B:702:PRO:HA	2:B:739:GLY:O	2.06	0.56
2:B:758:ASP:HA	2:B:761:VAL:HG22	1.88	0.56
1:A:122:VAL:CG1	2:B:488:VAL:HG13	2.35	0.56
1:A:271:TRP:NE1	1:A:273:GLU:HB2	2.21	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HG3	1:A:278:LEU:HD21	1.87	0.56
2:B:226:SER:OG	2:B:244:ASN:HA	2.05	0.56
2:B:634:LEU:HB3	2:B:639:SER:OG	2.05	0.56
2:B:71:THR:HG22	2:B:72:VAL:N	2.21	0.56
1:A:238:TYR:HA	1:A:251:VAL:HG11	1.88	0.55
2:B:366:PRO:C	2:B:367:LEU:HD22	2.27	0.55
1:A:287:HIS:CD2	1:A:288:PRO:HD2	2.41	0.55
2:B:514:SER:O	2:B:545:ARG:HG2	2.07	0.55
2:B:381:GLN:O	2:B:385:GLY:HA2	2.06	0.55
2:B:55:PRO:HA	2:B:62:LYS:HA	1.89	0.55
2:B:770:GLU:CG	2:B:771:ALA:H	2.19	0.55
2:B:221:LEU:CD2	2:B:386:ALA:HB2	2.36	0.55
2:B:527:ASP:HB3	2:B:528:PRO:HD2	1.89	0.55
2:B:38:VAL:C	2:B:40:PRO:HD3	2.27	0.55
1:A:96:PHE:CE1	2:B:567:ARG:HG3	2.42	0.54
1:A:94:SER:HB2	2:B:567:ARG:NH2	2.21	0.54
2:B:458:ASP:O	2:B:462:GLU:HG2	2.08	0.54
2:B:731:TYR:HD1	2:B:742:SER:HG	1.55	0.54
1:A:219:LEU:HB3	1:A:317:LEU:CD2	2.37	0.54
1:A:349:VAL:CG1	1:A:350:LEU:HD22	2.38	0.54
2:B:370:VAL:N	2:B:371:PRO:HD2	2.23	0.54
2:B:734:PRO:CB	2:B:735:PRO:HD3	2.37	0.54
2:B:530:ARG:HH11	2:B:530:ARG:HB2	1.72	0.54
2:B:239:MET:CE	2:B:355:GLU:HG3	2.37	0.54
1:A:343:LEU:HD13	2:B:509:GLU:O	2.07	0.54
2:B:509:GLU:HG3	2:B:510:VAL:N	2.22	0.54
2:B:757:ARG:CD	2:B:759:GLU:H	2.21	0.54
2:B:761:VAL:CG2	2:B:762:GLU:H	2.20	0.54
2:B:224:ALA:HB1	2:B:225:PRO:HD2	1.90	0.54
2:B:163:ASN:O	2:B:452:ASP:HB3	2.08	0.54
2:B:194:GLU:HB2	2:B:196:LEU:HD21	1.90	0.54
2:B:556:LEU:C	2:B:556:LEU:HD12	2.28	0.53
2:B:663:LEU:C	2:B:665:LEU:N	2.62	0.53
2:B:194:GLU:HB2	2:B:196:LEU:HD23	1.91	0.53
2:B:516:MET:HE3	2:B:545:ARG:HA	1.91	0.53
1:A:257:TYR:HB3	2:B:161:THR:CG2	2.36	0.53
2:B:702:PRO:HB2	2:B:704:PRO:HD2	1.90	0.53
2:B:707:TYR:O	2:B:707:TYR:CD1	2.62	0.53
2:B:773:ARG:C	2:B:775:ARG:N	2.62	0.53
1:A:242:GLN:OE1	1:A:247:PRO:HB3	2.09	0.53
2:B:650:GLY:HA3	2:B:673:LEU:HD13	1.90	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:669:HIS:C	2:B:670:LEU:HD13	2.29	0.53
2:B:275:ARG:O	2:B:299:VAL:HG12	2.08	0.53
2:B:575:ARG:HG2	2:B:581:GLU:HG2	1.90	0.53
2:B:498:LEU:O	2:B:498:LEU:HD12	2.08	0.52
2:B:523:ARG:NH1	2:B:523:ARG:HG3	2.23	0.52
1:A:281:GLY:HA2	4:A:1002:FYA:O3'	2.09	0.52
2:B:617:PHE:HB3	2:B:622:LEU:O	2.09	0.52
2:B:729:ASP:CG	2:B:730:LEU:N	2.62	0.52
1:A:148:MET:HE3	1:A:257:TYR:HE2	1.75	0.52
1:A:96:PHE:CZ	2:B:567:ARG:HG3	2.43	0.52
2:B:263:PHE:O	2:B:331:ILE:HB	2.10	0.52
2:B:728:PHE:N	2:B:728:PHE:CD1	2.78	0.52
2:B:20:VAL:O	2:B:24:ARG:HG2	2.10	0.52
2:B:285:THR:HG23	2:B:287:ASP:OD1	2.09	0.52
2:B:459:LEU:O	2:B:462:GLU:HB2	2.10	0.52
2:B:761:VAL:CG2	2:B:762:GLU:N	2.73	0.52
2:B:267:PHE:CE2	2:B:321:GLU:HG2	2.45	0.52
2:B:51:LEU:HD21	2:B:67:ASP:HB2	1.91	0.52
2:B:601:GLU:C	2:B:602:ARG:HD2	2.29	0.52
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.45	0.52
2:B:671:PHE:CD1	2:B:673:LEU:CD2	2.92	0.52
2:B:733:GLY:HA3	2:B:736:LEU:HD21	1.92	0.52
2:B:447:PRO:HB2	2:B:449:HIS:CE1	2.45	0.52
2:B:699:VAL:HG12	2:B:773:ARG:NH2	2.25	0.52
1:A:165:LEU:HD12	1:A:301:LEU:CD1	2.33	0.51
2:B:621:GLY:O	2:B:680:LYS:HE2	2.10	0.51
2:B:63:ARG:HD2	2:B:73:GLU:OE2	2.10	0.51
2:B:666:PRO:HB2	2:B:667:PRO:HD2	1.92	0.51
2:B:359:ARG:HG3	2:B:359:ARG:HH11	1.75	0.51
2:B:191:LEU:HD13	2:B:378:SER:HA	1.91	0.51
2:B:697:LEU:C	2:B:697:LEU:HD23	2.29	0.51
1:A:246:GLY:HA2	1:A:248:ASP:H	1.74	0.51
2:B:563:ASP:C	2:B:565:PRO:HD3	2.30	0.51
2:B:107:VAL:HA	2:B:112:ARG:HA	1.92	0.51
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.41	0.51
2:B:635:HIS:HB2	2:B:657:PRO:HD2	1.91	0.51
1:A:175:LEU:HB3	1:A:203:PHE:CD2	2.45	0.51
2:B:538:ALA:HB1	2:B:540:GLU:OE1	2.10	0.51
2:B:548:LEU:HD13	2:B:576:VAL:CG1	2.41	0.51
2:B:644:VAL:HG22	2:B:645:GLU:H	1.74	0.51
2:B:337:CYS:HB2	2:B:369:GLN:NE2	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLU:HG2	2:B:771:ALA:N	2.24	0.51
2:B:770:GLU:O	2:B:774:ALA:CB	2.58	0.51
1:A:283:ALA:HB2	1:A:315:PHE:CB	2.40	0.51
2:B:285:THR:HG22	2:B:291:ARG:HG3	1.93	0.51
2:B:723:GLU:OE1	2:B:750:ARG:HD2	2.10	0.51
2:B:770:GLU:HG3	2:B:771:ALA:N	2.24	0.51
1:A:94:SER:O	2:B:594:VAL:HB	2.11	0.51
2:B:643:LEU:C	2:B:644:VAL:O	2.47	0.51
1:A:271:TRP:CH2	1:A:274:GLY:HA3	2.45	0.51
2:B:409:GLU:OE1	2:B:413:ARG:NH1	2.43	0.51
2:B:762:GLU:C	2:B:765:VAL:HG12	2.31	0.51
2:B:530:ARG:NH1	2:B:530:ARG:HB2	2.25	0.50
2:B:635:HIS:CE1	2:B:636:PRO:O	2.64	0.50
1:A:101:HIS:CD2	1:A:103:ILE:HB	2.46	0.50
1:A:270:TRP:O	1:A:272:PRO:HD3	2.10	0.50
1:A:110:LEU:HD11	1:A:322:LEU:HD23	1.93	0.50
5:A:1006:HOH:O	2:B:31:GLU:HG3	2.11	0.50
2:B:773:ARG:HB2	2:B:773:ARG:NH1	2.27	0.50
2:B:105:GLU:HG3	2:B:114:PHE:CD1	2.47	0.50
2:B:286:LEU:HB3	2:B:317:MET:CE	2.42	0.50
2:B:36:GLU:O	2:B:154:VAL:HA	2.11	0.50
2:B:299:VAL:HG22	2:B:300:ILE:N	2.26	0.50
2:B:656:HIS:HB3	2:B:659:ILE:CD1	2.39	0.50
2:B:30:PHE:HA	5:B:976:HOH:O	2.10	0.50
2:B:274:VAL:HG12	2:B:298:LEU:HD21	1.92	0.50
2:B:2:ARG:HD2	5:B:828:HOH:O	2.12	0.50
2:B:262:ALA:HB1	2:B:331:ILE:HG13	1.94	0.50
1:A:105:LEU:HD22	1:A:349:VAL:CG1	2.41	0.50
2:B:253:MET:HG3	2:B:259:PRO:HA	1.93	0.50
2:B:557:LYS:HE3	2:B:664:GLU:OE2	2.11	0.50
2:B:72:VAL:HG21	2:B:114:PHE:CD2	2.47	0.50
2:B:649:VAL:CG2	2:B:674:ARG:H	2.24	0.50
2:B:188:GLU:HG3	2:B:188:GLU:O	2.12	0.49
1:A:198:VAL:N	1:A:220:GLU:O	2.38	0.49
2:B:46:VAL:HB	2:B:143:GLY:O	2.12	0.49
1:A:101:HIS:CB	2:B:509:GLU:HG2	2.32	0.49
2:B:92:PRO:HG3	2:B:114:PHE:O	2.13	0.49
2:B:598:TRP:CZ3	2:B:599:ALA:HB2	2.47	0.49
2:B:710:VAL:HG11	2:B:743:LEU:HD12	1.94	0.49
1:A:122:VAL:HG13	2:B:488:VAL:HG13	1.94	0.49
2:B:520:ASP:HA	2:B:523:ARG:HB2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:SER:OG	2:B:752:PRO:HA	2.13	0.49
2:B:50:VAL:HA	2:B:66:LEU:HD23	1.93	0.49
2:B:692:ALA:HA	2:B:749:PHE:O	2.12	0.49
1:A:134:PHE:CZ	1:A:151:THR:HG21	2.48	0.49
2:B:517:ASP:OD1	2:B:519:GLU:HB2	2.13	0.49
1:A:114:PHE:HA	1:A:117:LEU:HD13	1.95	0.49
2:B:765:VAL:HG13	2:B:766:SER:N	2.28	0.49
2:B:286:LEU:HB2	2:B:318:GLY:O	2.13	0.48
2:B:609:LEU:HD21	2:B:671:PHE:HD2	1.77	0.48
2:B:538:ALA:HB3	2:B:541:LYS:HG2	1.95	0.48
2:B:613:LEU:O	2:B:617:PHE:HD1	1.96	0.48
1:A:268:ALA:HA	1:A:278:LEU:O	2.12	0.48
2:B:355:GLU:O	2:B:359:ARG:HG3	2.13	0.48
2:B:532:LEU:N	2:B:532:LEU:HD22	2.28	0.48
2:B:509:GLU:HA	2:B:571:PHE:CE1	2.47	0.48
2:B:575:ARG:HG2	2:B:581:GLU:CG	2.44	0.48
2:B:587:GLY:HA3	2:B:671:PHE:CE2	2.47	0.48
1:A:283:ALA:HB2	1:A:315:PHE:HB3	1.95	0.48
1:A:213:GLU:HG2	1:A:214:ALA:N	2.28	0.48
1:A:104:THR:HG1	2:B:511:TYR:HH	1.62	0.48
1:A:86:VAL:HG23	1:A:87:ASP:N	2.29	0.48
2:B:119:SER:OG	2:B:129:GLY:HA2	2.14	0.48
2:B:721:TYR:N	2:B:721:TYR:CD1	2.81	0.48
2:B:703:ALA:N	2:B:704:PRO:HD2	2.28	0.47
2:B:331:ILE:HG12	2:B:332:ALA:N	2.29	0.47
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.43	0.47
2:B:596:LEU:HD13	2:B:598:TRP:CH2	2.50	0.47
1:A:205:PHE:HD1	1:A:205:PHE:O	1.97	0.47
1:A:342:PHE:O	1:A:345:GLN:HB2	2.15	0.47
2:B:303:TRP:CA	2:B:307:GLU:O	2.61	0.47
2:B:642:VAL:HG23	2:B:651:PHE:HA	1.96	0.47
1:A:337:GLY:O	1:A:339:ARG:N	2.41	0.47
1:A:339:ARG:NH1	2:B:562:LEU:HD22	2.30	0.47
1:A:349:VAL:O	1:A:349:VAL:CG1	2.63	0.47
2:B:244:ASN:O	2:B:248:VAL:HG23	2.15	0.47
2:B:486:ARG:HD3	2:B:486:ARG:HA	1.73	0.47
2:B:650:GLY:HA3	2:B:672:GLU:O	2.15	0.47
2:B:642:VAL:HG23	2:B:651:PHE:CA	2.45	0.47
1:A:208:THR:HG22	1:A:213:GLU:HA	1.96	0.47
2:B:253:MET:HE2	2:B:253:MET:HB3	1.67	0.47
2:B:293:LEU:CD1	2:B:293:LEU:N	2.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:LEU:HD22	2:B:652:LEU:CD1	2.45	0.47
2:B:105:GLU:HG3	2:B:114:PHE:HD1	1.79	0.47
2:B:615:ALA:O	2:B:618:ALA:HB3	2.15	0.47
2:B:661:GLN:C	2:B:663:LEU:N	2.68	0.47
2:B:671:PHE:C	2:B:671:PHE:CD1	2.88	0.47
2:B:702:PRO:O	2:B:741:LYS:HE2	2.15	0.47
2:B:751:HIS:HD2	2:B:752:PRO:CD	2.22	0.47
2:B:523:ARG:HH11	2:B:523:ARG:HG3	1.79	0.46
2:B:533:LEU:HB2	2:B:536:PRO:HG3	1.97	0.46
2:B:651:PHE:CE2	2:B:672:GLU:HB3	2.50	0.46
2:B:765:VAL:CG1	2:B:766:SER:N	2.78	0.46
1:A:209:ASP:C	1:A:333:ARG:HD2	2.35	0.46
2:B:243:ASN:ND2	2:B:243:ASN:C	2.69	0.46
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.97	0.46
1:A:221:GLY:O	1:A:314:ALA:HA	2.14	0.46
1:A:260:PHE:CD1	1:A:260:PHE:N	2.82	0.46
2:B:556:LEU:HD22	2:B:588:LEU:HD21	1.96	0.46
2:B:675:LEU:HB3	2:B:676:PRO:HA	1.96	0.46
2:B:731:TYR:CE2	2:B:733:GLY:HA2	2.50	0.46
2:B:374:ARG:HA	2:B:374:ARG:HD3	1.77	0.46
2:B:537:LEU:HA	2:B:537:LEU:HD23	1.60	0.46
1:A:147:ASP:N	1:A:147:ASP:OD1	2.49	0.46
1:A:94:SER:HB2	2:B:567:ARG:CZ	2.46	0.46
1:A:215:VAL:HG21	2:B:513:TYR:CD2	2.51	0.46
2:B:266:ARG:NH1	2:B:267:PHE:CE1	2.83	0.46
1:A:134:PHE:HZ	1:A:151:THR:HG21	1.81	0.46
1:A:169:VAL:HG22	1:A:170:GLU:N	2.31	0.46
1:A:213:GLU:HG3	1:A:214:ALA:N	2.01	0.46
2:B:93:GLY:O	2:B:102:LYS:HD3	2.16	0.46
2:B:417:THR:HG22	2:B:473:PRO:HD2	1.97	0.46
1:A:164:PRO:HG2	1:A:188:VAL:HG11	1.97	0.46
2:B:294:HIS:CD2	2:B:296:GLU:N	2.63	0.46
2:B:516:MET:HE1	2:B:546:THR:H	1.81	0.46
2:B:695:ARG:HH22	2:B:761:VAL:HG21	1.80	0.46
2:B:631:PHE:HB2	2:B:634:LEU:HB2	1.97	0.46
1:A:219:LEU:HB3	1:A:317:LEU:HD22	1.97	0.45
2:B:730:LEU:HD12	2:B:730:LEU:O	2.16	0.45
1:A:191:THR:HG22	1:A:192:PRO:HD2	1.98	0.45
1:A:238:TYR:HA	1:A:251:VAL:CG1	2.45	0.45
2:B:219:PHE:CZ	2:B:387:ARG:HB3	2.51	0.45
2:B:549:PHE:CD2	2:B:550:PRO:HD3	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:ALA:O	2:B:663:LEU:O	2.34	0.45
1:A:270:TRP:CE3	1:A:270:TRP:HA	2.51	0.45
2:B:164:ARG:O	2:B:167:ALA:HB3	2.16	0.45
2:B:243:ASN:HD21	2:B:246:VAL:HG23	1.82	0.45
2:B:695:ARG:HB2	2:B:747:LEU:HB2	1.99	0.45
2:B:509:GLU:HB2	2:B:571:PHE:CE1	2.52	0.45
2:B:600:LYS:N	2:B:600:LYS:HD2	2.31	0.45
2:B:617:PHE:HD2	2:B:622:LEU:HB2	1.81	0.45
2:B:757:ARG:HD3	2:B:758:ASP:N	2.31	0.45
1:A:287:HIS:CD2	1:A:289:LYS:H	2.16	0.45
1:A:315:PHE:C	1:A:315:PHE:CD1	2.89	0.45
1:A:271:TRP:HB2	1:A:278:LEU:HD11	1.98	0.45
2:B:219:PHE:CE2	2:B:387:ARG:NE	2.82	0.45
2:B:300:ILE:HD13	2:B:314:ALA:HA	1.97	0.45
1:A:258:PHE:CZ	4:A:1002:FYA:HD1	2.52	0.45
2:B:427:ILE:HG22	2:B:428:LEU:N	2.32	0.45
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.17	0.45
2:B:219:PHE:HE2	2:B:387:ARG:NE	2.12	0.45
2:B:399:LYS:HA	2:B:400:PRO:HD3	1.82	0.45
1:A:336:PHE:HB3	2:B:513:TYR:CE1	2.51	0.45
2:B:556:LEU:O	2:B:556:LEU:HD12	2.17	0.45
1:A:126:GLU:HB3	1:A:203:PHE:HE2	1.83	0.44
1:A:169:VAL:CG2	1:A:170:GLU:N	2.80	0.44
2:B:218:ALA:O	2:B:330:ALA:HA	2.17	0.44
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.98	0.44
2:B:623:ALA:O	2:B:645:GLU:HA	2.17	0.44
1:A:218:GLN:NE2	4:A:1002:FYA:C5'	2.75	0.44
2:B:121:ARG:HA	2:B:126:GLY:O	2.17	0.44
2:B:2:ARG:HH11	2:B:2:ARG:CG	2.30	0.44
2:B:701:VAL:CG2	2:B:702:PRO:HD2	2.42	0.44
1:A:105:LEU:HD22	1:A:349:VAL:HG12	1.98	0.44
2:B:35:ILE:O	2:B:36:GLU:HG2	2.16	0.44
2:B:657:PRO:O	2:B:660:ALA:HB3	2.18	0.44
1:A:180:SER:N	1:A:181:PRO:HD2	2.32	0.44
2:B:271:GLY:O	2:B:302:GLY:HA2	2.17	0.44
2:B:759:GLU:O	2:B:763:GLU:HB2	2.18	0.44
1:A:245:PHE:HE2	1:A:269:VAL:HG11	1.82	0.44
2:B:359:ARG:CG	2:B:359:ARG:HH11	2.30	0.44
2:B:549:PHE:CD1	2:B:550:PRO:N	2.86	0.44
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.48	0.44
2:B:603:LEU:C	2:B:603:LEU:CD1	2.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:VAL:CG1	2:B:736:LEU:HD13	2.47	0.44
2:B:721:TYR:CD2	2:B:756:LEU:HD21	2.53	0.44
1:A:242:GLN:O	1:A:245:PHE:O	2.35	0.44
1:A:326:ARG:HG2	1:A:327:TYR:CD1	2.52	0.44
2:B:235:PHE:CZ	2:B:241:PRO:HD2	2.53	0.44
2:B:609:LEU:CD2	2:B:652:LEU:HD13	2.47	0.44
2:B:730:LEU:HD12	2:B:731:TYR:N	2.33	0.44
2:B:695:ARG:HH12	2:B:761:VAL:HG23	1.82	0.44
1:A:225:GLY:O	1:A:228:ILE:HG12	2.17	0.44
1:A:160:ARG:N	2:B:579:GLU:O	2.45	0.44
2:B:643:LEU:HD13	2:B:648:GLU:HA	2.00	0.44
2:B:707:TYR:O	2:B:710:VAL:HB	2.18	0.44
1:A:143:HIS:CB	1:A:144:PRO:HD2	2.48	0.44
2:B:198:LEU:HA	2:B:199:PRO:HD2	1.54	0.44
1:A:339:ARG:NH1	2:B:563:ASP:OD1	2.51	0.44
2:B:728:PHE:O	2:B:729:ASP:HB2	2.18	0.44
1:A:277:TRP:O	1:A:278:LEU:HD23	2.17	0.43
2:B:42:PRO:HA	2:B:43:ARG:NH1	2.33	0.43
2:B:523:ARG:HH11	2:B:523:ARG:CG	2.30	0.43
2:B:557:LYS:HA	2:B:665:LEU:HD11	2.00	0.43
2:B:732:GLN:HA	2:B:732:GLN:OE1	2.14	0.43
2:B:276:ARG:NH1	2:B:296:GLU:O	2.38	0.43
2:B:368:GLY:O	2:B:371:PRO:HG2	2.17	0.43
2:B:598:TRP:CE3	2:B:599:ALA:HB2	2.53	0.43
2:B:253:MET:O	2:B:256:ARG:O	2.35	0.43
2:B:303:TRP:HB2	2:B:307:GLU:O	2.18	0.43
1:A:277:TRP:C	1:A:278:LEU:HD23	2.39	0.43
2:B:92:PRO:HD3	2:B:114:PHE:O	2.19	0.43
2:B:705:THR:HG23	2:B:706:PRO:HD2	2.00	0.43
2:B:575:ARG:HD3	2:B:581:GLU:OE2	2.18	0.43
2:B:90:ALA:HB2	2:B:118:LEU:HD11	2.00	0.43
1:A:237:ILE:O	1:A:240:LEU:HB3	2.18	0.43
2:B:379:LEU:HA	2:B:379:LEU:HD23	1.92	0.43
2:B:535:ASN:N	2:B:535:ASN:OD1	2.52	0.43
2:B:72:VAL:HG22	2:B:73:GLU:N	2.34	0.43
1:A:149:TRP:CD1	1:A:177:THR:CG2	2.98	0.43
1:A:229:ALA:H	1:A:232:HIS:CD2	2.27	0.43
1:A:230:MET:HB2	2:B:415:LEU:HA	2.01	0.43
2:B:265:LEU:HA	2:B:265:LEU:HD23	1.81	0.43
2:B:600:LYS:HG2	2:B:601:GLU:HG3	2.00	0.43
2:B:309:PHE:CD1	2:B:309:PHE:N	2.87	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:PHE:CD1	2:B:549:PHE:C	2.92	0.43
2:B:520:ASP:OD2	2:B:554:ARG:NH1	2.49	0.43
2:B:768:VAL:O	2:B:772:LEU:HB2	2.19	0.43
1:A:201:ARG:HD2	1:A:215:VAL:CG1	2.48	0.43
2:B:589:LEU:HB3	2:B:609:LEU:CD1	2.43	0.43
1:A:233:LEU:HB2	1:A:313:PHE:CG	2.54	0.43
1:A:341:LYS:HD3	1:A:341:LYS:HA	1.87	0.43
2:B:377:LEU:HD22	2:B:388:VAL:CG1	2.47	0.42
2:B:579:GLU:HG2	2:B:579:GLU:H	1.38	0.42
2:B:650:GLY:CA	2:B:672:GLU:O	2.67	0.42
2:B:286:LEU:HB3	2:B:317:MET:HE2	2.00	0.42
1:A:122:VAL:HG13	2:B:488:VAL:CG1	2.49	0.42
2:B:498:LEU:C	2:B:498:LEU:HD12	2.39	0.42
2:B:520:ASP:OD2	2:B:524:PHE:CE1	2.67	0.42
2:B:600:LYS:HB3	2:B:600:LYS:HE2	1.78	0.42
2:B:80:ASN:HD22	2:B:134:GLU:HG3	1.84	0.42
1:A:107:GLU:O	1:A:111:VAL:HG23	2.20	0.42
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.53	0.42
2:B:276:ARG:HB3	2:B:295:PRO:O	2.19	0.42
2:B:337:CYS:HB2	2:B:369:GLN:HE22	1.84	0.42
1:A:339:ARG:HH12	2:B:562:LEU:HD22	1.85	0.42
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.31	0.42
2:B:703:ALA:HA	2:B:741:LYS:HG2	2.00	0.42
1:A:177:THR:HG22	1:A:178:HIS:CD2	2.54	0.42
2:B:22:GLU:HG3	2:B:32:THR:HB	2.00	0.42
2:B:287:ASP:HB3	2:B:317:MET:HE1	2.01	0.42
2:B:717:ALA:C	2:B:768:VAL:HG22	2.40	0.42
2:B:80:ASN:O	2:B:82:ARG:HD3	2.19	0.42
2:B:171:LEU:HD23	2:B:171:LEU:HA	1.74	0.42
2:B:307:GLU:OE1	2:B:307:GLU:HA	2.14	0.42
2:B:589:LEU:HD21	2:B:608:LEU:HD23	2.01	0.42
2:B:651:PHE:O	2:B:671:PHE:HA	2.19	0.42
1:A:321:ARG:HA	1:A:324:MET:HE2	2.01	0.42
2:B:249:THR:HB	2:B:260:MET:HG3	2.02	0.42
2:B:430:ARG:NH2	5:B:786:HOH:O	2.53	0.42
2:B:700:VAL:HG12	2:B:736:LEU:CD1	2.49	0.42
2:B:98:GLY:HA3	5:B:975:HOH:O	2.19	0.42
1:A:113:ILE:O	1:A:117:LEU:HD12	2.19	0.42
2:B:538:ALA:HB3	2:B:541:LYS:CG	2.50	0.42
2:B:692:ALA:CA	2:B:749:PHE:O	2.68	0.42
2:B:524:PHE:O	2:B:526:LEU:HG	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:LEU:HD22	2:B:643:LEU:N	2.35	0.42
1:A:128:GLU:HG3	1:A:129:SER:H	1.84	0.41
2:B:519:GLU:O	2:B:522:ARG:HB2	2.20	0.41
2:B:535:ASN:N	2:B:536:PRO:HD3	2.35	0.41
2:B:509:GLU:CA	2:B:571:PHE:CE1	3.03	0.41
2:B:727:LEU:HA	2:B:744:ALA:O	2.20	0.41
2:B:277:ALA:O	2:B:295:PRO:HA	2.19	0.41
2:B:467:GLN:OE1	2:B:467:GLN:HA	2.20	0.41
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.55	0.41
2:B:294:HIS:CD2	2:B:296:GLU:CB	3.03	0.41
2:B:265:LEU:HD23	2:B:268:VAL:CG2	2.50	0.41
2:B:177:LEU:HA	2:B:177:LEU:HD23	1.83	0.41
2:B:572:GLU:HG3	2:B:573:VAL:N	2.36	0.41
2:B:636:PRO:C	2:B:638:VAL:H	2.24	0.41
2:B:505:LEU:HD12	2:B:505:LEU:HA	1.84	0.41
2:B:512:THR:HB	2:B:572:GLU:OE2	2.21	0.41
2:B:51:LEU:HD11	2:B:67:ASP:HB2	2.03	0.41
2:B:304:ARG:O	2:B:307:GLU:HB2	2.20	0.41
2:B:344:ARG:HG3	2:B:361:GLU:OE2	2.21	0.41
2:B:402:GLU:HG3	5:B:903:HOH:O	2.21	0.41
2:B:529:PRO:CB	2:B:543:ALA:HB1	2.50	0.41
2:B:52:GLU:HB3	2:B:54:HIS:CE1	2.55	0.41
2:B:600:LYS:H	2:B:600:LYS:HD2	1.85	0.41
1:A:144:PRO:HB2	2:B:162:PRO:HB3	2.03	0.41
2:B:633:PHE:HD1	2:B:634:LEU:HD13	1.85	0.41
2:B:730:LEU:CD1	2:B:730:LEU:C	2.77	0.41
2:B:766:SER:C	2:B:768:VAL:N	2.72	0.41
1:A:347:LYS:HZ2	1:A:347:LYS:HG2	1.71	0.41
2:B:145:PRO:O	2:B:148:GLU:HB2	2.21	0.41
2:B:609:LEU:HD23	2:B:613:LEU:CD2	2.51	0.41
2:B:71:THR:CG2	2:B:72:VAL:N	2.83	0.41
1:A:133:ASN:HD21	1:A:177:THR:HB	1.85	0.41
1:A:133:ASN:OD1	1:A:176:ARG:HA	2.21	0.41
2:B:520:ASP:HB3	2:B:524:PHE:CD1	2.55	0.41
2:B:669:HIS:C	2:B:670:LEU:CD1	2.89	0.41
2:B:267:PHE:CD2	2:B:321:GLU:HG2	2.56	0.41
1:A:126:GLU:CG	2:B:575:ARG:HD2	2.50	0.41
2:B:728:PHE:HE1	2:B:746:HIS:N	2.19	0.41
2:B:756:LEU:HA	2:B:756:LEU:HD23	1.82	0.41
2:B:699:VAL:CG1	2:B:773:ARG:NH2	2.84	0.41
2:B:90:ALA:O	2:B:103:VAL:HG11	2.21	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:NH2	2:B:308:SER:O	2.55	0.40
2:B:549:PHE:N	2:B:550:PRO:CD	2.84	0.40
2:B:588:LEU:C	2:B:588:LEU:CD2	2.88	0.40
2:B:656:HIS:HD2	2:B:657:PRO:CD	2.34	0.40
2:B:764:ALA:O	2:B:767:ARG:HB2	2.21	0.40
2:B:566:GLU:CG	2:B:592:GLU:HG2	2.51	0.40
1:A:278:LEU:HD13	1:A:325:LEU:HD11	2.01	0.40
1:A:244:LEU:O	1:A:326:ARG:NH2	2.53	0.40
2:B:108:ILE:HG22	2:B:109:GLN:H	1.81	0.40
2:B:35:ILE:C	2:B:36:GLU:HG2	2.42	0.40
2:B:41:ILE:HA	2:B:42:PRO:HD2	1.92	0.40
2:B:507:PHE:N	2:B:507:PHE:CD1	2.89	0.40
2:B:520:ASP:C	2:B:522:ARG:N	2.72	0.40
2:B:141:PRO:HG2	2:B:144:THR:CG2	2.51	0.40
2:B:531:LEU:C	2:B:532:LEU:HD22	2.42	0.40
2:B:773:ARG:HB2	2:B:773:ARG:HH11	1.86	0.40
1:A:195:ARG:HG2	1:A:223:VAL:HG22	2.03	0.40
1:A:113:ILE:HD13	1:A:243:ALA:CB	2.52	0.40
1:A:260:PHE:C	1:A:287:HIS:HB2	2.42	0.40
2:B:381:GLN:NE2	2:B:388:VAL:HG23	2.33	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	263/350 (75%)	244 (93%)	14 (5%)	5 (2%)	9	15
2	B	773/785 (98%)	695 (90%)	63 (8%)	15 (2%)	9	15
All	All	1036/1135 (91%)	939 (91%)	77 (7%)	20 (2%)	9	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU
1	A	338	GLY
2	B	708	GLY
1	A	94	SER
1	A	330	PRO
2	B	128	TYR
2	B	199	PRO
2	B	525	ARG
2	B	702	PRO
2	B	735	PRO
2	B	770	GLU
1	A	273	GLU
2	B	737	PRO
2	B	752	PRO
2	B	486	ARG
2	B	645	GLU
2	B	315	GLY
2	B	644	VAL

### 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	213/277 (77%)	176 (83%)	37 (17%)	2	4
2	B	623/630 (99%)	493 (79%)	130 (21%)	1	2
All	All	836/907 (92%)	669 (80%)	167 (20%)	1	2

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	122	VAL
1	A	129	SER
1	A	143	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	146	ARG
1	A	147	ASP
1	A	154	LEU
1	A	157	GLU
1	A	168	GLU
1	A	170	GLU
1	A	174	LEU
1	A	177	THR
1	A	178	HIS
1	A	183	GLN
1	A	201	ARG
1	A	204	ARG
1	A	211	THR
1	A	230	MET
1	A	245	PHE
1	A	249	SER
1	A	250	LYS
1	A	252	ARG
1	A	260	PHE
1	A	266	GLN
1	A	276	LYS
1	A	280	LEU
1	A	289	LYS
1	A	292	GLN
1	A	299	GLU
1	A	303	LEU
1	A	317	LEU
1	A	326	ARG
1	A	339	ARG
1	A	340	LEU
1	A	341	LYS
1	A	347	LYS
1	A	350	LEU
2	B	2	ARG
2	B	24	ARG
2	B	33	ASP
2	B	37	ARG
2	B	38	VAL
2	B	43	ARG
2	B	46	VAL
2	B	49	ARG
2	B	56	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	60	ARG
2	B	61	LEU
2	B	63	ARG
2	B	70	ARG
2	B	89	LEU
2	B	95	GLU
2	B	96	LEU
2	B	99	LEU
2	B	106	ARG
2	B	108	ILE
2	B	109	GLN
2	B	111	VAL
2	B	118	LEU
2	B	127	GLU
2	B	144	THR
2	B	148	GLU
2	B	152	GLU
2	B	153	GLU
2	B	157	ASP
2	B	161	THR
2	B	171	LEU
2	B	188	GLU
2	B	196	LEU
2	B	203	LYS
2	B	208	GLU
2	B	222	ARG
2	B	226	SER
2	B	230	MET
2	B	239	MET
2	B	243	ASN
2	B	256	ARG
2	B	283	LEU
2	B	284	LYS
2	B	285	THR
2	B	286	LEU
2	B	293	LEU
2	B	294	HIS
2	B	298	LEU
2	B	307	GLU
2	B	313	LEU
2	B	322	SER
2	B	326	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	329	GLU
2	B	331	ILE
2	B	339	ASP
2	B	345	LYS
2	B	357	SER
2	B	361	GLU
2	B	364	VAL
2	B	397	SER
2	B	399	LYS
2	B	438	GLU
2	B	441	THR
2	B	451	LEU
2	B	459	LEU
2	B	461	GLU
2	B	484	ASP
2	B	486	ARG
2	B	494	LYS
2	B	497	ARG
2	B	499	ARG
2	B	512	THR
2	B	523	ARG
2	B	525	ARG
2	B	526	LEU
2	B	541	LYS
2	B	545	ARG
2	B	548	LEU
2	B	556	LEU
2	B	558	GLU
2	B	562	LEU
2	B	567	ARG
2	B	570	LEU
2	B	571	PHE
2	B	575	ARG
2	B	579	GLU
2	B	588	LEU
2	B	590	PHE
2	B	592	GLU
2	B	600	LYS
2	B	602	ARG
2	B	603	LEU
2	B	609	LEU
2	B	613	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	624	PHE
2	B	633	PHE
2	B	634	LEU
2	B	635	HIS
2	B	638	VAL
2	B	639	SER
2	B	645	GLU
2	B	648	GLU
2	B	649	VAL
2	B	661	GLN
2	B	662	GLU
2	B	663	LEU
2	B	670	LEU
2	B	673	LEU
2	B	674	ARG
2	B	682	LEU
2	B	685	GLN
2	B	688	SER
2	B	689	ARG
2	B	700	VAL
2	B	701	VAL
2	B	707	TYR
2	B	713	LEU
2	B	715	ARG
2	B	716	GLU
2	B	727	LEU
2	B	728	PHE
2	B	730	LEU
2	B	731	TYR
2	B	732	GLN
2	B	738	GLU
2	B	741	LYS
2	B	746	HIS
2	B	748	ARG
2	B	767	ARG
2	B	770	GLU
2	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	120	GLN
1	A	138	ASN
1	A	142	HIS
1	A	178	HIS
1	A	183	GLN
1	A	218	GLN
1	A	232	HIS
1	A	287	HIS
2	B	54	HIS
2	B	109	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	243	ASN
2	B	258	GLN
2	B	261	HIS
2	B	294	HIS
2	B	350	HIS
2	B	449	HIS
2	B	656	HIS
2	B	751	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	FYA	A	1002	-	33,36,36	1.19	3 (9%)	31,52,52	0.64	0

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	FYA	A	1002	-	-	0/16/36/36	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FYA	O3P-C	-4.32	1.27	1.44
4	A	1002	FYA	C8-N7	-2.00	1.30	1.34
4	A	1002	FYA	O4'-C1'	2.52	1.44	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	FYA	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	265/350 (75%)	0.07	8 (3%) 51 53	27, 54, 103, 129	0
2	B	775/785 (98%)	0.08	39 (5%) 30 31	21, 59, 108, 128	0
All	All	1040/1135 (91%)	0.08	47 (4%) 34 36	21, 58, 107, 129	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	5.6
2	B	718	ALA	5.0
1	A	350	LEU	4.9
2	B	753	LYS	4.8
2	B	739	GLY	4.7
2	B	736	LEU	4.5
1	A	142	HIS	4.3
2	B	732	GLN	4.3
2	B	731	TYR	4.2
2	B	99	LEU	4.1
2	B	700	VAL	4.1
2	B	743	LEU	4.1
2	B	697	LEU	3.9
2	B	768	VAL	3.8
2	B	759	GLU	3.8
1	A	148	MET	3.8
2	B	756	LEU	3.6
2	B	696	ASP	3.5
2	B	713	LEU	3.4
2	B	689	ARG	3.4
1	A	158	GLY	3.2
2	B	100	GLY	3.1
2	B	638	VAL	3.1
2	B	693	ALA	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	699	VAL	3.0
2	B	733	GLY	3.0
2	B	772	LEU	3.0
2	B	701	VAL	2.9
2	B	633	PHE	2.8
2	B	771	ALA	2.7
1	A	207	GLN	2.7
2	B	705	THR	2.6
2	B	282	ARG	2.6
2	B	734	PRO	2.6
2	B	752	PRO	2.6
2	B	694	PHE	2.6
2	B	692	ALA	2.6
2	B	745	PHE	2.4
2	B	761	VAL	2.4
1	A	143	HIS	2.4
1	A	271	TRP	2.3
2	B	738	GLU	2.2
2	B	704	PRO	2.2
2	B	751	HIS	2.1
2	B	749	PHE	2.1
2	B	757	ARG	2.0
2	B	775	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	1001	1/1	0.84	0.26	9.14	42,42,42,42	0
4	FYA	A	1002	33/33	0.97	0.15	-0.01	40,65,73,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.