



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:11 am GMT

PDB ID : 1O5W
Title : The structure basis of specific recognitions for substrates and inhibitors of rat monoamine oxidase A
Authors : Ma, J.; Yoshimura, M.; Yamashita, E.; Nakagawa, A.; Ito, A.; Tsukihara, T.
Deposited on : 2003-10-06
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

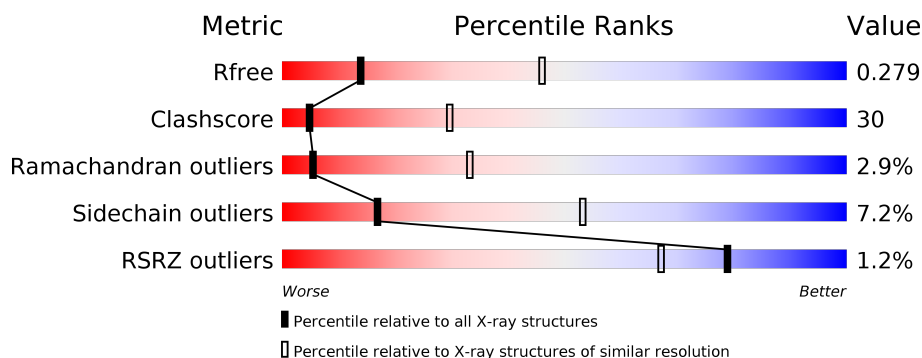
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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

Mol	Chain	Length	Quality of chain
1	A	534	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>40%</div> <div>5%</div> <div></div> </div> </div>
1	B	534	<div> <div></div> <div> <div>47%</div> <div>41%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	534	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>40%</div> <div>5%</div> <div></div> </div> </div>
1	D	534	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>5%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLG	B	1709	-	-	-	X
2	MLG	C	2709	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16456 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 Amine oxidase [flavin-containing] A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4071	2620	691	738	22			
1	B	503	Total	C	N	O	S	0	0	0
			4002	2570	682	729	21			
1	C	512	Total	C	N	O	S	0	0	0
			4079	2626	692	739	22			
1	D	506	Total	C	N	O	S	0	0	0
			4024	2585	685	732	22			

There are 44 discrepancies between the modelled and reference sequences:

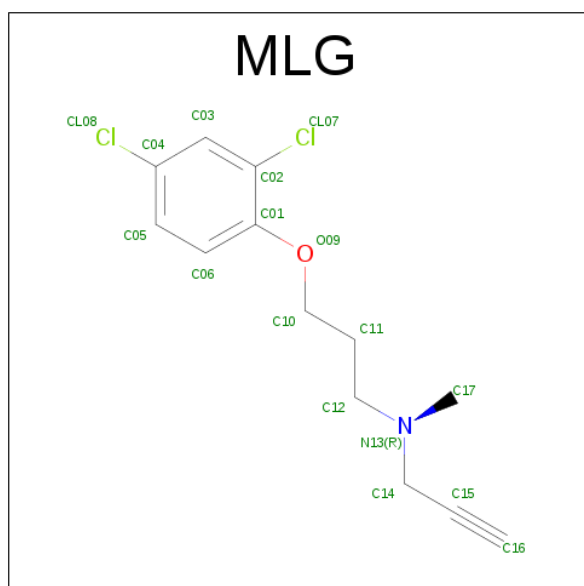
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP P21396
A	-6	GLY	-	EXPRESSION TAG	UNP P21396
A	-5	HIS	-	EXPRESSION TAG	UNP P21396
A	-4	HIS	-	EXPRESSION TAG	UNP P21396
A	-3	HIS	-	EXPRESSION TAG	UNP P21396
A	-2	HIS	-	EXPRESSION TAG	UNP P21396
A	-1	HIS	-	EXPRESSION TAG	UNP P21396
A	0	HIS	-	EXPRESSION TAG	UNP P21396
A	17	VAL	GLY	SEE REMARK 999	UNP P21396
A	18	VAL	LEU	SEE REMARK 999	UNP P21396
A	361	LEU	GLN	SEE REMARK 999	UNP P21396
B	993	MET	-	EXPRESSION TAG	UNP P21396
B	994	GLY	-	EXPRESSION TAG	UNP P21396
B	995	HIS	-	EXPRESSION TAG	UNP P21396
B	996	HIS	-	EXPRESSION TAG	UNP P21396
B	997	HIS	-	EXPRESSION TAG	UNP P21396
B	998	HIS	-	EXPRESSION TAG	UNP P21396
B	999	HIS	-	EXPRESSION TAG	UNP P21396
B	1000	HIS	-	EXPRESSION TAG	UNP P21396
B	1017	VAL	GLY	SEE REMARK 999	UNP P21396
B	1018	VAL	LEU	SEE REMARK 999	UNP P21396

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1361	LEU	GLN	SEE REMARK 999	UNP P21396
C	1993	MET	-	EXPRESSION TAG	UNP P21396
C	1994	GLY	-	EXPRESSION TAG	UNP P21396
C	1995	HIS	-	EXPRESSION TAG	UNP P21396
C	1996	HIS	-	EXPRESSION TAG	UNP P21396
C	1997	HIS	-	EXPRESSION TAG	UNP P21396
C	1998	HIS	-	EXPRESSION TAG	UNP P21396
C	1999	HIS	-	EXPRESSION TAG	UNP P21396
C	2000	HIS	-	EXPRESSION TAG	UNP P21396
C	2017	VAL	GLY	SEE REMARK 999	UNP P21396
C	2018	VAL	LEU	SEE REMARK 999	UNP P21396
C	2361	LEU	GLN	SEE REMARK 999	UNP P21396
D	2993	MET	-	EXPRESSION TAG	UNP P21396
D	2994	GLY	-	EXPRESSION TAG	UNP P21396
D	2995	HIS	-	EXPRESSION TAG	UNP P21396
D	2996	HIS	-	EXPRESSION TAG	UNP P21396
D	2997	HIS	-	EXPRESSION TAG	UNP P21396
D	2998	HIS	-	EXPRESSION TAG	UNP P21396
D	2999	HIS	-	EXPRESSION TAG	UNP P21396
D	3000	HIS	-	EXPRESSION TAG	UNP P21396
D	3017	VAL	GLY	SEE REMARK 999	UNP P21396
D	3018	VAL	LEU	SEE REMARK 999	UNP P21396
D	3361	LEU	GLN	SEE REMARK 999	UNP P21396

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: MLG, FAD) (formula: $C_{13}H_{15}Cl_2NO$, $C_{27}H_{33}N_9O_{15}P_2$).

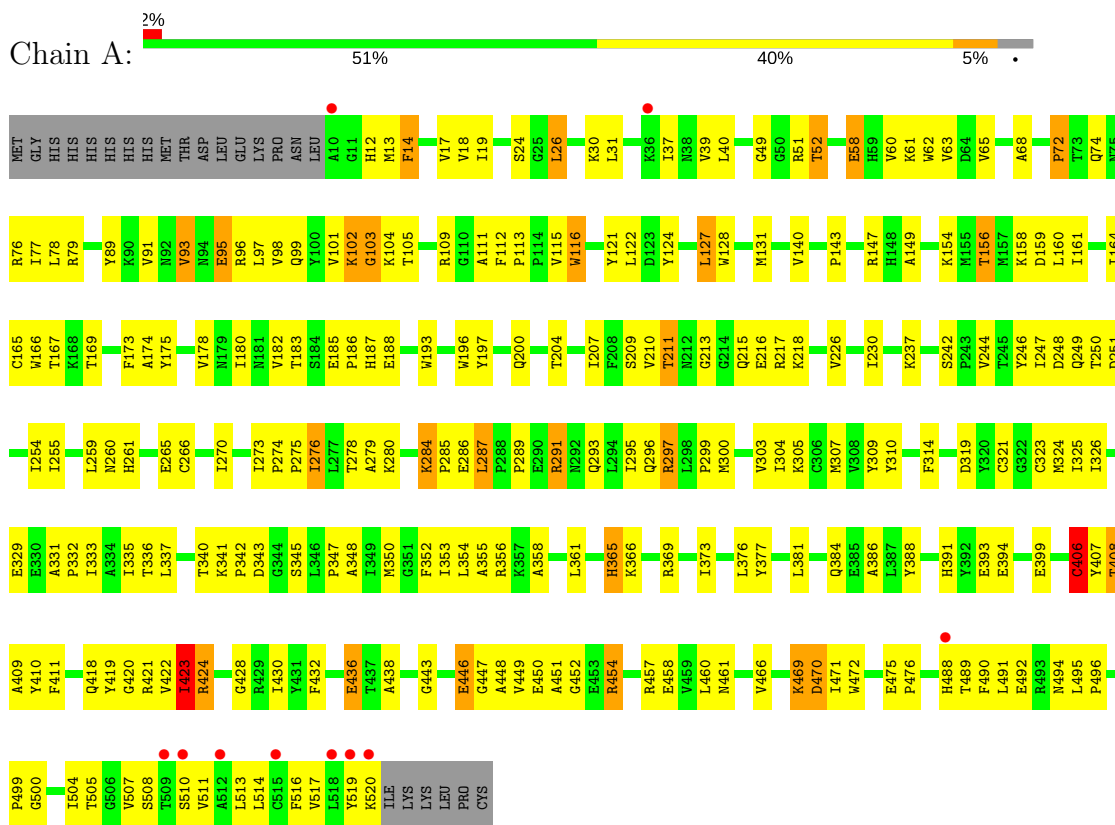


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	B	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	C	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		
2	D	2	Total	C	Cl	N	O	P	0	0
			70	40	2	10	16	2		

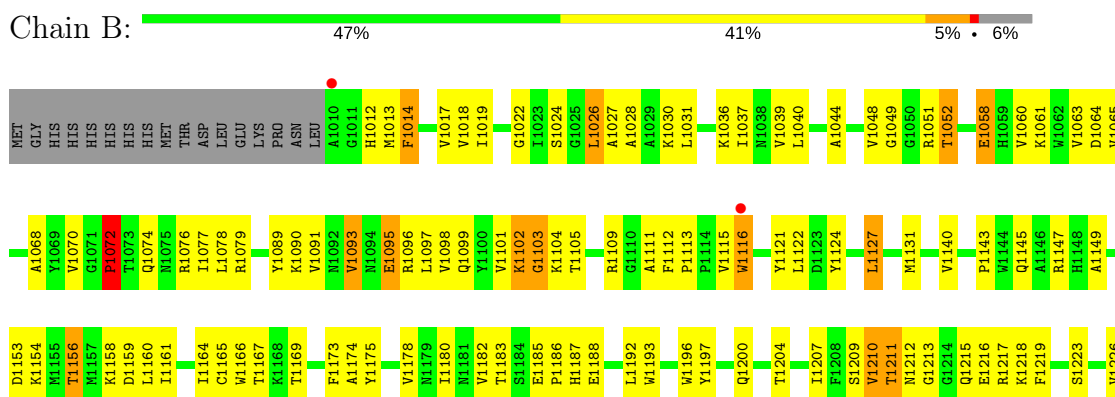
3 Residue-property plots

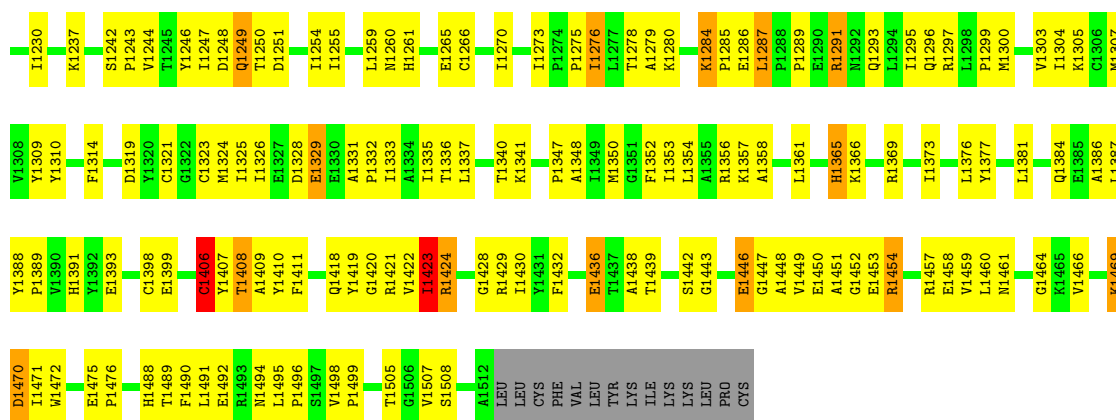
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Amine oxidase [flavin-containing] A

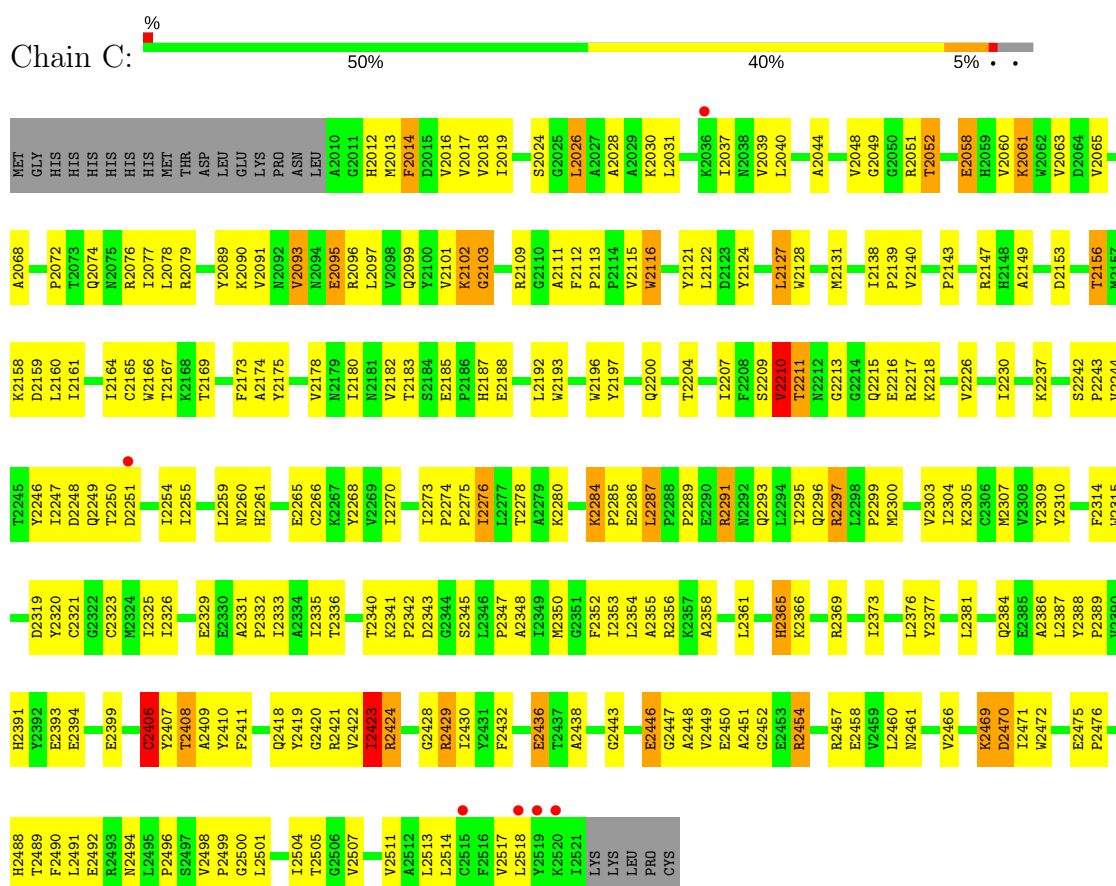


• Molecule 1: Amine oxidase [flavin-containing] A

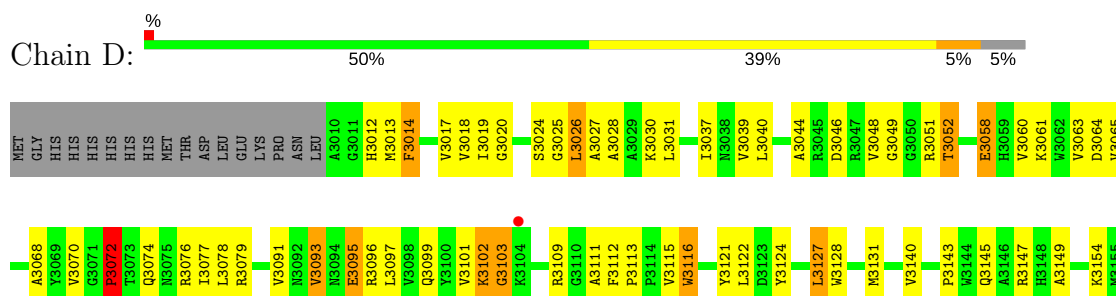




• Molecule 1: Amine oxidase [flavin-containing] A



• Molecule 1: Amine oxidase [flavin-containing] A



E3475	H3391	F3314	K3237	T3156
T3487	Y3392	W3315	S3241	K3157
H3488	E3393		S3242	K3158
T3489	E3394		P3243	D3159
F3490		D3319	V3244	L3160
L3491	E3399	Y3320	T3245	I3161
E3492		C3321	Y3246	I3164
H3493	C3406	G3322	I3247	C3165
N3494	Y3407	C3323	D3248	W3166
L3495	T3408	M3324	Q3249	T3167
P3496	A3409	I3325	T3250	K3168
S3497	Y3410	I3326	D3251	T3169
V3498	F3411	F3327		
P3499		D3328	I3254	F3173
	Q3418	E3329	I3255	A3174
	Y3419	E3330	I3256	Y3175
	G3420	A3331		
	R3421	P3332	L3259	V3178
	V3422	I3333	N3260	H3179
	I3423	A3334	H3261	I3180
	R3424	I3335	E3265	N3181
		T3336	C3266	V3182
	G3428			T3183
	R3429	T3340	I3270	S3184
	I3430	K3341		E3185
	Y3431		I3273	P3186
	F3432	P3347	P3274	H3187
		A3348	P3275	E3188
	E3436	I3349	T3276	V3189
	LEU	M3350	L3277	
	TYR	G3351	T3278	W3193
	LYS	F3352	A3279	
	ILE	I3353		W3196
	LYS	L3354	K3284	Y3197
	LYS	A3355	P3285	
	LEU	R3356	E3286	Q3200
	PRO	K3357	L3287	
	CYS	A3358	P3288	T3204
			P3289	
		L3361	E3290	I3207
			R3291	F3208
		H3365	N3292	S3209
		K3366	Q3293	V3210
			L3294	T3211
		R3369	I3295	N3212
			Q3296	G3213
		I3373	R3297	G3214
			L3298	Q3215
		L3376	P3299	E3216
		Y3377	M3300	R3217
				K3218
		L3381	V3303	F3219
			I3304	
		Q3384	K3305	
		E3385	C3306	S3223
		A3386	M3307	
		L3387	V3308	V3226
		F3388	Y3309	
		P3389	Y3310	I3230
		V3390		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.56Å 157.56Å 257.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.19 – 3.20 16.18 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (16.19-3.20) 98.9 (16.18-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.282 0.221 , 0.279	Depositor DCC
R_{free} test set	2684 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	106.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16456	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/4171	0.65	1/5657 (0.0%)
1	B	0.39	1/4100 (0.0%)	0.64	2/5561 (0.0%)
1	C	0.39	1/4179 (0.0%)	0.65	2/5668 (0.0%)
1	D	0.39	1/4122 (0.0%)	0.65	1/5591 (0.0%)
All	All	0.40	3/16572 (0.0%)	0.65	6/22477 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3210	VAL	CB-CG1	-5.23	1.41	1.52
1	C	2210	VAL	CB-CG2	-5.17	1.42	1.52
1	B	1210	VAL	CB-CG1	-5.06	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	CYS	N-CA-C	6.98	129.84	111.00
1	C	2406	CYS	N-CA-C	6.91	129.66	111.00
1	B	1406	CYS	N-CA-C	6.83	129.46	111.00
1	D	3406	CYS	N-CA-C	6.79	129.35	111.00
1	B	1406	CYS	CA-CB-SG	-5.38	104.31	114.00
1	C	2406	CYS	CA-CB-SG	-5.03	104.94	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4071	0	4085	256	0
1	B	4002	0	4007	270	0
1	C	4079	0	4096	260	0
1	D	4024	0	4034	257	0
2	A	70	0	44	4	0
2	B	70	0	44	3	0
2	C	70	0	44	2	0
2	D	70	0	44	2	0
All	All	16456	0	16398	997	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 30.

All (997) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1464:GLY:HA3	1:D:3145:GLN:HG2	1.18	1.15
1:A:458:GLU:HA	1:A:471:ILE:HD11	1.33	1.10
1:C:2458:GLU:HA	1:C:2471:ILE:HD11	1.33	1.10
1:D:3458:GLU:HA	1:D:3471:ILE:HD11	1.34	1.06
1:B:1458:GLU:HA	1:B:1471:ILE:HD11	1.34	1.03
1:A:275:PRO:HD3	1:A:436:GLU:HG3	1.37	1.02
1:B:1275:PRO:HD3	1:B:1436:GLU:HG3	1.39	1.02
1:D:3275:PRO:HD3	1:D:3436:GLU:HG3	1.39	1.02
1:A:284:LYS:HB3	1:A:285:PRO:HD3	1.42	1.01
1:C:2275:PRO:HD3	1:C:2436:GLU:HG3	1.41	1.01
1:D:3284:LYS:HB3	1:D:3285:PRO:HD3	1.42	1.01
1:B:1145:GLN:HG2	1:D:3464:GLY:HA3	1.41	1.00
1:C:2284:LYS:HB3	1:C:2285:PRO:HD3	1.44	0.99
1:B:1284:LYS:HB3	1:B:1285:PRO:HD3	1.45	0.98
1:D:3408:THR:HG23	1:D:3443:GLY:HA2	1.50	0.93
1:C:2156:THR:HG22	1:C:2158:LYS:H	1.33	0.93
1:C:2408:THR:CG2	1:C:2443:GLY:HA2	1.99	0.93
1:D:3408:THR:CG2	1:D:3443:GLY:HA2	1.99	0.92
1:B:1408:THR:CG2	1:B:1443:GLY:HA2	2.00	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:NE2	1:B:1356:ARG:HA	1.85	0.91
1:C:2408:THR:HG23	1:C:2443:GLY:HA2	1.51	0.90
1:A:408:THR:CG2	1:A:443:GLY:HA2	2.01	0.90
1:A:408:THR:HG23	1:A:443:GLY:HA2	1.54	0.90
1:B:1408:THR:HG23	1:B:1443:GLY:HA2	1.52	0.89
1:B:1464:GLY:HA3	1:D:3145:GLN:CG	2.04	0.88
1:D:3156:THR:HG22	1:D:3158:LYS:H	1.38	0.88
1:A:156:THR:HG22	1:A:158:LYS:H	1.38	0.87
1:B:1156:THR:HG22	1:B:1158:LYS:H	1.40	0.87
1:A:63:VAL:HG11	1:A:309:TYR:OH	1.77	0.83
1:C:2063:VAL:HG11	1:C:2309:TYR:OH	1.79	0.83
1:B:1063:VAL:HG11	1:B:1309:TYR:OH	1.78	0.82
1:C:2418:GLN:NE2	1:D:3356:ARG:HA	1.95	0.82
1:A:356:ARG:HA	1:B:1418:GLN:NE2	1.95	0.82
1:D:3063:VAL:HG11	1:D:3309:TYR:OH	1.79	0.82
1:B:1505:THR:O	1:B:1507:VAL:HG23	1.80	0.81
1:B:1145:GLN:CG	1:D:3464:GLY:HA3	2.10	0.81
1:B:1464:GLY:CA	1:D:3145:GLN:HG2	2.07	0.81
1:D:3300:MET:CE	1:D:3409:ALA:HB2	2.12	0.80
1:D:3275:PRO:CD	1:D:3436:GLU:HG3	2.12	0.80
1:A:275:PRO:CD	1:A:436:GLU:HG3	2.12	0.80
1:A:296:GLN:HE21	1:B:1300:MET:H	1.28	0.79
1:B:1275:PRO:CD	1:B:1436:GLU:HG3	2.13	0.79
1:A:26:LEU:HB3	1:A:230:ILE:HD13	1.64	0.79
1:C:2335:ILE:HB	2:C:2709:MLG:CL07	2.20	0.79
1:B:1300:MET:CE	1:B:1409:ALA:HB2	2.14	0.78
1:C:2026:LEU:HB3	1:C:2230:ILE:HD13	1.64	0.78
1:C:2356:ARG:HA	1:D:3418:GLN:NE2	1.98	0.78
1:C:2418:GLN:HE22	1:D:3356:ARG:HA	1.49	0.77
1:C:2275:PRO:CD	1:C:2436:GLU:HG3	2.13	0.77
1:D:3026:LEU:HB3	1:D:3230:ILE:HD13	1.67	0.77
1:A:300:MET:CE	1:A:409:ALA:HB2	2.13	0.77
1:A:296:GLN:NE2	1:B:1300:MET:H	1.81	0.77
1:B:1242:SER:HA	1:B:1260:ASN:HD21	1.49	0.76
1:C:2300:MET:CE	1:C:2409:ALA:HB2	2.15	0.76
1:B:1424:ARG:HB3	1:B:1424:ARG:NH1	2.01	0.76
1:D:3242:SER:HA	1:D:3260:ASN:HD21	1.49	0.76
1:A:242:SER:HA	1:A:260:ASN:HD21	1.48	0.75
1:B:1026:LEU:HB3	1:B:1230:ILE:HD13	1.68	0.75
1:A:356:ARG:HA	1:B:1418:GLN:HE22	1.51	0.75
1:D:3424:ARG:HB3	1:D:3424:ARG:NH1	2.01	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:O	1:A:200:GLN:HG3	1.87	0.75
1:A:418:GLN:HE22	1:B:1356:ARG:HA	1.49	0.75
1:C:2156:THR:HG22	1:C:2158:LYS:N	2.00	0.75
1:D:3335:ILE:HB	2:D:3709:MLG:CL07	2.24	0.75
1:C:2242:SER:HA	1:C:2260:ASN:HD21	1.52	0.75
1:B:1156:THR:CG2	1:B:1187:HIS:HA	2.18	0.74
1:A:300:MET:H	1:B:1296:GLN:HE21	1.35	0.74
1:A:156:THR:HG22	1:A:158:LYS:N	2.02	0.74
1:A:300:MET:HE2	1:A:409:ALA:HB2	1.68	0.74
1:C:2296:GLN:NE2	1:D:3300:MET:H	1.85	0.74
1:A:424:ARG:NH1	1:A:424:ARG:HB3	2.02	0.74
1:A:489:THR:HG22	1:A:491:LEU:H	1.53	0.74
1:C:2091:VAL:HG23	1:C:2217:ARG:HA	1.70	0.74
1:D:3156:THR:HG22	1:D:3158:LYS:N	2.02	0.74
1:A:519:TYR:HD2	1:A:520:LYS:HG3	1.53	0.73
1:C:2513:LEU:O	1:C:2517:VAL:HG23	1.88	0.73
1:C:2296:GLN:HE21	1:D:3300:MET:H	1.35	0.73
1:C:2300:MET:H	1:D:3296:GLN:HE21	1.36	0.73
1:C:2489:THR:HG22	1:C:2491:LEU:H	1.53	0.73
1:C:2424:ARG:NH1	1:C:2424:ARG:HB3	2.03	0.73
1:A:424:ARG:HB3	1:A:424:ARG:HH11	1.54	0.72
1:D:3091:VAL:HG23	1:D:3217:ARG:HA	1.70	0.72
1:A:91:VAL:HG23	1:A:217:ARG:HA	1.71	0.72
1:B:1091:VAL:HG23	1:B:1217:ARG:HA	1.70	0.72
1:B:1156:THR:HG22	1:B:1158:LYS:N	2.03	0.72
1:B:1424:ARG:HB3	1:B:1424:ARG:HH11	1.54	0.72
1:B:1489:THR:HG22	1:B:1491:LEU:H	1.54	0.72
1:A:226:VAL:O	1:A:230:ILE:HG22	1.89	0.72
1:B:1197:TYR:O	1:B:1200:GLN:HG3	1.90	0.72
1:D:3489:THR:HG22	1:D:3491:LEU:H	1.53	0.71
1:C:2156:THR:CG2	1:C:2187:HIS:HA	2.20	0.71
1:D:3156:THR:CG2	1:D:3187:HIS:HA	2.19	0.71
1:A:156:THR:CG2	1:A:187:HIS:HA	2.20	0.71
1:C:2424:ARG:HH11	1:C:2424:ARG:HB3	1.55	0.71
1:C:2197:TYR:O	1:C:2200:GLN:HG3	1.90	0.71
1:B:1300:MET:HE2	1:B:1409:ALA:HB2	1.72	0.70
1:D:3424:ARG:HB3	1:D:3424:ARG:HH11	1.54	0.70
1:A:250:THR:HG23	1:A:285:PRO:HG3	1.73	0.70
1:C:2300:MET:HE2	1:C:2409:ALA:HB2	1.72	0.70
1:C:2356:ARG:HA	1:D:3418:GLN:HE22	1.55	0.70
1:B:1457:ARG:HD2	1:B:1471:ILE:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1226:VAL:O	1:B:1230:ILE:HG22	1.91	0.70
1:A:507:VAL:O	1:A:511:VAL:HG23	1.92	0.70
1:B:1352:PHE:HB3	1:B:1354:LEU:HD21	1.74	0.70
1:C:2017:VAL:HG23	1:C:2266:CYS:HB3	1.74	0.70
1:C:2352:PHE:HB3	1:C:2354:LEU:HD21	1.72	0.70
1:D:3197:TYR:O	1:D:3200:GLN:HG3	1.92	0.70
1:C:2156:THR:CG2	1:C:2158:LYS:H	2.03	0.69
1:D:3300:MET:HE2	1:D:3409:ALA:HB2	1.74	0.69
1:B:1469:LYS:C	1:B:1469:LYS:HD3	2.13	0.69
1:C:2300:MET:H	1:D:3296:GLN:NE2	1.90	0.69
1:D:3093:VAL:O	1:D:3093:VAL:HG12	1.93	0.69
1:A:116:TRP:CE3	1:A:116:TRP:HA	2.28	0.69
1:A:278:THR:HG21	1:A:295:ILE:HD13	1.75	0.69
1:A:156:THR:CG2	1:A:158:LYS:H	2.05	0.68
1:B:1093:VAL:O	1:B:1093:VAL:HG12	1.94	0.68
1:A:17:VAL:HG23	1:A:266:CYS:HB3	1.75	0.68
1:B:1145:GLN:HG2	1:D:3464:GLY:CA	2.19	0.68
1:A:19:ILE:HD11	1:A:247:ILE:HD11	1.74	0.68
1:A:335:ILE:HB	2:A:709:MLG:CL07	2.29	0.68
1:A:408:THR:HG22	1:A:436:GLU:OE1	1.94	0.68
1:A:457:ARG:HD2	1:A:471:ILE:O	1.94	0.68
1:C:2250:THR:HG23	1:C:2285:PRO:HG3	1.76	0.68
1:B:1260:ASN:O	1:B:1261:HIS:HB2	1.94	0.68
1:A:352:PHE:HB3	1:A:354:LEU:HD21	1.75	0.68
1:D:3352:PHE:HB3	1:D:3354:LEU:HD21	1.76	0.68
1:B:1116:TRP:HE3	1:B:1116:TRP:HA	1.60	0.67
1:C:2019:ILE:HD11	1:C:2247:ILE:HD11	1.75	0.67
1:A:116:TRP:HA	1:A:116:TRP:HE3	1.59	0.67
1:A:469:LYS:HD3	1:A:469:LYS:C	2.14	0.67
1:D:3116:TRP:CE3	1:D:3116:TRP:HA	2.29	0.67
1:C:2514:LEU:O	1:C:2518:LEU:HG	1.95	0.67
1:A:284:LYS:CB	1:A:285:PRO:HD3	2.23	0.67
1:A:489:THR:HB	1:A:492:GLU:HG3	1.76	0.67
1:D:3116:TRP:HE3	1:D:3116:TRP:HA	1.59	0.67
1:A:300:MET:H	1:B:1296:GLN:NE2	1.92	0.67
1:B:1156:THR:HG21	1:B:1187:HIS:HA	1.75	0.67
1:D:3156:THR:CG2	1:D:3158:LYS:H	2.07	0.67
1:D:3226:VAL:O	1:D:3230:ILE:HG22	1.95	0.67
1:C:2469:LYS:HD3	1:C:2469:LYS:C	2.15	0.67
1:D:3469:LYS:C	1:D:3469:LYS:HD3	2.14	0.67
1:B:1116:TRP:CE3	1:B:1116:TRP:HA	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:LEU:HD12	1:B:1287:LEU:H	1.59	0.66
1:D:3489:THR:HB	1:D:3492:GLU:HG3	1.76	0.66
1:C:2489:THR:HB	1:C:2492:GLU:HG3	1.77	0.66
1:D:3407:TYR:CZ	2:D:3709:MLG:H142	2.29	0.66
1:C:2116:TRP:CE3	1:C:2116:TRP:HA	2.29	0.66
1:C:2287:LEU:H	1:C:2287:LEU:HD12	1.59	0.66
1:C:2408:THR:HG22	1:C:2436:GLU:OE1	1.94	0.66
1:A:93:VAL:O	1:A:93:VAL:HG12	1.95	0.66
1:B:1242:SER:CA	1:B:1260:ASN:HD21	2.08	0.66
1:C:2093:VAL:O	1:C:2093:VAL:HG12	1.95	0.66
1:C:2391:HIS:CE1	1:C:2393:GLU:HG2	2.31	0.66
1:C:2457:ARG:HD2	1:C:2471:ILE:O	1.96	0.66
1:D:3408:THR:HG22	1:D:3436:GLU:OE1	1.95	0.66
1:B:1391:HIS:CE1	1:B:1393:GLU:HG2	2.30	0.66
1:D:3019:ILE:HG12	1:D:3244:VAL:HG21	1.76	0.66
1:A:391:HIS:CE1	1:A:393:GLU:HG2	2.31	0.66
1:B:1156:THR:CG2	1:B:1158:LYS:H	2.08	0.66
1:B:1408:THR:HG22	1:B:1436:GLU:OE1	1.96	0.66
1:A:289:PRO:HG3	1:B:1399:GLU:HG2	1.77	0.66
1:B:1017:VAL:HG23	1:B:1266:CYS:HB3	1.76	0.66
1:D:3250:THR:HG23	1:D:3285:PRO:HG3	1.76	0.66
1:C:2116:TRP:HE3	1:C:2116:TRP:HA	1.60	0.66
1:A:242:SER:CA	1:A:260:ASN:HD21	2.08	0.66
1:C:2226:VAL:O	1:C:2230:ILE:HG22	1.97	0.65
1:A:260:ASN:O	1:A:261:HIS:HB2	1.96	0.65
1:B:1250:THR:HG23	1:B:1285:PRO:HG3	1.77	0.65
1:B:1489:THR:HB	1:B:1492:GLU:HG3	1.76	0.65
1:D:3030:LYS:HB2	1:D:3230:ILE:HD11	1.79	0.65
1:C:2278:THR:HG21	1:C:2295:ILE:HD13	1.78	0.65
1:D:3278:THR:HG21	1:D:3295:ILE:HD13	1.79	0.65
1:A:30:LYS:HB2	1:A:230:ILE:HD11	1.77	0.65
1:D:3287:LEU:H	1:D:3287:LEU:HD12	1.59	0.65
1:D:3408:THR:HG21	1:D:3443:GLY:HA2	1.79	0.65
1:A:287:LEU:H	1:A:287:LEU:HD12	1.61	0.65
1:C:2260:ASN:O	1:C:2261:HIS:HB2	1.95	0.65
1:D:3019:ILE:HD11	1:D:3247:ILE:HD11	1.78	0.64
1:D:3156:THR:HG21	1:D:3187:HIS:HA	1.79	0.64
1:D:3242:SER:CA	1:D:3260:ASN:HD21	2.08	0.64
1:D:3017:VAL:HG23	1:D:3266:CYS:HB3	1.79	0.64
1:D:3260:ASN:O	1:D:3261:HIS:HB2	1.96	0.64
1:D:3391:HIS:CE1	1:D:3393:GLU:HG2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2030:LYS:HB2	1:C:2230:ILE:HD11	1.79	0.64
1:B:1408:THR:HG21	1:B:1443:GLY:HA2	1.80	0.64
1:D:3156:THR:HB	1:D:3159:ASP:OD1	1.97	0.64
1:C:2156:THR:HB	1:C:2159:ASP:OD1	1.97	0.64
1:B:1156:THR:HB	1:B:1159:ASP:OD1	1.98	0.64
1:A:284:LYS:HB3	1:A:285:PRO:CD	2.22	0.64
1:D:3457:ARG:HD2	1:D:3471:ILE:O	1.98	0.64
1:B:1013:MET:HG2	1:B:1265:GLU:HB2	1.79	0.64
1:C:2185:GLU:OE2	1:C:2356:ARG:HG2	1.98	0.64
1:B:1143:PRO:HG3	1:B:1196:TRP:CD1	2.32	0.63
1:B:1284:LYS:CB	1:B:1285:PRO:HD3	2.26	0.63
1:C:2242:SER:CA	1:C:2260:ASN:HD21	2.11	0.63
1:C:2408:THR:HG21	1:C:2443:GLY:HA2	1.78	0.63
1:B:1248:ASP:HA	1:B:1284:LYS:HB2	1.79	0.63
1:A:156:THR:HB	1:A:159:ASP:OD1	1.98	0.63
1:B:1014:PHE:CD1	1:B:1040:LEU:HB2	2.33	0.63
1:B:1284:LYS:HB3	1:B:1285:PRO:CD	2.25	0.63
1:A:408:THR:HG21	1:A:443:GLY:HA2	1.80	0.63
1:A:14:PHE:CD1	1:A:40:LEU:HB2	2.34	0.63
1:D:3284:LYS:HB3	1:D:3285:PRO:CD	2.22	0.63
1:A:156:THR:HG21	1:A:187:HIS:HA	1.80	0.63
1:A:519:TYR:HD2	1:A:520:LYS:CG	2.12	0.63
1:D:3248:ASP:HA	1:D:3284:LYS:HB2	1.81	0.63
1:B:1030:LYS:HB2	1:B:1230:ILE:HD11	1.81	0.63
1:B:1505:THR:O	1:B:1505:THR:HG22	1.99	0.62
1:B:1278:THR:HG21	1:B:1295:ILE:HD13	1.80	0.62
1:D:3284:LYS:CB	1:D:3285:PRO:HD3	2.25	0.62
1:C:2156:THR:HG21	1:C:2187:HIS:HA	1.79	0.62
1:A:293:GLN:HG2	1:A:419:TYR:CZ	2.35	0.62
1:C:2407:TYR:CZ	2:C:2709:MLG:H142	2.35	0.62
1:C:2143:PRO:HG3	1:C:2196:TRP:CD1	2.35	0.62
1:A:143:PRO:HG3	1:A:196:TRP:CD1	2.35	0.62
1:A:248:ASP:HB3	1:A:255:ILE:HB	1.82	0.62
1:C:2182:VAL:HG12	1:C:2182:VAL:O	2.00	0.62
1:D:3013:MET:HG2	1:D:3265:GLU:HB2	1.82	0.62
1:A:101:VAL:O	1:A:103:GLY:N	2.34	0.61
1:B:1049:GLY:O	1:B:1052:THR:HG22	1.99	0.61
1:B:1247:ILE:HG21	1:B:1430:ILE:HD11	1.81	0.61
1:A:247:ILE:HG21	1:A:430:ILE:HD11	1.80	0.61
1:D:3432:PHE:O	1:D:3454:ARG:NH2	2.34	0.61
1:C:2210:VAL:CG1	1:C:2211:THR:N	2.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2293:GLN:HG2	1:C:2419:TYR:CZ	2.36	0.61
1:B:1293:GLN:HG2	1:B:1419:TYR:CZ	2.36	0.61
1:C:2019:ILE:HG12	1:C:2244:VAL:HG21	1.83	0.61
1:D:3014:PHE:CD1	1:D:3040:LEU:HB2	2.36	0.61
1:A:291:ARG:O	1:A:295:ILE:HG13	2.01	0.61
1:A:296:GLN:HE22	1:B:1300:MET:HB2	1.64	0.61
1:B:1019:ILE:HD11	1:B:1247:ILE:HD11	1.83	0.61
1:C:2284:LYS:HB3	1:C:2285:PRO:CD	2.23	0.61
1:B:1019:ILE:HG12	1:B:1244:VAL:HG21	1.81	0.61
1:B:1248:ASP:HA	1:B:1284:LYS:CB	2.30	0.61
1:D:3469:LYS:HD3	1:D:3470:ASP:N	2.16	0.60
1:B:1242:SER:CB	1:B:1260:ASN:HD21	2.14	0.60
1:C:2013:MET:HG2	1:C:2265:GLU:HB2	1.82	0.60
1:D:3242:SER:CB	1:D:3260:ASN:HD21	2.14	0.60
1:D:3143:PRO:HG3	1:D:3196:TRP:CD1	2.37	0.60
1:C:2248:ASP:HA	1:C:2284:LYS:HB2	1.81	0.60
1:C:2399:GLU:HG2	1:D:3289:PRO:HG3	1.83	0.60
1:D:3101:VAL:O	1:D:3103:GLY:N	2.34	0.60
1:A:13:MET:HG2	1:A:265:GLU:HB2	1.83	0.60
1:D:3300:MET:HE1	1:D:3409:ALA:HB2	1.83	0.60
1:A:248:ASP:HA	1:A:284:LYS:HB2	1.82	0.60
1:A:293:GLN:O	1:A:296:GLN:HG2	2.01	0.60
1:C:2101:VAL:O	1:C:2103:GLY:N	2.35	0.60
1:A:19:ILE:HG12	1:A:244:VAL:HG21	1.84	0.60
1:D:3185:GLU:OE2	1:D:3356:ARG:HG2	2.01	0.60
1:D:3293:GLN:O	1:D:3296:GLN:HG2	2.02	0.60
1:A:209:SER:O	1:A:213:GLY:HA3	2.01	0.60
1:C:2284:LYS:CB	1:C:2285:PRO:HD3	2.25	0.59
1:D:3182:VAL:O	1:D:3182:VAL:HG12	2.02	0.59
1:D:3293:GLN:HG2	1:D:3419:TYR:CZ	2.36	0.59
1:A:49:GLY:O	1:A:52:THR:HG22	2.02	0.59
1:C:2166:TRP:CE2	1:C:2499:PRO:HG3	2.37	0.59
1:C:2248:ASP:HA	1:C:2284:LYS:CB	2.32	0.59
1:D:3248:ASP:HA	1:D:3284:LYS:CB	2.32	0.59
1:D:3166:TRP:CE2	1:D:3499:PRO:HG3	2.38	0.59
1:B:1185:GLU:OE2	1:B:1356:ARG:HG2	2.02	0.59
1:C:2077:ILE:H	1:C:2446:GLU:HG2	1.67	0.59
1:A:469:LYS:HD3	1:A:470:ASP:N	2.16	0.59
1:C:2408:THR:HG22	1:C:2436:GLU:CD	2.22	0.59
1:B:1293:GLN:O	1:B:1296:GLN:HG2	2.01	0.59
1:C:2469:LYS:HD3	1:C:2470:ASP:N	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3049:GLY:O	1:D:3052:THR:HG22	2.01	0.59
1:B:1291:ARG:O	1:B:1295:ILE:HG13	2.02	0.59
1:C:2247:ILE:HG21	1:C:2430:ILE:HD11	1.84	0.59
1:C:2353:ILE:CG2	1:C:2361:LEU:HD12	2.33	0.59
1:C:2489:THR:HG22	1:C:2491:LEU:N	2.18	0.59
1:A:299:PRO:O	1:A:409:ALA:HA	2.03	0.59
1:B:1407:TYR:CZ	2:B:1709:MLG:H142	2.37	0.59
1:A:489:THR:HG22	1:A:491:LEU:N	2.17	0.59
1:B:1469:LYS:HD3	1:B:1470:ASP:N	2.17	0.59
1:C:2293:GLN:O	1:C:2296:GLN:HG2	2.02	0.59
1:C:2471:ILE:HG23	1:C:2472:TRP:CD1	2.38	0.59
1:D:3193:TRP:CG	1:D:3411:PHE:HB2	2.37	0.59
1:D:3489:THR:HG22	1:D:3491:LEU:N	2.18	0.59
1:A:185:GLU:OE2	1:A:356:ARG:HG2	2.03	0.59
1:C:2458:GLU:CA	1:C:2471:ILE:HD11	2.20	0.59
1:D:3247:ILE:HG21	1:D:3430:ILE:HD11	1.84	0.59
1:A:432:PHE:O	1:A:454:ARG:NH2	2.37	0.58
1:B:1101:VAL:O	1:B:1103:GLY:N	2.36	0.58
1:B:1408:THR:HG22	1:B:1436:GLU:CD	2.24	0.58
1:A:408:THR:HG22	1:A:436:GLU:CD	2.24	0.58
1:A:407:TYR:CZ	2:A:709:MLG:H142	2.39	0.58
1:B:1335:ILE:HB	2:B:1709:MLG:CL07	2.41	0.58
1:A:248:ASP:HA	1:A:284:LYS:CB	2.33	0.58
1:C:2014:PHE:CD1	1:C:2040:LEU:HB2	2.38	0.58
1:C:2049:GLY:O	1:C:2052:THR:HG22	2.04	0.58
1:C:2299:PRO:O	1:C:2409:ALA:HA	2.03	0.58
1:D:3353:ILE:HG22	1:D:3358:ALA:HA	1.85	0.58
1:C:2242:SER:CB	1:C:2260:ASN:HD21	2.17	0.58
1:D:3180:ILE:HA	1:D:3354:LEU:CD1	2.34	0.58
1:C:2291:ARG:O	1:C:2295:ILE:HG13	2.03	0.57
1:D:3077:ILE:H	1:D:3446:GLU:HG2	1.69	0.57
1:B:1424:ARG:HH11	1:B:1424:ARG:CB	2.16	0.57
1:A:424:ARG:CB	1:A:424:ARG:HH11	2.18	0.57
1:B:1432:PHE:O	1:B:1454:ARG:NH2	2.38	0.57
1:D:3095:GLU:HB2	1:D:3321:CYS:N	2.19	0.57
1:B:1166:TRP:CE2	1:B:1499:PRO:HG3	2.40	0.57
1:C:2193:TRP:CG	1:C:2411:PHE:HB2	2.39	0.57
1:D:3424:ARG:CB	1:D:3424:ARG:HH11	2.17	0.57
1:A:166:TRP:CE2	1:A:499:PRO:HG3	2.40	0.57
1:B:1077:ILE:H	1:B:1446:GLU:HG2	1.70	0.57
1:B:1051:ARG:HG2	1:B:1406:CYS:SG	2.45	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:HG2	1:B:1289:PRO:HG3	1.84	0.57
1:A:156:THR:HG23	1:A:187:HIS:HA	1.86	0.57
1:A:242:SER:CB	1:A:260:ASN:HD21	2.17	0.57
1:D:3156:THR:HG23	1:D:3187:HIS:HA	1.87	0.57
1:D:3291:ARG:O	1:D:3295:ILE:HG13	2.04	0.57
1:D:3408:THR:HG22	1:D:3436:GLU:CD	2.24	0.57
1:A:246:TYR:HB2	1:B:1259:LEU:HD11	1.87	0.57
1:B:1209:SER:O	1:B:1213:GLY:HA3	2.05	0.57
1:B:1097:LEU:HD23	1:B:1321:CYS:SG	2.45	0.57
1:D:3074:GLN:O	1:D:3077:ILE:HG22	2.04	0.57
1:D:3299:PRO:O	1:D:3409:ALA:HA	2.05	0.57
1:D:3471:ILE:HG23	1:D:3472:TRP:CD1	2.39	0.57
1:B:1193:TRP:CG	1:B:1411:PHE:HB2	2.40	0.56
1:C:2113:PRO:HG3	1:C:2325:ILE:HD12	1.87	0.56
1:D:3209:SER:O	1:D:3213:GLY:HA3	2.04	0.56
1:A:77:ILE:H	1:A:446:GLU:HG2	1.70	0.56
1:C:2180:ILE:HA	1:C:2354:LEU:CD1	2.35	0.56
1:B:1471:ILE:HG23	1:B:1472:TRP:CD1	2.40	0.56
1:B:1095:GLU:HB2	1:B:1321:CYS:N	2.21	0.56
1:C:2182:VAL:CG1	1:C:2182:VAL:O	2.52	0.56
1:C:2248:ASP:HB3	1:C:2255:ILE:HB	1.87	0.56
1:C:2432:PHE:O	1:C:2454:ARG:NH2	2.38	0.56
1:D:3097:LEU:HD22	1:D:3323:CYS:HB3	1.87	0.56
1:A:278:THR:CG2	1:A:295:ILE:HD13	2.35	0.56
1:A:300:MET:HB2	1:B:1296:GLN:HE22	1.70	0.56
1:B:1182:VAL:O	1:B:1182:VAL:HG12	2.04	0.56
1:C:2017:VAL:HG23	1:C:2266:CYS:CB	2.35	0.56
1:C:2051:ARG:HG2	1:C:2406:CYS:SG	2.46	0.56
1:A:275:PRO:O	1:A:278:THR:HB	2.05	0.56
1:A:97:LEU:HD22	1:A:323:CYS:HB3	1.88	0.56
1:D:3113:PRO:HG3	1:D:3325:ILE:HD12	1.86	0.56
1:A:51:ARG:HG2	1:A:406:CYS:SG	2.46	0.56
1:B:1489:THR:HG22	1:B:1491:LEU:N	2.19	0.56
1:D:3182:VAL:CG1	1:D:3182:VAL:O	2.54	0.56
1:A:182:VAL:HG12	1:A:182:VAL:O	2.04	0.56
1:B:1180:ILE:HA	1:B:1354:LEU:CD1	2.35	0.56
1:C:2156:THR:HG23	1:C:2187:HIS:HA	1.88	0.56
1:A:333:ILE:HG21	1:A:336:THR:HG22	1.88	0.56
1:C:2095:GLU:HB2	1:C:2321:CYS:N	2.21	0.56
1:A:26:LEU:HB3	1:A:230:ILE:CD1	2.35	0.56
1:A:471:ILE:HG23	1:A:472:TRP:CD1	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:ARG:HG2	1:B:1076:ARG:HH11	1.71	0.55
1:B:1353:ILE:HG22	1:B:1358:ALA:HA	1.86	0.55
1:B:1193:TRP:CZ2	1:B:1410:TYR:HA	2.42	0.55
1:A:276:ILE:HD13	1:A:295:ILE:O	2.06	0.55
1:A:353:ILE:HG22	1:A:358:ALA:HA	1.88	0.55
1:C:2333:ILE:HG21	1:C:2336:THR:HG22	1.88	0.55
1:D:3458:GLU:CA	1:D:3471:ILE:HD11	2.22	0.55
1:A:95:GLU:HB2	1:A:321:CYS:N	2.21	0.55
1:B:1297:ARG:O	1:B:1299:PRO:HD3	2.05	0.55
1:C:2353:ILE:HD13	1:C:2361:LEU:HD13	1.88	0.55
1:D:3333:ILE:HG21	1:D:3336:THR:HG22	1.87	0.55
1:D:3353:ILE:CG2	1:D:3361:LEU:HD12	2.36	0.55
1:A:17:VAL:HG23	1:A:266:CYS:CB	2.36	0.55
1:C:2209:SER:O	1:C:2213:GLY:HA3	2.05	0.55
1:A:160:LEU:O	1:A:164:ILE:HG12	2.07	0.55
1:B:1299:PRO:O	1:B:1409:ALA:HA	2.06	0.55
1:A:193:TRP:CG	1:A:411:PHE:HB2	2.41	0.55
1:B:1242:SER:HA	1:B:1260:ASN:ND2	2.21	0.55
1:B:1275:PRO:O	1:B:1278:THR:HB	2.07	0.55
1:C:2127:LEU:HG	1:C:2131:MET:HE2	1.88	0.55
1:D:3097:LEU:HD23	1:D:3321:CYS:SG	2.47	0.55
1:B:1113:PRO:HG3	1:B:1325:ILE:HD12	1.89	0.55
1:C:2248:ASP:OD2	1:C:2284:LYS:HG2	2.07	0.55
1:C:2014:PHE:O	1:C:2266:CYS:HA	2.06	0.55
1:C:2300:MET:HB2	1:D:3296:GLN:HE22	1.72	0.55
1:D:3127:LEU:HG	1:D:3131:MET:HE2	1.89	0.55
1:B:1017:VAL:HG23	1:B:1266:CYS:CB	2.36	0.55
1:B:1297:ARG:C	1:B:1299:PRO:HD3	2.28	0.55
1:B:1309:TYR:CD2	1:B:1348:ALA:HB2	2.42	0.55
1:B:1335:ILE:O	1:B:1335:ILE:HD12	2.07	0.55
1:D:3018:VAL:HG22	1:D:3270:ILE:HB	1.89	0.55
1:A:353:ILE:CG2	1:A:361:LEU:HD12	2.37	0.54
1:A:406:CYS:O	1:A:408:THR:N	2.40	0.54
1:C:2124:TYR:O	1:C:2127:LEU:HB3	2.07	0.54
1:C:2335:ILE:O	1:C:2335:ILE:HD12	2.07	0.54
1:C:2296:GLN:HE22	1:D:3300:MET:HB2	1.72	0.54
1:A:79:ARG:HD3	1:A:475:GLU:OE2	2.07	0.54
1:B:1074:GLN:O	1:B:1077:ILE:HG22	2.07	0.54
1:B:1182:VAL:O	1:B:1182:VAL:CG1	2.55	0.54
1:D:3248:ASP:HB3	1:D:3255:ILE:HB	1.89	0.54
1:D:3333:ILE:HG21	1:D:3336:THR:CG2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:O	1:A:127:LEU:HB3	2.07	0.54
1:B:1068:ALA:HB1	1:B:1218:LYS:HE3	1.88	0.54
1:B:1097:LEU:HD22	1:B:1323:CYS:HB3	1.89	0.54
1:B:1248:ASP:HB3	1:B:1255:ILE:HB	1.89	0.54
1:C:2160:LEU:O	1:C:2164:ILE:HG12	2.07	0.54
1:C:2074:GLN:O	1:C:2077:ILE:HG22	2.07	0.54
1:D:3242:SER:HA	1:D:3260:ASN:ND2	2.21	0.54
1:A:305:LYS:HG3	1:A:352:PHE:CE2	2.42	0.54
1:A:97:LEU:HD23	1:A:321:CYS:SG	2.48	0.54
1:A:449:VAL:O	1:A:450:GLU:C	2.46	0.54
1:D:3024:SER:HB2	1:D:3448:ALA:HB1	1.89	0.54
1:B:1276:ILE:HD13	1:B:1295:ILE:O	2.08	0.54
1:B:1278:THR:CG2	1:B:1295:ILE:HD13	2.38	0.54
1:C:2278:THR:CG2	1:C:2295:ILE:HD13	2.37	0.54
1:C:2289:PRO:HG3	1:D:3399:GLU:HG2	1.88	0.54
1:A:309:TYR:CD2	1:A:348:ALA:HB2	2.43	0.54
1:C:2424:ARG:HH11	1:C:2424:ARG:CB	2.19	0.54
1:C:2259:LEU:HD11	1:D:3246:TYR:HB2	1.89	0.54
1:D:3291:ARG:HE	1:D:3422:VAL:HG12	1.73	0.54
1:C:2097:LEU:HD22	1:C:2323:CYS:HB3	1.89	0.54
1:C:2326:ILE:CD1	1:C:2376:LEU:HD21	2.38	0.54
1:D:3336:THR:HG21	1:D:3377:TYR:HE1	1.73	0.54
1:B:1156:THR:HG23	1:B:1187:HIS:HA	1.87	0.54
1:A:297:ARG:O	1:A:299:PRO:HD3	2.08	0.53
1:B:1300:MET:HE1	1:B:1409:ALA:HB2	1.88	0.53
1:C:2353:ILE:HG23	1:C:2361:LEU:HD12	1.90	0.53
1:A:68:ALA:HB1	1:A:218:LYS:HE3	1.90	0.53
1:D:3160:LEU:O	1:D:3164:ILE:HG12	2.08	0.53
1:D:3305:LYS:HG3	1:D:3352:PHE:CE2	2.43	0.53
1:D:3309:TYR:CD2	1:D:3348:ALA:HB2	2.43	0.53
1:A:242:SER:HA	1:A:260:ASN:ND2	2.20	0.53
1:B:1332:PRO:HB3	1:B:1361:LEU:CD1	2.38	0.53
1:C:2026:LEU:HB3	1:C:2230:ILE:CD1	2.36	0.53
1:D:3193:TRP:CZ2	1:D:3410:TYR:HA	2.43	0.53
1:A:291:ARG:HE	1:A:422:VAL:HG12	1.73	0.53
1:D:3275:PRO:O	1:D:3278:THR:HB	2.09	0.53
1:A:323:CYS:SG	2:A:709:MLG:CL08	3.04	0.53
1:B:1406:CYS:O	1:B:1408:THR:N	2.42	0.53
1:C:2309:TYR:CD2	1:C:2348:ALA:HB2	2.44	0.53
1:D:3310:TYR:O	1:D:3347:PRO:HG2	2.09	0.53
1:A:248:ASP:OD2	1:A:284:LYS:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1305:LYS:HG3	1:B:1352:PHE:CE2	2.43	0.53
1:B:1353:ILE:CG2	1:B:1361:LEU:HD12	2.39	0.53
1:C:2310:TYR:O	1:C:2347:PRO:HG2	2.09	0.53
1:C:2501:LEU:HA	1:C:2504:ILE:HD12	1.91	0.53
1:A:180:ILE:HA	1:A:354:LEU:CD1	2.39	0.53
1:B:1099:GLN:HG2	1:B:1101:VAL:HG23	1.91	0.53
1:B:1127:LEU:HG	1:B:1131:MET:HE2	1.90	0.53
1:C:2097:LEU:HD23	1:C:2321:CYS:SG	2.49	0.53
1:A:336:THR:HG21	1:A:377:TYR:HE1	1.74	0.53
1:B:1248:ASP:OD2	1:B:1284:LYS:HG2	2.09	0.53
1:C:2079:ARG:HD3	1:C:2475:GLU:OE2	2.09	0.53
1:A:182:VAL:O	1:A:182:VAL:CG1	2.56	0.52
1:B:1079:ARG:HD3	1:B:1475:GLU:OE2	2.09	0.52
1:B:1210:VAL:O	1:B:1216:GLU:HA	2.09	0.52
1:C:2068:ALA:HB1	1:C:2218:LYS:HE3	1.90	0.52
1:C:2275:PRO:O	1:C:2278:THR:HB	2.08	0.52
1:C:2406:CYS:O	1:C:2408:THR:N	2.42	0.52
1:C:2454:ARG:HG3	1:C:2454:ARG:HH11	1.74	0.52
1:B:1458:GLU:CA	1:B:1471:ILE:HD11	2.23	0.52
1:D:3099:GLN:HG2	1:D:3101:VAL:HG23	1.91	0.52
1:D:3278:THR:CG2	1:D:3295:ILE:HD13	2.38	0.52
1:A:113:PRO:HG3	1:A:325:ILE:HD12	1.90	0.52
1:A:14:PHE:O	1:A:266:CYS:HA	2.10	0.52
1:D:3197:TYR:HA	1:D:3200:GLN:HG2	1.91	0.52
1:A:18:VAL:HG22	1:A:270:ILE:HB	1.91	0.52
1:A:454:ARG:HH11	1:A:454:ARG:HG3	1.74	0.52
1:B:1160:LEU:O	1:B:1164:ILE:HG12	2.10	0.52
1:D:3332:PRO:HB3	1:D:3361:LEU:CD1	2.39	0.52
1:D:3365:HIS:ND1	1:D:3366:LYS:N	2.58	0.52
1:B:1332:PRO:HB3	1:B:1361:LEU:HD11	1.92	0.52
1:C:2297:ARG:C	1:C:2299:PRO:HD3	2.30	0.52
1:D:3051:ARG:HG2	1:D:3406:CYS:SG	2.50	0.52
1:B:1018:VAL:HG22	1:B:1270:ILE:HB	1.90	0.52
1:C:2076:ARG:HH11	1:C:2076:ARG:HG2	1.75	0.52
1:C:2210:VAL:O	1:C:2216:GLU:HA	2.10	0.52
1:C:2353:ILE:HD13	1:C:2361:LEU:CD1	2.40	0.52
1:D:3077:ILE:HG23	1:D:3078:LEU:N	2.25	0.52
1:D:3276:ILE:HD13	1:D:3295:ILE:O	2.09	0.52
1:A:210:VAL:CG1	1:A:211:THR:N	2.72	0.52
1:A:76:ARG:HH11	1:A:76:ARG:HG2	1.74	0.52
1:C:2115:VAL:HG23	1:C:2121:TYR:HD1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TYR:O	1:A:347:PRO:HG2	2.10	0.52
1:C:2333:ILE:HG21	1:C:2336:THR:CG2	2.40	0.52
1:A:297:ARG:C	1:A:299:PRO:HD3	2.30	0.52
1:B:1340:THR:HG23	1:B:1347:PRO:HA	1.90	0.52
1:B:1350:MET:C	1:B:1350:MET:SD	2.88	0.52
1:C:2353:ILE:HG22	1:C:2358:ALA:HA	1.92	0.52
1:C:2300:MET:HE1	1:C:2409:ALA:HB2	1.91	0.52
1:C:2291:ARG:HE	1:C:2422:VAL:HG12	1.74	0.52
1:A:513:LEU:O	1:A:517:VAL:HG23	2.10	0.51
1:A:259:LEU:HD11	1:B:1246:TYR:HB2	1.91	0.51
1:B:1024:SER:HB2	1:B:1448:ALA:HB1	1.91	0.51
1:A:193:TRP:CZ2	1:A:410:TYR:HA	2.45	0.51
1:A:210:VAL:O	1:A:216:GLU:HA	2.10	0.51
1:A:39:VAL:O	1:A:237:LYS:HD2	2.09	0.51
1:A:74:GLN:O	1:A:77:ILE:HG22	2.10	0.51
1:C:2336:THR:HG21	1:C:2377:TYR:HE1	1.76	0.51
1:D:3336:THR:HG21	1:D:3377:TYR:CE1	2.46	0.51
1:A:115:VAL:HG23	1:A:121:TYR:HD1	1.76	0.51
1:A:154:LYS:HA	1:B:1187:HIS:CD2	2.45	0.51
1:C:2365:HIS:ND1	1:C:2366:LYS:N	2.59	0.51
1:D:3076:ARG:HH11	1:D:3076:ARG:HG2	1.76	0.51
1:B:1115:VAL:HG23	1:B:1121:TYR:HD1	1.76	0.51
1:A:297:ARG:NH2	1:B:1300:MET:O	2.43	0.51
1:D:3254:ILE:O	1:D:3265:GLU:HA	2.11	0.51
1:D:3340:THR:HG23	1:D:3347:PRO:HA	1.92	0.51
1:A:335:ILE:HD12	1:A:335:ILE:O	2.10	0.51
1:D:3124:TYR:O	1:D:3127:LEU:HB3	2.11	0.51
1:C:2018:VAL:HG22	1:C:2270:ILE:HB	1.93	0.51
1:C:2310:TYR:CE2	1:C:2386:ALA:HA	2.46	0.51
1:D:3353:ILE:HG23	1:D:3361:LEU:HD12	1.92	0.51
1:C:2197:TYR:HA	1:C:2200:GLN:HG2	1.91	0.51
1:C:2276:ILE:HD13	1:C:2295:ILE:O	2.10	0.51
1:C:2350:MET:C	1:C:2350:MET:SD	2.88	0.51
1:D:3115:VAL:HG23	1:D:3121:TYR:HD1	1.75	0.51
1:C:2507:VAL:O	1:C:2511:VAL:HG23	2.10	0.51
1:C:2332:PRO:HB3	1:C:2361:LEU:HD11	1.93	0.51
1:D:3017:VAL:HG23	1:D:3266:CYS:CB	2.41	0.51
1:D:3026:LEU:HB3	1:D:3230:ILE:CD1	2.39	0.51
1:A:310:TYR:CE2	1:A:386:ALA:HA	2.46	0.51
1:A:336:THR:HG21	1:A:377:TYR:CE1	2.45	0.51
1:B:1310:TYR:O	1:B:1347:PRO:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2332:PRO:HB3	1:C:2361:LEU:CD1	2.41	0.51
1:D:3079:ARG:HD3	1:D:3475:GLU:OE2	2.10	0.51
1:B:1365:HIS:ND1	1:B:1366:LYS:N	2.59	0.50
1:D:3068:ALA:HB1	1:D:3218:LYS:HE3	1.93	0.50
1:A:197:TYR:HA	1:A:200:GLN:HG2	1.93	0.50
1:A:254:ILE:O	1:A:265:GLU:HA	2.10	0.50
1:B:1336:THR:HG21	1:B:1377:TYR:CE1	2.47	0.50
1:C:2039:VAL:O	1:C:2237:LYS:HD2	2.11	0.50
1:D:3014:PHE:O	1:D:3266:CYS:HA	2.10	0.50
1:B:1336:THR:HG21	1:B:1377:TYR:HE1	1.77	0.50
1:C:2122:LEU:HD22	1:C:2496:PRO:O	2.11	0.50
1:A:340:THR:HG23	1:A:347:PRO:HA	1.94	0.50
1:B:1076:ARG:HB2	1:B:1446:GLU:HG2	1.93	0.50
1:C:2340:THR:HG23	1:C:2347:PRO:HA	1.93	0.50
1:D:3406:CYS:O	1:D:3408:THR:N	2.44	0.50
1:A:285:PRO:O	1:A:286:GLU:C	2.50	0.50
1:B:1291:ARG:HE	1:B:1422:VAL:HG12	1.75	0.50
1:C:2093:VAL:HG21	1:C:2210:VAL:HG11	1.94	0.50
1:D:3310:TYR:CE2	1:D:3386:ALA:HA	2.46	0.50
1:D:3210:VAL:HG23	1:D:3215:GLN:HB2	1.94	0.50
1:D:3335:ILE:O	1:D:3335:ILE:HD12	2.11	0.50
1:A:127:LEU:HG	1:A:131:MET:HE2	1.94	0.50
1:A:458:GLU:CA	1:A:471:ILE:HD11	2.22	0.50
1:B:1039:VAL:O	1:B:1237:LYS:HD2	2.11	0.50
1:C:2336:THR:HG21	1:C:2377:TYR:CE1	2.47	0.50
1:D:3076:ARG:HB2	1:D:3446:GLU:HG2	1.94	0.50
1:D:3454:ARG:HG3	1:D:3454:ARG:HH11	1.77	0.50
1:A:340:THR:HG22	1:A:341:LYS:N	2.27	0.50
1:A:365:HIS:ND1	1:A:366:LYS:N	2.60	0.50
1:B:1469:LYS:C	1:B:1471:ILE:H	2.15	0.50
1:C:2254:ILE:O	1:C:2265:GLU:HA	2.12	0.50
1:A:332:PRO:HB3	1:A:361:LEU:CD1	2.41	0.50
1:B:1210:VAL:CG1	1:B:1211:THR:N	2.75	0.50
1:A:350:MET:SD	1:A:350:MET:C	2.90	0.49
1:B:1112:PHE:HB3	1:B:1124:TYR:OH	2.12	0.49
1:B:1124:TYR:O	1:B:1127:LEU:HB3	2.11	0.49
1:C:2242:SER:HA	1:C:2260:ASN:ND2	2.23	0.49
1:A:510:SER:O	1:A:514:LEU:HB2	2.12	0.49
1:B:1420:GLY:O	1:B:1422:VAL:N	2.45	0.49
1:C:2099:GLN:HG2	1:C:2101:VAL:HG23	1.93	0.49
1:D:3326:ILE:CD1	1:D:3376:LEU:HD21	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3332:PRO:HB3	1:D:3361:LEU:HD11	1.94	0.49
1:A:326:ILE:CD1	1:A:376:LEU:HD21	2.42	0.49
1:A:353:ILE:HG23	1:A:361:LEU:HD12	1.93	0.49
1:B:1326:ILE:CD1	1:B:1376:LEU:HD21	2.41	0.49
1:D:3511:VAL:O	1:D:3511:VAL:HG12	2.13	0.49
1:A:101:VAL:O	1:A:102:LYS:C	2.51	0.49
1:A:333:ILE:HG21	1:A:336:THR:CG2	2.42	0.49
1:B:1158:LYS:O	1:B:1159:ASP:C	2.50	0.49
1:B:1014:PHE:O	1:B:1266:CYS:HA	2.13	0.49
1:C:2275:PRO:O	1:C:2295:ILE:HG23	2.12	0.49
1:D:3210:VAL:O	1:D:3216:GLU:HA	2.11	0.49
1:C:2246:TYR:HB2	1:D:3259:LEU:HD11	1.94	0.49
1:A:99:GLN:HG2	1:A:101:VAL:HG23	1.94	0.49
1:D:3469:LYS:C	1:D:3471:ILE:H	2.16	0.49
1:B:1180:ILE:O	1:B:1407:TYR:HE1	1.96	0.49
1:C:2175:TYR:O	1:C:2178:VAL:HB	2.12	0.49
1:D:3112:PHE:HB3	1:D:3124:TYR:OH	2.13	0.49
1:B:1333:ILE:HG21	1:B:1336:THR:HG22	1.95	0.49
1:C:2469:LYS:C	1:C:2471:ILE:H	2.16	0.49
1:D:3420:GLY:O	1:D:3422:VAL:N	2.46	0.49
1:B:1026:LEU:HB3	1:B:1230:ILE:CD1	2.40	0.48
1:A:418:GLN:HE21	1:B:1356:ARG:HA	1.74	0.48
1:C:2112:PHE:HB3	1:C:2124:TYR:OH	2.13	0.48
1:C:2024:SER:HB2	1:C:2448:ALA:HB1	1.95	0.48
1:D:3074:GLN:O	1:D:3446:GLU:HG3	2.13	0.48
1:D:3449:VAL:O	1:D:3450:GLU:C	2.50	0.48
1:D:3127:LEU:HG	1:D:3131:MET:CE	2.44	0.48
1:D:3183:THR:HG23	1:D:3407:TYR:CD1	2.49	0.48
1:A:332:PRO:HB3	1:A:361:LEU:HD11	1.96	0.48
1:C:2284:LYS:CB	1:C:2285:PRO:CD	2.90	0.48
1:C:2500:GLY:O	1:C:2504:ILE:HG13	2.13	0.48
1:D:3314:PHE:HE1	1:D:3381:LEU:HD13	1.78	0.48
1:A:112:PHE:HB3	1:A:124:TYR:OH	2.13	0.48
1:A:505:THR:O	1:A:508:SER:N	2.43	0.48
1:A:76:ARG:HD2	1:A:446:GLU:CD	2.34	0.48
1:D:3297:ARG:O	1:D:3299:PRO:HD3	2.14	0.48
1:D:3350:MET:C	1:D:3350:MET:SD	2.91	0.48
1:D:3388:TYR:CD1	1:D:3388:TYR:N	2.81	0.48
1:A:122:LEU:HD22	1:A:496:PRO:O	2.13	0.48
1:B:1353:ILE:HG23	1:B:1361:LEU:HD12	1.94	0.48
1:A:76:ARG:HB2	1:A:446:GLU:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:ILE:HG23	1:B:1078:LEU:N	2.29	0.48
1:A:280:LYS:HD3	1:B:1279:ALA:O	2.13	0.48
1:B:1285:PRO:O	1:B:1286:GLU:C	2.51	0.48
1:C:2019:ILE:CD1	1:C:2247:ILE:HD11	2.42	0.48
1:C:2091:VAL:HG23	1:C:2216:GLU:O	2.14	0.48
1:C:2303:VAL:HG22	1:C:2304:ILE:N	2.29	0.48
1:C:2449:VAL:O	1:C:2450:GLU:C	2.52	0.48
1:A:77:ILE:HG23	1:A:78:LEU:N	2.28	0.48
1:B:1210:VAL:HG23	1:B:1215:GLN:HB2	1.96	0.48
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.79	0.48
1:B:1310:TYR:CE2	1:B:1386:ALA:HA	2.48	0.48
1:B:1333:ILE:HG21	1:B:1336:THR:CG2	2.44	0.48
1:A:156:THR:CG2	1:A:158:LYS:HB3	2.44	0.48
1:A:275:PRO:O	1:A:295:ILE:HG23	2.14	0.48
1:B:1275:PRO:O	1:B:1295:ILE:HG23	2.14	0.48
1:B:1314:PHE:HE1	1:B:1381:LEU:HD13	1.78	0.48
1:D:3128:TRP:CE3	1:D:3131:MET:HE3	2.49	0.48
1:A:388:TYR:CD1	1:A:388:TYR:N	2.82	0.47
1:C:2101:VAL:O	1:C:2102:LYS:C	2.52	0.47
1:C:2505:THR:C	1:C:2507:VAL:N	2.66	0.47
1:D:3158:LYS:O	1:D:3159:ASP:C	2.52	0.47
1:A:76:ARG:HD2	1:A:446:GLU:OE1	2.14	0.47
1:B:1254:ILE:O	1:B:1265:GLU:HA	2.14	0.47
1:C:2291:ARG:CG	1:C:2291:ARG:HH11	2.27	0.47
1:C:2077:ILE:HG23	1:C:2078:LEU:N	2.29	0.47
1:C:2127:LEU:HG	1:C:2131:MET:CE	2.44	0.47
1:D:3101:VAL:O	1:D:3102:LYS:C	2.52	0.47
1:D:3356:ARG:HH11	1:D:3356:ARG:HG3	1.80	0.47
1:B:1340:THR:HG22	1:B:1341:LYS:N	2.30	0.47
1:C:2297:ARG:O	1:C:2299:PRO:HD3	2.13	0.47
1:A:104:LYS:HB3	1:A:105:THR:H	1.59	0.47
1:A:204:THR:O	1:A:207:ILE:HG22	2.15	0.47
1:B:1014:PHE:N	1:B:1014:PHE:CD2	2.82	0.47
1:B:1014:PHE:CE1	1:B:1040:LEU:HB2	2.48	0.47
1:A:469:LYS:C	1:A:471:ILE:H	2.17	0.47
1:B:1284:LYS:CB	1:B:1285:PRO:CD	2.91	0.47
1:B:1388:TYR:CD1	1:B:1388:TYR:N	2.83	0.47
1:B:1454:ARG:HG3	1:B:1454:ARG:HH11	1.80	0.47
1:C:2210:VAL:HG12	1:C:2211:THR:N	2.30	0.47
1:D:3122:LEU:HD22	1:D:3496:PRO:O	2.14	0.47
1:D:3019:ILE:CD1	1:D:3247:ILE:HD11	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2280:LYS:HD3	1:D:3279:ALA:O	2.15	0.47
1:C:2183:THR:HG23	1:C:2407:TYR:CD1	2.50	0.47
1:A:300:MET:HE1	1:A:409:ALA:HB2	1.93	0.47
1:B:1356:ARG:HG3	1:B:1356:ARG:HH11	1.79	0.47
1:C:2076:ARG:HB2	1:C:2446:GLU:HG2	1.97	0.47
1:D:3039:VAL:O	1:D:3237:LYS:HD2	2.14	0.47
1:A:14:PHE:CD2	1:A:14:PHE:N	2.83	0.47
1:A:293:GLN:HG2	1:A:419:TYR:CE1	2.50	0.47
1:A:353:ILE:HD13	1:A:361:LEU:HD13	1.97	0.47
1:B:1167:THR:HG22	1:B:1169:THR:H	1.80	0.47
1:A:19:ILE:CD1	1:A:247:ILE:HD11	2.43	0.46
1:B:1122:LEU:HD22	1:B:1496:PRO:O	2.15	0.46
1:C:2285:PRO:O	1:C:2286:GLU:C	2.52	0.46
1:C:2305:LYS:HG3	1:C:2352:PHE:CE2	2.50	0.46
1:B:1197:TYR:HA	1:B:1200:GLN:HG2	1.95	0.46
1:B:1204:THR:O	1:B:1207:ILE:HG22	2.15	0.46
1:B:1303:VAL:HG22	1:B:1304:ILE:N	2.31	0.46
1:C:2158:LYS:O	1:C:2159:ASP:C	2.53	0.46
1:D:3193:TRP:O	1:D:3196:TRP:HB3	2.15	0.46
1:A:91:VAL:HG23	1:A:216:GLU:O	2.16	0.46
1:D:3248:ASP:OD2	1:D:3284:LYS:HG2	2.15	0.46
1:D:3297:ARG:C	1:D:3299:PRO:HD3	2.35	0.46
1:D:3353:ILE:HD13	1:D:3361:LEU:HD13	1.98	0.46
1:D:3471:ILE:HG23	1:D:3472:TRP:HD1	1.80	0.46
1:D:3504:ILE:C	1:D:3506:GLY:N	2.68	0.46
1:A:158:LYS:O	1:A:159:ASP:C	2.52	0.46
1:B:1060:VAL:O	1:B:1061:LYS:HB2	2.16	0.46
1:D:3326:ILE:HD13	1:D:3376:LEU:HD11	1.98	0.46
1:C:2156:THR:CG2	1:C:2158:LYS:HB3	2.45	0.46
1:C:2127:LEU:HD13	1:C:2165:CYS:SG	2.55	0.46
1:C:2356:ARG:HH11	1:C:2356:ARG:HG3	1.79	0.46
1:C:2193:TRP:CZ2	1:C:2410:TYR:HA	2.50	0.46
1:D:3026:LEU:HD21	1:D:3048:VAL:CG2	2.45	0.46
1:D:3307:MET:SD	1:D:3307:MET:N	2.89	0.46
1:D:3369:ARG:O	1:D:3373:ILE:HG13	2.16	0.46
1:A:24:SER:HB2	1:A:448:ALA:HB1	1.98	0.46
1:B:1101:VAL:O	1:B:1102:LYS:C	2.53	0.46
1:C:2326:ILE:HD13	1:C:2376:LEU:HD11	1.97	0.46
1:A:89:TYR:O	1:A:217:ARG:HB2	2.16	0.46
1:B:1127:LEU:HG	1:B:1131:MET:CE	2.45	0.46
1:D:3093:VAL:O	1:D:3093:VAL:CG1	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3180:ILE:O	1:D:3407:TYR:HE1	1.98	0.46
1:A:210:VAL:HG23	1:A:215:GLN:HB2	1.98	0.46
1:B:1127:LEU:HD13	1:B:1165:CYS:SG	2.56	0.46
1:D:3451:ALA:O	1:D:3452:GLY:C	2.54	0.46
1:A:128:TRP:CE3	1:A:131:MET:HE3	2.51	0.46
1:A:185:GLU:HB2	1:A:188:GLU:HG3	1.97	0.46
1:B:1156:THR:CG2	1:B:1158:LYS:HB3	2.46	0.46
1:C:2340:THR:HG22	1:C:2341:LYS:N	2.31	0.46
1:D:3014:PHE:CE1	1:D:3040:LEU:HB2	2.51	0.46
1:B:1104:LYS:HB3	1:B:1105:THR:H	1.59	0.45
1:C:2014:PHE:N	1:C:2014:PHE:CD2	2.84	0.45
1:C:2422:VAL:O	1:C:2423:ILE:C	2.55	0.45
1:D:3014:PHE:N	1:D:3014:PHE:CD2	2.84	0.45
1:D:3060:VAL:O	1:D:3061:LYS:HB2	2.16	0.45
1:D:3115:VAL:HG21	1:D:3121:TYR:HA	1.99	0.45
1:C:2161:ILE:HD13	1:C:2174:ALA:CB	2.46	0.45
1:B:1353:ILE:HD13	1:B:1361:LEU:HD13	1.98	0.45
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.29	0.45
1:D:3285:PRO:O	1:D:3286:GLU:C	2.55	0.45
1:D:3303:VAL:HG22	1:D:3304:ILE:N	2.30	0.45
1:D:3420:GLY:C	1:D:3422:VAL:H	2.20	0.45
1:C:2099:GLN:CG	1:C:2101:VAL:HG23	2.47	0.45
1:C:2204:THR:O	1:C:2207:ILE:HG22	2.16	0.45
1:D:3099:GLN:CG	1:D:3101:VAL:HG23	2.46	0.45
1:D:3332:PRO:HD2	1:D:3376:LEU:HD22	1.98	0.45
1:C:2314:PHE:HE1	1:C:2381:LEU:HD13	1.82	0.45
1:D:3291:ARG:CG	1:D:3291:ARG:HH11	2.30	0.45
1:D:3296:GLN:C	1:D:3297:ARG:HG2	2.37	0.45
1:A:303:VAL:HG22	1:A:304:ILE:N	2.32	0.45
1:A:510:SER:O	1:A:514:LEU:CB	2.64	0.45
1:B:1026:LEU:HD21	1:B:1048:VAL:CG2	2.47	0.45
1:B:1183:THR:HG23	1:B:1407:TYR:CD1	2.52	0.45
1:B:1273:ILE:HD11	1:B:1278:THR:HA	1.98	0.45
1:C:2167:THR:HG22	1:C:2169:THR:H	1.81	0.45
1:C:2471:ILE:HG23	1:C:2472:TRP:HD1	1.79	0.45
1:D:3185:GLU:HB2	1:D:3188:GLU:HG3	1.99	0.45
1:D:3340:THR:HG22	1:D:3341:LYS:N	2.32	0.45
1:D:3373:ILE:HG22	1:D:3377:TYR:CE2	2.51	0.45
1:A:127:LEU:HD13	1:A:165:CYS:SG	2.57	0.45
1:A:422:VAL:O	1:A:423:ILE:C	2.54	0.45
1:A:451:ALA:O	1:A:452:GLY:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1331:ALA:HA	1:B:1332:PRO:HD3	1.78	0.45
1:C:2166:TRP:NE1	1:C:2499:PRO:HG3	2.32	0.45
1:C:2340:THR:OG1	1:C:2347:PRO:HA	2.16	0.45
1:A:167:THR:HG22	1:A:169:THR:H	1.81	0.45
1:A:340:THR:OG1	1:A:347:PRO:HA	2.16	0.45
1:B:1115:VAL:HG21	1:B:1121:TYR:HA	1.98	0.45
1:B:1175:TYR:O	1:B:1178:VAL:HB	2.16	0.45
1:C:2420:GLY:O	1:C:2422:VAL:N	2.50	0.45
1:D:3037:ILE:HD12	1:D:3460:LEU:CD2	2.47	0.45
1:D:3291:ARG:HD2	1:D:3422:VAL:HG11	1.98	0.45
1:A:183:THR:HG22	1:A:354:LEU:HD22	1.98	0.45
1:A:331:ALA:HA	1:A:332:PRO:HD3	1.77	0.45
1:A:505:THR:C	1:A:507:VAL:N	2.69	0.45
1:C:2193:TRP:O	1:C:2196:TRP:HB3	2.17	0.45
1:C:2307:MET:SD	1:C:2307:MET:N	2.90	0.44
1:A:332:PRO:HD2	1:A:376:LEU:HD22	1.99	0.44
1:B:1026:LEU:O	1:B:1027:ALA:C	2.56	0.44
1:B:1293:GLN:HG2	1:B:1419:TYR:CE1	2.52	0.44
1:B:1369:ARG:O	1:B:1373:ILE:HG13	2.17	0.44
1:B:1451:ALA:O	1:B:1452:GLY:C	2.53	0.44
1:D:3210:VAL:CG1	1:D:3211:THR:N	2.80	0.44
1:D:3293:GLN:HG2	1:D:3419:TYR:CE1	2.52	0.44
1:B:1096:ARG:HB2	1:B:1319:ASP:O	2.17	0.44
1:B:1019:ILE:CD1	1:B:1247:ILE:HD11	2.46	0.44
1:C:2089:TYR:CD1	1:C:2342:PRO:HG3	2.53	0.44
1:B:1156:THR:HG22	1:B:1158:LYS:HB3	2.00	0.44
1:C:2293:GLN:HG2	1:C:2419:TYR:CE1	2.52	0.44
1:C:2451:ALA:O	1:C:2452:GLY:C	2.54	0.44
1:C:2300:MET:O	1:D:3297:ARG:NH2	2.50	0.44
1:A:175:TYR:O	1:A:178:VAL:HB	2.17	0.44
1:A:337:LEU:HG	2:A:709:MLG:CL07	2.55	0.44
1:A:384:GLN:C	1:A:386:ALA:N	2.71	0.44
1:B:1391:HIS:HE1	1:B:1393:GLU:HG2	1.80	0.44
1:C:2026:LEU:HD21	1:C:2048:VAL:CG2	2.47	0.44
1:C:2388:TYR:CD1	1:C:2388:TYR:N	2.84	0.44
1:D:3115:VAL:O	1:D:3115:VAL:HG23	2.17	0.44
1:D:3204:THR:O	1:D:3207:ILE:HG22	2.17	0.44
1:A:180:ILE:O	1:A:407:TYR:HE1	2.01	0.44
1:B:1076:ARG:HD2	1:B:1446:GLU:CD	2.38	0.44
1:A:279:ALA:O	1:B:1280:LYS:HD3	2.18	0.44
1:B:1420:GLY:C	1:B:1422:VAL:H	2.20	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2296:GLN:C	1:C:2297:ARG:HG2	2.38	0.44
1:C:2353:ILE:HG21	1:C:2361:LEU:HD12	1.98	0.44
1:D:3353:ILE:HD13	1:D:3361:LEU:CD1	2.48	0.44
1:B:1077:ILE:H	1:B:1446:GLU:CG	2.31	0.44
1:C:2115:VAL:HG21	1:C:2121:TYR:HA	2.00	0.44
1:C:2156:THR:HG22	1:C:2158:LYS:HB3	1.99	0.44
1:D:3156:THR:CG2	1:D:3158:LYS:HB3	2.47	0.44
1:A:99:GLN:CG	1:A:101:VAL:HG23	2.48	0.44
1:A:127:LEU:HG	1:A:131:MET:CE	2.48	0.44
1:B:1340:THR:OG1	1:B:1347:PRO:HA	2.18	0.44
1:B:1028:ALA:HB2	1:B:1452:GLY:O	2.18	0.44
1:C:2490:PHE:CE1	1:C:2494:ASN:ND2	2.86	0.44
1:A:460:LEU:HB3	1:A:466:VAL:HG23	2.00	0.44
1:A:516:PHE:O	1:A:519:TYR:HB3	2.18	0.44
1:B:1161:ILE:HD13	1:B:1174:ALA:HB1	1.99	0.44
1:C:2096:ARG:HB2	1:C:2319:ASP:O	2.18	0.44
1:C:2138:ILE:HA	1:C:2139:PRO:HD3	1.88	0.44
1:C:2391:HIS:HE1	1:C:2393:GLU:HG2	1.79	0.44
1:A:156:THR:HG22	1:A:158:LYS:HB3	1.98	0.43
1:A:307:MET:N	1:A:307:MET:SD	2.91	0.43
1:B:1058:GLU:OE1	1:B:1058:GLU:N	2.51	0.43
1:B:1017:VAL:CG2	1:B:1266:CYS:HB3	2.47	0.43
1:C:2093:VAL:HG21	1:C:2210:VAL:CG1	2.47	0.43
1:D:3076:ARG:HD2	1:D:3446:GLU:OE1	2.17	0.43
1:D:3167:THR:HG22	1:D:3169:THR:H	1.83	0.43
1:A:353:ILE:HD13	1:A:361:LEU:CD1	2.48	0.43
1:B:1249:GLN:HE21	1:B:1249:GLN:HB2	1.68	0.43
1:D:3219:PHE:HD1	1:D:3223:SER:HA	1.83	0.43
1:B:1070:VAL:HG11	1:B:1219:PHE:CZ	2.53	0.43
1:B:1161:ILE:HD13	1:B:1174:ALA:CB	2.47	0.43
1:B:1185:GLU:HB2	1:B:1188:GLU:HG3	2.01	0.43
1:C:2331:ALA:HA	1:C:2332:PRO:HD3	1.76	0.43
1:C:2180:ILE:O	1:C:2407:TYR:HE1	2.01	0.43
1:A:17:VAL:CG2	1:A:266:CYS:HB3	2.47	0.43
1:A:300:MET:O	1:B:1297:ARG:NH2	2.51	0.43
1:C:2076:ARG:HD2	1:C:2446:GLU:CD	2.38	0.43
1:C:2076:ARG:HD2	1:C:2446:GLU:OE1	2.18	0.43
1:C:2161:ILE:HD13	1:C:2174:ALA:HB1	2.01	0.43
1:C:2210:VAL:HG23	1:C:2215:GLN:HB2	2.00	0.43
1:D:3147:ARG:C	1:D:3149:ALA:H	2.22	0.43
1:D:3384:GLN:C	1:D:3386:ALA:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:TRP:O	1:B:1196:TRP:HB3	2.17	0.43
1:B:1384:GLN:C	1:B:1386:ALA:N	2.71	0.43
1:D:3183:THR:HG22	1:D:3354:LEU:HD22	1.99	0.43
1:D:3340:THR:OG1	1:D:3347:PRO:HA	2.18	0.43
1:A:115:VAL:HG23	1:A:115:VAL:O	2.18	0.43
1:A:89:TYR:CD1	1:A:342:PRO:HG3	2.54	0.43
1:A:14:PHE:CE1	1:A:40:LEU:HB2	2.53	0.43
1:B:1438:ALA:HB2	1:B:1447:GLY:O	2.18	0.43
1:B:1449:VAL:O	1:B:1450:GLU:C	2.53	0.43
1:B:1471:ILE:HG23	1:B:1472:TRP:HD1	1.83	0.43
1:C:2115:VAL:O	1:C:2115:VAL:HG23	2.18	0.43
1:C:2326:ILE:HD12	1:C:2376:LEU:HD21	2.00	0.43
1:A:289:PRO:HB3	1:B:1398:CYS:HB2	2.00	0.43
1:B:1460:LEU:HB3	1:B:1466:VAL:HG23	2.01	0.43
1:C:2044:ALA:HB1	1:C:2243:PRO:HG3	2.01	0.43
1:C:2090:LYS:HA	1:C:2217:ARG:HB3	2.00	0.43
1:A:289:PRO:CG	1:B:1399:GLU:HG2	2.47	0.43
1:C:2089:TYR:O	1:C:2217:ARG:HB2	2.18	0.43
1:D:3422:VAL:O	1:D:3423:ILE:C	2.57	0.43
1:B:1335:ILE:HD11	1:B:1352:PHE:HD1	1.84	0.43
1:D:3249:GLN:HE21	1:D:3249:GLN:HB2	1.70	0.43
1:D:3387:LEU:O	1:D:3389:PRO:HD3	2.19	0.43
1:A:422:VAL:O	1:A:424:ARG:N	2.52	0.43
1:B:1099:GLN:CG	1:B:1101:VAL:HG23	2.48	0.43
1:B:1115:VAL:HG23	1:B:1115:VAL:O	2.18	0.43
1:B:1158:LYS:O	1:B:1161:ILE:N	2.51	0.43
1:B:1291:ARG:HH11	1:B:1291:ARG:CG	2.31	0.43
1:C:2420:GLY:C	1:C:2422:VAL:H	2.23	0.43
1:D:3439:THR:HB	1:D:3450:GLU:OE1	2.19	0.43
1:D:3200:GLN:NE2	1:D:3442:SER:HB3	2.34	0.43
1:A:490:PHE:CE1	1:A:494:ASN:ND2	2.87	0.42
1:A:505:THR:O	1:A:507:VAL:N	2.52	0.42
1:B:1022:GLY:O	1:B:1026:LEU:HD22	2.19	0.42
1:B:1353:ILE:HD13	1:B:1361:LEU:CD1	2.49	0.42
1:B:1387:LEU:C	1:B:1389:PRO:HD3	2.39	0.42
1:C:2210:VAL:HG12	1:C:2211:THR:H	1.84	0.42
1:C:2303:VAL:CG2	1:C:2304:ILE:N	2.81	0.42
1:C:2384:GLN:C	1:C:2386:ALA:N	2.72	0.42
1:A:37:ILE:HD12	1:A:460:LEU:CD2	2.48	0.42
1:B:1076:ARG:HG2	1:B:1076:ARG:NH1	2.34	0.42
1:B:1166:TRP:NE1	1:B:1499:PRO:HG3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1296:GLN:C	1:B:1297:ARG:HG2	2.38	0.42
1:C:2460:LEU:HB3	1:C:2466:VAL:HG23	2.01	0.42
1:D:3076:ARG:HD2	1:D:3446:GLU:CD	2.40	0.42
1:D:3058:GLU:OE1	1:D:3058:GLU:N	2.53	0.42
1:D:3096:ARG:HB2	1:D:3319:ASP:O	2.19	0.42
1:D:3127:LEU:HD13	1:D:3165:CYS:SG	2.59	0.42
1:D:3315:TRP:O	1:D:3320:TYR:HB2	2.19	0.42
1:A:326:ILE:HD13	1:A:376:LEU:HD11	2.02	0.42
1:B:1183:THR:HG22	1:B:1354:LEU:HD22	2.01	0.42
1:C:2153:ASP:HB2	1:C:2192:LEU:CD2	2.49	0.42
1:D:3044:ALA:HB1	1:D:3243:PRO:HG3	2.00	0.42
1:D:3175:TYR:O	1:D:3178:VAL:HB	2.19	0.42
1:D:3490:PHE:CE1	1:D:3494:ASN:ND2	2.87	0.42
1:B:1291:ARG:HD2	1:B:1422:VAL:HG11	2.02	0.42
1:B:1307:MET:SD	1:B:1307:MET:N	2.93	0.42
1:B:1373:ILE:O	1:B:1376:LEU:HB3	2.20	0.42
1:C:2074:GLN:O	1:C:2446:GLU:HG3	2.18	0.42
1:C:2147:ARG:C	1:C:2149:ALA:H	2.23	0.42
1:C:2369:ARG:O	1:C:2373:ILE:HG13	2.20	0.42
1:D:3072:PRO:HD2	1:D:3213:GLY:O	2.20	0.42
1:D:3303:VAL:CG2	1:D:3304:ILE:N	2.82	0.42
1:A:115:VAL:HG21	1:A:121:TYR:HA	2.01	0.42
1:D:3166:TRP:NE1	1:D:3499:PRO:HG3	2.34	0.42
1:D:3391:HIS:HE1	1:D:3393:GLU:HG2	1.81	0.42
1:A:147:ARG:C	1:A:149:ALA:H	2.23	0.42
1:A:58:GLU:OE1	1:A:58:GLU:N	2.53	0.42
1:C:2060:VAL:O	1:C:2061:LYS:HB2	2.18	0.42
1:C:2369:ARG:NH1	1:C:2394:GLU:OE1	2.53	0.42
1:D:3091:VAL:HG23	1:D:3216:GLU:O	2.20	0.42
1:A:60:VAL:O	1:A:61:LYS:HB2	2.19	0.42
1:B:1036:LYS:HA	1:B:1036:LYS:HE2	2.02	0.42
1:B:1156:THR:HG23	1:B:1186:PRO:O	2.19	0.42
1:B:1248:ASP:HA	1:B:1284:LYS:HB3	2.01	0.42
1:B:1270:ILE:HD11	1:B:1459:VAL:HG21	2.02	0.42
1:C:2153:ASP:HB2	1:C:2192:LEU:HD23	2.01	0.42
1:C:2287:LEU:H	1:C:2287:LEU:CD1	2.24	0.42
1:C:2291:ARG:HD2	1:C:2422:VAL:HG11	2.01	0.42
1:D:3248:ASP:HA	1:D:3284:LYS:HB3	2.02	0.42
1:A:193:TRP:O	1:A:196:TRP:HB3	2.20	0.42
1:A:475:GLU:HA	1:A:476:PRO:HD3	1.82	0.42
1:B:1422:VAL:O	1:B:1423:ILE:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2268:TYR:CE2	1:C:2429:ARG:HG2	2.55	0.42
1:D:3156:THR:HG22	1:D:3158:LYS:HB3	2.02	0.42
1:A:408:THR:HB	1:A:409:ALA:H	1.61	0.42
1:A:166:TRP:NE1	1:A:499:PRO:HG3	2.35	0.42
1:C:2336:THR:HA	1:C:2350:MET:O	2.20	0.42
1:C:2387:LEU:C	1:C:2389:PRO:HD3	2.40	0.42
1:C:2505:THR:C	1:C:2507:VAL:H	2.24	0.42
1:D:3274:PRO:HA	1:D:3275:PRO:HD3	1.92	0.42
1:D:3331:ALA:HA	1:D:3332:PRO:HD3	1.76	0.42
1:B:1147:ARG:C	1:B:1149:ALA:H	2.23	0.41
1:B:1303:VAL:CG2	1:B:1304:ILE:N	2.83	0.41
1:B:1498:VAL:HB	1:B:1499:PRO:HD3	2.02	0.41
1:C:2273:ILE:HD11	1:C:2278:THR:HA	2.00	0.41
1:C:2369:ARG:HD2	1:C:2394:GLU:OE2	2.21	0.41
1:D:3077:ILE:H	1:D:3446:GLU:CG	2.32	0.41
1:C:2187:HIS:CD2	1:D:3154:LYS:HA	2.55	0.41
1:D:3051:ARG:NH2	1:D:3274:PRO:HG3	2.35	0.41
1:D:3498:VAL:HB	1:D:3499:PRO:HD3	2.01	0.41
1:A:343:ASP:OD2	1:A:345:SER:HB2	2.20	0.41
1:B:1076:ARG:HD2	1:B:1446:GLU:OE1	2.19	0.41
1:B:1072:PRO:HG2	1:B:1212:ASN:O	2.20	0.41
1:C:2422:VAL:O	1:C:2424:ARG:N	2.53	0.41
1:D:3469:LYS:C	1:D:3469:LYS:CD	2.88	0.41
1:A:296:GLN:C	1:A:297:ARG:HG2	2.40	0.41
1:A:369:ARG:HD2	1:A:394:GLU:OE2	2.20	0.41
1:A:98:VAL:CG2	1:A:324:MET:HG2	2.50	0.41
1:B:1037:ILE:HD12	1:B:1460:LEU:CD2	2.50	0.41
1:B:1097:LEU:CD2	1:B:1321:CYS:SG	3.08	0.41
1:B:1332:PRO:HD2	1:B:1376:LEU:HD22	2.02	0.41
1:B:1469:LYS:O	1:B:1471:ILE:N	2.52	0.41
1:B:1337:LEU:HG	2:B:1709:MLG:CL07	2.57	0.41
1:D:3028:ALA:HB2	1:D:3452:GLY:O	2.19	0.41
1:D:3249:GLN:NE2	1:D:3428:GLY:O	2.48	0.41
1:A:161:ILE:HD13	1:A:174:ALA:CB	2.51	0.41
1:B:1373:ILE:HG22	1:B:1377:TYR:CE2	2.55	0.41
1:C:2093:VAL:O	1:C:2093:VAL:CG1	2.66	0.41
1:C:2183:THR:HG22	1:C:2354:LEU:HD22	2.02	0.41
1:C:2343:ASP:OD2	1:C:2345:SER:HB2	2.21	0.41
1:D:3070:VAL:HG11	1:D:3219:PHE:CZ	2.56	0.41
1:D:3273:ILE:HD11	1:D:3278:THR:HA	2.01	0.41
1:D:3460:LEU:HB3	1:D:3466:VAL:HG23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HA	1:A:275:PRO:HD3	1.92	0.41
1:C:2128:TRP:CE3	1:C:2131:MET:HE3	2.56	0.41
1:C:2335:ILE:HD11	1:C:2352:PHE:HD1	1.85	0.41
1:A:51:ARG:NH2	1:A:274:PRO:HG3	2.34	0.41
1:A:291:ARG:HD2	1:A:422:VAL:HG11	2.02	0.41
1:A:96:ARG:HB2	1:A:319:ASP:O	2.21	0.41
1:B:1064:ASP:HB3	1:B:1068:ALA:HB2	2.02	0.41
1:A:187:HIS:CD2	1:B:1154:LYS:HA	2.55	0.41
1:B:1387:LEU:O	1:B:1389:PRO:HD3	2.19	0.41
1:C:2210:VAL:HG13	1:C:2211:THR:N	2.36	0.41
1:D:3020:GLY:O	1:D:3025:GLY:HA3	2.21	0.41
1:D:3026:LEU:O	1:D:3027:ALA:C	2.57	0.41
1:A:183:THR:HG23	1:A:407:TYR:CD1	2.56	0.41
1:A:420:GLY:O	1:A:422:VAL:N	2.53	0.41
1:A:60:VAL:O	1:A:62:TRP:N	2.54	0.41
1:B:1490:PHE:CE1	1:B:1494:ASN:ND2	2.88	0.41
1:C:2014:PHE:CE1	1:C:2040:LEU:HB2	2.56	0.41
1:C:2077:ILE:H	1:C:2446:GLU:CG	2.32	0.41
1:C:2185:GLU:HB2	1:C:2188:GLU:HG3	2.03	0.41
1:D:3387:LEU:C	1:D:3389:PRO:HD3	2.40	0.41
1:A:273:ILE:HD11	1:A:278:THR:HA	2.01	0.41
1:A:519:TYR:CD2	1:A:520:LYS:HG3	2.44	0.41
1:B:1091:VAL:HG23	1:B:1216:GLU:O	2.20	0.41
1:B:1098:VAL:CG2	1:B:1324:MET:HG2	2.51	0.41
1:C:2028:ALA:HB2	1:C:2452:GLY:O	2.21	0.41
1:D:3333:ILE:N	1:D:3333:ILE:HD12	2.36	0.41
1:A:156:THR:HG23	1:A:186:PRO:O	2.21	0.41
1:A:158:LYS:O	1:A:161:ILE:N	2.54	0.41
1:A:353:ILE:HG21	1:A:361:LEU:HD12	2.02	0.41
1:A:471:ILE:HG23	1:A:472:TRP:HD1	1.83	0.41
1:B:1090:LYS:HA	1:B:1217:ARG:HB3	2.03	0.41
1:B:1495:LEU:HA	1:B:1496:PRO:HD3	1.87	0.41
1:C:2315:TRP:O	1:C:2320:TYR:HB2	2.21	0.41
1:B:1044:ALA:HB1	1:B:1243:PRO:HG3	2.02	0.41
1:B:1356:ARG:NH1	1:B:1357:LYS:HE3	2.36	0.41
1:D:3161:ILE:HD13	1:D:3174:ALA:CB	2.51	0.41
1:A:287:LEU:H	1:A:287:LEU:CD1	2.26	0.41
1:A:369:ARG:O	1:A:373:ILE:HG13	2.21	0.41
1:C:2475:GLU:HA	1:C:2476:PRO:HD3	1.83	0.41
1:C:2498:VAL:HB	1:C:2499:PRO:HD3	2.02	0.41
1:D:3046:ASP:OD1	1:D:3046:ASP:C	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:CG1	1:A:309:TYR:OH	2.61	0.40
1:A:438:ALA:HB2	1:A:447:GLY:O	2.21	0.40
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.88	0.40
1:A:500:GLY:O	1:A:504:ILE:HG13	2.20	0.40
1:C:2016:VAL:O	1:C:2039:VAL:HG23	2.20	0.40
1:C:2248:ASP:HA	1:C:2284:LYS:HB3	2.02	0.40
1:C:2332:PRO:HD2	1:C:2376:LEU:HD22	2.02	0.40
1:C:2387:LEU:O	1:C:2389:PRO:HD3	2.21	0.40
1:D:3328:ASP:O	1:D:3329:GLU:C	2.59	0.40
1:B:1074:GLN:O	1:B:1446:GLU:HG3	2.21	0.40
1:B:1089:TYR:O	1:B:1217:ARG:HB2	2.21	0.40
1:B:1153:ASP:HB2	1:B:1192:LEU:CD2	2.51	0.40
1:B:1200:GLN:NE2	1:B:1442:SER:HB3	2.36	0.40
1:B:1328:ASP:O	1:B:1329:GLU:C	2.60	0.40
1:B:1449:VAL:O	1:B:1453:GLU:HG3	2.21	0.40
1:C:2058:GLU:OE1	1:C:2058:GLU:N	2.54	0.40
1:C:2017:VAL:CG2	1:C:2266:CYS:HB3	2.47	0.40
1:D:3218:LYS:HB3	1:D:3218:LYS:HE2	1.79	0.40
1:D:3291:ARG:HD2	1:D:3422:VAL:CG1	2.52	0.40
1:A:74:GLN:O	1:A:446:GLU:HG3	2.20	0.40
1:A:76:ARG:NH1	1:A:76:ARG:HG2	2.36	0.40
1:B:1219:PHE:HD1	1:B:1223:SER:HA	1.86	0.40
1:B:1475:GLU:HA	1:B:1476:PRO:HD3	1.82	0.40
1:C:2037:ILE:HD12	1:C:2460:LEU:CD2	2.52	0.40
1:D:3026:LEU:HD21	1:D:3048:VAL:HG21	2.04	0.40
1:A:326:ILE:HD12	1:A:376:LEU:HD21	2.03	0.40
1:B:1439:THR:HB	1:B:1450:GLU:OE1	2.22	0.40
1:D:3241:SER:O	1:D:3260:ASN:OD1	2.39	0.40
1:D:3369:ARG:HD2	1:D:3394:GLU:OE2	2.20	0.40
1:D:3457:ARG:HA	1:D:3460:LEU:HD12	2.03	0.40
1:A:314:PHE:HE1	1:A:381:LEU:HD13	1.86	0.40
1:A:436:GLU:HG2	1:A:436:GLU:H	1.64	0.40
1:C:2438:ALA:HB2	1:C:2447:GLY:O	2.22	0.40
1:D:3064:ASP:HB3	1:D:3068:ALA:HB2	2.04	0.40
1:D:3335:ILE:HD11	1:D:3352:PHE:HD1	1.85	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	509/534 (95%)	428 (84%)	67 (13%)	14 (3%)	6	34
1	B	501/534 (94%)	416 (83%)	70 (14%)	15 (3%)	5	32
1	C	510/534 (96%)	422 (83%)	73 (14%)	15 (3%)	5	33
1	D	504/534 (94%)	418 (83%)	71 (14%)	15 (3%)	5	32
All	All	2024/2136 (95%)	1684 (83%)	281 (14%)	59 (3%)	5	33

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	408	THR
1	A	423	ILE
1	B	1102	LYS
1	B	1127	LEU
1	B	1408	THR
1	B	1423	ILE
1	C	2102	LYS
1	C	2127	LEU
1	C	2408	THR
1	C	2423	ILE
1	D	3102	LYS
1	D	3127	LEU
1	D	3408	THR
1	D	3423	ILE
1	A	103	GLY
1	A	127	LEU
1	A	329	GLU
1	A	428	GLY
1	B	1103	GLY
1	B	1421	ARG
1	B	1428	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2103	GLY
1	C	2421	ARG
1	C	2428	GLY
1	D	3103	GLY
1	D	3329	GLU
1	D	3421	ARG
1	D	3428	GLY
1	A	111	ALA
1	A	421	ARG
1	A	470	ASP
1	B	1111	ALA
1	B	1329	GLU
1	B	1470	ASP
1	C	2111	ALA
1	C	2329	GLU
1	C	2470	ASP
1	D	3470	ASP
1	D	3508	SER
1	B	1429	ARG
1	B	1508	SER
1	D	3111	ALA
1	A	284	LYS
1	A	355	ALA
1	B	1284	LYS
1	C	2061	LYS
1	C	2284	LYS
1	C	2355	ALA
1	C	2429	ARG
1	D	3284	LYS
1	D	3355	ALA
1	A	72	PRO
1	A	93	VAL
1	B	1072	PRO
1	B	1093	VAL
1	C	2093	VAL
1	D	3093	VAL
1	D	3072	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	433/455 (95%)	402 (93%)	31 (7%)	17	53
1	B	425/455 (93%)	395 (93%)	30 (7%)	17	54
1	C	434/455 (95%)	401 (92%)	33 (8%)	15	51
1	D	428/455 (94%)	398 (93%)	30 (7%)	18	54
All	All	1720/1820 (94%)	1596 (93%)	124 (7%)	17	53

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	14	PHE
1	A	26	LEU
1	A	31	LEU
1	A	52	THR
1	A	58	GLU
1	A	65	VAL
1	A	72	PRO
1	A	95	GLU
1	A	109	ARG
1	A	116	TRP
1	A	140	VAL
1	A	156	THR
1	A	173	PHE
1	A	211	THR
1	A	249	GLN
1	A	251	ASP
1	A	276	ILE
1	A	287	LEU
1	A	291	ARG
1	A	297	ARG
1	A	365	HIS
1	A	406	CYS
1	A	423	ILE
1	A	424	ARG
1	A	436	GLU
1	A	446	GLU
1	A	454	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	461	ASN
1	A	469	LYS
1	A	488	HIS
1	B	1012	HIS
1	B	1014	PHE
1	B	1026	LEU
1	B	1031	LEU
1	B	1052	THR
1	B	1058	GLU
1	B	1065	VAL
1	B	1072	PRO
1	B	1095	GLU
1	B	1109	ARG
1	B	1116	TRP
1	B	1140	VAL
1	B	1156	THR
1	B	1173	PHE
1	B	1211	THR
1	B	1249	GLN
1	B	1251	ASP
1	B	1276	ILE
1	B	1287	LEU
1	B	1291	ARG
1	B	1365	HIS
1	B	1406	CYS
1	B	1423	ILE
1	B	1424	ARG
1	B	1436	GLU
1	B	1446	GLU
1	B	1454	ARG
1	B	1461	ASN
1	B	1469	LYS
1	B	1488	HIS
1	C	2012	HIS
1	C	2014	PHE
1	C	2026	LEU
1	C	2031	LEU
1	C	2052	THR
1	C	2058	GLU
1	C	2065	VAL
1	C	2072	PRO
1	C	2095	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2109	ARG
1	C	2116	TRP
1	C	2140	VAL
1	C	2156	THR
1	C	2173	PHE
1	C	2210	VAL
1	C	2211	THR
1	C	2249	GLN
1	C	2251	ASP
1	C	2274	PRO
1	C	2276	ILE
1	C	2287	LEU
1	C	2291	ARG
1	C	2297	ARG
1	C	2365	HIS
1	C	2406	CYS
1	C	2423	ILE
1	C	2424	ARG
1	C	2436	GLU
1	C	2446	GLU
1	C	2454	ARG
1	C	2461	ASN
1	C	2469	LYS
1	C	2488	HIS
1	D	3012	HIS
1	D	3014	PHE
1	D	3026	LEU
1	D	3031	LEU
1	D	3052	THR
1	D	3058	GLU
1	D	3065	VAL
1	D	3072	PRO
1	D	3095	GLU
1	D	3109	ARG
1	D	3116	TRP
1	D	3140	VAL
1	D	3156	THR
1	D	3173	PHE
1	D	3189	VAL
1	D	3211	THR
1	D	3249	GLN
1	D	3251	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3276	ILE
1	D	3287	LEU
1	D	3291	ARG
1	D	3297	ARG
1	D	3365	HIS
1	D	3406	CYS
1	D	3424	ARG
1	D	3436	GLU
1	D	3446	GLU
1	D	3461	ASN
1	D	3469	LYS
1	D	3488	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	293	GLN
1	A	296	GLN
1	A	391	HIS
1	A	401	GLN
1	A	418	GLN
1	A	494	ASN
1	B	1260	ASN
1	B	1293	GLN
1	B	1296	GLN
1	B	1391	HIS
1	B	1418	GLN
1	B	1494	ASN
1	C	2260	ASN
1	C	2293	GLN
1	C	2296	GLN
1	C	2391	HIS
1	C	2401	GLN
1	C	2418	GLN
1	D	3260	ASN
1	D	3293	GLN
1	D	3296	GLN
1	D	3391	HIS
1	D	3418	GLN
1	D	3494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	652	1,2	51,58,58	2.61	14 (27%)	54,89,89	2.36	8 (14%)
2	MLG	A	709	2	16,17,17	3.87	10 (62%)	20,21,21	9.80	5 (25%)
2	FAD	B	1652	1,2	51,58,58	2.68	13 (25%)	54,89,89	2.40	8 (14%)
2	MLG	B	1709	2	16,17,17	3.85	9 (56%)	20,21,21	9.97	5 (25%)
2	FAD	C	2652	1,2	51,58,58	2.66	13 (25%)	54,89,89	2.39	13 (24%)
2	MLG	C	2709	2	16,17,17	3.86	10 (62%)	20,21,21	9.83	5 (25%)
2	FAD	D	3652	1,2	51,58,58	2.65	13 (25%)	54,89,89	2.34	10 (18%)
2	MLG	D	3709	2	16,17,17	3.88	10 (62%)	20,21,21	9.90	5 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	652	1,2	-	0/28/50/50	0/6/6/6
2	MLG	A	709	2	-	0/9/10/10	0/1/1/1
2	FAD	B	1652	1,2	-	0/28/50/50	0/6/6/6
2	MLG	B	1709	2	-	0/9/10/10	0/1/1/1
2	FAD	C	2652	1,2	-	0/28/50/50	0/6/6/6
2	MLG	C	2709	2	-	0/9/10/10	0/1/1/1
2	FAD	D	3652	1,2	-	0/28/50/50	0/6/6/6
2	MLG	D	3709	2	-	0/9/10/10	0/1/1/1

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1709	MLG	C14-C15	-7.90	1.37	1.47
2	D	3709	MLG	C14-C15	-7.74	1.37	1.47
2	C	2709	MLG	C14-C15	-7.26	1.38	1.47
2	A	709	MLG	C14-C15	-7.07	1.38	1.47
2	C	2652	FAD	C1'-N10	-5.58	1.42	1.48
2	B	1652	FAD	C1'-N10	-4.37	1.43	1.48
2	D	3652	FAD	C1'-N10	-4.17	1.44	1.48
2	B	1652	FAD	C5A-C4A	-3.97	1.31	1.40
2	A	652	FAD	C1'-N10	-3.92	1.44	1.48
2	A	652	FAD	C5A-C4A	-3.81	1.31	1.40
2	D	3652	FAD	C5A-C4A	-3.63	1.32	1.40
2	C	2652	FAD	C5A-C4A	-3.57	1.32	1.40
2	B	1709	MLG	C12-N13	-3.29	1.37	1.46
2	A	709	MLG	C12-N13	-3.28	1.37	1.46
2	D	3709	MLG	C12-N13	-3.26	1.37	1.46
2	C	2709	MLG	C12-N13	-3.16	1.38	1.46
2	C	2652	FAD	C5'-C4'	-3.04	1.47	1.51
2	D	3652	FAD	C5'-C4'	-3.03	1.47	1.51
2	A	652	FAD	C5'-C4'	-3.00	1.47	1.51
2	B	1652	FAD	C2B-C3B	-2.83	1.45	1.53
2	B	1652	FAD	C5'-C4'	-2.81	1.47	1.51
2	A	652	FAD	C2B-C3B	-2.76	1.46	1.53
2	C	2652	FAD	C2B-C3B	-2.56	1.46	1.53
2	D	3652	FAD	C2B-C3B	-2.37	1.47	1.53
2	D	3652	FAD	C8A-N7A	-2.30	1.30	1.34
2	B	1652	FAD	C8A-N7A	-2.28	1.30	1.34
2	A	652	FAD	C8A-N7A	-2.17	1.30	1.34
2	C	2652	FAD	C8A-N7A	-2.08	1.30	1.34
2	A	652	FAD	C2'-C3'	-2.07	1.49	1.53
2	C	2709	MLG	C05-C06	2.02	1.42	1.38
2	A	709	MLG	C05-C06	2.03	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3709	MLG	C05-C06	2.04	1.42	1.38
2	C	2709	MLG	C01-C02	2.37	1.43	1.39
2	A	709	MLG	C01-C02	2.50	1.44	1.39
2	B	1709	MLG	C01-C02	2.51	1.44	1.39
2	D	3709	MLG	C01-C02	2.53	1.44	1.39
2	A	709	MLG	C03-C04	2.56	1.42	1.38
2	A	709	MLG	C06-C01	2.68	1.45	1.39
2	A	652	FAD	C9A-C5X	2.72	1.48	1.42
2	B	1709	MLG	C06-C01	2.79	1.45	1.39
2	B	1709	MLG	C03-C04	2.83	1.43	1.38
2	C	2709	MLG	C03-C04	2.84	1.43	1.38
2	C	2652	FAD	C9A-C5X	2.88	1.48	1.42
2	C	2709	MLG	C06-C01	2.91	1.45	1.39
2	D	3709	MLG	C03-C04	2.95	1.43	1.38
2	D	3709	MLG	C06-C01	3.05	1.46	1.39
2	B	1652	FAD	C9A-C5X	3.05	1.48	1.42
2	D	3652	FAD	C9A-C5X	3.06	1.48	1.42
2	A	709	MLG	C05-C04	3.15	1.44	1.38
2	D	3709	MLG	C05-C04	3.27	1.44	1.38
2	C	2709	MLG	C05-C04	3.29	1.44	1.38
2	B	1709	MLG	C05-C04	3.38	1.44	1.38
2	D	3709	MLG	C11-C12	3.42	1.66	1.51
2	A	709	MLG	C11-C12	3.43	1.66	1.51
2	B	1709	MLG	C11-C12	3.45	1.66	1.51
2	C	2709	MLG	C11-C12	3.49	1.66	1.51
2	B	1709	MLG	C03-C02	3.91	1.45	1.38
2	D	3709	MLG	C03-C02	4.02	1.45	1.38
2	A	709	MLG	C03-C02	4.09	1.45	1.38
2	C	2709	MLG	C03-C02	4.10	1.45	1.38
2	D	3652	FAD	C10-N1	4.45	1.39	1.33
2	D	3652	FAD	C4-N3	4.50	1.41	1.33
2	B	1652	FAD	C10-N1	4.55	1.39	1.33
2	A	652	FAD	C4-N3	4.60	1.41	1.33
2	C	2652	FAD	C4-N3	4.64	1.41	1.33
2	B	1652	FAD	C4-N3	4.67	1.41	1.33
2	C	2652	FAD	C10-N1	4.70	1.39	1.33
2	A	652	FAD	C2A-N3A	4.89	1.40	1.32
2	A	652	FAD	C10-N1	5.00	1.40	1.33
2	B	1652	FAD	C4A-N3A	5.09	1.43	1.35
2	D	3652	FAD	C5X-N5	5.10	1.43	1.35
2	A	652	FAD	C4A-N3A	5.19	1.43	1.35
2	D	3652	FAD	C4A-N3A	5.27	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2652	FAD	C5X-N5	5.28	1.43	1.35
2	A	652	FAD	C5X-N5	5.33	1.43	1.35
2	B	1652	FAD	C2A-N3A	5.40	1.41	1.32
2	C	2652	FAD	C2A-N3A	5.43	1.41	1.32
2	B	1652	FAD	C5X-N5	5.45	1.43	1.35
2	C	2652	FAD	C4A-N3A	5.83	1.44	1.35
2	D	3652	FAD	C2A-N3A	5.87	1.41	1.32
2	C	2652	FAD	C9A-N10	7.37	1.48	1.38
2	A	652	FAD	C4X-N5	7.86	1.44	1.33
2	D	3652	FAD	C4X-N5	8.14	1.45	1.33
2	B	1652	FAD	C4X-N5	8.19	1.45	1.33
2	C	2652	FAD	C4X-N5	8.21	1.45	1.33
2	A	652	FAD	C9A-N10	8.26	1.49	1.38
2	D	3652	FAD	C9A-N10	8.38	1.49	1.38
2	B	1652	FAD	C9A-N10	8.58	1.50	1.38
2	B	1709	MLG	C15-C16	9.67	1.40	1.18
2	D	3709	MLG	C15-C16	9.84	1.41	1.18
2	C	2709	MLG	C15-C16	10.24	1.41	1.18
2	A	709	MLG	C15-C16	10.48	1.42	1.18

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1709	MLG	C14-C15-C16	-44.08	121.67	177.74
2	D	3709	MLG	C14-C15-C16	-43.81	122.02	177.74
2	C	2709	MLG	C14-C15-C16	-43.50	122.40	177.74
2	A	709	MLG	C14-C15-C16	-43.37	122.58	177.74
2	C	2652	FAD	N3A-C2A-N1A	-6.97	122.79	128.86
2	B	1652	FAD	N3A-C2A-N1A	-6.96	122.79	128.86
2	A	652	FAD	N3A-C2A-N1A	-6.69	123.03	128.86
2	D	3652	FAD	N3A-C2A-N1A	-5.77	123.83	128.86
2	B	1652	FAD	C4X-C4-N3	-5.19	116.10	123.48
2	C	2652	FAD	C4X-C4-N3	-5.10	116.22	123.48
2	D	3652	FAD	C4X-C4-N3	-4.93	116.46	123.48
2	A	652	FAD	C4X-C4-N3	-4.67	116.84	123.48
2	D	3652	FAD	C5X-C9A-N10	-3.87	114.79	117.66
2	A	652	FAD	C5X-C9A-N10	-3.87	114.79	117.66
2	A	652	FAD	C4X-C10-N10	-3.57	118.04	120.52
2	B	1652	FAD	C5X-C9A-N10	-3.25	115.24	117.66
2	D	3652	FAD	C4X-C10-N10	-3.11	118.36	120.52
2	B	1652	FAD	C4X-C10-N10	-2.95	118.47	120.52
2	C	2652	FAD	C5X-C9A-N10	-2.79	115.59	117.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1709	MLG	C17-N13-C12	-2.64	103.27	110.60
2	A	709	MLG	C17-N13-C12	-2.62	103.32	110.60
2	C	2709	MLG	C17-N13-C12	-2.55	103.53	110.60
2	D	3709	MLG	C17-N13-C12	-2.50	103.66	110.60
2	C	2652	FAD	C4X-C10-N10	-2.42	118.84	120.52
2	C	2652	FAD	C6-C7-C8	-2.33	115.79	119.95
2	A	652	FAD	C1'-N10-C9A	-2.32	116.22	118.35
2	B	1709	MLG	O09-C01-C06	-2.25	119.15	124.00
2	D	3652	FAD	C1'-N10-C9A	-2.21	116.32	118.35
2	A	709	MLG	O09-C01-C06	-2.21	119.24	124.00
2	C	2709	MLG	O09-C01-C06	-2.20	119.27	124.00
2	C	2652	FAD	C1'-N10-C9A	-2.16	116.36	118.35
2	D	3709	MLG	O09-C01-C06	-2.15	119.36	124.00
2	D	3652	FAD	O2'-C2'-C1'	-2.08	104.98	109.79
2	C	2652	FAD	O2'-C2'-C1'	-2.02	105.11	109.79
2	A	652	FAD	O2B-C2B-C3B	2.04	118.36	111.83
2	B	1652	FAD	C4'-C3'-C2'	2.07	117.87	113.41
2	D	3652	FAD	C4'-C3'-C2'	2.08	117.89	113.41
2	C	2652	FAD	C4'-C3'-C2'	2.12	117.97	113.41
2	C	2652	FAD	C9-C8-C7	2.14	123.76	119.95
2	B	1652	FAD	O2B-C2B-C3B	2.22	118.96	111.83
2	C	2652	FAD	O2B-C2B-C3B	2.38	119.44	111.83
2	C	2652	FAD	C10-C4X-N5	2.47	123.44	120.59
2	D	3652	FAD	C10-C4X-N5	2.49	123.46	120.59
2	B	1652	FAD	C10-C4X-N5	2.60	123.58	120.59
2	C	2652	FAD	C1'-N10-C10	2.70	121.27	118.50
2	D	3652	FAD	O2B-C2B-C3B	2.71	120.50	111.83
2	C	2709	MLG	C01-C02-CL07	2.77	122.62	119.42
2	A	709	MLG	C01-C02-CL07	2.84	122.69	119.42
2	A	652	FAD	C10-C4X-N5	2.86	123.88	120.59
2	D	3709	MLG	C01-C02-CL07	2.90	122.76	119.42
2	B	1709	MLG	C01-C02-CL07	3.06	122.95	119.42
2	C	2709	MLG	O09-C01-C02	3.62	120.84	116.38
2	D	3709	MLG	O09-C01-C02	3.65	120.88	116.38
2	B	1709	MLG	O09-C01-C02	3.68	120.91	116.38
2	A	709	MLG	O09-C01-C02	3.70	120.94	116.38
2	A	652	FAD	C4-N3-C2	11.66	125.36	115.16
2	C	2652	FAD	C4-N3-C2	11.78	125.46	115.16
2	D	3652	FAD	C4-N3-C2	11.78	125.46	115.16
2	B	1652	FAD	C4-N3-C2	12.05	125.70	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	709	MLG	4	0
2	B	1709	MLG	3	0
2	C	2709	MLG	2	0
2	D	3709	MLG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	511/534 (95%)	-0.50	10 (1%) 65 50	41, 78, 146, 201	0
1	B	503/534 (94%)	-0.46	2 (0%) 92 89	43, 93, 152, 188	0
1	C	512/534 (95%)	-0.50	6 (1%) 79 67	41, 87, 151, 201	0
1	D	506/534 (94%)	-0.48	6 (1%) 79 67	48, 89, 150, 201	0
All	All	2032/2136 (95%)	-0.49	24 (1%) 79 67	41, 86, 150, 201	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3515	CYS	6.7
1	C	2519	TYR	6.5
1	C	2518	LEU	5.6
1	A	10	ALA	5.0
1	A	519	TYR	4.5
1	A	509	THR	3.8
1	C	2520	LYS	3.7
1	C	2036	LYS	3.6
1	D	3513	LEU	3.3
1	A	510	SER	3.1
1	A	518	LEU	2.7
1	B	1010	ALA	2.7
1	A	515	CYS	2.6
1	D	3323	CYS	2.5
1	D	3104	LYS	2.5
1	A	520	LYS	2.5
1	C	2515	CYS	2.4
1	D	3493	ARG	2.4
1	C	2251	ASP	2.3
1	A	512	ALA	2.2
1	A	488	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1116	TRP	2.2
1	D	3487	THR	2.2
1	A	36	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MLG	C	2709	17/17	0.73	0.35	3.47	62,91,140,149	0
2	MLG	B	1709	17/17	0.76	0.34	2.31	46,121,168,184	0
2	MLG	A	709	17/17	0.79	0.28	1.70	48,67,114,126	0
2	MLG	D	3709	17/17	0.74	0.31	1.70	61,111,159,175	0
2	FAD	A	652	53/53	0.97	0.16	0.09	32,62,102,113	0
2	FAD	C	2652	53/53	0.96	0.15	-0.07	33,67,98,126	0
2	FAD	B	1652	53/53	0.95	0.17	-0.21	34,72,138,153	0
2	FAD	D	3652	53/53	0.96	0.16	-0.25	35,75,119,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.