



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:32 am BST

PDB ID : 4B1B
Title : Crystal structure of Plasmodium falciparum oxidised Thioredoxin Reductase at 2.9 angstrom
Authors : Boumis, G.; Giardina, G.; Dimastrogiovanni, D.; Angelucci, F.; Saccoccia, F.; Brunori, M.; Bellelli, A.; Miele, A.E.
Deposited on : 2012-07-09
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

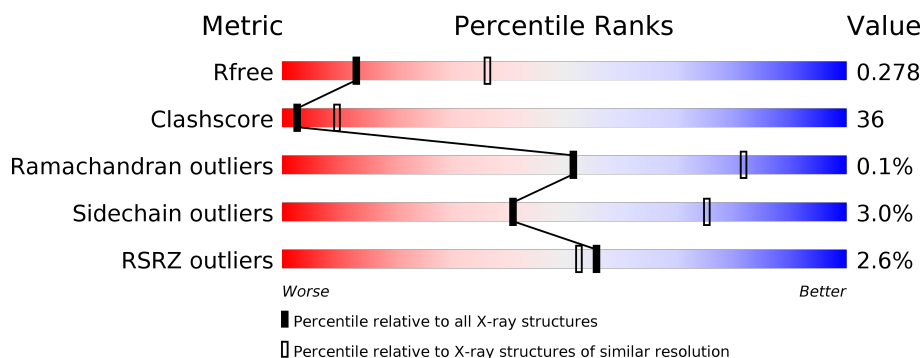
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	542	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	542	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>33%</div> <div>•</div> <div>19%</div> </div> </div>

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.

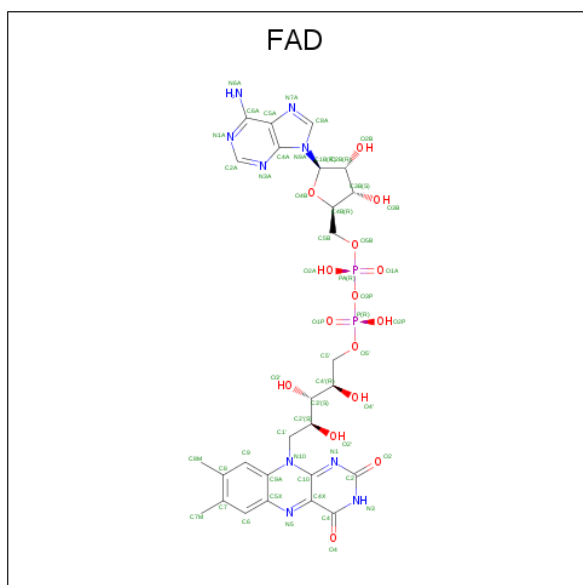
- Molecule 1 is a protein called THIOREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total 3389	C 2167	N 562	O 639	S 21	0	1	0
1	B	437	Total 3389	C 2167	N 562	O 639	S 21	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q25861
A	1	SER	-	expression tag	UNP Q25861
B	0	GLY	-	expression tag	UNP Q25861
B	1	SER	-	expression tag	UNP Q25861

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

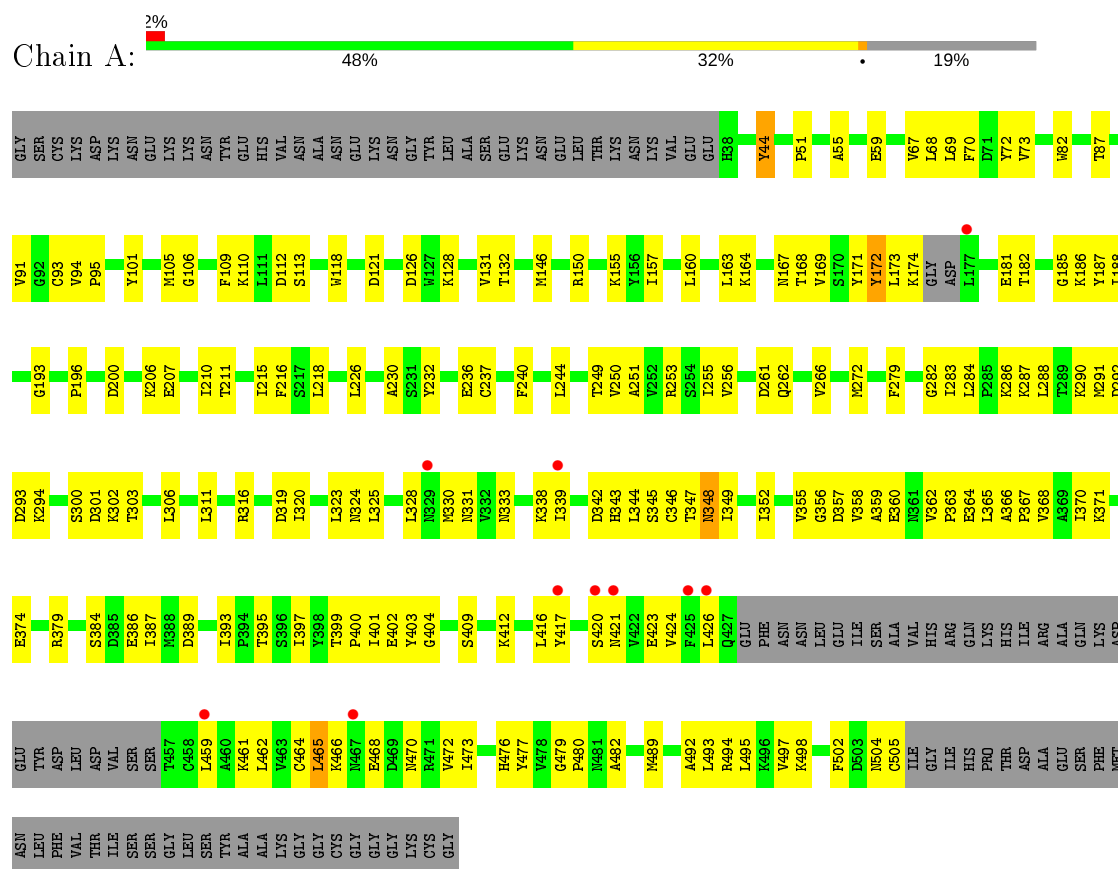
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		

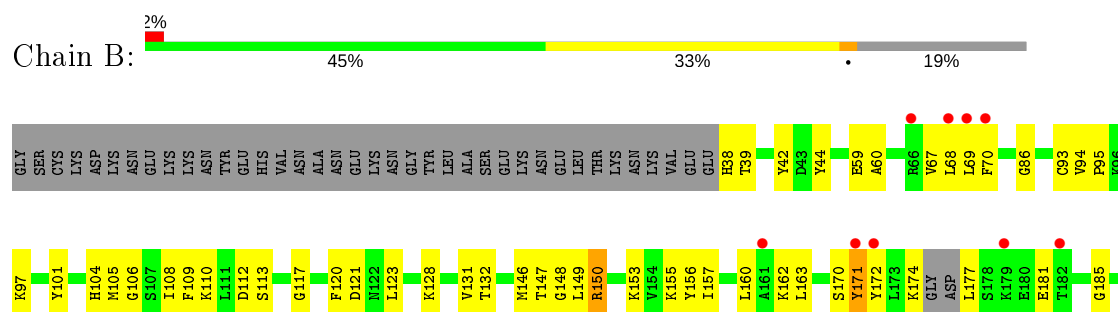
3 Residue-property plots

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: THIOREDOXIN REDUCTASE



• Molecule 1: THIOREDOXIN REDUCTASE



PRO	THR	ASP	ALA	GLU	SER	PHE	MET	ASN	LEU	PHE	VAL	THR	ILE	SER	SER	GLY	LEU	SER	TYR	ALA	GLY	GLY	CYS	GLY	GLY	LYS	CYS	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
LVS	HIS	ILE	ARG	ALA	GLN	LYS	ASP	GLU	TYR	ASP	VAL	ASP	VAL	SER	SER	T457	C458	L459	A460	R461	L462	V463	C464	L465	R466	N467	E468	D469	N470	R471	V472	I473	G474	F475	H476	Y477	V478	G479	N489	A492	L493	R494	L495	K496	V497	K498	K499	K500	D501	F502	D503	N504	C505	I506	G507	I508	G509	H510	L511	S512	L513	S514	L515	S516	L517	S518	L519	S520	L521	S522	L523	S524	L525	S526	L527	S528	L529	S530	L531	S532	L533	S534	L535	S536	L537	S538	L539	S540	L541	S542	L543	S544	L545	S546	L547	S548	L549	S550	L551	S552	L553	S554	L555	S556	L557	S558	L559	S560	L561	S562	L563	S564	L565	S566	L567	S568	L569	S570	L571	S572	L573	S574	L575	S576	L577	S578	L579	S580	L581	S582	L583	S584	L585	S586	L587	S588	L589	S590	L591	S592	L593	S594	L595	S596	L597	S598	L599	S600	L601	S602	L603	S604	L605	S606	L607	S608	L609	S610	L611	S612	L613	S614	L615	S616	L617	S618	L619	S620	L621	S622	L623	S624	L625	S626	L627	S628	L629	S630	L631	S632	L633	S634	L635	S636	L637	S638	L639	S640	L641	S642	L643	S644	L645	S646	L647	S648	L649	S650	L651	S652	L653	S654	L655	S656	L657	S658	L659	S660	L661	S662	L663	S664	L665	S666	L667	S668	L669	S670	L671	S672	L673	S674	L675	S676	L677	S678	L679	S680	L681	S682	L683	S684	L685	S686	L687	S688	L689	S690	L691	S692	L693	S694	L695	S696	L697	S698	L699	S700	L701	S702	L703	S704	L705	S706	L707	S708	L709	S710	L711	S712	L713	S714	L715	S716	L717	S718	L719	S720	L721	S722	L723	S724	L725	S726	L727	S728	L729	S730	L731	S732	L733	S734	L735	S736	L737	S738	L739	S740	L741	S742	L743	S744	L745	S746	L747	S748	L749	S750	L751	S752	L753	S754	L755	S756	L757	S758	L759	S760	L761	S762	L763	S764	L765	S766	L767	S768	L769	S770	L771	S772	L773	S774	L775	S776	L777	S778	L779	S780	L781	S782	L783	S784	L785	S786	L787	S788	L789	S790	L791	S792	L793	S794	L795	S796	L797	S798	L799	S800	L801	S802	L803	S804	L805	S806	L807	S808	L809	S810	L811	S812	L813	S814	L815	S816	L817	S818	L819	S820	L821	S822	L823	S824	L825	S826	L827	S828	L829	S830	L831	S832	L833	S834	L835	S836	L837	S838	L839	S840	L841	S842	L843	S844	L845	S846	L847	S848	L849	S850	L851	S852	L853	S854	L855	S856	L857	S858	L859	S860	L861	S862	L863	S864	L865	S866	L867	S868	L869	S870	L871	S872	L873	S874	L875	S876	L877	S878	L879	S880	L881	S882	L883	S884	L885	S886	L887	S888	L889	S890	L891	S892	L893	S894	L895	S896	L897	S898	L899	S900	L901	S902	L903	S904	L905	S906	L907	S908	L909	S910	L911	S912	L913	S914	L915	S916	L917	S918	L919	S920	L921	S922	L923	S924	L925	S926	L927	S928	L929	S930	L931	S932	L933	S934	L935	S936	L937	S938	L939	S940	L941	S942	L943	S944	L945	S946	L947	S948	L949	S950	L951	S952	L953	S954	L955	S956	L957	S958	L959	S960	L961	S962	L963	S964	L965	S966	L967	S968	L969	S970	L971	S972	L973	S974	L975	S976	L977	S978	L979	S980	L981	S982	L983	S984	L985	S986	L987	S988	L989	S990	L991	S992	L993	S994	L995	S996	L997	S998	L999	S1000
K371	E374	I375	R378	D383	S384	D385	E386	I387	K388	E389	Y390	Y391	Y392	I393	E394	T395	S396	I397	Y398	T399	P400	I401	E402	Y403	C406	G407	Y408	Y414	E415	L416	Y417	C418	K419	S420	N421	V422	E423	Y424	F425	L426	Q427	GLU	PHE	ASN	ASN	LEU	GLU	ILE	SER	ALA	VAL	HIS	ARG	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
D801	K302	T303	I306	Y307	D308	L311	I314	G318	E319	I320	L325	E326	S327	I328	N329	N330	N331	K334	S335	N336	N337	K338	I339	I340	A341	D342	H343	L344	S345	G346	T347	N348	I349	P350	S351	I352	P353	G356	D357	V358	A359	E360	N361	V362	P363	E364	I365	L366	P367	V368	A369	I370																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L189	G193	C194	I198	P199	D200	K206	T211	I215	K220	D221	V227	A230	C237	S238	G239	F240	L241	N242	S243	L244	V248	V252	R253	S254	I255	V256	L257	R258	Q262	V266	V277	I283	L284	P285	K286	K287	L288	D292	D293	K294	F299	S300																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.19Å 109.24Å 182.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.90 46.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.91-2.90) 96.7 (46.91-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.265 , 0.288 0.259 , 0.278	Depositor DCC
R_{free} test set	1394 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: 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	0.35	0/3455	0.36	0/4659
1	B	0.38	0/3455	0.41	2/4659 (0.0%)
All	All	0.36	0/6910	0.39	2/9318 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	GLY	C-N-CD	5.80	140.57	128.40
1	B	458	CYS	O-C-N	5.26	131.12	122.70

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	3389	0	3427	246	1
1	B	3389	0	3427	279	1
2	A	53	0	31	4	0
2	B	53	0	31	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	6887	0	6916	497	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (497) 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:489:MET:HE1	1:B:502:PHE:CZ	1.68	1.27
1:B:489:MET:CE	1:B:502:PHE:HZ	1.49	1.26
1:A:489:MET:CE	1:A:502:PHE:CZ	2.23	1.20
1:B:162:LYS:CE	1:B:172:TYR:HE1	1.56	1.17
1:B:492:ALA:HB1	1:B:497:VAL:HG21	1.22	1.16
1:B:489:MET:CE	1:B:502:PHE:CZ	2.25	1.15
1:A:109:PHE:CE1	1:B:109:PHE:CE1	2.34	1.15
1:A:186:LYS:HE3	1:A:187:TYR:CE2	1.81	1.15
1:A:497:VAL:HG22	1:B:495:LEU:CD1	1.77	1.14
1:A:489:MET:HE2	1:A:502:PHE:HZ	0.98	1.14
1:B:425:PHE:CE2	1:B:499:LYS:HD2	1.82	1.13
1:B:162:LYS:HE3	1:B:172:TYR:HE1	1.08	1.13
1:A:489:MET:CE	1:A:502:PHE:HZ	1.59	1.12
1:A:495:LEU:CD1	1:B:497:VAL:HG22	1.80	1.10
1:A:331:ASN:N	1:A:348:ASN:HD21	1.49	1.09
1:B:365:LEU:HD21	1:B:395:THR:HG22	1.35	1.09
1:A:497:VAL:HG22	1:B:495:LEU:HD11	1.10	1.08
1:B:162:LYS:HE3	1:B:172:TYR:CE1	1.88	1.07
1:A:489:MET:HE1	1:A:502:PHE:CZ	1.85	1.07
1:A:426:LEU:CD2	1:A:461:LYS:HD2	1.82	1.07
1:B:150:ARG:HG3	1:B:150:ARG:HH11	0.90	1.06
1:B:230:ALA:HB1	1:B:256:VAL:HA	1.38	1.06
1:A:489:MET:HE2	1:A:502:PHE:CZ	1.86	1.05
1:A:495:LEU:HD11	1:B:497:VAL:CG2	1.85	1.05
1:A:417:TYR:HE2	1:A:465:LEU:HD21	1.17	1.03
1:A:472:VAL:HG23	1:A:493:LEU:HD22	1.38	1.01
1:A:105:MET:HE1	1:B:113:SER:HA	1.42	1.01
1:B:150:ARG:NH1	1:B:150:ARG:HG3	1.68	1.01
1:B:492:ALA:O	1:B:497:VAL:HG23	1.57	1.00
1:A:68:LEU:HD11	1:A:157:ILE:HD13	1.42	1.00
1:A:384:SER:OG	1:A:386:GLU:HG2	1.62	0.99
1:A:420:SER:O	1:A:466:LYS:HD2	1.63	0.96
1:A:113:SER:HA	1:B:105:MET:HE1	1.45	0.95
1:A:320:ILE:HG23	1:A:325:LEU:HD12	1.49	0.94
1:B:306:LEU:O	1:B:306:LEU:HD12	1.67	0.94
1:B:253:ARG:HB2	1:B:284:LEU:HD11	1.45	0.94
1:A:495:LEU:HD11	1:B:497:VAL:HG22	0.95	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:HA	1:B:206:LYS:HE2	1.47	0.94
1:B:359:ALA:HB3	1:B:362:VAL:HG11	1.49	0.94
1:A:113:SER:HA	1:B:105:MET:CE	1.97	0.94
1:B:160:LEU:O	1:B:160:LEU:HD12	1.68	0.93
1:B:150:ARG:CG	1:B:150:ARG:HH11	1.81	0.93
1:B:359:ALA:O	1:B:362:VAL:HG12	1.69	0.92
1:A:342:ASP:HB3	1:A:346[A]:CYS:H	1.34	0.92
1:A:472:VAL:CG2	1:A:493:LEU:CD2	2.48	0.92
1:B:162:LYS:CE	1:B:172:TYR:CE1	2.49	0.92
1:A:331:ASN:H	1:A:348:ASN:HD21	1.00	0.91
1:B:465:LEU:HG	1:B:473:ILE:HD11	1.52	0.91
1:A:359:ALA:O	1:A:362:VAL:HG12	1.69	0.91
1:B:330:MET:CE	1:B:339:ILE:HG23	2.00	0.91
1:A:342:ASP:HB3	1:A:346[B]:CYS:H	1.34	0.91
1:A:417:TYR:CE2	1:A:465:LEU:HD21	2.05	0.90
1:B:347:THR:HG22	1:B:348:ASN:N	1.87	0.89
1:A:421:ASN:O	1:A:466:LYS:HB2	1.74	0.88
1:A:389:ASP:CG	1:A:494:ARG:NH2	2.26	0.88
1:A:109:PHE:CZ	1:B:109:PHE:CE1	2.61	0.88
1:A:331:ASN:H	1:A:348:ASN:ND2	1.72	0.87
1:A:294:LYS:HD3	1:A:306:LEU:HD13	1.57	0.87
1:A:365:LEU:HD21	1:A:395:THR:HG22	1.55	0.87
1:A:426:LEU:HD22	1:A:461:LYS:HD2	1.54	0.86
1:A:105:MET:CE	1:B:113:SER:HA	2.05	0.86
1:A:186:LYS:HE3	1:A:187:TYR:HE2	1.40	0.85
1:B:42:TYR:O	1:B:185:GLY:HA2	1.76	0.85
1:A:472:VAL:CG2	1:A:493:LEU:HD22	2.06	0.85
1:A:465:LEU:O	1:A:470:ASN:HA	1.77	0.85
1:A:417:TYR:CD2	1:A:465:LEU:HD11	2.11	0.84
1:B:162:LYS:HE2	1:B:172:TYR:HE1	1.43	0.83
1:B:38:HIS:ND1	1:B:39:THR:HG23	1.93	0.83
1:A:146:MET:HG3	1:A:150:ARG:NH1	1.93	0.83
1:B:347:THR:HG22	1:B:348:ASN:H	1.43	0.83
1:B:489:MET:HE2	1:B:502:PHE:CZ	2.12	0.83
1:B:334:LYS:H	1:B:334:LYS:HD2	1.42	0.83
1:A:328:LEU:HB3	1:A:349:ILE:HD11	1.59	0.82
1:A:424:VAL:HG11	1:A:461:LYS:HE3	1.62	0.82
1:A:163:LEU:HD12	1:A:325:LEU:HD23	1.62	0.82
1:A:320:ILE:CG2	1:A:325:LEU:HD12	2.10	0.82
1:B:283:ILE:HD13	1:B:301:ASP:CG	2.00	0.82
1:A:344:LEU:HD13	1:A:379:ARG:NH2	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LEU:CD1	1:B:473:ILE:HD11	2.10	0.81
1:B:492:ALA:HB1	1:B:497:VAL:CG2	2.08	0.81
1:B:465:LEU:CG	1:B:473:ILE:HD11	2.09	0.80
1:A:472:VAL:HG21	1:A:493:LEU:CD2	2.10	0.80
1:A:492:ALA:HB1	1:A:497:VAL:HG21	1.62	0.80
1:A:492:ALA:O	1:A:497:VAL:HG23	1.81	0.80
1:A:109:PHE:CE1	1:B:109:PHE:CD1	2.70	0.80
1:B:320:ILE:CG2	1:B:325:LEU:HD12	2.13	0.79
1:B:320:ILE:HG23	1:B:325:LEU:HD12	1.65	0.79
1:A:344:LEU:HD13	1:A:379:ARG:HH22	1.46	0.78
1:A:94:VAL:HB	1:A:95:PRO:CD	2.13	0.78
1:B:162:LYS:HZ1	1:B:170:SER:HB2	1.50	0.77
1:A:389:ASP:CB	1:A:494:ARG:HH22	1.98	0.77
1:A:426:LEU:CD2	1:A:461:LYS:CD	2.62	0.77
1:B:330:MET:HE1	1:B:339:ILE:CG2	2.15	0.77
1:A:328:LEU:CB	1:A:349:ILE:HD11	2.15	0.76
1:A:465:LEU:HD23	1:A:468:GLU:OE2	1.86	0.76
1:A:426:LEU:HD22	1:A:461:LYS:CD	2.14	0.76
1:A:389:ASP:HB3	1:A:494:ARG:HH22	1.47	0.76
1:A:387:ILE:C	1:A:387:ILE:HD12	2.06	0.76
1:B:86:GLY:HA2	2:B:1506:FAD:O3B	1.84	0.75
1:A:331:ASN:N	1:A:348:ASN:ND2	2.30	0.75
1:A:472:VAL:HG23	1:A:493:LEU:CD2	2.08	0.75
1:B:384:SER:OG	1:B:386:GLU:HG2	1.86	0.75
1:B:330:MET:HE1	1:B:339:ILE:HG23	1.68	0.75
1:A:330:MET:CE	1:A:339:ILE:HD12	2.15	0.74
1:B:109:PHE:HA	1:B:113:SER:HB2	1.67	0.74
1:A:237:CYS:HA	1:A:240:PHE:CE2	2.23	0.74
1:A:387:ILE:HD12	1:A:387:ILE:O	1.87	0.74
1:B:425:PHE:CZ	1:B:499:LYS:HD2	2.23	0.74
1:A:160:LEU:O	1:A:160:LEU:HD12	1.87	0.73
1:A:186:LYS:CE	1:A:187:TYR:CE2	2.67	0.73
1:A:330:MET:HE3	1:A:339:ILE:HG23	1.69	0.73
1:B:68:LEU:HD11	1:B:157:ILE:HD13	1.71	0.73
1:B:465:LEU:O	1:B:470:ASN:HA	1.88	0.73
1:A:497:VAL:CG2	1:B:495:LEU:CD1	2.64	0.73
1:A:109:PHE:CZ	1:B:109:PHE:CD1	2.77	0.72
1:B:489:MET:HE1	1:B:502:PHE:HZ	1.14	0.72
1:B:472:VAL:HG22	1:B:497:VAL:O	1.90	0.72
1:B:331:ASN:O	1:B:340:ILE:HG12	1.90	0.72
1:B:242:ASN:HB2	1:B:248:VAL:HG21	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LYS:HB3	1:B:358:VAL:O	1.91	0.71
1:B:420:SER:O	1:B:466:LYS:HD2	1.90	0.71
1:A:306:LEU:HD12	1:A:306:LEU:O	1.90	0.71
1:B:326:GLU:H	1:B:326:GLU:CD	1.94	0.71
1:B:489:MET:CE	1:B:502:PHE:CE2	2.73	0.71
1:A:255:ILE:HD12	1:A:262:GLN:NE2	2.05	0.70
1:A:301:ASP:O	1:A:302:LYS:HB2	1.91	0.70
1:B:330:MET:HE2	1:B:339:ILE:HG23	1.73	0.70
1:B:283:ILE:HD13	1:B:301:ASP:OD2	1.90	0.70
1:B:465:LEU:HG	1:B:473:ILE:CD1	2.21	0.70
1:B:301:ASP:O	1:B:302:LYS:HB2	1.92	0.69
1:B:320:ILE:HD12	1:B:337:ASN:O	1.92	0.69
1:A:55:ALA:CB	1:A:370:ILE:HG23	2.21	0.69
1:A:355:VAL:HG12	1:A:356:GLY:N	2.05	0.69
1:B:352:ILE:N	1:B:352:ILE:HD12	2.08	0.69
1:A:371:LYS:NZ	1:B:504:ASN:O	2.26	0.68
1:B:368:VAL:HG21	1:B:393:ILE:HD12	1.75	0.68
1:A:94:VAL:HB	1:A:95:PRO:HD3	1.73	0.68
1:B:359:ALA:HB3	1:B:362:VAL:CG1	2.22	0.68
1:A:167:ASN:HB2	1:A:185:GLY:O	1.93	0.68
1:B:252:VAL:HG11	1:B:256:VAL:HG12	1.76	0.68
1:B:425:PHE:HE2	1:B:464:CYS:SG	2.15	0.68
1:A:359:ALA:HB3	1:A:362:VAL:HG11	1.75	0.68
1:A:253:ARG:HG3	1:A:284:LEU:HD11	1.75	0.68
1:A:399:THR:HB	1:A:400:PRO:HD2	1.75	0.67
1:A:330:MET:CE	1:A:339:ILE:HG23	2.23	0.67
1:B:347:THR:CG2	1:B:348:ASN:H	2.06	0.67
1:A:109:PHE:CE1	1:B:109:PHE:CZ	2.82	0.67
1:B:425:PHE:CE2	1:B:464:CYS:SG	2.88	0.67
1:B:347:THR:CG2	1:B:348:ASN:N	2.56	0.66
1:A:146:MET:HG3	1:A:150:ARG:HH12	1.58	0.66
1:B:349:ILE:N	1:B:349:ILE:HD12	2.10	0.65
1:A:364:GLU:C	1:A:365:LEU:HD12	2.16	0.65
1:A:68:LEU:CD1	1:A:157:ILE:HD13	2.22	0.65
1:A:497:VAL:HG12	1:A:498:LYS:N	2.12	0.65
1:B:38:HIS:CE1	1:B:39:THR:HG23	2.32	0.65
1:A:338:LYS:HE2	1:A:357:ASP:O	1.97	0.65
1:A:355:VAL:CG1	1:A:356:GLY:N	2.59	0.65
1:A:404:GLY:H	1:A:482:ALA:HB1	1.61	0.65
1:B:330:MET:HG2	1:B:349:ILE:HD13	1.79	0.65
1:A:495:LEU:CD1	1:B:497:VAL:CG2	2.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:THR:HB	1:B:400:PRO:HD2	1.79	0.65
1:A:409:SER:OG	1:A:412:LYS:HB2	1.96	0.64
1:A:155:LYS:HE3	1:A:157:ILE:HD11	1.78	0.64
1:A:105:MET:HB3	1:A:109:PHE:HE2	1.63	0.64
1:B:294:LYS:HE3	1:B:306:LEU:CD1	2.28	0.64
1:B:359:ALA:O	1:B:362:VAL:CG1	2.45	0.63
1:A:389:ASP:CG	1:A:494:ARG:HH22	1.99	0.63
1:A:363:PRO:HG2	1:A:368:VAL:HG11	1.79	0.63
1:B:408:TYR:CD2	1:B:473:ILE:CG2	2.81	0.63
1:B:497:VAL:HG11	1:B:502:PHE:CE1	2.34	0.63
1:B:101:TYR:O	1:B:105:MET:HG3	1.99	0.63
1:B:364:GLU:C	1:B:365:LEU:HD12	2.19	0.62
1:B:489:MET:HE2	1:B:502:PHE:CE2	2.33	0.62
1:A:211:THR:HA	1:A:311:LEU:CD1	2.29	0.62
1:B:344:LEU:O	1:B:345:SER:HB2	1.98	0.62
1:A:55:ALA:HB2	1:A:370:ILE:HG23	1.80	0.62
1:B:162:LYS:NZ	1:B:170:SER:HB2	2.15	0.62
1:B:334:LYS:CD	1:B:334:LYS:H	2.12	0.62
1:A:69:LEU:HD23	1:A:69:LEU:C	2.19	0.62
1:B:162:LYS:HG3	1:B:170:SER:OG	1.99	0.62
1:B:155:LYS:HD2	1:B:157:ILE:HD11	1.82	0.62
1:A:504:ASN:O	1:B:371:LYS:NZ	2.33	0.61
1:B:320:ILE:HG23	1:B:325:LEU:CD1	2.31	0.61
1:A:109:PHE:HA	1:A:113:SER:HB3	1.83	0.61
1:A:342:ASP:OD1	1:A:343:HIS:N	2.34	0.61
1:B:489:MET:HE1	1:B:502:PHE:CE2	2.32	0.61
1:A:363:PRO:HG3	1:A:393:ILE:HD11	1.83	0.61
1:B:162:LYS:HE2	1:B:172:TYR:CE1	2.26	0.60
1:B:366:ALA:HB3	1:B:367:PRO:HD3	1.83	0.60
1:A:171:TYR:CE2	1:A:181:GLU:HB3	2.35	0.60
1:A:379:ARG:HD3	1:A:386:GLU:O	2.00	0.60
1:A:472:VAL:HG21	1:A:493:LEU:HD23	1.83	0.60
1:B:408:TYR:CD2	1:B:473:ILE:HG22	2.35	0.60
1:A:320:ILE:HG23	1:A:325:LEU:CD1	2.28	0.60
1:B:128:LYS:O	1:B:132:THR:HG23	2.02	0.60
1:B:406:CYS:SG	1:B:493:LEU:HD12	2.42	0.60
1:A:113:SER:HA	1:B:105:MET:HE3	1.83	0.60
1:B:306:LEU:HD12	1:B:306:LEU:C	2.20	0.60
1:A:363:PRO:HG3	1:A:393:ILE:CD1	2.31	0.60
1:B:375:ILE:HG12	1:B:378:ARG:NH2	2.16	0.60
1:B:171:TYR:CZ	1:B:181:GLU:HB3	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:HE2	1:A:300:SER:HA	1.85	0.59
1:B:465:LEU:HD11	1:B:473:ILE:HD11	1.83	0.59
1:B:294:LYS:HE3	1:B:306:LEU:HD11	1.85	0.59
1:A:330:MET:HE1	1:A:339:ILE:HD12	1.85	0.59
1:B:329:ASN:O	1:B:348:ASN:ND2	2.36	0.59
1:A:193:GLY:HA2	1:A:357:ASP:HB2	1.85	0.59
1:A:404:GLY:N	1:A:482:ALA:HB1	2.18	0.59
1:A:417:TYR:O	1:A:421:ASN:ND2	2.26	0.58
1:B:200:ASP:CA	1:B:206:LYS:HE2	2.28	0.58
1:B:416:LEU:HB3	1:B:417:TYR:CE1	2.37	0.58
1:B:336:ASN:HD22	1:B:336:ASN:C	2.06	0.58
1:A:230:ALA:HB1	1:A:256:VAL:HA	1.84	0.58
1:B:155:LYS:HD2	1:B:157:ILE:CD1	2.33	0.58
1:A:370:ILE:O	1:A:374:GLU:HG3	2.03	0.58
1:B:492:ALA:C	1:B:497:VAL:HG23	2.23	0.58
1:B:425:PHE:CD2	1:B:499:LYS:HD2	2.35	0.58
1:A:69:LEU:HD23	1:A:70:PHE:N	2.19	0.58
1:B:155:LYS:CD	1:B:157:ILE:HD11	2.34	0.58
1:A:403:TYR:OH	1:A:476:HIS:HD2	1.87	0.57
1:B:465:LEU:HG	1:B:473:ILE:CG1	2.34	0.57
1:B:211:THR:HA	1:B:311:LEU:HD12	1.86	0.57
1:B:421:ASN:CG	1:B:467:ASN:HD21	2.07	0.57
1:B:69:LEU:HD23	1:B:69:LEU:C	2.25	0.57
1:A:193:GLY:N	1:A:358:VAL:HG13	2.18	0.57
1:B:370:ILE:O	1:B:374:GLU:HG2	2.04	0.57
1:B:120:PHE:HE2	1:B:123:LEU:HB2	1.70	0.57
1:B:462:LEU:CD2	1:B:475:PHE:HD1	2.17	0.57
1:B:403:TYR:OH	1:B:476:HIS:HD2	1.88	0.57
1:B:360:GLU:O	1:B:361:ASN:HB2	2.05	0.57
1:A:401:ILE:HG23	1:A:401:ILE:O	2.04	0.57
1:A:497:VAL:CG1	1:A:498:LYS:N	2.68	0.57
1:B:120:PHE:CE2	1:B:123:LEU:HB2	2.40	0.57
1:B:171:TYR:C	1:B:171:TYR:CD1	2.79	0.57
1:B:378:ARG:HB3	1:B:384:SER:HB2	1.86	0.57
1:B:162:LYS:NZ	1:B:170:SER:CB	2.67	0.56
1:A:389:ASP:CB	1:A:494:ARG:NH2	2.65	0.56
1:B:256:VAL:O	1:B:257:LEU:HB2	2.05	0.56
1:A:389:ASP:HB3	1:A:494:ARG:NH2	2.19	0.56
1:B:240:PHE:O	1:B:244:LEU:HG	2.06	0.56
1:B:365:LEU:HB3	1:B:367:PRO:HD2	1.88	0.56
1:B:408:TYR:HD2	1:B:473:ILE:HG22	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HB	1:B:95:PRO:HD3	1.87	0.56
1:A:489:MET:HE1	1:A:502:PHE:CE1	2.39	0.56
1:A:121:ASP:O	1:B:121:ASP:N	2.37	0.56
1:A:333:ASN:ND2	1:A:360:GLU:OE2	2.39	0.56
1:B:283:ILE:CG2	1:B:299:PHE:HB3	2.35	0.55
1:A:101:TYR:O	1:A:105:MET:HG3	2.07	0.55
1:A:319:ASP:C	1:A:320:ILE:HD12	2.27	0.55
1:B:149:LEU:HD13	1:B:156:TYR:HB2	1.88	0.55
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.89	0.55
1:B:283:ILE:CD1	1:B:301:ASP:CG	2.74	0.55
1:B:425:PHE:CZ	1:B:499:LYS:CD	2.89	0.55
1:A:424:VAL:HG11	1:A:461:LYS:CE	2.33	0.55
1:A:109:PHE:CD1	1:B:109:PHE:CZ	2.94	0.55
1:B:292:ASP:O	1:B:293:ASP:HB2	2.07	0.55
1:B:286:LYS:HE2	1:B:300:SER:HA	1.88	0.54
1:B:294:LYS:HG2	1:B:306:LEU:HD13	1.88	0.54
1:B:211:THR:HA	1:B:311:LEU:CD1	2.37	0.54
1:B:330:MET:CE	1:B:347:THR:CG2	2.85	0.54
1:A:342:ASP:CB	1:A:346[B]:CYS:HB2	2.37	0.54
1:A:417:TYR:HD2	1:A:465:LEU:HD11	1.68	0.54
1:B:336:ASN:ND2	1:B:338:LYS:HG3	2.23	0.54
1:B:255:ILE:HD11	1:B:258:ARG:NH1	2.22	0.54
1:A:146:MET:CG	1:A:150:ARG:HH12	2.20	0.54
1:B:301:ASP:HB3	1:B:303:THR:OG1	2.08	0.54
1:A:193:GLY:H	1:A:358:VAL:HG13	1.72	0.54
1:A:301:ASP:HB3	1:A:303:THR:OG1	2.07	0.54
1:A:113:SER:CA	1:B:105:MET:CE	2.81	0.54
1:B:477:TYR:CZ	1:B:479:GLY:HA3	2.43	0.54
1:A:423:GLU:HG3	1:A:424:VAL:N	2.22	0.54
1:B:349:ILE:CG2	1:B:352:ILE:HD13	2.38	0.54
1:A:186:LYS:CE	1:A:187:TYR:HE2	2.14	0.54
1:B:193:GLY:N	1:B:358:VAL:HG13	2.23	0.54
1:A:287:LYS:C	1:A:288:LEU:HD12	2.28	0.53
1:B:408:TYR:HB2	1:B:473:ILE:HG22	1.90	0.53
1:A:169:VAL:HG23	1:A:188:ILE:HD13	1.90	0.53
1:B:416:LEU:CB	1:B:417:TYR:CE1	2.92	0.53
1:B:364:GLU:O	1:B:365:LEU:HD12	2.09	0.53
1:A:210:ILE:HG13	1:A:311:LEU:HD13	1.90	0.53
1:B:366:ALA:O	1:B:370:ILE:HG13	2.09	0.53
1:B:336:ASN:HD21	1:B:338:LYS:HB2	1.74	0.53
1:A:272:MET:HG2	1:A:400:PRO:HG2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASN:O	1:A:504:ASN:OD1	2.26	0.53
1:A:262:GLN:O	1:A:266:VAL:HG23	2.09	0.52
1:A:366:ALA:O	1:A:370:ILE:HG13	2.08	0.52
1:A:59:GLU:OE1	1:A:59:GLU:HA	2.09	0.52
1:B:128:LYS:HA	1:B:131:VAL:HG22	1.90	0.52
1:B:156:TYR:C	1:B:157:ILE:HD12	2.29	0.52
1:B:171:TYR:OH	1:B:181:GLU:HG2	2.09	0.52
1:B:351:SER:HB2	1:B:352:ILE:HD12	1.91	0.52
1:A:290:LYS:O	1:A:291:MET:CG	2.58	0.52
1:B:198:ILE:HG23	1:B:199:PRO:HD2	1.90	0.52
1:B:349:ILE:N	1:B:349:ILE:CD1	2.73	0.52
1:B:363:PRO:HG2	1:B:393:ILE:HD11	1.92	0.52
1:B:163:LEU:HD12	1:B:325:LEU:HD23	1.92	0.52
1:B:342:ASP:OD1	1:B:344:LEU:HB2	2.10	0.52
1:B:462:LEU:HD23	1:B:475:PHE:HD1	1.75	0.52
1:B:237:CYS:HA	1:B:240:PHE:CE2	2.45	0.51
1:B:262:GLN:O	1:B:266:VAL:HG23	2.10	0.51
1:B:365:LEU:HD21	1:B:395:THR:CG2	2.23	0.51
1:A:128:LYS:O	1:A:131:VAL:HG22	2.09	0.51
1:A:362:VAL:HG13	1:A:362:VAL:O	2.11	0.51
1:B:104:HIS:O	1:B:108:ILE:HG13	2.10	0.51
1:A:465:LEU:O	1:A:470:ASN:CA	2.56	0.51
1:B:68:LEU:HD12	1:B:155:LYS:O	2.10	0.51
1:A:397:ILE:HG22	1:A:399:THR:HG23	1.93	0.51
1:A:409:SER:OG	1:A:412:LYS:HE2	2.11	0.51
1:A:106:GLY:O	1:A:110:LYS:HG2	2.11	0.51
1:A:328:LEU:HB2	1:A:349:ILE:HD11	1.92	0.51
1:A:366:ALA:N	1:A:367:PRO:CD	2.73	0.51
1:B:131:VAL:HG23	1:B:132:THR:N	2.26	0.51
1:A:172:TYR:N	1:A:172:TYR:CD1	2.79	0.51
1:A:328:LEU:HB3	1:A:349:ILE:CD1	2.34	0.51
1:B:255:ILE:HD11	1:B:258:ARG:CZ	2.41	0.51
1:A:44:TYR:HB3	1:A:67:VAL:HG22	1.93	0.51
1:A:211:THR:HA	1:A:311:LEU:HD12	1.93	0.51
1:A:389:ASP:CG	1:A:494:ARG:HH21	2.11	0.51
1:B:401:ILE:O	1:B:401:ILE:HG23	2.10	0.51
1:A:365:LEU:HB3	1:A:367:PRO:HD2	1.93	0.50
1:B:254:SER:OG	1:B:255:ILE:HG12	2.10	0.50
1:A:171:TYR:CZ	1:A:181:GLU:HB3	2.47	0.50
1:B:283:ILE:CD1	1:B:301:ASP:OD2	2.59	0.50
1:A:226:LEU:HD12	1:A:249:THR:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HE1	1:B:339:ILE:HG21	1.92	0.50
1:B:94:VAL:HB	1:B:95:PRO:CD	2.41	0.50
1:B:146:MET:C	1:B:148:GLY:H	2.13	0.50
1:B:193:GLY:H	1:B:358:VAL:HG13	1.75	0.50
1:A:105:MET:HE1	1:B:113:SER:CA	2.29	0.50
1:A:417:TYR:CE2	1:A:465:LEU:HD11	2.46	0.50
1:B:150:ARG:NH1	1:B:150:ARG:CG	2.49	0.50
1:A:109:PHE:CD1	1:B:109:PHE:CE1	2.96	0.50
1:B:366:ALA:N	1:B:367:PRO:CD	2.74	0.50
1:B:408:TYR:CE1	1:B:416:LEU:HD12	2.47	0.50
1:B:162:LYS:NZ	1:B:170:SER:OG	2.38	0.49
1:B:254:SER:OG	1:B:255:ILE:N	2.44	0.49
1:A:55:ALA:HB1	1:A:370:ILE:HG23	1.93	0.49
1:B:356:GLY:O	1:B:362:VAL:HG11	2.13	0.49
1:B:109:PHE:O	1:B:113:SER:HB3	2.13	0.49
1:B:330:MET:SD	1:B:347:THR:HG21	2.53	0.49
1:A:384:SER:OG	1:A:386:GLU:CG	2.49	0.49
1:B:497:VAL:HG12	1:B:498:LYS:N	2.27	0.49
1:A:251:ALA:HB1	1:A:283:ILE:O	2.13	0.49
1:A:426:LEU:HD23	1:A:461:LYS:HD2	1.87	0.49
1:B:128:LYS:O	1:B:131:VAL:HG22	2.13	0.48
1:A:328:LEU:HD13	1:A:349:ILE:HD13	1.94	0.48
1:B:248:VAL:HG21	1:B:277:VAL:HG22	1.94	0.48
1:B:416:LEU:CB	1:B:417:TYR:CD1	2.96	0.48
1:A:292:ASP:O	1:A:293:ASP:HB2	2.14	0.48
1:B:163:LEU:HD12	1:B:325:LEU:CD2	2.43	0.48
1:B:199:PRO:HD3	1:B:314:ILE:HD11	1.96	0.48
1:B:469:ASP:OD1	1:B:500:LYS:HE3	2.14	0.48
1:B:162:LYS:HG3	1:B:170:SER:HG	1.78	0.48
1:B:352:ILE:N	1:B:352:ILE:CD1	2.76	0.48
1:B:320:ILE:CD1	1:B:337:ASN:O	2.61	0.47
1:A:290:LYS:O	1:A:291:MET:HG2	2.14	0.47
1:B:340:ILE:HD12	1:B:360:GLU:OE1	2.12	0.47
1:B:336:ASN:ND2	1:B:338:LYS:H	2.13	0.47
1:B:227:VAL:HG21	1:B:238:SER:HB3	1.96	0.47
1:A:210:ILE:O	1:A:311:LEU:HD12	2.13	0.47
1:B:388:MET:HG2	1:B:390:TYR:CZ	2.49	0.47
1:B:417:TYR:CD1	1:B:417:TYR:N	2.82	0.47
1:B:471:ARG:HA	1:B:498:LYS:HG2	1.96	0.47
1:A:424:VAL:HA	1:A:462:LEU:O	2.15	0.47
1:A:118:TRP:CZ2	1:B:106:GLY:HA3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:CD2	1:A:160:LEU:HD23	2.50	0.47
1:A:387:ILE:C	1:A:387:ILE:CD1	2.77	0.47
1:B:106:GLY:O	1:B:110:LYS:HG3	2.15	0.47
1:B:471:ARG:HD2	1:B:496:LYS:HB3	1.96	0.46
1:A:384:SER:HG	1:A:386:GLU:HG2	1.77	0.46
1:B:408:TYR:HD2	1:B:473:ILE:CG2	2.25	0.46
1:A:128:LYS:O	1:A:132:THR:HG23	2.15	0.46
1:B:359:ALA:C	1:B:362:VAL:HG12	2.33	0.46
1:A:253:ARG:O	1:A:282:GLY:HA2	2.14	0.46
1:A:173:LEU:O	1:A:174:LYS:HG3	2.16	0.46
1:A:421:ASN:O	1:A:466:LYS:CB	2.56	0.46
1:A:426:LEU:HD21	1:A:461:LYS:HD2	1.86	0.46
1:A:109:PHE:O	1:A:113:SER:OG	2.28	0.46
1:A:155:LYS:CE	1:A:157:ILE:HD11	2.45	0.46
1:A:325:LEU:CD1	1:A:339:ILE:HD11	2.46	0.46
1:A:421:ASN:O	1:A:466:LYS:N	2.39	0.46
1:A:472:VAL:CG2	1:A:493:LEU:HD23	2.38	0.46
1:B:423:GLU:HG2	1:B:425:PHE:CZ	2.51	0.46
1:B:392:TYR:CD1	1:B:493:LEU:HB3	2.50	0.46
1:A:261:ASP:OD2	1:A:461:LYS:NZ	2.49	0.45
1:B:472:VAL:HG21	1:B:493:LEU:HD23	1.98	0.45
1:B:146:MET:C	1:B:148:GLY:N	2.70	0.45
1:B:416:LEU:C	1:B:417:TYR:CD1	2.89	0.45
1:A:477:TYR:CZ	1:A:479:GLY:HA3	2.51	0.45
1:B:59:GLU:HA	1:B:59:GLU:OE1	2.16	0.45
1:A:155:LYS:CD	1:A:157:ILE:HD11	2.46	0.45
1:A:331:ASN:HB2	1:A:348:ASN:OD1	2.16	0.45
1:B:403:TYR:OH	1:B:476:HIS:CD2	2.69	0.45
1:B:414:TYR:CD1	1:B:419:LYS:HA	2.51	0.45
1:B:472:VAL:CG2	1:B:493:LEU:CD2	2.94	0.45
1:A:240:PHE:O	1:A:244:LEU:HG	2.17	0.45
1:A:196:PRO:HD3	1:A:316:ARG:NH1	2.31	0.45
1:B:294:LYS:CG	1:B:306:LEU:HD13	2.47	0.45
1:A:105:MET:O	1:A:109:PHE:CD2	2.70	0.45
1:A:342:ASP:CB	1:A:346[A]:CYS:HB2	2.46	0.45
1:A:402:GLU:OE1	1:A:480:PRO:O	2.34	0.45
1:B:330:MET:CE	1:B:347:THR:HG21	2.46	0.45
1:A:113:SER:CA	1:B:105:MET:HE3	2.45	0.45
1:A:417:TYR:HD2	1:A:465:LEU:CD1	2.27	0.45
1:B:252:VAL:HG11	1:B:256:VAL:CG1	2.45	0.45
1:A:169:VAL:CG2	1:A:188:ILE:HD13	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HA	1:B:348:ASN:HD22	1.81	0.45
1:A:51:PRO:HD2	2:A:1506:FAD:O5'	2.16	0.44
1:B:331:ASN:O	1:B:340:ILE:CG1	2.63	0.44
1:B:340:ILE:CD1	1:B:360:GLU:OE1	2.65	0.44
1:A:417:TYR:CD2	1:A:465:LEU:CD1	2.92	0.44
1:B:160:LEU:HD12	1:B:160:LEU:C	2.37	0.44
1:B:330:MET:HE2	1:B:339:ILE:HD12	2.00	0.44
1:B:94:VAL:N	1:B:95:PRO:HD2	2.33	0.44
1:B:320:ILE:HG21	1:B:325:LEU:HD12	1.97	0.44
1:B:421:ASN:C	1:B:466:LYS:HB2	2.38	0.44
1:A:423:GLU:HG3	1:A:424:VAL:H	1.83	0.44
1:A:113:SER:CA	1:B:105:MET:HE1	2.33	0.44
1:B:97:LYS:HE2	1:B:398:TYR:CE2	2.52	0.44
1:B:397:ILE:HG22	1:B:399:THR:HG23	2.00	0.44
1:A:232:TYR:O	1:A:236:GLU:HG3	2.17	0.44
1:B:194:CYS:SG	1:B:318:GLY:HA2	2.58	0.44
1:B:330:MET:CE	1:B:347:THR:HG23	2.47	0.44
1:B:465:LEU:HD13	1:B:468:GLU:OE2	2.17	0.44
1:A:416:LEU:HB3	1:A:417:TYR:CD1	2.52	0.44
1:A:319:ASP:O	1:A:320:ILE:HD12	2.18	0.44
1:A:403:TYR:OH	1:A:476:HIS:CD2	2.69	0.44
1:B:171:TYR:CE1	1:B:181:GLU:HB3	2.51	0.44
1:B:334:LYS:HD2	1:B:334:LYS:N	2.22	0.44
1:B:348:ASN:C	1:B:349:ILE:HD12	2.39	0.44
1:A:160:LEU:C	1:A:160:LEU:HD12	2.38	0.43
1:A:416:LEU:C	1:A:417:TYR:HD1	2.21	0.43
1:B:459:LEU:O	1:B:477:TYR:CD1	2.70	0.43
1:B:356:GLY:O	1:B:362:VAL:CG1	2.67	0.43
1:B:399:THR:O	1:B:400:PRO:C	2.56	0.43
1:B:69:LEU:HD23	1:B:70:PHE:N	2.33	0.43
1:A:347:THR:OG1	1:A:352:ILE:O	2.32	0.43
1:A:323:LEU:O	1:A:324:ASN:HB3	2.19	0.43
1:B:416:LEU:HB2	1:B:417:TYR:CD1	2.53	0.43
1:A:330:MET:HE2	1:A:339:ILE:HD12	1.99	0.43
1:A:459:LEU:HD23	1:A:459:LEU:C	2.39	0.43
1:B:338:LYS:HE2	1:B:357:ASP:O	2.19	0.43
1:A:328:LEU:CB	1:A:349:ILE:CD1	2.91	0.43
1:A:359:ALA:O	1:A:362:VAL:CG1	2.54	0.43
1:B:287:LYS:C	1:B:288:LEU:HD12	2.40	0.43
1:A:94:VAL:CB	1:A:95:PRO:CD	2.87	0.43
1:A:461:LYS:HB3	1:A:461:LYS:HE2	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:CYS:C	1:B:239:GLY:N	2.71	0.42
1:B:320:ILE:HD13	1:B:339:ILE:HD13	2.00	0.42
1:B:378:ARG:HE	1:B:386:GLU:CD	2.21	0.42
1:A:73:VAL:HG11	1:A:82:TRP:CE2	2.53	0.42
1:A:68:LEU:HD13	1:A:155:LYS:HD2	2.02	0.42
1:B:352:ILE:HG22	1:B:353:PHE:N	2.34	0.42
1:A:365:LEU:N	1:A:365:LEU:HD12	2.35	0.42
1:B:383:ASP:OD1	1:B:383:ASP:O	2.37	0.42
1:A:250:VAL:HB	1:A:279:PHE:CD1	2.55	0.42
1:A:489:MET:CE	1:A:502:PHE:CE1	2.93	0.42
1:B:349:ILE:HG21	1:B:352:ILE:HD13	2.00	0.42
1:A:105:MET:CE	1:B:113:SER:CA	2.88	0.42
1:A:364:GLU:O	2:A:1506:FAD:H1'2	2.20	0.42
1:A:160:LEU:HA	2:A:1506:FAD:N1A	2.34	0.42
1:A:253:ARG:CG	1:A:284:LEU:HD11	2.45	0.42
1:A:126:ASP:N	1:B:117:GLY:O	2.43	0.42
1:B:344:LEU:O	1:B:345:SER:CB	2.68	0.42
1:A:200:ASP:HA	1:A:206:LYS:HE2	2.01	0.42
1:A:157:ILE:N	1:A:157:ILE:HD12	2.35	0.42
1:B:153:LYS:HD3	1:B:153:LYS:HA	1.86	0.42
1:B:215:ILE:HD12	1:B:311:LEU:HD22	2.02	0.42
1:B:198:ILE:HD11	1:B:211:THR:HG23	2.02	0.41
1:B:68:LEU:CD1	1:B:157:ILE:HD13	2.46	0.41
1:A:366:ALA:HA	2:A:1506:FAD:H4'	2.02	0.41
1:A:325:LEU:HD13	1:A:339:ILE:CD1	2.50	0.41
1:B:60:ALA:HB3	1:B:67:VAL:HG21	2.03	0.41
1:A:355:VAL:CG1	1:A:356:GLY:H	2.30	0.41
1:B:112:ASP:O	1:B:113:SER:C	2.58	0.41
1:B:427:GLN:HB2	1:B:427:GLN:HE21	1.63	0.41
1:B:497:VAL:CG1	1:B:498:LYS:N	2.83	0.41
1:B:256:VAL:O	1:B:256:VAL:HG23	2.19	0.41
1:B:174:LYS:NZ	1:B:177:LEU:O	2.54	0.41
1:B:200:ASP:HB3	1:B:206:LYS:CE	2.50	0.41
1:B:408:TYR:O	1:B:476:HIS:HE1	2.04	0.41
1:B:44:TYR:OH	1:B:189:LEU:HD22	2.21	0.41
1:A:215:ILE:HG23	1:A:216:PHE:N	2.36	0.41
1:A:320:ILE:HG21	1:A:325:LEU:HD12	1.99	0.41
1:A:342:ASP:HB3	1:A:346[B]:CYS:HB2	2.02	0.41
2:B:1506:FAD:H1'1	2:B:1506:FAD:H9	1.76	0.41
1:B:426:LEU:HA	1:B:460:ALA:O	2.21	0.40
1:A:164:LYS:HB3	1:A:168:THR:HG22	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:VAL:O	1:A:473:ILE:HD13	2.21	0.40
1:A:87:THR:HG23	1:A:91:VAL:HG23	2.02	0.40
1:B:220:LYS:HG2	1:B:221:ASP:N	2.36	0.40
1:A:112:ASP:O	1:A:113:SER:C	2.60	0.40
1:A:330:MET:HE1	1:A:339:ILE:HG23	2.02	0.40
1:B:237:CYS:C	1:B:239:GLY:H	2.24	0.40
1:A:344:LEU:O	1:A:345:SER:HB2	2.22	0.40
1:A:504:ASN:C	1:A:504:ASN:OD1	2.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:HIS:CG	1:B:38:HIS:CD2[3_544]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/542 (80%)	399 (92%)	33 (8%)	0	100	100
1	B	432/542 (80%)	402 (93%)	29 (7%)	1 (0%)	47	78
All	All	864/1084 (80%)	801 (93%)	62 (7%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	THR

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	371/457 (81%)	361 (97%)	10 (3%)	44	77
1	B	371/457 (81%)	359 (97%)	12 (3%)	39	73
All	All	742/914 (81%)	720 (97%)	22 (3%)	41	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	A	93	CYS
1	A	172	TYR
1	A	182	THR
1	A	207	GLU
1	A	218	LEU
1	A	348	ASN
1	A	464	CYS
1	A	465	LEU
1	A	505	CYS
1	B	93	CYS
1	B	150	ARG
1	B	171	TYR
1	B	253	ARG
1	B	301	ASP
1	B	308	ASP
1	B	334	LYS
1	B	336	ASN
1	B	337	ASN
1	B	427	GLN
1	B	459	LEU
1	B	464	CYS

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

Mol	Chain	Res	Type
1	A	63	HIS
1	A	90	ASN
1	A	262	GLN
1	A	348	ASN
1	A	427	GLN
1	A	476	HIS
1	A	487	GLN
1	B	158	ASN
1	B	242	ASN
1	B	336	ASN
1	B	348	ASN
1	B	427	GLN
1	B	467	ASN
1	B	476	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	B	1506	-	51,58,58	1.34	6 (11%)	60,89,89	1.54	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	1506	-	51,58,58	1.33	6 (11%)	60,89,89	1.53	7 (11%)

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	B	1506	-	-	8/30/50/50	0/6/6/6
2	FAD	A	1506	-	-	9/30/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1506	FAD	C10-N1	4.03	1.38	1.33
2	A	1506	FAD	C10-N1	3.98	1.38	1.33
2	B	1506	FAD	C2A-N3A	3.95	1.38	1.32
2	A	1506	FAD	C2A-N3A	3.94	1.38	1.32
2	B	1506	FAD	C4X-N5	3.63	1.38	1.33
2	A	1506	FAD	C4X-N5	3.52	1.38	1.33
2	B	1506	FAD	C4-N3	3.04	1.38	1.33
2	A	1506	FAD	C4-N3	3.02	1.38	1.33
2	A	1506	FAD	C2A-N1A	2.47	1.38	1.33
2	B	1506	FAD	C2A-N1A	2.46	1.38	1.33
2	A	1506	FAD	C1'-N10	2.26	1.50	1.48
2	B	1506	FAD	C1'-N10	2.21	1.50	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	FAD	C4-N3-C2	5.95	120.16	115.14
2	A	1506	FAD	C4-N3-C2	5.93	120.15	115.14
2	A	1506	FAD	N3A-C2A-N1A	-5.52	120.06	128.68
2	B	1506	FAD	N3A-C2A-N1A	-5.42	120.20	128.68
2	B	1506	FAD	P-O3P-PA	-3.47	120.90	132.83
2	A	1506	FAD	P-O3P-PA	-3.39	121.19	132.83
2	A	1506	FAD	C4X-N5-C5X	3.25	120.02	116.77
2	B	1506	FAD	C5X-C9A-N10	3.25	120.07	117.72
2	B	1506	FAD	C4X-N5-C5X	3.08	119.85	116.77
2	A	1506	FAD	C5X-C9A-N10	3.06	119.93	117.72
2	B	1506	FAD	C4X-C4-N3	-2.63	119.83	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	FAD	C3B-C2B-C1B	2.57	104.84	100.98
2	A	1506	FAD	C4X-C4-N3	-2.55	119.94	123.43
2	A	1506	FAD	C1'-N10-C9A	2.25	120.06	118.29
2	B	1506	FAD	C1'-N10-C9A	2.16	120.00	118.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1506	FAD	C3'-C4'-C5'-O5'
2	B	1506	FAD	O4'-C4'-C5'-O5'
2	B	1506	FAD	C5'-O5'-P-O2P
2	B	1506	FAD	PA-O3P-P-O5'
2	A	1506	FAD	O4B-C4B-C5B-O5B
2	A	1506	FAD	C3'-C4'-C5'-O5'
2	A	1506	FAD	O4'-C4'-C5'-O5'
2	A	1506	FAD	C5'-O5'-P-O1P
2	A	1506	FAD	C5'-O5'-P-O2P
2	A	1506	FAD	PA-O3P-P-O5'
2	B	1506	FAD	O4B-C4B-C5B-O5B
2	B	1506	FAD	C3B-C4B-C5B-O5B
2	A	1506	FAD	C3B-C4B-C5B-O5B
2	B	1506	FAD	C5'-O5'-P-O3P
2	A	1506	FAD	C5'-O5'-P-O3P
2	B	1506	FAD	C5'-O5'-P-O1P
2	A	1506	FAD	C1'-C2'-C3'-O3'

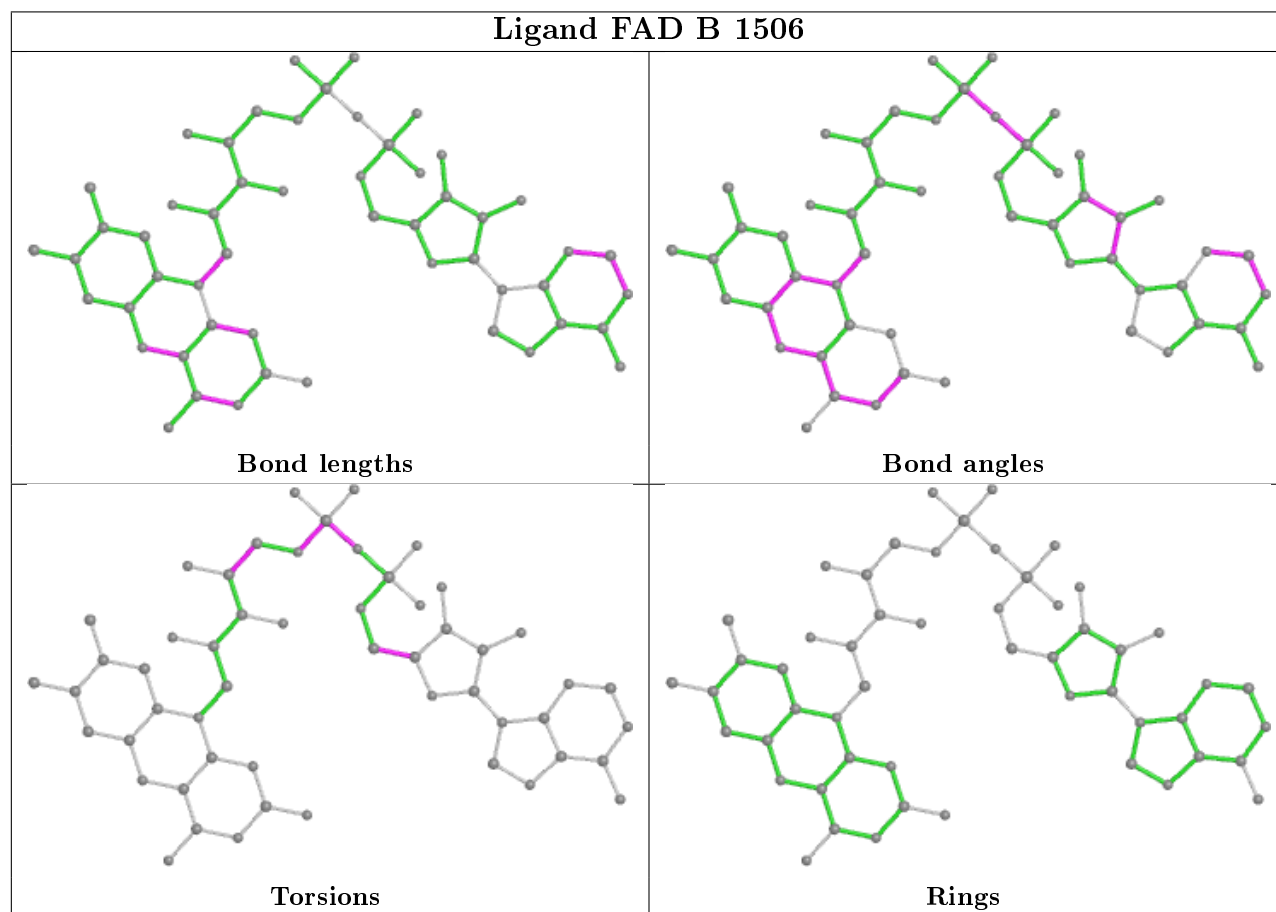
There are no ring outliers.

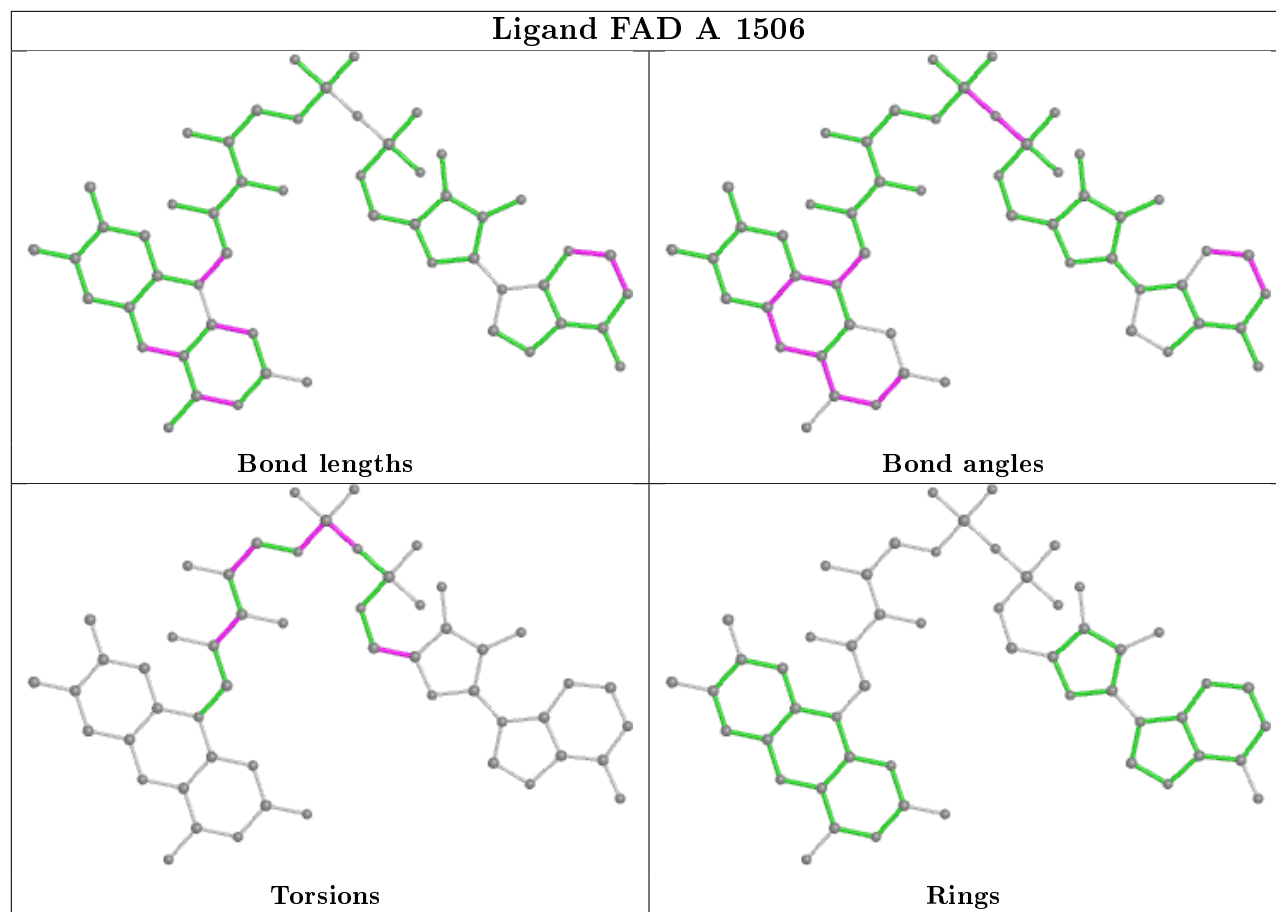
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1506	FAD	2	0
2	A	1506	FAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	437/542 (80%)	0.12	10 (2%) 60 58	17, 27, 66, 77	2 (0%)
1	B	437/542 (80%)	0.21	13 (2%) 50 45	17, 34, 64, 86	6 (1%)
All	All	874/1084 (80%)	0.17	23 (2%) 56 52	17, 30, 65, 86	8 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	4.7
1	A	426	LEU	4.2
1	B	172	TYR	4.1
1	A	459	LEU	3.7
1	A	467	ASN	3.6
1	B	179	LYS	3.5
1	B	505	CYS	3.4
1	A	420	SER	3.0
1	B	343	HIS	2.9
1	B	327	SER	2.8
1	B	69	LEU	2.7
1	B	182	THR	2.7
1	B	171	TYR	2.6
1	B	331	ASN	2.4
1	A	417	TYR	2.2
1	B	161	ALA	2.2
1	A	339	ILE	2.2
1	B	66	ARG	2.1
1	B	68	LEU	2.1
1	A	421	ASN	2.1
1	A	425	PHE	2.1
1	B	70	PHE	2.1
1	A	329	ASN	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](#)

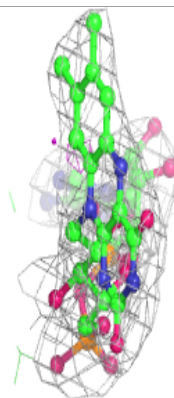
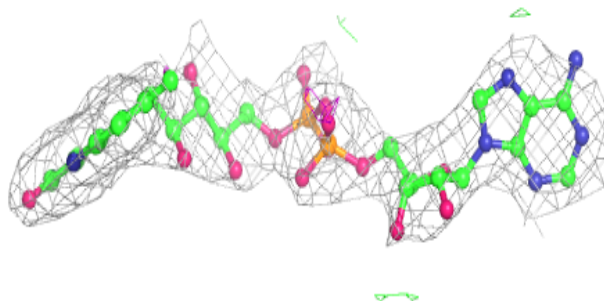
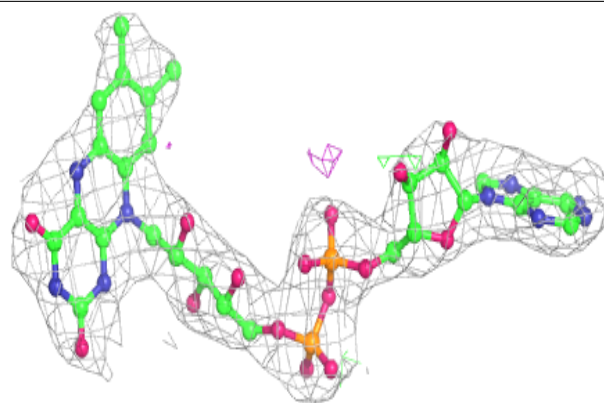
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	1506	53/53	0.95	0.18	26,30,37,39	0
2	FAD	A	1506	53/53	0.96	0.17	18,19,20,20	0

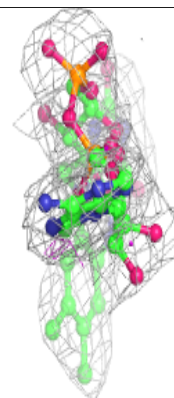
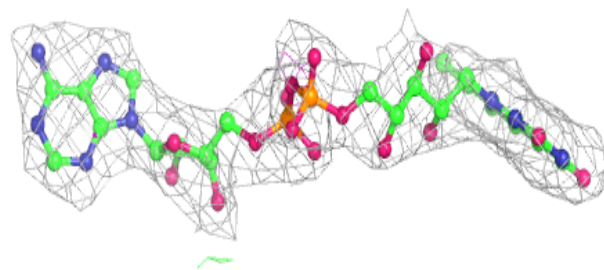
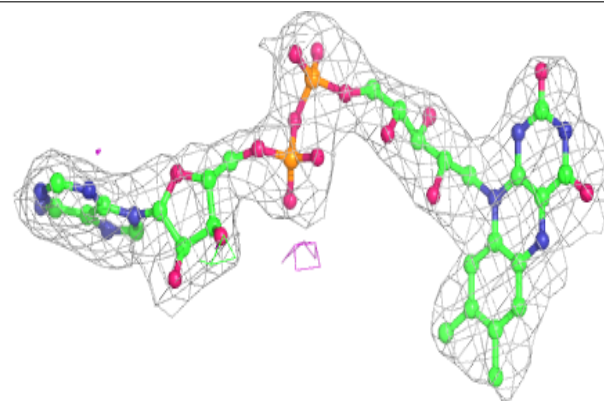
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1506:

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

**Electron density around FAD A 1506:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.