



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:13 AM UTC

PDB ID : 2ZXH / pdb_00002zxh
Title : Structure of Aquifex aeolicus GidA in the form I crystal
Authors : Numata, T.; Osawa, T.
Deposited on : 2008-12-24
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

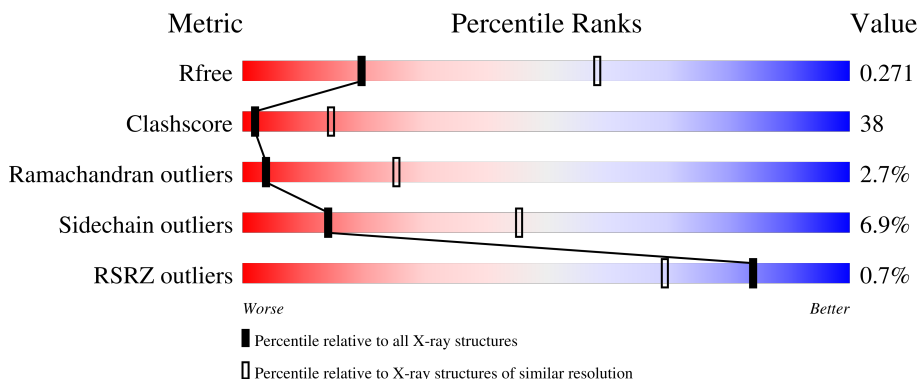
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of 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	637	
1	B	637	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9714 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4804	3080	816	893	15			
1	B	601	Total	C	N	O	S	0	0	0
			4789	3070	813	891	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66962
A	-18	GLY	-	expression tag	UNP O66962
A	-17	SER	-	expression tag	UNP O66962
A	-16	SER	-	expression tag	UNP O66962
A	-15	HIS	-	expression tag	UNP O66962
A	-14	HIS	-	expression tag	UNP O66962
A	-13	HIS	-	expression tag	UNP O66962
A	-12	HIS	-	expression tag	UNP O66962
A	-11	HIS	-	expression tag	UNP O66962
A	-10	HIS	-	expression tag	UNP O66962
A	-9	SER	-	expression tag	UNP O66962
A	-8	SER	-	expression tag	UNP O66962
A	-7	GLY	-	expression tag	UNP O66962
A	-6	LEU	-	expression tag	UNP O66962
A	-5	VAL	-	expression tag	UNP O66962
A	-4	PRO	-	expression tag	UNP O66962
A	-3	ALA	-	expression tag	UNP O66962
A	-2	GLY	-	expression tag	UNP O66962
A	-1	SER	-	expression tag	UNP O66962
A	0	HIS	-	expression tag	UNP O66962
B	-19	MET	-	expression tag	UNP O66962
B	-18	GLY	-	expression tag	UNP O66962
B	-17	SER	-	expression tag	UNP O66962
B	-16	SER	-	expression tag	UNP O66962

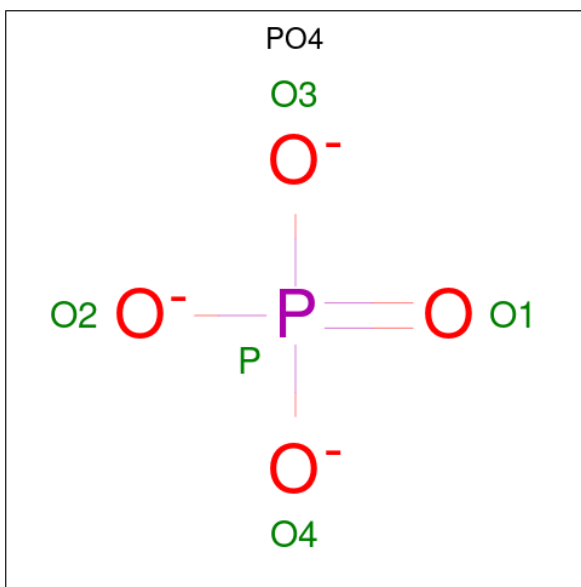
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP O66962
B	-14	HIS	-	expression tag	UNP O66962
B	-13	HIS	-	expression tag	UNP O66962
B	-12	HIS	-	expression tag	UNP O66962
B	-11	HIS	-	expression tag	UNP O66962
B	-10	HIS	-	expression tag	UNP O66962
B	-9	SER	-	expression tag	UNP O66962
B	-8	SER	-	expression tag	UNP O66962
B	-7	GLY	-	expression tag	UNP O66962
B	-6	LEU	-	expression tag	UNP O66962
B	-5	VAL	-	expression tag	UNP O66962
B	-4	PRO	-	expression tag	UNP O66962
B	-3	ALA	-	expression tag	UNP O66962
B	-2	GLY	-	expression tag	UNP O66962
B	-1	SER	-	expression tag	UNP O66962
B	0	HIS	-	expression tag	UNP O66962

- # FAD

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

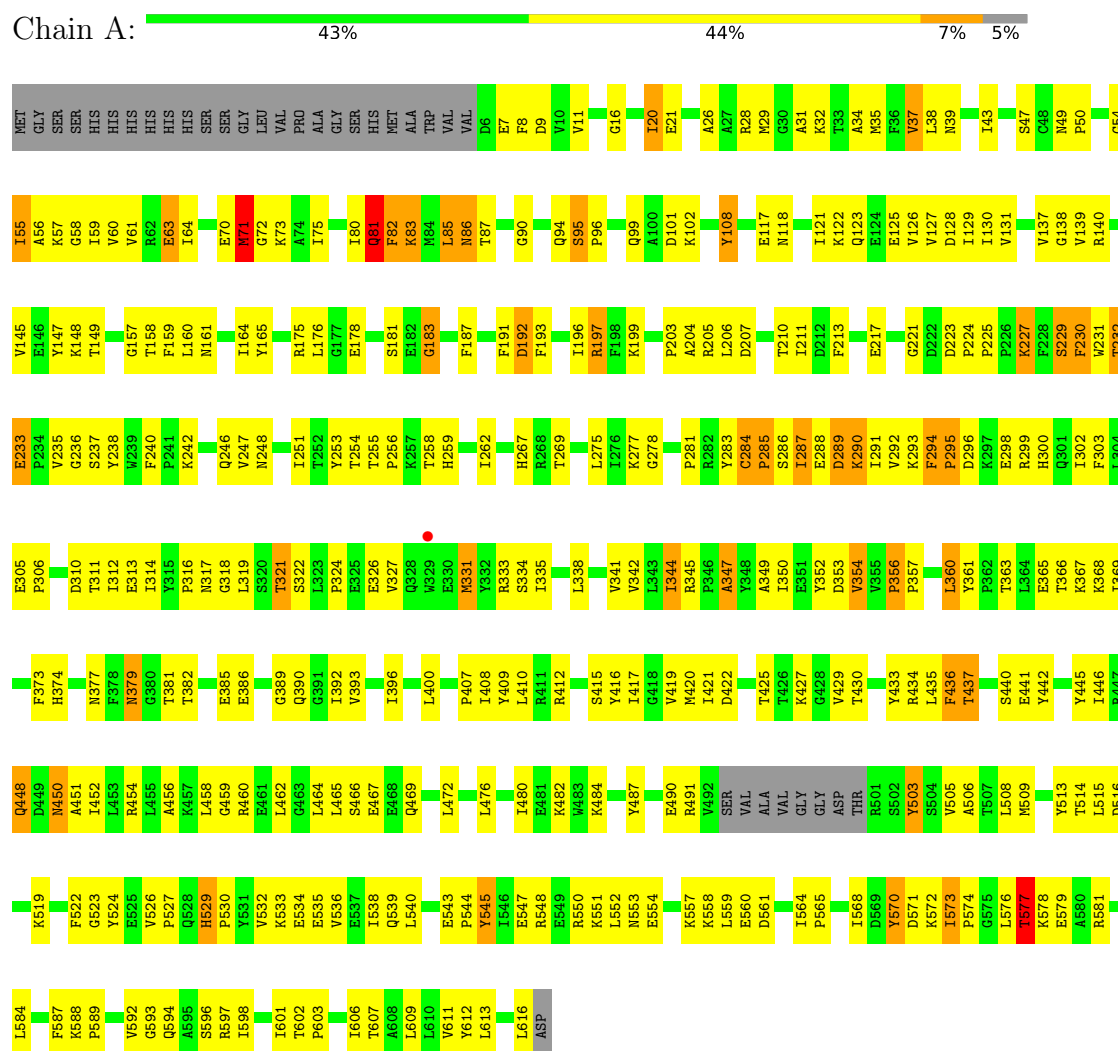


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

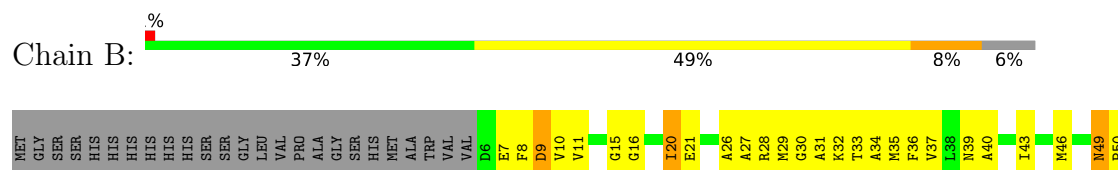
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mmmG



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mmmG



E554	K555	L559	E560	D561	I564	P565	I568	D569	Y570	D571	K572	I573	P574	G575	L576	T577	A580	R581	E582	K583	L584	K585	K586	F587	K588	P589	I590	T591	V592	G593	Q594	R597	I598	I601	T602	P603	I606	T607	A608	L609	L610	V611	Y612	L613	G614	LYS	LEU	ASP									
V492	SER	VAL	ALA	VAL	GLY	GLY	ASP	THR	R501	S502	Y503	S504	V505	A506	T507	L508	M509	T510	M511	N512	Y513	T514	L515	D516	D517	V518	K519	E520	K521	F522	Q523	Y524	E525	V526	P527	Q528	H529	P530	Y531	E534	V535	V536	E537	I538	Q539	L540	E543	P544	Y545	I546	E547	R548	E549	R550	K551	L552	N553
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
L119	Y120	Q123	Y126	Y127	D128	I129	I130	G138	V139	Y147	K148	T149	K150	A151	V154	F159	L160	V163	I164	Y165	I166	M170	G174	R175	E178	P179	G183	D186	F187	Y188	R189	R190	F191	D192	F193	F194	L195	I196	R197	K199	T202	P203	A204	R205	E117	N118											
D207	K208	R209	T210	I211	D212	F213	E217	A219	P220	G221	D222	D223	P224	P225	P226	K227	F228	S229	F230	W231	V235	G236	Y237	Y238	Y239	F240	P241	K242	Q246	V247	N248	W249	I251	T252	Y253	T254	T255	P256	K257	T258	H259	E260	I261	I262	R263	K264	H267	R268	T269	A270	L271	L275					
I276	P281	Y282	Y283	C284	P285	S286	I287	D288	D289	K290	I291	V292	K293	F294	P295	Q301	I302	E305	P306	L309	D310	T311	T312	E313	I314	Y315	P316	R317	G318	L319	S320	T321	P324	E325	E326	V327	Q328	V329	E330	M331	Y332	R333	S334	T335	P336	G337	L338	E339	R340	V341	V342	L343	T344	R345			
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
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V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
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P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
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V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
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V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365	T366	K367	K368	I369	F378	N379	G380	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425							
V429	T430	E431	A432	Y433	R434	L435	F436	T437	S438	R439	S440	E441	Y442	R443	L444	R447	Q448	D449	N450	A451	L452	L453	R454	L455	A456	T381	T382	E385	E386	G389	I392	I396	N397	A398	A399	L400	R401	P407	I408	Y409	L410	R411	R412	Y416	L417	G418	V419	M420	T421	D422	T425						
P346	A347	Y348	A349	I350	D353	Y354	V355	P356	P357	T358	E359	L360	Y361	P362	T363	L364	E365																																								

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.64Å 213.27Å 231.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.20 19.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-3.20) 99.0 (19.97-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.271 0.247 , 0.271	Depositor DCC
R_{free} test set	3801 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9714	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, PO4

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	0.51	0/4904	1.02	29/6624 (0.4%)
1	B	0.51	0/4889	1.02	30/6605 (0.5%)
All	All	0.51	0/9793	1.02	59/13229 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLY	N-CA-C	8.09	122.90	112.54
1	B	287	ILE	N-CA-C	-7.49	104.01	113.22
1	B	526	VAL	CA-C-N	7.31	128.98	119.84
1	B	526	VAL	C-N-CA	7.31	128.98	119.84
1	B	573	ILE	CA-C-N	7.27	127.25	119.76
1	B	573	ILE	C-N-CA	7.27	127.25	119.76
1	A	251	ILE	N-CA-C	7.14	118.17	107.75
1	B	251	ILE	N-CA-C	7.06	118.05	107.75
1	B	334	SER	N-CA-C	-7.03	104.74	113.38
1	A	334	SER	N-CA-C	-7.02	104.74	113.38
1	B	183	GLY	N-CA-C	6.76	120.34	112.50
1	A	573	ILE	CA-C-N	6.73	126.69	119.76
1	A	573	ILE	C-N-CA	6.73	126.69	119.76
1	B	344	ILE	N-CA-C	-6.69	106.06	111.81
1	A	183	GLY	N-CA-C	6.66	120.23	112.50
1	B	95	SER	CA-C-N	6.63	126.39	119.76
1	B	95	SER	C-N-CA	6.63	126.39	119.76
1	A	95	SER	CA-C-N	6.12	125.88	119.76
1	A	95	SER	C-N-CA	6.12	125.88	119.76
1	B	230	PHE	N-CA-C	-6.09	106.11	112.93
1	B	292	VAL	N-CA-C	-6.07	107.02	112.12
1	A	283	TYR	N-CA-C	-6.04	106.89	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	THR	N-CA-C	-5.80	106.84	114.04
1	A	230	PHE	N-CA-C	-5.75	106.60	113.21
1	B	458	LEU	N-CA-C	-5.73	105.12	111.71
1	B	529	HIS	CA-C-N	5.69	126.95	119.84
1	B	529	HIS	C-N-CA	5.69	126.95	119.84
1	A	289	ASP	N-CA-C	-5.61	104.56	111.40
1	A	344	ILE	N-CA-C	-5.60	106.99	111.81
1	A	347	ALA	N-CA-C	-5.57	103.03	110.55
1	A	47	SER	N-CA-C	5.54	120.10	113.23
1	A	287	ILE	N-CA-C	-5.53	106.06	112.98
1	B	159	PHE	N-CA-C	5.52	120.28	112.93
1	B	9	ASP	N-CA-C	-5.50	104.69	111.40
1	B	347	ALA	N-CA-C	-5.48	103.15	110.55
1	A	335	ILE	CA-C-N	5.47	126.67	119.84
1	A	335	ILE	C-N-CA	5.47	126.67	119.84
1	B	335	ILE	CA-C-N	5.47	126.67	119.84
1	B	335	ILE	C-N-CA	5.47	126.67	119.84
1	A	9	ASP	N-CA-C	-5.37	104.85	111.40
1	A	294	PHE	CA-C-N	5.36	126.54	119.84
1	A	294	PHE	C-N-CA	5.36	126.54	119.84
1	B	378	PHE	N-CA-C	-5.26	106.69	113.01
1	B	229	SER	N-CA-C	5.22	117.59	108.76
1	A	482	LYS	N-CA-C	-5.21	105.29	110.97
1	A	284	CYS	CA-C-N	5.21	126.35	119.84
1	A	284	CYS	C-N-CA	5.21	126.35	119.84
1	A	197	ARG	N-CA-C	5.20	117.88	109.40
1	B	51	ALA	N-CA-C	5.19	117.08	109.24
1	B	437	THR	N-CA-C	-5.17	107.64	114.31
1	A	229	SER	N-CA-C	5.17	117.49	108.76
1	B	355	VAL	CA-C-N	5.17	125.70	120.38
1	B	355	VAL	C-N-CA	5.17	125.70	120.38
1	B	49	ASN	CA-C-N	5.15	126.28	119.84
1	B	49	ASN	C-N-CA	5.15	126.28	119.84
1	B	197	ARG	N-CA-C	5.08	117.18	108.90
1	A	458	LEU	N-CA-C	-5.07	105.88	111.71
1	A	529	HIS	CA-C-N	5.01	126.11	119.84
1	A	529	HIS	C-N-CA	5.01	126.11	119.84

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	4804	0	4871	343	0
1	B	4789	0	4854	400	1
2	A	53	0	31	3	0
2	B	53	0	31	1	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
All	All	9714	0	9787	737	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 38.

All (737) 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:466:SER:HB3	1:B:469:GLN:HG3	1.32	1.06
1:B:480:ILE:HD13	1:B:535:GLU:HG2	1.44	1.00
1:A:311:THR:HG22	1:A:313:GLU:H	1.26	0.97
1:B:20:ILE:HG21	1:B:109:MET:HE3	1.46	0.95
1:B:311:THR:HG22	1:B:313:GLU:H	1.30	0.94
1:B:7:GLU:HG2	1:B:148:LYS:HB2	1.52	0.91
1:B:87:THR:HA	1:B:94:GLN:HE21	1.36	0.90
1:B:254:THR:HG23	1:B:302:ILE:HD11	1.53	0.90
1:A:254:THR:HG23	1:A:302:ILE:HD11	1.55	0.88
1:B:211:ILE:HB	1:B:213:PHE:CE1	2.09	0.88
1:B:32:LYS:HZ2	1:B:120:TYR:HE1	1.20	0.87
1:A:71:MET:HE1	1:A:385:GLU:HA	1.56	0.86
1:B:478:ARG:HH12	1:B:482:LYS:HE2	1.40	0.85
1:B:362:PRO:HG2	1:B:594:GLN:HE22	1.42	0.84
1:A:122:LYS:HZ3	1:A:147:TYR:HE2	1.23	0.83
1:A:127:VAL:HG13	1:A:183:GLY:HA3	1.58	0.83
1:B:210:THR:HG21	1:B:342:VAL:HG23	1.59	0.83
1:A:225:PRO:HG2	1:A:240:PHE:HB2	1.60	0.82
1:A:29:MET:HE1	1:A:396:ILE:HG12	1.59	0.82
1:A:87:THR:HA	1:A:94:GLN:HE21	1.45	0.81
1:B:257:LYS:O	1:B:260:GLU:HG2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LEU:HA	1:B:511:MET:HE3	1.62	0.81
1:A:302:ILE:HD13	1:A:319:LEU:HD11	1.65	0.79
1:B:10:VAL:HG23	1:B:33:THR:HG23	1.64	0.78
1:B:466:SER:H	1:B:469:GLN:HE21	1.31	0.78
1:B:8:PHE:CE2	1:B:34:ALA:HB2	2.19	0.78
1:B:483:TRP:HE1	1:B:528:GLN:HE21	1.32	0.77
1:B:20:ILE:HG21	1:B:109:MET:CE	2.13	0.77
1:B:412:ARG:HD2	1:B:597:ARG:NH1	2.00	0.77
1:A:29:MET:HE1	1:A:396:ILE:HA	1.67	0.76
1:A:357:PRO:O	1:A:360:LEU:HD12	1.86	0.76
1:A:392:ILE:O	1:A:396:ILE:HG13	1.84	0.76
1:A:287:ILE:HD12	1:A:290:LYS:HD2	1.69	0.75
1:A:7:GLU:HG2	1:A:148:LYS:HB2	1.68	0.75
1:B:52:ILE:HG23	1:B:71:MET:HE2	1.68	0.75
1:B:362:PRO:CG	1:B:594:GLN:HE22	1.98	0.75
1:B:505:VAL:HA	1:B:508:LEU:HG	1.69	0.75
1:B:224:PRO:HD3	1:B:242:LYS:HE2	1.68	0.75
1:B:476:LEU:O	1:B:480:ILE:HG13	1.87	0.74
1:A:210:THR:HG21	1:A:342:VAL:HG23	1.68	0.74
1:B:29:MET:HE1	1:B:396:ILE:HG12	1.68	0.74
1:B:221:GLY:HA3	1:B:246:GLN:OE1	1.88	0.73
1:A:122:LYS:NZ	1:A:147:TYR:HE2	1.87	0.73
1:B:329:TRP:CD1	1:B:343:LEU:HD12	2.24	0.73
1:B:57:LYS:HZ3	1:B:436:PHE:HE1	1.35	0.73
1:A:161:ASN:O	1:A:197:ARG:NH2	2.21	0.73
1:B:565:PRO:HB2	1:B:568:ILE:HG23	1.69	0.73
1:A:360:LEU:HD21	1:A:374:HIS:HB2	1.71	0.73
1:B:8:PHE:CD2	1:B:34:ALA:HB2	2.23	0.73
1:B:521:LYS:C	1:B:522:PHE:HD2	1.96	0.72
1:A:324:PRO:HB2	1:A:327:VAL:HG23	1.71	0.72
1:B:10:VAL:HG12	1:B:151:ALA:HB3	1.71	0.72
1:B:545:TYR:HD1	1:B:545:TYR:H	1.36	0.72
1:B:573:ILE:HA	1:B:612:TYR:HD1	1.54	0.72
1:A:311:THR:HG22	1:A:313:GLU:N	2.03	0.72
1:A:476:LEU:O	1:A:480:ILE:HG13	1.90	0.72
1:A:505:VAL:HA	1:A:508:LEU:HD12	1.71	0.71
1:B:329:TRP:HD1	1:B:343:LEU:HD12	1.55	0.71
1:B:483:TRP:CZ2	1:B:527:PRO:HA	2.24	0.71
1:A:386:GLU:HG3	1:A:435:LEU:HG	1.72	0.71
1:B:20:ILE:HD13	1:B:109:MET:HE3	1.71	0.71
1:A:211:ILE:HB	1:A:213:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:GLN:HA	1:B:597:ARG:NH2	2.06	0.71
1:B:29:MET:HE1	1:B:396:ILE:HA	1.72	0.70
1:A:275:LEU:HD11	1:B:441:GLU:HG3	1.72	0.70
1:A:160:LEU:HB3	1:A:353:ASP:HB2	1.72	0.70
1:A:363:THR:HG22	1:A:408:ILE:O	1.89	0.70
1:B:37:VAL:HG12	1:B:39:ASN:H	1.57	0.70
1:A:505:VAL:O	1:A:508:LEU:HB2	1.91	0.69
1:B:55:ILE:HG22	1:B:56:ALA:N	2.07	0.69
1:B:472:LEU:O	1:B:476:LEU:HG	1.92	0.69
1:B:476:LEU:HD22	1:B:529:HIS:NE2	2.07	0.69
1:A:420:MET:HG3	1:A:433:TYR:HE1	1.57	0.69
1:B:412:ARG:HD2	1:B:597:ARG:HH11	1.55	0.69
1:A:565:PRO:HB2	1:A:568:ILE:HG23	1.75	0.69
1:A:476:LEU:HD21	1:A:529:HIS:CE1	2.27	0.68
1:A:85:LEU:HD23	1:A:86:ASN:H	1.58	0.68
1:B:70:GLU:O	1:B:72:GLY:N	2.26	0.68
1:B:207:ASP:OD1	1:B:312:ILE:HD12	1.94	0.68
1:B:138:GLY:HA2	1:B:149:THR:HG22	1.75	0.68
1:B:466:SER:H	1:B:469:GLN:NE2	1.91	0.68
1:B:478:ARG:NH1	1:B:482:LYS:HE2	2.09	0.68
1:A:313:GLU:HG2	1:A:344:ILE:HD12	1.75	0.68
1:A:589:PRO:HG3	1:A:598:ILE:HD11	1.76	0.68
1:A:603:PRO:O	1:A:606:ILE:HG22	1.94	0.67
1:B:108:TYR:C	1:B:108:TYR:HD2	2.03	0.67
1:B:336:PRO:HA	1:B:339:GLU:OE2	1.94	0.67
1:B:46:MET:HE1	1:B:100:ALA:HB3	1.77	0.67
1:B:204:ALA:N	1:B:347:ALA:HB2	2.08	0.67
1:A:480:ILE:HD13	1:A:535:GLU:HG2	1.75	0.66
1:B:382:THR:OG1	1:B:432:PRO:HB3	1.95	0.66
1:B:480:ILE:HG23	1:B:536:VAL:HG23	1.77	0.66
1:B:450:ASN:HD22	1:B:451:ALA:N	1.93	0.66
1:A:381:THR:HG21	1:A:390:GLN:NE2	2.10	0.66
1:B:225:PRO:HG2	1:B:240:PHE:HB2	1.77	0.66
1:A:545:TYR:HD1	1:A:545:TYR:H	1.43	0.66
1:B:211:ILE:HB	1:B:213:PHE:HE1	1.59	0.66
1:A:70:GLU:O	1:A:72:GLY:N	2.28	0.65
1:A:420:MET:HG3	1:A:433:TYR:CE1	2.29	0.65
1:A:37:VAL:O	1:A:123:GLN:HA	1.96	0.65
1:B:37:VAL:HG12	1:B:39:ASN:N	2.12	0.65
1:B:60:VAL:HG21	1:B:435:LEU:CD1	2.27	0.65
1:B:612:TYR:CD2	1:B:612:TYR:C	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:NZ	1:A:587:PHE:HA	2.11	0.65
1:A:247:VAL:HG12	1:A:248:ASN:N	2.12	0.64
1:B:206:LEU:HD23	1:B:343:LEU:HD23	1.78	0.64
1:A:294:PHE:N	1:A:295:PRO:HD3	2.13	0.64
1:A:357:PRO:HG3	1:A:379:ASN:O	1.97	0.64
1:B:87:THR:HG22	1:B:94:GLN:NE2	2.13	0.64
1:A:568:ILE:HD11	1:A:570:TYR:CE1	2.33	0.64
1:B:362:PRO:HG2	1:B:594:GLN:NE2	2.12	0.64
1:B:573:ILE:HG12	1:B:612:TYR:CD1	2.33	0.64
1:A:204:ALA:N	1:A:347:ALA:HB2	2.12	0.64
1:B:191:PHE:O	1:B:192:ASP:HB2	1.98	0.64
1:B:250:TRP:C	1:B:251:ILE:HD12	2.22	0.64
1:B:452:ILE:O	1:B:456:ALA:HB2	1.98	0.64
1:B:90:GLY:O	1:B:94:GLN:HG3	1.98	0.64
1:B:328:GLN:O	1:B:332:TYR:HD2	1.81	0.63
1:A:130:ILE:N	1:A:130:ILE:HD12	2.13	0.63
1:B:59:ILE:HG12	1:B:448:GLN:HB3	1.81	0.63
1:B:67:LEU:HD21	1:B:458:LEU:HD23	1.81	0.63
1:A:434:ARG:HG2	1:A:434:ARG:HH11	1.63	0.63
1:A:448:GLN:NE2	1:A:448:GLN:O	2.31	0.63
1:B:52:ILE:HD12	1:B:71:MET:CE	2.28	0.63
1:A:8:PHE:O	1:A:149:THR:HA	1.99	0.63
1:A:60:VAL:HG21	1:A:435:LEU:CD1	2.28	0.63
1:A:435:LEU:C	1:A:437:THR:H	2.06	0.63
1:B:360:LEU:O	1:B:367:LYS:HE3	1.99	0.63
1:B:37:VAL:O	1:B:123:GLN:HA	1.99	0.62
1:B:452:ILE:HD11	1:B:473:VAL:HG21	1.80	0.62
1:B:466:SER:HB3	1:B:469:GLN:CG	2.19	0.62
1:A:57:LYS:HB3	1:A:385:GLU:HG2	1.82	0.62
1:B:311:THR:HG22	1:B:313:GLU:N	2.09	0.62
1:B:492:VAL:HG12	1:B:492:VAL:O	1.97	0.62
1:B:108:TYR:C	1:B:108:TYR:CD2	2.75	0.62
1:A:60:VAL:O	1:A:64:ILE:HG13	2.00	0.62
1:B:247:VAL:HG12	1:B:248:ASN:N	2.14	0.62
1:A:514:THR:C	1:A:516:ASP:H	2.05	0.62
1:B:275:LEU:N	1:B:275:LEU:HD22	2.14	0.62
1:A:460:ARG:CZ	1:A:467:GLU:HG2	2.29	0.62
1:B:9:ASP:OD1	1:B:150:LYS:HE3	2.00	0.62
1:B:225:PRO:HB3	1:B:246:GLN:HE22	1.64	0.62
1:B:514:THR:C	1:B:516:ASP:H	2.07	0.62
1:B:260:GLU:O	1:B:264:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:HIS:CE1	1:B:531:TYR:HB3	2.34	0.61
1:A:231:TRP:CZ3	1:A:469:GLN:HG2	2.35	0.61
1:A:366:THR:HG22	1:A:368:LYS:N	2.15	0.61
1:A:138:GLY:HA2	1:A:149:THR:HG22	1.82	0.61
1:A:284:CYS:SG	1:A:293:LYS:HD2	2.41	0.61
1:B:594:GLN:N	1:B:597:ARG:HH21	1.98	0.61
1:A:29:MET:CE	1:A:396:ILE:HG12	2.30	0.61
1:A:129:ILE:HB	1:A:187:PHE:CE1	2.35	0.61
1:A:122:LYS:NZ	1:A:147:TYR:CE2	2.66	0.61
1:B:570:TYR:CD2	1:B:584:LEU:HB3	2.36	0.61
1:A:71:MET:HE1	1:A:385:GLU:CA	2.30	0.60
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.17	0.60
1:B:357:PRO:HG3	1:B:379:ASN:O	2.01	0.60
1:B:52:ILE:CG2	1:B:71:MET:HE2	2.31	0.60
1:B:57:LYS:NZ	1:B:436:PHE:HE1	1.98	0.60
1:A:573:ILE:HG21	1:A:576:LEU:HD22	1.83	0.60
1:A:554:GLU:O	1:A:558:LYS:HG3	2.02	0.60
1:A:287:ILE:HD13	1:A:318:GLY:O	2.01	0.60
1:B:8:PHE:HE1	1:B:147:TYR:HD2	1.50	0.60
1:B:159:PHE:CD2	1:B:174:GLY:HA3	2.36	0.60
1:B:363:THR:HG22	1:B:408:ILE:O	2.02	0.60
1:B:381:THR:CG2	1:B:382:THR:N	2.65	0.60
1:B:589:PRO:HA	1:B:594:GLN:OE1	2.00	0.60
1:A:196:ILE:HG13	1:A:354:VAL:HG12	1.83	0.59
1:A:551:LYS:HA	1:A:554:GLU:HG3	1.83	0.59
1:B:564:ILE:HD11	1:B:592:VAL:HA	1.84	0.59
1:B:366:THR:HG22	1:B:368:LYS:N	2.17	0.59
1:B:251:ILE:HD12	1:B:251:ILE:N	2.16	0.59
1:A:204:ALA:O	1:A:205:ARG:HD2	2.01	0.59
1:A:450:ASN:N	1:A:450:ASN:HD22	1.99	0.59
1:B:11:VAL:HG23	1:B:149:THR:OG1	2.01	0.59
1:A:574:PRO:HD3	1:A:612:TYR:HD1	1.66	0.59
1:B:227:LYS:NZ	1:B:229:SER:O	2.36	0.59
1:A:480:ILE:HG23	1:A:536:VAL:HG23	1.84	0.59
1:B:267:HIS:CD2	1:B:267:HIS:H	2.19	0.59
1:A:82:PHE:CD1	1:A:82:PHE:N	2.70	0.59
1:A:286:SER:HB2	1:A:288:GLU:OE1	2.03	0.59
1:B:8:PHE:O	1:B:149:THR:HA	2.03	0.59
1:B:435:LEU:C	1:B:437:THR:H	2.10	0.59
1:A:28:ARG:HH12	1:A:70:GLU:HG2	1.68	0.59
1:A:196:ILE:CG1	1:A:354:VAL:HG12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASN:O	1:B:454:ARG:HG3	2.02	0.58
1:A:108:TYR:C	1:A:108:TYR:CD2	2.81	0.58
1:B:29:MET:CE	1:B:464:LEU:HD21	2.32	0.58
1:A:8:PHE:CD2	1:A:34:ALA:HB2	2.38	0.58
1:A:247:VAL:HG12	1:A:248:ASN:H	1.68	0.58
1:B:29:MET:CE	1:B:396:ILE:HG12	2.33	0.58
1:A:81:GLN:HB3	1:A:99:GLN:HB2	1.84	0.58
1:B:589:PRO:HG3	1:B:598:ILE:HD11	1.86	0.58
1:B:396:ILE:O	1:B:400:LEU:HG	2.04	0.58
1:B:62:ARG:NH1	1:B:238:TYR:CD1	2.72	0.58
1:B:362:PRO:CG	1:B:594:GLN:NE2	2.67	0.58
1:B:573:ILE:HA	1:B:612:TYR:CD1	2.37	0.58
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.39	0.58
1:A:160:LEU:HD23	1:A:353:ASP:CB	2.34	0.58
1:B:210:THR:HB	1:B:341:VAL:HA	1.86	0.58
1:B:420:MET:HG3	1:B:433:TYR:CE1	2.38	0.58
1:A:224:PRO:HD3	1:A:242:LYS:HE2	1.84	0.57
1:A:452:ILE:O	1:A:456:ALA:HB2	2.03	0.57
1:B:225:PRO:HB3	1:B:246:GLN:NE2	2.19	0.57
1:B:442:TYR:HA	1:B:549:GLU:OE2	2.04	0.57
1:B:359:GLU:OE1	1:B:368:LYS:HE3	2.04	0.57
1:B:381:THR:HG22	1:B:382:THR:N	2.19	0.57
1:A:206:LEU:HB2	1:A:314:ILE:HB	1.86	0.57
1:B:262:ILE:HB	1:B:291:ILE:HD13	1.84	0.57
1:B:430:THR:HG23	1:B:431:GLU:HG2	1.87	0.57
1:B:191:PHE:CD2	1:B:369:ILE:HD11	2.39	0.57
1:B:329:TRP:HD1	1:B:343:LEU:CD1	2.17	0.57
1:B:63:GLU:O	1:B:67:LEU:HD12	2.05	0.57
1:A:60:VAL:HA	1:A:63:GLU:HG3	1.85	0.57
1:A:160:LEU:HA	1:A:181:SER:OG	2.04	0.57
1:B:453:LEU:HD11	1:B:535:GLU:OE2	2.05	0.57
1:A:589:PRO:HA	1:A:594:GLN:OE1	2.04	0.57
1:A:81:GLN:HG3	1:A:247:VAL:O	2.04	0.57
1:A:365:GLU:HG3	1:A:373:PHE:CE2	2.40	0.57
1:B:492:VAL:C	1:B:502:SER:HA	2.30	0.57
1:A:584:LEU:HG	1:A:601:ILE:HD11	1.87	0.56
1:A:450:ASN:HD22	1:A:451:ALA:N	2.03	0.56
1:A:293:LYS:C	1:A:295:PRO:HD3	2.31	0.56
1:B:81:GLN:HG3	1:B:247:VAL:O	2.05	0.56
1:B:594:GLN:CA	1:B:597:ARG:NH2	2.69	0.56
1:A:20:ILE:HA	1:A:35:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PRO:HG3	1:B:434:ARG:NH2	2.21	0.56
1:A:560:GLU:OE1	1:A:597:ARG:NH2	2.38	0.56
1:B:319:LEU:HD11	1:B:335:ILE:CD1	2.36	0.56
1:B:82:PHE:O	1:B:83:LYS:HB3	2.06	0.56
1:B:392:ILE:O	1:B:396:ILE:HG13	2.06	0.56
1:B:545:TYR:N	1:B:545:TYR:CD1	2.74	0.56
1:A:389:GLY:O	1:A:392:ILE:HG22	2.05	0.56
1:A:108:TYR:C	1:A:108:TYR:HD2	2.14	0.56
1:A:367:LYS:HZ1	1:A:587:PHE:HA	1.71	0.56
1:A:534:GLU:O	1:A:538:ILE:HG13	2.05	0.56
1:A:71:MET:HE1	1:A:385:GLU:HG3	1.88	0.56
1:B:450:ASN:ND2	1:B:454:ARG:HE	2.03	0.56
1:A:221:GLY:HA3	1:A:246:GLN:OE1	2.06	0.55
1:A:230:PHE:HZ	1:A:476:LEU:HD13	1.71	0.55
1:A:90:GLY:O	1:A:94:GLN:HG3	2.07	0.55
1:A:275:LEU:HD23	1:A:292:VAL:HG13	1.87	0.55
1:B:480:ILE:HD13	1:B:535:GLU:CG	2.28	0.55
1:A:210:THR:HG21	1:A:342:VAL:CG2	2.35	0.55
1:A:290:LYS:HB3	1:A:300:HIS:CE1	2.41	0.55
1:B:199:LYS:HA	1:B:350:ILE:O	2.07	0.55
1:B:275:LEU:HD22	1:B:275:LEU:H	1.72	0.55
1:B:483:TRP:CE3	1:B:527:PRO:HG3	2.41	0.55
1:B:509:MET:CE	1:B:515:LEU:HG	2.37	0.55
1:A:229:SER:HB3	1:A:232:THR:OG1	2.06	0.55
1:A:360:LEU:HD11	1:A:379:ASN:HD21	1.70	0.55
1:A:63:GLU:OE2	1:A:454:ARG:NH2	2.38	0.55
1:A:85:LEU:HD23	1:A:86:ASN:N	2.20	0.55
1:A:573:ILE:HA	1:A:612:TYR:CD1	2.41	0.55
1:B:224:PRO:HB3	1:B:242:LYS:HG2	1.88	0.55
1:B:247:VAL:HG12	1:B:248:ASN:H	1.69	0.55
1:A:102:LYS:NZ	1:A:205:ARG:HH21	2.04	0.55
1:A:233:GLU:OE1	1:A:235:VAL:HG23	2.06	0.55
1:A:440:SER:C	1:A:442:TYR:H	2.15	0.55
1:A:570:TYR:CE2	1:A:584:LEU:HB3	2.42	0.55
1:A:275:LEU:CD1	1:B:441:GLU:HG3	2.37	0.55
1:A:545:TYR:N	1:A:545:TYR:CD1	2.76	0.55
1:A:547:GLU:HA	1:A:547:GLU:OE1	2.07	0.55
1:B:117:GLU:HG2	1:B:118:ASN:OD1	2.07	0.54
1:B:519:LYS:HD2	1:B:526:VAL:CG2	2.37	0.54
1:B:262:ILE:HD13	1:B:287:ILE:HG23	1.89	0.54
1:B:440:SER:C	1:B:442:TYR:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:VAL:HG21	1:B:26:ALA:HB1	1.90	0.54
1:B:160:LEU:HD23	1:B:353:ASP:CB	2.38	0.54
1:A:386:GLU:CG	1:A:435:LEU:HG	2.36	0.54
1:B:29:MET:HE2	1:B:464:LEU:HD21	1.89	0.54
1:B:259:HIS:N	1:B:259:HIS:CD2	2.74	0.54
1:B:508:LEU:O	1:B:513:TYR:HB2	2.07	0.54
1:B:509:MET:HE3	1:B:537:GLU:HG3	1.89	0.54
1:B:480:ILE:HG23	1:B:536:VAL:CG2	2.37	0.54
1:A:390:GLN:HG3	1:A:420:MET:HE3	1.90	0.54
1:A:199:LYS:HA	1:A:350:ILE:O	2.08	0.54
1:B:514:THR:HG22	1:B:537:GLU:OE2	2.07	0.54
1:A:204:ALA:HB1	1:A:345:ARG:O	2.07	0.54
1:A:547:GLU:OE1	1:A:550:ARG:HD3	2.07	0.53
1:B:548:ARG:O	1:B:552:LEU:HG	2.08	0.53
1:A:29:MET:HE1	1:A:396:ILE:CG1	2.36	0.53
1:A:396:ILE:O	1:A:400:LEU:HG	2.09	0.53
1:B:28:ARG:HH12	1:B:70:GLU:HG2	1.73	0.53
1:A:294:PHE:C	1:A:296:ASP:H	2.15	0.53
1:A:341:VAL:HG22	1:A:342:VAL:N	2.24	0.53
1:A:514:THR:C	1:A:516:ASP:N	2.67	0.53
1:B:484:LYS:HE3	1:B:540:LEU:HD23	1.91	0.53
1:A:225:PRO:HG2	1:A:240:PHE:CB	2.35	0.53
1:A:366:THR:HG22	1:A:368:LYS:H	1.74	0.53
1:A:574:PRO:CD	1:A:612:TYR:HD1	2.21	0.53
1:B:204:ALA:HB1	1:B:345:ARG:O	2.08	0.53
1:B:366:THR:HG22	1:B:368:LYS:H	1.73	0.53
1:B:397:ASN:OD1	1:B:408:ILE:N	2.36	0.53
1:A:352:TYR:CD1	1:A:352:TYR:N	2.77	0.53
1:B:409:TYR:CE2	1:B:590:ILE:HD12	2.44	0.53
1:A:82:PHE:O	1:A:83:LYS:HB3	2.07	0.53
1:B:160:LEU:HD23	1:B:353:ASP:HB3	1.91	0.53
1:B:258:THR:HB	1:B:259:HIS:HD2	1.73	0.53
1:B:46:MET:SD	1:B:105:TYR:CD2	3.02	0.53
1:A:396:ILE:HD13	1:A:462:LEU:HD13	1.90	0.52
1:B:286:SER:HB2	1:B:288:GLU:HG2	1.91	0.52
1:B:505:VAL:CA	1:B:508:LEU:HG	2.39	0.52
1:B:507:THR:HG22	1:B:511:MET:HE2	1.91	0.52
1:B:335:ILE:HB	1:B:338:LEU:HD12	1.91	0.52
1:B:460:ARG:HD3	1:B:467:GLU:HA	1.91	0.52
1:B:510:THR:HG22	1:B:510:THR:O	2.07	0.52
1:A:128:ASP:OD1	1:A:129:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:HIS:N	1:A:259:HIS:CD2	2.78	0.52
1:A:526:VAL:HG11	1:A:533:LYS:HE3	1.91	0.52
1:B:60:VAL:HG21	1:B:435:LEU:HD13	1.91	0.52
1:B:81:GLN:HB3	1:B:99:GLN:HB2	1.91	0.52
1:B:534:GLU:O	1:B:538:ILE:HG13	2.08	0.52
1:A:460:ARG:NH2	1:A:467:GLU:HG2	2.25	0.52
1:A:56:ALA:HB3	1:A:435:LEU:HB3	1.91	0.52
1:A:381:THR:HG21	1:A:390:GLN:HE22	1.73	0.52
1:B:484:LYS:HE3	1:B:540:LEU:CD2	2.40	0.52
1:A:71:MET:CE	1:A:385:GLU:HG3	2.39	0.51
1:A:275:LEU:HD23	1:A:292:VAL:CG1	2.40	0.51
1:B:218:VAL:CG1	1:B:248:ASN:HD22	2.23	0.51
1:B:166:ILE:HD11	1:B:348:TYR:HB3	1.91	0.51
1:A:288:GLU:O	1:A:292:VAL:HG23	2.10	0.51
1:B:82:PHE:CD1	1:B:82:PHE:N	2.79	0.51
1:B:410:LEU:HD12	1:B:417:ILE:CG2	2.40	0.51
1:B:286:SER:CB	1:B:288:GLU:HG2	2.41	0.51
1:B:361:TYR:O	1:B:425:THR:HG21	2.10	0.51
1:B:126:VAL:HG13	1:B:139:VAL:CG1	2.41	0.51
1:B:416:TYR:O	1:B:419:VAL:HB	2.10	0.51
1:B:514:THR:C	1:B:516:ASP:N	2.69	0.51
1:A:160:LEU:HD23	1:A:353:ASP:HB3	1.92	0.51
1:B:8:PHE:CE1	1:B:147:TYR:HD2	2.29	0.51
1:B:154:VAL:HG21	1:B:188:TYR:OH	2.11	0.51
1:A:361:TYR:OH	1:A:588:LYS:HD2	2.10	0.51
1:A:393:VAL:HG21	1:A:421:ILE:HD11	1.93	0.51
1:A:466:SER:HB3	1:A:469:GLN:HB2	1.92	0.51
1:A:60:VAL:HG21	1:A:435:LEU:HD13	1.92	0.50
1:A:357:PRO:HA	1:A:360:LEU:HD12	1.94	0.50
1:B:28:ARG:HH22	1:B:70:GLU:CD	2.18	0.50
1:A:126:VAL:HG13	1:A:139:VAL:CG1	2.41	0.50
1:B:268:ARG:O	1:B:324:PRO:HD3	2.10	0.50
1:A:450:ASN:N	1:A:450:ASN:ND2	2.58	0.50
1:B:289:ASP:C	1:B:291:ILE:H	2.19	0.50
1:B:460:ARG:NH1	1:B:467:GLU:N	2.59	0.50
1:A:38:LEU:HD21	1:A:125:GLU:HG3	1.94	0.50
1:B:487:TYR:CE2	1:B:515:LEU:HD11	2.47	0.50
1:A:39:ASN:HA	1:A:123:GLN:OE1	2.12	0.50
1:A:255:THR:HB	1:A:256:PRO:HD2	1.93	0.50
1:B:28:ARG:NH2	1:B:70:GLU:OE2	2.44	0.50
1:B:508:LEU:C	1:B:513:TYR:HB2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:VAL:O	1:B:524:TYR:HB2	2.12	0.50
1:A:381:THR:CG2	1:A:390:GLN:HE22	2.24	0.50
1:A:506:ALA:HB1	1:A:540:LEU:HD22	1.92	0.50
1:B:360:LEU:HD23	1:B:366:THR:HA	1.94	0.50
1:B:434:ARG:HD3	1:B:436:PHE:CE2	2.46	0.50
1:B:612:TYR:C	1:B:612:TYR:HD2	2.20	0.50
1:B:560:GLU:HA	1:B:591:THR:HG21	1.94	0.49
1:B:509:MET:CE	1:B:537:GLU:HG3	2.42	0.49
1:B:551:LYS:HA	1:B:554:GLU:HG3	1.94	0.49
1:A:290:LYS:O	1:A:300:HIS:CE1	2.66	0.49
1:A:412:ARG:HD2	1:A:597:ARG:NH1	2.26	0.49
1:A:480:ILE:HD13	1:A:535:GLU:CG	2.41	0.49
1:B:324:PRO:O	1:B:328:GLN:HG3	2.12	0.49
1:B:480:ILE:HG21	1:B:535:GLU:HG3	1.93	0.49
1:B:483:TRP:CH2	1:B:527:PRO:HA	2.46	0.49
1:A:94:GLN:O	1:A:448:GLN:HG2	2.11	0.49
1:A:230:PHE:CE1	1:A:236:GLY:O	2.65	0.49
1:B:7:GLU:O	1:B:32:LYS:HD3	2.13	0.49
1:A:365:GLU:HG3	1:A:373:PHE:CZ	2.47	0.49
1:A:539:GLN:O	1:A:543:GLU:HB2	2.11	0.49
1:B:16:GLY:O	1:B:20:ILE:HG13	2.11	0.49
1:A:159:PHE:CE1	1:A:175:ARG:HG3	2.48	0.49
1:A:366:THR:HG22	1:A:369:ILE:H	1.78	0.49
1:B:509:MET:HE1	1:B:515:LEU:HG	1.93	0.49
1:A:350:ILE:O	1:A:350:ILE:HG23	2.13	0.49
1:B:203:PRO:O	1:B:205:ARG:NH1	2.46	0.49
1:A:484:LYS:NZ	1:A:539:GLN:HB3	2.27	0.49
1:B:492:VAL:O	1:B:492:VAL:CG1	2.60	0.49
1:B:209:ARG:HD3	1:B:312:ILE:HD12	1.95	0.49
1:B:570:TYR:CE2	1:B:584:LEU:HB3	2.47	0.49
1:A:159:PHE:HE1	1:A:175:ARG:HG3	1.78	0.48
1:A:230:PHE:CE2	1:A:452:ILE:HG12	2.47	0.48
1:B:26:ALA:O	1:B:31:ALA:HB3	2.13	0.48
1:B:130:ILE:HD12	1:B:130:ILE:H	1.78	0.48
1:B:70:GLU:O	1:B:71:MET:C	2.56	0.48
1:B:108:TYR:HE2	1:B:112:VAL:CG2	2.26	0.48
1:B:547:GLU:OE1	1:B:550:ARG:HD3	2.13	0.48
1:B:587:PHE:O	1:B:588:LYS:C	2.55	0.48
1:B:9:ASP:OD2	1:B:32:LYS:N	2.34	0.48
1:B:286:SER:OG	1:B:288:GLU:HG2	2.13	0.48
1:B:326:GLU:HA	1:B:329:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:CD	1:B:597:ARG:NH1	2.74	0.48
1:B:519:LYS:O	1:B:523:GLY:HA2	2.13	0.48
1:A:213:PHE:CD1	1:A:213:PHE:N	2.81	0.48
1:A:460:ARG:NH1	1:A:467:GLU:HG2	2.28	0.48
1:A:484:LYS:HZ2	1:A:539:GLN:HB3	1.78	0.48
1:B:539:GLN:O	1:B:543:GLU:HB2	2.13	0.48
1:B:544:PRO:HB2	1:B:545:TYR:HD1	1.79	0.48
1:A:338:LEU:O	1:A:341:VAL:HG12	2.13	0.48
1:A:550:ARG:O	1:A:550:ARG:HG2	2.13	0.48
1:B:452:ILE:HG23	1:B:453:LEU:HD23	1.95	0.48
1:A:71:MET:CE	1:A:385:GLU:HA	2.37	0.48
1:A:191:PHE:O	1:A:192:ASP:HB2	2.12	0.48
1:A:363:THR:HG21	1:A:407:PRO:HB2	1.94	0.48
1:A:564:ILE:HD11	1:A:592:VAL:HA	1.95	0.48
1:B:130:ILE:HD12	1:B:130:ILE:N	2.29	0.48
1:B:363:THR:O	1:B:364:LEU:HB2	2.13	0.48
1:B:519:LYS:HG3	1:B:524:TYR:O	2.13	0.48
1:A:102:LYS:HZ1	1:A:205:ARG:HH21	1.60	0.48
1:A:587:PHE:O	1:A:588:LYS:C	2.56	0.48
1:B:253:TYR:CE2	1:B:301:GLN:HG3	2.49	0.48
1:A:39:ASN:OD1	1:A:39:ASN:C	2.57	0.48
1:A:175:ARG:NE	1:A:178:GLU:OE2	2.42	0.48
1:A:230:PHE:CD2	1:A:452:ILE:HG12	2.48	0.48
1:B:29:MET:HG3	1:B:464:LEU:HD21	1.96	0.48
1:B:130:ILE:HD13	1:B:138:GLY:C	2.39	0.48
1:B:230:PHE:HZ	1:B:476:LEU:HD12	1.77	0.48
1:B:389:GLY:O	1:B:392:ILE:HG22	2.14	0.48
1:B:519:LYS:HD2	1:B:526:VAL:HG23	1.96	0.48
1:B:545:TYR:HD1	1:B:545:TYR:N	2.07	0.48
1:A:460:ARG:HD3	1:A:467:GLU:HA	1.96	0.48
1:B:52:ILE:HD12	1:B:71:MET:HE2	1.93	0.48
1:B:594:GLN:CA	1:B:597:ARG:HH21	2.26	0.48
1:A:80:ILE:O	1:A:81:GLN:HB2	2.13	0.47
1:A:140:ARG:HG2	1:A:145:VAL:O	2.13	0.47
1:B:51:ALA:HB1	1:B:98:ALA:O	2.14	0.47
1:B:318:GLY:O	1:B:319:LEU:HD23	2.14	0.47
1:A:480:ILE:HG23	1:A:536:VAL:CG2	2.44	0.47
1:B:72:GLY:O	1:B:73:LYS:C	2.57	0.47
1:B:128:ASP:CG	1:B:190:ARG:HH22	2.22	0.47
1:B:476:LEU:HD22	1:B:529:HIS:CD2	2.48	0.47
1:A:574:PRO:HD3	1:A:612:TYR:CD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASP:O	1:B:190:ARG:HB2	2.14	0.47
1:B:224:PRO:HB3	1:B:242:LYS:CG	2.45	0.47
1:B:294:PHE:N	1:B:295:PRO:HD3	2.29	0.47
1:A:357:PRO:HA	1:A:360:LEU:CD1	2.45	0.47
1:A:422:ASP:OD2	1:A:597:ARG:NH1	2.48	0.47
1:A:607:THR:O	1:A:611:VAL:HG23	2.13	0.47
1:B:543:GLU:N	1:B:544:PRO:CD	2.78	0.47
1:B:28:ARG:HH22	1:B:70:GLU:CG	2.28	0.47
1:B:29:MET:HE1	1:B:396:ILE:CG1	2.40	0.47
1:B:218:VAL:HG12	1:B:220:PRO:HD3	1.95	0.47
1:A:11:VAL:HG11	1:A:139:VAL:HG21	1.96	0.47
1:A:289:ASP:O	1:A:291:ILE:N	2.48	0.47
1:B:11:VAL:HG13	1:B:36:PHE:CE1	2.50	0.47
1:B:193:PHE:CZ	1:B:366:THR:HG21	2.50	0.47
1:A:161:ASN:HB3	1:A:197:ARG:NH2	2.30	0.47
1:B:396:ILE:HG12	1:B:464:LEU:HD11	1.97	0.47
1:A:593:GLY:O	1:A:596:SER:OG	2.28	0.47
1:B:62:ARG:NH1	1:B:238:TYR:CG	2.82	0.47
1:B:72:GLY:O	1:B:75:ILE:HG22	2.14	0.47
1:B:210:THR:CB	1:B:341:VAL:HA	2.44	0.47
1:B:420:MET:HG3	1:B:433:TYR:HE1	1.79	0.47
1:A:613:LEU:HA	1:A:616:LEU:CD1	2.45	0.47
1:B:57:LYS:HD3	1:B:385:GLU:CD	2.40	0.47
1:B:165:TYR:CE1	1:B:170:MET:HG2	2.50	0.47
1:B:223:ASP:OD1	1:B:242:LYS:HA	2.15	0.47
1:B:289:ASP:C	1:B:291:ILE:N	2.71	0.47
1:A:290:LYS:O	1:A:300:HIS:HE1	1.98	0.46
1:A:509:MET:SD	1:A:515:LEU:HD23	2.55	0.46
1:B:178:GLU:HB3	1:B:179:PRO:HD2	1.97	0.46
1:A:361:TYR:O	1:A:425:THR:HG21	2.15	0.46
1:A:472:LEU:HD12	1:A:472:LEU:O	2.15	0.46
1:B:471:LYS:O	1:B:475:GLU:HB2	2.15	0.46
1:B:522:PHE:N	1:B:522:PHE:CD2	2.83	0.46
1:A:294:PHE:O	1:A:296:ASP:N	2.48	0.46
1:A:356:PRO:HA	1:A:357:PRO:HD3	1.77	0.46
1:B:29:MET:CE	1:B:396:ILE:HA	2.43	0.46
1:B:54:GLY:O	1:B:55:ILE:C	2.59	0.46
1:B:505:VAL:HA	1:B:508:LEU:CG	2.41	0.46
1:B:582:GLU:HG3	1:B:586:LYS:HE3	1.98	0.46
1:A:70:GLU:O	1:A:71:MET:C	2.58	0.46
1:B:11:VAL:HG23	1:B:149:THR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HG3	1:A:579:GLU:OE2	2.16	0.46
1:A:87:THR:HA	1:A:94:GLN:NE2	2.21	0.46
1:A:293:LYS:HB2	1:A:294:PHE:CD2	2.51	0.46
1:A:446:ILE:O	1:A:446:ILE:HG22	2.16	0.46
1:A:576:LEU:O	1:A:577:THR:C	2.58	0.46
1:A:247:VAL:CG1	1:A:248:ASN:N	2.78	0.46
1:A:303:PHE:HB2	1:A:317:ASN:HB3	1.97	0.46
1:A:437:THR:CG2	1:B:276:ILE:HG23	2.46	0.46
1:B:287:ILE:CD1	1:B:290:LYS:HD2	2.45	0.46
1:B:381:THR:CG2	1:B:386:GLU:HB2	2.46	0.46
1:B:522:PHE:HD2	1:B:522:PHE:N	2.13	0.46
1:A:203:PRO:HB3	1:A:316:PRO:HG2	1.98	0.46
1:A:480:ILE:HG12	1:A:532:VAL:HG13	1.98	0.46
1:A:602:THR:HG21	1:B:165:TYR:CZ	2.51	0.46
1:B:40:ALA:O	1:B:43:ILE:HG13	2.15	0.46
1:B:361:TYR:OH	1:B:588:LYS:HD2	2.15	0.46
1:A:60:VAL:HG21	1:A:435:LEU:HD11	1.97	0.46
1:A:415:SER:HA	1:A:454:ARG:HH21	1.80	0.46
1:A:529:HIS:C	1:A:529:HIS:CD2	2.94	0.46
1:B:483:TRP:O	1:B:487:TYR:CD2	2.69	0.46
1:B:576:LEU:O	1:B:577:THR:C	2.57	0.46
1:A:60:VAL:HG12	1:A:64:ILE:HD11	1.98	0.45
1:A:333:ARG:HG2	1:A:338:LEU:O	2.16	0.45
1:A:460:ARG:NH1	1:A:467:GLU:N	2.64	0.45
1:A:526:VAL:HG13	1:A:527:PRO:HD2	1.98	0.45
1:A:551:LYS:O	1:A:554:GLU:HG3	2.16	0.45
1:B:480:ILE:O	1:B:536:VAL:HG22	2.15	0.45
1:A:277:LYS:HG2	1:B:439:ARG:NH1	2.31	0.45
1:A:72:GLY:O	1:A:73:LYS:C	2.59	0.45
1:A:157:GLY:HA2	1:A:377:ASN:HB2	1.98	0.45
1:A:588:LYS:N	1:A:589:PRO:HD3	2.31	0.45
1:B:160:LEU:HB3	1:B:353:ASP:HB2	1.98	0.45
1:B:570:TYR:HB2	1:B:585:LYS:HE2	1.98	0.45
1:A:503:TYR:N	1:A:503:TYR:CD2	2.85	0.45
1:B:447:ARG:NH2	1:B:450:ASN:HB3	2.32	0.45
1:B:366:THR:HG22	1:B:369:ILE:H	1.80	0.45
1:B:80:ILE:O	1:B:81:GLN:HB2	2.15	0.45
1:B:191:PHE:CE2	1:B:369:ILE:HD11	2.51	0.45
1:B:230:PHE:CE1	1:B:236:GLY:O	2.69	0.45
1:B:491:ARG:HD2	1:B:502:SER:O	2.17	0.45
1:A:26:ALA:O	1:A:31:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD22	1:A:331:MET:HE1	1.99	0.45
1:B:71:MET:O	1:B:75:ILE:HG22	2.16	0.45
1:B:287:ILE:HD12	1:B:287:ILE:HA	1.80	0.45
1:B:287:ILE:HD12	1:B:290:LYS:HD2	1.98	0.45
1:B:324:PRO:HB2	1:B:327:VAL:HG23	1.99	0.45
1:B:487:TYR:CE1	1:B:515:LEU:HD21	2.51	0.45
1:B:607:THR:O	1:B:611:VAL:HG23	2.17	0.45
1:A:117:GLU:O	1:A:118:ASN:HB2	2.17	0.45
1:B:86:ASN:ND2	1:B:89:LYS:HD2	2.31	0.45
1:B:319:LEU:HD13	1:B:331:MET:CE	2.47	0.45
1:B:573:ILE:HA	1:B:574:PRO:HD3	1.74	0.45
1:A:505:VAL:HA	1:A:508:LEU:CD1	2.42	0.45
1:A:519:LYS:O	1:A:523:GLY:HA2	2.16	0.45
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.74	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:B:267:HIS:H	1:B:267:HIS:HD2	1.62	0.45
1:B:487:TYR:OH	1:B:527:PRO:HD3	2.17	0.45
1:A:20:ILE:O	1:A:21:GLU:C	2.58	0.45
1:B:319:LEU:HD13	1:B:331:MET:HE1	1.99	0.45
1:A:29:MET:CE	1:A:464:LEU:HD21	2.47	0.44
1:A:366:THR:CG2	1:A:369:ILE:H	2.30	0.44
1:A:442:TYR:OH	1:A:557:LYS:HE3	2.17	0.44
1:A:553:ASN:O	1:A:554:GLU:C	2.60	0.44
1:B:94:GLN:O	1:B:448:GLN:HG2	2.17	0.44
1:A:82:PHE:N	1:A:82:PHE:HD1	2.14	0.44
1:A:158:THR:HB	1:A:350:ILE:HG12	1.99	0.44
1:A:609:LEU:HD12	1:A:609:LEU:O	2.17	0.44
1:B:29:MET:HE1	1:B:396:ILE:CA	2.44	0.44
1:A:159:PHE:HB2	2:A:618:FAD:H8A	2.00	0.44
1:A:262:ILE:HD13	1:A:287:ILE:HG23	1.99	0.44
1:A:503:TYR:N	1:A:503:TYR:HD2	2.16	0.44
1:A:589:PRO:CG	1:A:598:ILE:HD11	2.45	0.44
1:B:20:ILE:O	1:B:21:GLU:C	2.61	0.44
1:B:553:ASN:O	1:B:554:GLU:C	2.59	0.44
1:A:29:MET:HE2	1:A:464:LEU:HD21	2.00	0.44
1:A:159:PHE:CE2	2:A:618:FAD:H2B	2.53	0.44
1:A:253:TYR:CD1	1:A:253:TYR:N	2.85	0.44
1:A:289:ASP:C	1:A:291:ILE:N	2.74	0.44
1:A:385:GLU:H	1:A:385:GLU:CD	2.26	0.44
1:A:400:LEU:CD1	1:A:408:ILE:HG23	2.47	0.44
1:A:519:LYS:HB2	1:A:526:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLU:OE1	1:A:550:ARG:CD	2.66	0.44
1:B:261:ILE:HD13	1:B:330:GLU:HG2	2.00	0.44
1:B:305:GLU:HA	1:B:306:PRO:HD3	1.75	0.44
1:B:452:ILE:HD11	1:B:473:VAL:CG2	2.46	0.44
1:A:227:LYS:HG2	1:A:238:TYR:C	2.42	0.44
1:A:410:LEU:HD12	1:A:417:ILE:CG2	2.48	0.44
1:A:435:LEU:C	1:A:437:THR:N	2.73	0.44
1:A:577:THR:O	1:A:581:ARG:HG3	2.18	0.44
1:B:87:THR:HA	1:B:94:GLN:NE2	2.18	0.44
1:B:101:ASP:O	1:B:102:LYS:C	2.60	0.44
1:A:29:MET:HE1	1:A:396:ILE:CA	2.43	0.44
1:A:59:ILE:HG12	1:A:448:GLN:HB3	2.00	0.44
1:B:223:ASP:HA	1:B:224:PRO:C	2.42	0.44
1:B:507:THR:HG22	1:B:507:THR:O	2.16	0.44
1:A:262:ILE:HB	1:A:291:ILE:HD13	1.99	0.44
1:A:480:ILE:O	1:A:484:LYS:HG3	2.18	0.44
1:A:573:ILE:HA	1:A:574:PRO:HD3	1.75	0.44
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.78	0.44
1:A:165:TYR:CZ	1:B:602:THR:HG21	2.54	0.43
1:A:305:GLU:HA	1:A:306:PRO:HD3	1.81	0.43
1:A:568:ILE:HD12	1:A:568:ILE:O	2.18	0.43
1:B:8:PHE:HE1	1:B:147:TYR:CD2	2.32	0.43
1:B:57:LYS:O	1:B:58:GLY:C	2.60	0.43
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.82	0.43
1:A:86:ASN:HD22	1:A:86:ASN:HA	1.61	0.43
1:A:259:HIS:CD2	1:A:259:HIS:H	2.34	0.43
1:A:460:ARG:HA	1:A:460:ARG:HD2	1.91	0.43
1:B:511:MET:O	1:B:513:TYR:HD1	2.01	0.43
1:B:573:ILE:HD13	1:B:609:LEU:HD12	1.99	0.43
1:A:229:SER:C	1:A:231:TRP:H	2.26	0.43
1:A:275:LEU:CD2	1:A:292:VAL:HG13	2.49	0.43
1:A:559:LEU:C	1:A:561:ASP:N	2.76	0.43
1:B:483:TRP:CE2	1:B:527:PRO:HA	2.53	0.43
1:B:559:LEU:C	1:B:561:ASP:N	2.76	0.43
1:A:175:ARG:HE	1:A:178:GLU:CD	2.25	0.43
1:B:29:MET:HE2	1:B:464:LEU:HD11	1.99	0.43
1:B:56:ALA:CB	1:B:435:LEU:HB3	2.49	0.43
1:B:422:ASP:OD2	1:B:597:ARG:NH1	2.52	0.43
1:A:57:LYS:O	1:A:58:GLY:C	2.62	0.43
1:A:61:VAL:HA	1:A:64:ILE:HD12	2.01	0.43
1:A:164:ILE:N	1:A:164:ILE:HD12	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH1	1:B:353:ASP:OD1	2.50	0.43
1:B:230:PHE:CD2	1:B:452:ILE:HG12	2.54	0.43
1:B:235:VAL:HG12	1:B:236:GLY:N	2.33	0.43
1:B:281:PRO:C	1:B:283:TYR:H	2.27	0.43
1:B:110:LYS:HE2	1:B:114:GLU:OE2	2.19	0.43
1:A:548:ARG:O	1:A:552:LEU:HG	2.19	0.43
1:B:287:ILE:O	1:B:291:ILE:HG23	2.18	0.43
1:B:341:VAL:HG22	1:B:342:VAL:N	2.33	0.43
1:B:519:LYS:HB2	1:B:526:VAL:HG23	2.00	0.43
1:B:568:ILE:O	1:B:568:ILE:HG13	2.19	0.43
1:A:85:LEU:CD2	1:A:86:ASN:N	2.82	0.43
1:A:367:LYS:HZ3	1:A:587:PHE:HA	1.84	0.43
1:A:526:VAL:CG1	1:A:527:PRO:HD2	2.49	0.43
1:B:163:VAL:O	1:B:350:ILE:HD12	2.18	0.43
1:B:223:ASP:OD1	1:B:224:PRO:HA	2.19	0.43
1:B:440:SER:C	1:B:442:TYR:N	2.76	0.43
1:A:572:LYS:O	1:A:612:TYR:HE1	2.01	0.43
1:B:610:LEU:HD23	1:B:610:LEU:HA	1.73	0.43
1:A:204:ALA:C	1:A:205:ARG:HD2	2.43	0.42
1:A:408:ILE:HG13	1:A:409:TYR:N	2.31	0.42
1:B:108:TYR:HE2	1:B:112:VAL:HG21	1.84	0.42
1:A:16:GLY:O	1:A:20:ILE:HG13	2.19	0.42
1:A:258:THR:HB	1:A:259:HIS:HD2	1.84	0.42
1:B:381:THR:HG23	1:B:386:GLU:HB2	2.00	0.42
1:A:459:GLY:HA3	1:A:465:LEU:HD12	2.01	0.42
1:B:56:ALA:HB3	1:B:435:LEU:HB3	2.00	0.42
1:B:175:ARG:NE	1:B:178:GLU:OE2	2.52	0.42
1:B:229:SER:C	1:B:231:TRP:H	2.27	0.42
1:B:509:MET:HE1	1:B:515:LEU:N	2.33	0.42
1:B:594:GLN:HA	1:B:597:ARG:CZ	2.49	0.42
1:A:193:PHE:CZ	1:A:366:THR:HG21	2.55	0.42
1:B:108:TYR:CE2	1:B:112:VAL:CG2	3.02	0.42
1:B:588:LYS:N	1:B:589:PRO:HD3	2.35	0.42
1:A:293:LYS:HB2	1:A:294:PHE:CE2	2.54	0.42
1:A:445:TYR:O	1:A:445:TYR:CG	2.73	0.42
1:B:396:ILE:O	1:B:399:ALA:HB3	2.19	0.42
1:A:7:GLU:O	1:A:32:LYS:HE3	2.20	0.42
1:A:43:ILE:HD11	1:A:121:ILE:HD13	2.00	0.42
1:A:287:ILE:HG12	1:A:319:LEU:HD23	2.01	0.42
1:B:397:ASN:O	1:B:398:ALA:C	2.63	0.42
1:A:203:PRO:CB	1:A:316:PRO:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:O	1:A:536:VAL:HG23	2.19	0.42
1:B:70:GLU:C	1:B:72:GLY:N	2.76	0.42
1:B:203:PRO:HB2	1:B:316:PRO:HG2	2.02	0.42
1:B:204:ALA:H	1:B:347:ALA:HB2	1.82	0.42
1:B:275:LEU:N	1:B:275:LEU:CD2	2.83	0.42
1:B:509:MET:SD	1:B:513:TYR:O	2.78	0.42
1:B:580:ALA:HB1	1:B:601:ILE:CD1	2.49	0.42
1:A:54:GLY:O	1:A:55:ILE:C	2.63	0.42
1:A:159:PHE:CD2	2:A:618:FAD:H2B	2.55	0.42
1:A:440:SER:C	1:A:442:TYR:N	2.77	0.42
1:B:60:VAL:O	1:B:64:ILE:HG13	2.19	0.42
1:A:299:ARG:O	1:A:299:ARG:HG3	2.18	0.42
1:A:377:ASN:HD21	1:A:382:THR:HA	1.84	0.42
1:A:613:LEU:HA	1:A:616:LEU:HG	2.01	0.42
1:B:491:ARG:HA	1:B:503:TYR:O	2.20	0.42
1:B:603:PRO:O	1:B:606:ILE:HG22	2.20	0.42
1:A:95:SER:HA	1:A:96:PRO:HD2	1.93	0.41
1:A:175:ARG:O	1:A:176:LEU:C	2.62	0.41
1:A:255:THR:HB	1:A:256:PRO:CD	2.50	0.41
1:A:522:PHE:HB3	1:A:524:TYR:CE1	2.55	0.41
1:B:444:LEU:HD12	1:B:549:GLU:OE1	2.20	0.41
1:B:569:ASP:C	1:B:571:ASP:H	2.28	0.41
1:A:321:THR:OG1	1:A:322:SER:N	2.53	0.41
1:A:415:SER:HA	1:A:454:ARG:NH2	2.35	0.41
1:A:602:THR:HB	1:A:603:PRO:HD2	2.02	0.41
1:A:613:LEU:HD23	1:A:616:LEU:HD11	2.00	0.41
1:B:319:LEU:HD11	1:B:335:ILE:HD11	2.00	0.41
1:B:490:GLU:HB2	1:B:505:VAL:HG23	2.00	0.41
1:B:504:SER:O	1:B:508:LEU:HG	2.20	0.41
1:A:247:VAL:CG1	1:A:248:ASN:H	2.32	0.41
1:B:367:LYS:NZ	1:B:587:PHE:HA	2.36	0.41
1:B:602:THR:HB	1:B:603:PRO:HD2	2.01	0.41
1:A:7:GLU:O	1:A:32:LYS:CE	2.68	0.41
1:A:70:GLU:C	1:A:72:GLY:N	2.78	0.41
1:A:71:MET:O	1:A:75:ILE:HG22	2.21	0.41
1:A:101:ASP:O	1:A:102:LYS:C	2.62	0.41
1:A:416:TYR:O	1:A:419:VAL:HB	2.21	0.41
1:B:202:THR:CA	1:B:320:SER:HB3	2.50	0.41
1:B:410:LEU:HD12	1:B:417:ILE:HG21	2.00	0.41
1:B:487:TYR:CZ	1:B:515:LEU:HD21	2.56	0.41
1:B:560:GLU:OE1	1:B:597:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:HA	1:B:285:PRO:HD3	1.87	0.41
1:B:357:PRO:C	1:B:359:GLU:N	2.78	0.41
1:A:416:TYR:O	1:A:416:TYR:HD1	2.03	0.41
1:A:509:MET:HA	1:A:513:TYR:O	2.21	0.41
1:B:82:PHE:N	1:B:82:PHE:HD1	2.18	0.41
1:B:213:PHE:CD1	1:B:213:PHE:N	2.89	0.41
1:A:434:ARG:HD3	1:A:436:PHE:CZ	2.54	0.41
1:A:487:TYR:HD1	1:A:505:VAL:HG11	1.84	0.41
1:B:355:VAL:HG23	1:B:378:PHE:CZ	2.56	0.41
1:A:267:HIS:NE2	1:B:555:LYS:HD2	2.36	0.41
1:A:490:GLU:C	1:A:491:ARG:HG2	2.46	0.41
1:B:62:ARG:HE	1:B:96:PRO:HG3	1.86	0.41
1:B:492:VAL:HG11	1:B:522:PHE:HE1	1.85	0.41
1:A:281:PRO:HG3	1:A:294:PHE:CD1	2.55	0.41
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.80	0.41
1:A:312:ILE:O	1:A:312:ILE:HG13	2.19	0.41
1:A:527:PRO:HB2	1:A:533:LYS:HB2	2.02	0.41
1:A:571:ASP:C	1:A:573:ILE:H	2.29	0.41
1:B:289:ASP:O	1:B:291:ILE:N	2.54	0.41
1:B:293:LYS:C	1:B:295:PRO:HD3	2.46	0.41
1:B:356:PRO:HA	1:B:357:PRO:HD3	1.86	0.41
1:B:363:THR:HG21	1:B:407:PRO:HB2	2.02	0.41
1:B:386:GLU:O	1:B:420:MET:HE1	2.20	0.41
1:B:450:ASN:HD22	1:B:450:ASN:N	2.17	0.41
1:B:559:LEU:C	1:B:561:ASP:H	2.29	0.41
1:B:591:THR:HB	1:B:594:GLN:H	1.86	0.41
1:A:123:GLN:O	1:A:123:GLN:HG2	2.21	0.41
1:B:227:LYS:HG2	1:B:238:TYR:C	2.46	0.41
1:B:435:LEU:C	1:B:437:THR:N	2.74	0.41
1:B:450:ASN:ND2	1:B:450:ASN:N	2.67	0.41
1:A:57:LYS:HD3	1:A:385:GLU:OE1	2.21	0.40
1:A:130:ILE:N	1:A:130:ILE:CD1	2.80	0.40
1:A:508:LEU:O	1:A:513:TYR:HB2	2.21	0.40
1:A:602:THR:HB	1:A:603:PRO:CD	2.51	0.40
1:B:11:VAL:HG13	1:B:36:PHE:HE1	1.86	0.40
1:B:82:PHE:HB2	1:B:225:PRO:HB2	2.03	0.40
1:B:15:GLY:HA3	1:B:37:VAL:HG22	2.03	0.40
1:B:338:LEU:O	1:B:341:VAL:HG12	2.21	0.40
1:A:56:ALA:CB	1:A:435:LEU:HB3	2.51	0.40
1:A:422:ASP:CG	1:A:597:ARG:NH1	2.78	0.40
1:A:450:ASN:ND2	1:A:454:ARG:HH11	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:C	1:A:561:ASP:H	2.29	0.40
1:B:27:ALA:O	1:B:30:GLY:N	2.43	0.40
1:B:189:ARG:CG	1:B:195:LEU:HD12	2.50	0.40
1:B:207:ASP:HB3	1:B:210:THR:OG1	2.21	0.40
1:B:269:THR:C	1:B:271:LEU:H	2.28	0.40
1:B:509:MET:HA	1:B:513:TYR:O	2.22	0.40
1:A:207:ASP:HB3	1:A:210:THR:OG1	2.22	0.40
1:A:227:LYS:HE3	1:A:229:SER:O	2.21	0.40
1:A:235:VAL:HG12	1:A:236:GLY:N	2.36	0.40
1:A:322:SER:HB3	1:A:349:ALA:HB2	2.04	0.40
1:A:570:TYR:CD2	1:A:584:LEU:HB3	2.55	0.40
1:B:505:VAL:O	1:B:508:LEU:HB2	2.20	0.40
1:B:529:HIS:CE1	1:B:531:TYR:CB	3.03	0.40
2:B:618:FAD:O1A	2:B:618:FAD:H4'	2.21	0.40
1:A:237:SER:OG	1:A:238:TYR:N	2.53	0.40
1:A:450:ASN:HD21	1:A:454:ARG:HH11	1.69	0.40
1:B:7:GLU:HG2	1:B:148:LYS:CB	2.35	0.40
1:B:29:MET:HE3	1:B:464:LEU:HD21	2.02	0.40
1:B:203:PRO:CB	1:B:316:PRO:HG2	2.51	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:B:107:GLU:OE1	1:B:107:GLU:OE1[8_565]	1.59	0.61

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	599/637 (94%)	500 (84%)	84 (14%)	15 (2%)	4 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	597/637 (94%)	497 (83%)	83 (14%)	17 (3%)	4	25
All	All	1196/1274 (94%)	997 (83%)	167 (14%)	32 (3%)	4	25

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	285	PRO
1	B	55	ILE
1	B	71	MET
1	B	285	PRO
1	B	527	PRO
1	A	55	ILE
1	A	81	GLN
1	A	290	LYS
1	A	577	THR
1	B	81	GLN
1	B	577	THR
1	A	295	PRO
1	B	436	PHE
1	B	528	GLN
1	A	436	PHE
1	B	270	ALA
1	B	544	PRO
1	A	83	LYS
1	A	530	PRO
1	A	544	PRO
1	A	570	TYR
1	B	83	LYS
1	B	290	LYS
1	A	217	GLU
1	B	217	GLU
1	A	20	ILE
1	B	20	ILE
1	A	356	PRO
1	B	179	PRO
1	B	356	PRO
1	B	530	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	511/540 (95%)	478 (94%)	33 (6%)	15	47
1	B	510/540 (94%)	473 (93%)	37 (7%)	13	43
All	All	1021/1080 (94%)	951 (93%)	70 (7%)	14	45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	63	GLU
1	A	71	MET
1	A	81	GLN
1	A	82	PHE
1	A	85	LEU
1	A	86	ASN
1	A	108	TYR
1	A	131	VAL
1	A	137	VAL
1	A	192	ASP
1	A	223	ASP
1	A	227	LYS
1	A	232	THR
1	A	233	GLU
1	A	269	THR
1	A	298	GLU
1	A	310	ASP
1	A	321	THR
1	A	326	GLU
1	A	331	MET
1	A	354	VAL
1	A	360	LEU
1	A	379	ASN
1	A	427	LYS
1	A	429	VAL
1	A	430	THR

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Mol	Chain	Res	Type
1	A	441	GLU
1	A	448	GLN
1	A	450	ASN
1	A	503	TYR
1	A	545	TYR
1	A	577	THR
1	B	35	MET
1	B	67	LEU
1	B	81	GLN
1	B	82	PHE
1	B	86	ASN
1	B	104	ARG
1	B	108	TYR
1	B	116	GLN
1	B	164	ILE
1	B	192	ASP
1	B	256	PRO
1	B	267	HIS
1	B	269	THR
1	B	288	GLU
1	B	291	ILE
1	B	309	LEU
1	B	310	ASP
1	B	314	ILE
1	B	320	SER
1	B	321	THR
1	B	331	MET
1	B	342	VAL
1	B	379	ASN
1	B	382	THR
1	B	386	GLU
1	B	401	ARG
1	B	429	VAL
1	B	441	GLU
1	B	448	GLN
1	B	450	ASN
1	B	452	ILE
1	B	527	PRO
1	B	530	PRO
1	B	545	TYR
1	B	577	THR
1	B	591	THR

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Mol	Chain	Res	Type
1	B	606	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	81	GLN
1	A	86	ASN
1	A	94	GLN
1	A	259	HIS
1	A	265	ASN
1	A	300	HIS
1	A	340	ASN
1	A	377	ASN
1	A	379	ASN
1	A	448	GLN
1	A	450	ASN
1	A	529	HIS
1	B	45	GLN
1	B	81	GLN
1	B	86	ASN
1	B	94	GLN
1	B	248	ASN
1	B	259	HIS
1	B	267	HIS
1	B	340	ASN
1	B	377	ASN
1	B	448	GLN
1	B	450	ASN
1	B	469	GLN
1	B	528	GLN
1	B	594	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	618	-	58,58,58	1.81	16 (27%)	85,89,89	1.96	23 (27%)
3	PO4	A	619	-	4,4,4	1.63	0	6,6,6	0.47	0
3	PO4	A	620	-	4,4,4	1.65	0	6,6,6	0.47	0
2	FAD	B	618	-	58,58,58	1.88	17 (29%)	85,89,89	2.00	23 (27%)
3	PO4	B	619	-	4,4,4	1.32	1 (25%)	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	618	-	-	6/34/50/50	0/6/6/6
2	FAD	B	618	-	-	8/34/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	618	FAD	C4X-N5	4.48	1.40	1.30
2	B	618	FAD	C6-C7	4.36	1.45	1.39
2	A	618	FAD	C4X-N5	4.32	1.40	1.30
2	A	618	FAD	P-O3P	-3.65	1.55	1.59
2	B	618	FAD	C10-N10	3.49	1.44	1.37
2	A	618	FAD	C6-C7	3.48	1.44	1.39
2	B	618	FAD	O4-C4	-3.20	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	618	FAD	C6-C5X	3.19	1.44	1.40
2	A	618	FAD	PA-O3P	-3.13	1.56	1.59
2	B	618	FAD	C9-C9A	3.03	1.44	1.39
2	A	618	FAD	C9-C9A	2.96	1.44	1.39
2	B	618	FAD	P-O2P	-2.94	1.41	1.55
2	B	618	FAD	P-O3P	-2.91	1.56	1.59
2	A	618	FAD	O4-C4	-2.89	1.18	1.23
2	A	618	FAD	C6-C5X	2.87	1.44	1.40
2	B	618	FAD	O4B-C4B	-2.81	1.38	1.45
2	A	618	FAD	O4B-C4B	-2.79	1.38	1.45
2	A	618	FAD	C10-N10	2.76	1.43	1.37
2	A	618	FAD	P-O2P	-2.75	1.42	1.55
2	B	618	FAD	C1'-C2'	2.73	1.56	1.52
2	B	618	FAD	PA-O2A	-2.72	1.42	1.55
2	B	618	FAD	C10-N1	2.71	1.38	1.33
2	A	618	FAD	C10-N1	2.58	1.38	1.33
2	B	618	FAD	C2'-C3'	2.54	1.57	1.53
2	A	618	FAD	PA-O2A	-2.49	1.43	1.55
3	B	619	PO4	P-O1	2.47	1.56	1.50
2	A	618	FAD	C2'-C3'	2.37	1.57	1.53
2	A	618	FAD	PA-O1A	-2.34	1.42	1.50
2	B	618	FAD	C9A-C5X	2.27	1.44	1.41
2	B	618	FAD	PA-O1A	-2.26	1.43	1.50
2	A	618	FAD	O3'-C3'	-2.22	1.37	1.43
2	A	618	FAD	P-O1P	-2.11	1.43	1.50
2	B	618	FAD	O3'-C3'	-2.09	1.37	1.43
2	B	618	FAD	P-O1P	-2.04	1.43	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	FAD	C5A-C4A-N3A	-5.56	119.07	126.72
2	A	618	FAD	C4'-C3'-C2'	5.07	122.00	113.57
2	A	618	FAD	C5A-C4A-N3A	-4.94	119.91	126.72
2	B	618	FAD	N3A-C4A-N9A	4.86	135.44	127.17
2	A	618	FAD	N3A-C2A-N1A	-4.63	121.58	128.58
2	B	618	FAD	N3A-C2A-N1A	-4.56	121.67	128.58
2	A	618	FAD	C4-N3-C2	-4.37	117.88	125.64
2	B	618	FAD	C4-N3-C2	-4.35	117.92	125.64
2	A	618	FAD	N3A-C4A-N9A	4.17	134.25	127.17
2	B	618	FAD	C5A-N7A-C8A	4.04	109.80	103.45
2	B	618	FAD	C2A-N3A-C4A	3.86	121.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	FAD	C10-C4X-N5	-3.81	117.04	124.81
2	A	618	FAD	C2A-N3A-C4A	3.69	120.85	111.83
2	B	618	FAD	C4'-C3'-C2'	3.60	119.56	113.57
2	B	618	FAD	C4-C4X-N5	3.56	123.13	118.21
2	A	618	FAD	C5A-N7A-C8A	3.53	109.00	103.45
2	A	618	FAD	C10-C4X-N5	-3.51	117.64	124.81
2	A	618	FAD	C4X-C4-N3	3.39	121.87	113.25
2	B	618	FAD	C4X-C10-N1	-3.35	116.37	124.59
2	B	618	FAD	C4A-C5A-N7A	-3.32	106.78	110.58
2	B	618	FAD	C4X-C4-N3	3.32	121.70	113.25
2	B	618	FAD	C4X-C10-N10	3.32	121.23	116.48
2	B	618	FAD	C5X-N5-C4X	3.30	123.43	118.09
2	A	618	FAD	C5X-N5-C4X	3.26	123.36	118.09
2	A	618	FAD	C4-C4X-N5	3.20	122.63	118.21
2	A	618	FAD	C4X-C10-N10	3.09	120.91	116.48
2	A	618	FAD	C4A-N9A-C1B	-3.07	119.45	126.63
2	A	618	FAD	C4X-C10-N1	-3.04	117.14	124.59
2	A	618	FAD	C4A-C5A-N7A	-2.89	107.28	110.58
2	B	618	FAD	O4-C4-N3	-2.85	114.75	120.11
2	B	618	FAD	C10-N1-C2	2.84	123.00	116.85
2	A	618	FAD	C10-N1-C2	2.81	122.93	116.85
2	B	618	FAD	C9A-C9-C8	2.71	124.67	119.22
2	A	618	FAD	C9A-C9-C8	2.70	124.64	119.22
2	B	618	FAD	N9A-C8A-N7A	-2.67	110.16	113.94
2	A	618	FAD	C1B-N9A-C8A	2.62	132.91	127.09
2	A	618	FAD	C9A-C5X-N5	-2.53	119.77	122.45
2	A	618	FAD	N9A-C8A-N7A	-2.52	110.36	113.94
2	B	618	FAD	C4A-N9A-C1B	-2.42	120.98	126.63
2	A	618	FAD	O2'-C2'-C3'	2.41	114.89	109.25
2	A	618	FAD	O3'-C3'-C2'	-2.36	103.56	108.93
2	A	618	FAD	O4-C4-N3	-2.36	115.69	120.11
2	B	618	FAD	C9A-C5X-N5	-2.14	120.18	122.45
2	B	618	FAD	O2-C2-N1	-2.10	118.31	121.80
2	B	618	FAD	O5'-C5'-C4'	2.08	114.92	109.36
2	B	618	FAD	O2'-C2'-C3'	2.03	114.00	109.25

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	618	FAD	C3'-C4'-C5'-O5'
2	A	618	FAD	O4'-C4'-C5'-O5'

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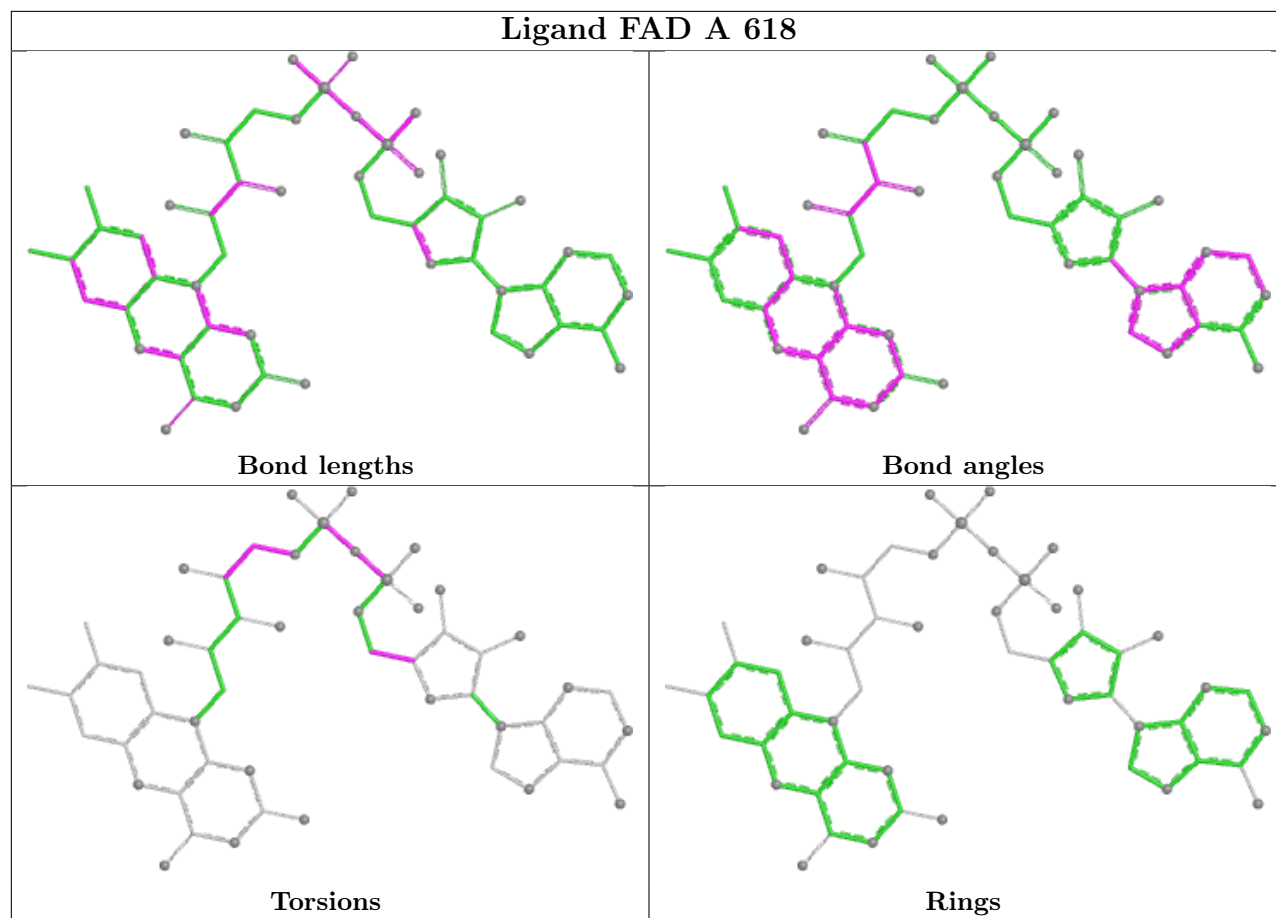
Mol	Chain	Res	Type	Atoms
2	B	618	FAD	C3'-C4'-C5'-O5'
2	B	618	FAD	O4'-C4'-C5'-O5'
2	B	618	FAD	PA-O3P-P-O5'
2	B	618	FAD	C2'-C3'-C4'-O4'
2	B	618	FAD	O3'-C3'-C4'-C5'
2	B	618	FAD	C2'-C3'-C4'-C5'
2	B	618	FAD	C4'-C5'-O5'-P
2	B	618	FAD	O3'-C3'-C4'-O4'
2	A	618	FAD	C4'-C5'-O5'-P
2	A	618	FAD	PA-O3P-P-O5'
2	A	618	FAD	O4B-C4B-C5B-O5B
2	A	618	FAD	P-O3P-PA-O1A

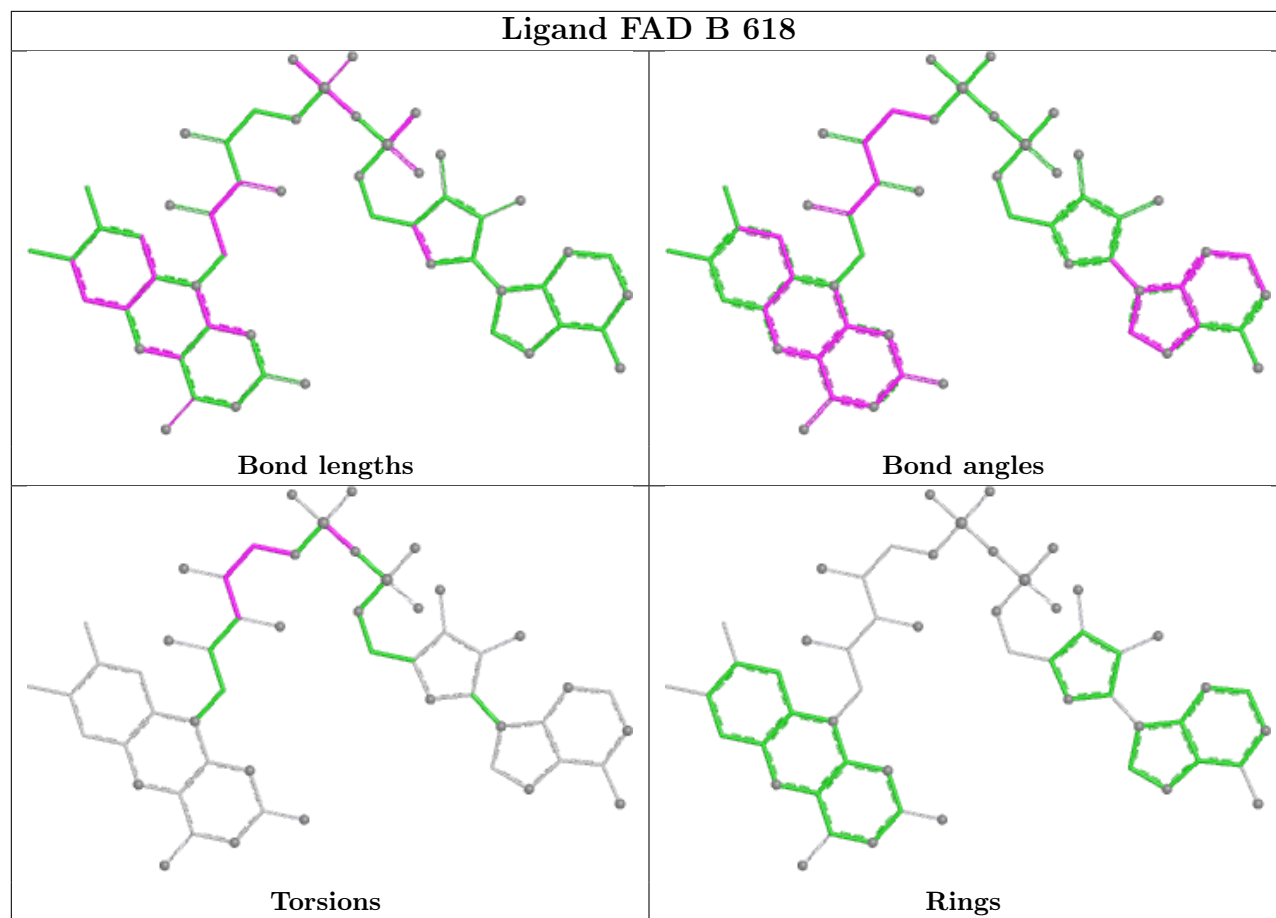
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	618	FAD	3	0
2	B	618	FAD	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	603/637 (94%)	-0.24	1 (0%) 91 85	31, 60, 99, 118	0
1	B	601/637 (94%)	-0.00	8 (1%) 75 55	32, 72, 123, 147	0
All	All	1204/1274 (94%)	-0.12	9 (0%) 84 69	31, 67, 112, 147	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	PHE	4.2
1	A	329	TRP	3.1
1	B	329	TRP	2.9
1	B	525	GLU	2.5
1	B	526	VAL	2.4
1	B	513	TYR	2.3
1	B	506	ALA	2.0
1	B	502	SER	2.0
1	B	540	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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,

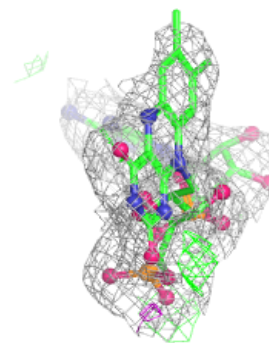
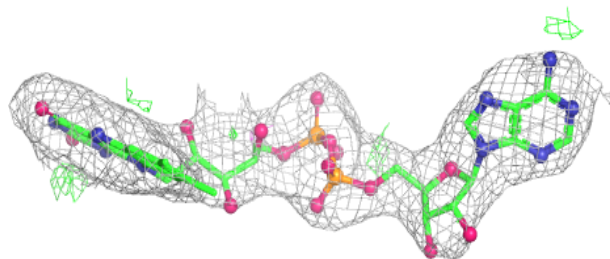
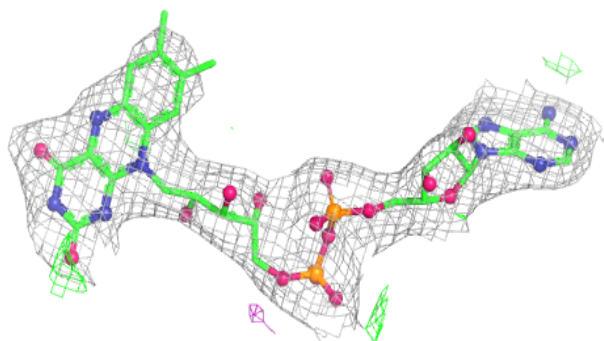
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

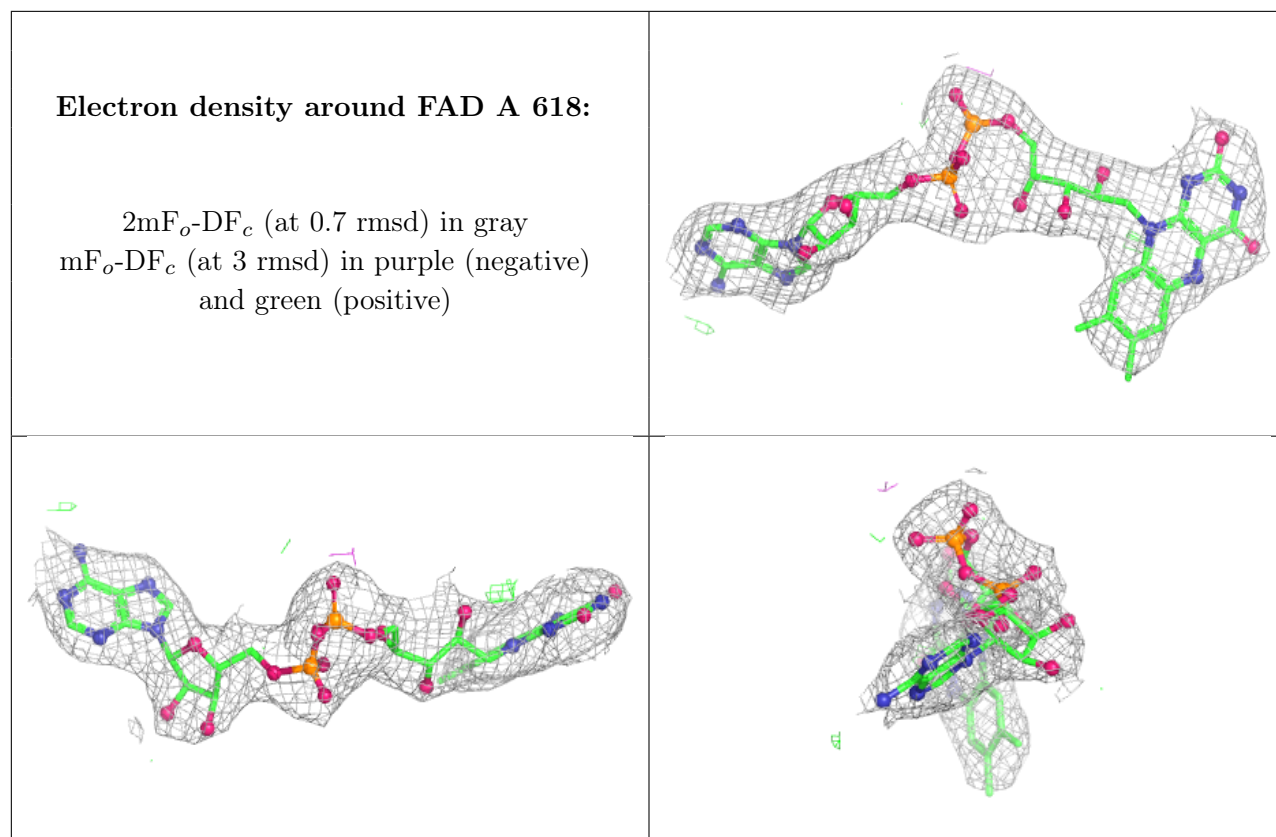
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	A	620	5/5	0.64	0.12	120,122,126,127	0
3	PO4	A	619	5/5	0.71	0.10	118,119,123,127	0
3	PO4	B	619	5/5	0.88	0.13	123,124,128,130	0
2	FAD	B	618	53/53	0.96	0.10	39,65,78,78	0
2	FAD	A	618	53/53	0.97	0.08	23,47,66,73	0

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 618:

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 [i](#)

There are no such residues in this entry.