



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DWK
Title : Identification of Dynamic Structural Motifs Involved in Peptidoglycan Glycosyltransfer
Authors : Lovering, A.L.; De Castro, L.; Strynadka, N.C.J.
Deposited on : 2008-07-22
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

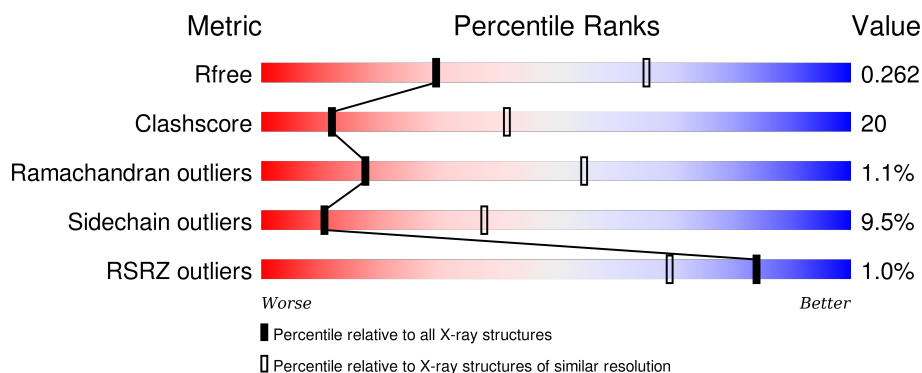
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	625	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>• •</div> </div> </div>
1	B	625	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
1	C	625	<div> <div></div> <div> <div>61%</div> <div>34%</div> <div>5%</div> </div> </div>
1	D	625	<div> <div></div> <div> <div>60%</div> <div>32%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	11	-	-	X	-
2	SO4	A	15	-	-	X	-
2	SO4	A	17	-	-	X	-
2	SO4	A	27	-	-	-	X
2	SO4	A	41	-	-	X	-
2	SO4	B	38	-	-	X	-
2	SO4	C	31	-	-	X	-
2	SO4	D	39	-	-	X	-
3	LDA	D	1	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19474 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4712	2953	809	938	12			
1	B	621	Total	C	N	O	S	0	0	0
			4874	3051	839	972	12			
1	C	623	Total	C	N	O	S	0	0	0
			4891	3060	843	976	12			
1	D	602	Total	C	N	O	S	0	0	0
			4751	2977	817	945	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	MET	LYS	ENGINEERED	UNP Q5HFX3
B	68	MET	LYS	ENGINEERED	UNP Q5HFX3
C	68	MET	LYS	ENGINEERED	UNP Q5HFX3
D	68	MET	LYS	ENGINEERED	UNP Q5HFX3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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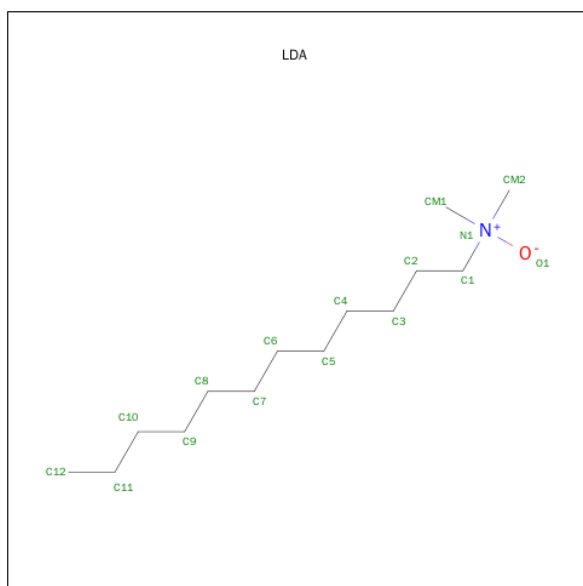
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

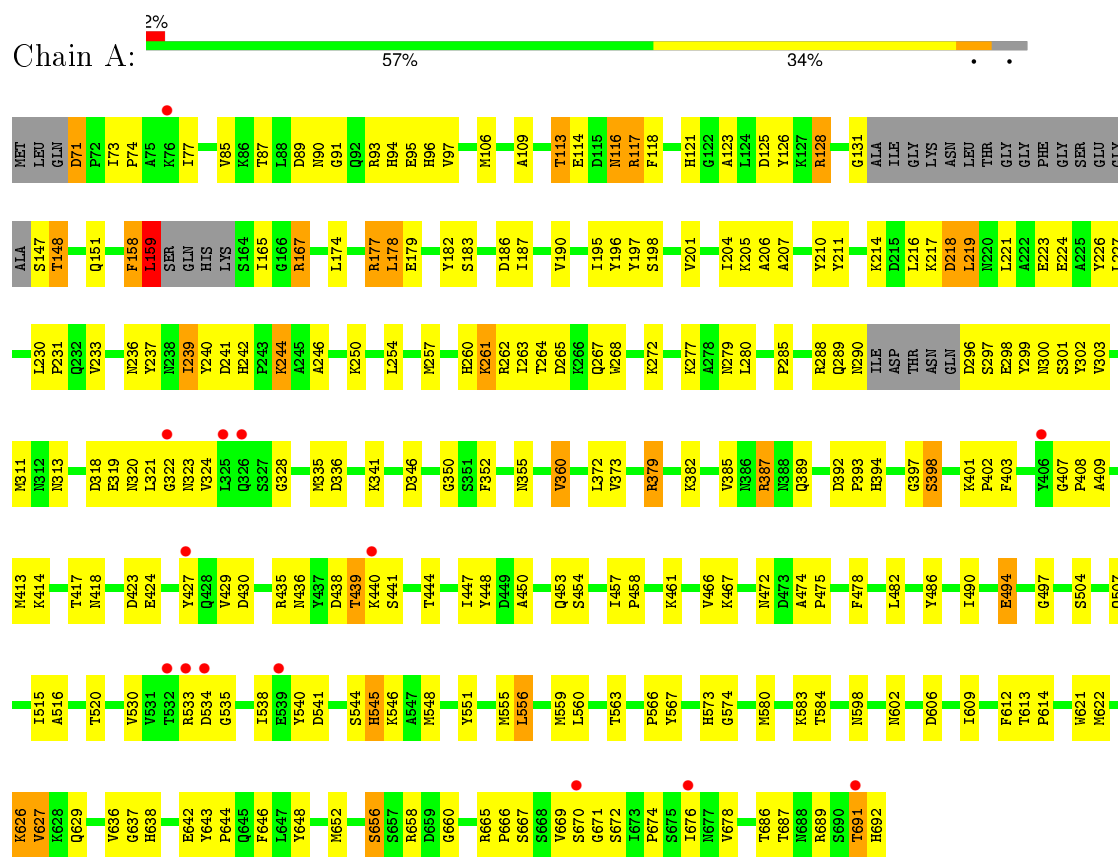


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			16	14	1	1		

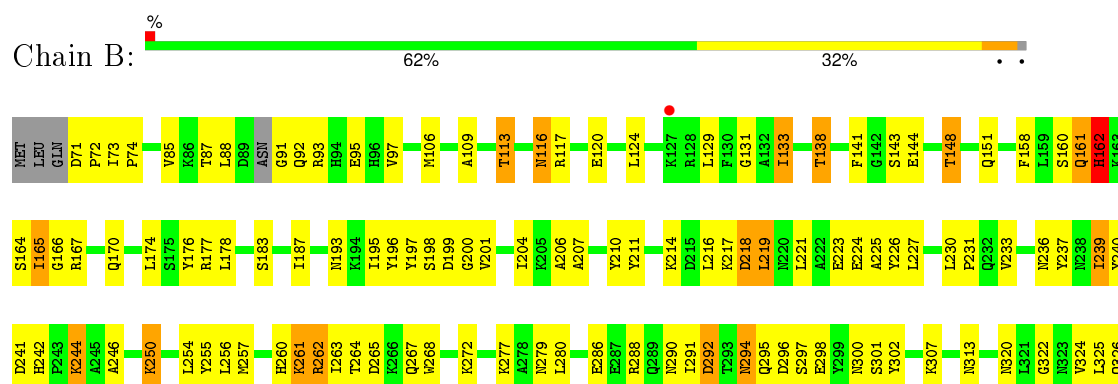
3 Residue-property plots

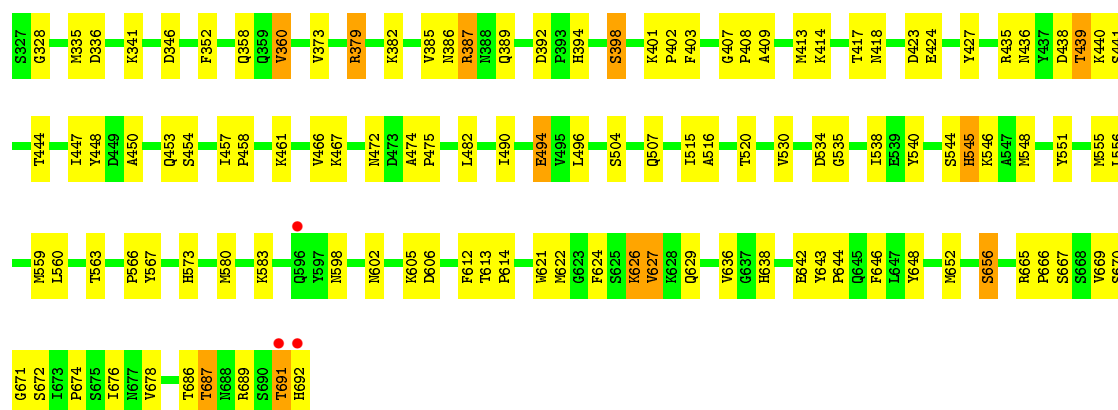
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Penicillin-binding protein 2



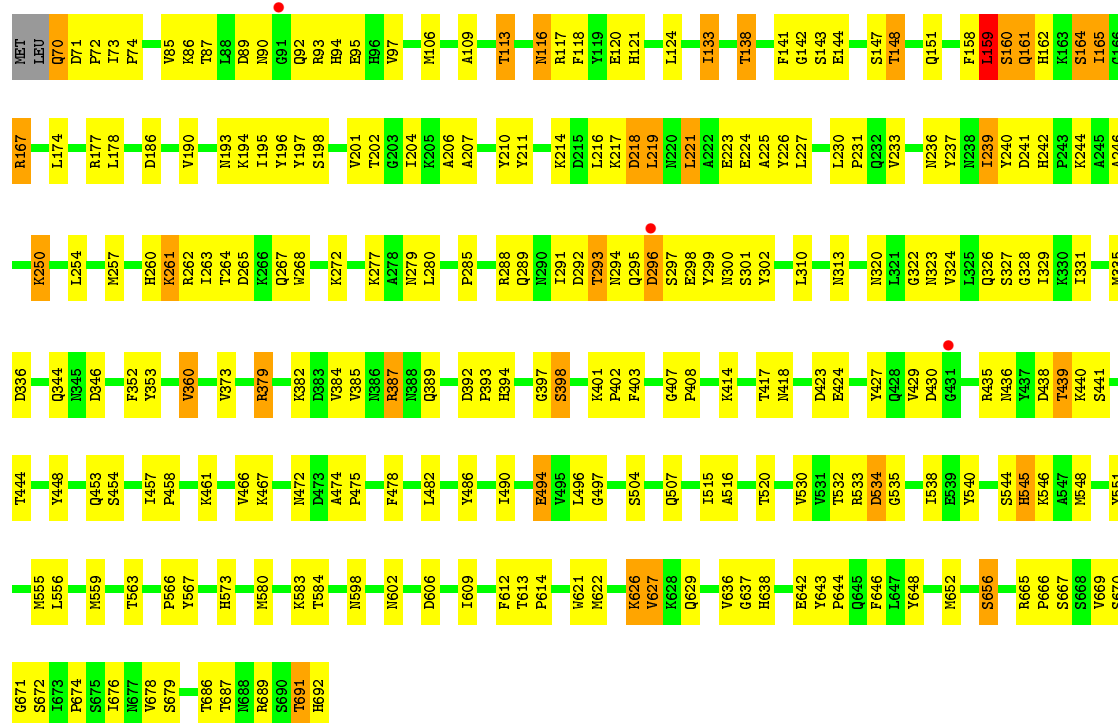
• Molecule 1: Penicillin-binding protein 2





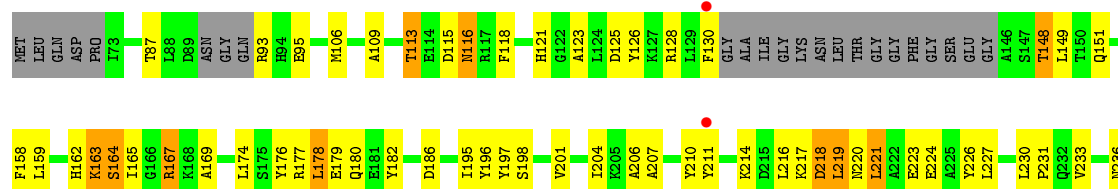
• Molecule 1: Penicillin-binding protein 2

Chain C: 61% 34% 5%



• Molecule 1: Penicillin-binding protein 2

Chain D: 60% 32% 8%



P644	I538	M436	V324	P645	P539	Y437	I237	P646	Y540	D438	I239	L647	S544	K440	T439	Y240	P648	H545	S441	D336	D241	P649	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P650	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P651	M551	Y448	D449	I345	D346	G344	S345	T331	I238	P652	M555	A450	Q453	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323
P653	P538	Y437	I237	P654	Y540	D438	I239	P655	Y551	Y448	I238	L647	S544	K440	T439	Y240	P656	H545	S441	D336	D241	P657	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P658	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P659	M555	A450	Q453	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323										
P654	P539	Y437	I237	P655	Y540	D438	I239	P656	Y551	Y448	I238	L647	S544	K440	T439	Y240	P657	H545	S441	D336	D241	P658	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P659	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P660	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P655	P538	Y437	I237	P656	Y540	D438	I239	P657	Y551	Y448	I238	L647	S544	K440	T439	Y240	P658	H545	S441	D336	D241	P659	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P660	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P661	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P656	P539	Y437	I237	P657	Y540	D438	I239	P666	Y551	Y448	I238	L647	S544	K440	T439	Y240	P667	H545	S441	D336	D241	P668	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P668	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P669	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P667	P539	Y437	I237	P668	Y540	D438	I239	P669	Y551	Y448	I238	L647	S544	K440	T439	Y240	P670	H545	S441	D336	D241	P671	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P672	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P673	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P678	P538	Y437	I237	P679	Y540	D438	I239	P674	Y551	Y448	I238	L647	S544	K440	T439	Y240	P675	H545	S441	D336	D241	P676	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P677	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P678	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P679	P539	Y437	I237	P686	P538	Y437	I237	P687	Y540	D438	I239	L647	S544	K440	T439	Y240	P688	H545	S441	D336	D241	P689	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P688	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P689	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P686	P539	Y437	I237	P687	P538	Y437	I237	P688	Y540	D438	I239	L647	S544	K440	T439	Y240	P689	H545	S441	D336	D241	P690	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P690	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P691	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P687	P538	Y437	I237	P688	P539	Y437	I237	P689	Y540	D438	I239	L647	S544	K440	T439	Y240	P690	H545	S441	D336	D241	P691	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P691	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P692	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P688	P539	Y437	I237	P689	P538	Y437	I237	P690	Y540	D438	I239	L647	S544	K440	T439	Y240	P691	H545	S441	D336	D241	P692	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P692	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P693	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P689	P538	Y437	I237	P690	P539	Y437	I237	P691	Y540	D438	I239	L647	S544	K440	T439	Y240	P692	H545	S441	D336	D241	P693	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P693	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P694	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P690	P539	Y437	I237	P691	P538	Y437	I237	P692	Y540	D438	I239	L647	S544	K440	T439	Y240	P693	H545	S441	D336	D241	P694	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P694	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P695	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P691	P538	Y437	I237	P692	P539	Y437	I237	P693	Y540	D438	I239	L647	S544	K440	T439	Y240	P694	H545	S441	D336	D241	P695	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P695	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P696	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P692	P539	Y437	I237	P693	P538	Y437	I237	P694	Y540	D438	I239	L647	S544	K440	T439	Y240	P695	H545	S441	D336	D241	P696	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P696	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P697	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P693	P538	Y437	I237	P694	P539	Y437	I237	P695	Y540	D438	I239	L647	S544	K440	T439	Y240	P696	H545	S441	D336	D241	P697	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P697	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P698	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P694	P539	Y437	I237	P695	P538	Y437	I237	P696	Y540	D438	I239	L647	S544	K440	T439	Y240	P697	H545	S441	D336	D241	P698	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P698	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P699	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394	S398	I291	D292	T293	N294	Q295	D296	S297	E298	Y299	M300	S301	Y302	K307	L310	M313	M320	L321	G322	M323								
P695	P538	Y437	I237	P696	P539	Y437	I237	P697	Y540	D438	I239	L647	S544	K440	T439	Y240	P698	H545	S441	D336	D241	P699	M547	T444	K341	Q344	D346	G350	S351	F352	M257	P699	L254	K250	A246	A245	K244	P243	H242	D241	Y240	I239	P700	M559	L560	T563	P458	I457	S454	F352	V360	V373	R379	K382	I383	V384	V385	N386	R387	N388	Q389	D392	P393	H394																												

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.35Å 217.47Å 95.73Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	41.88 – 3.10 41.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.88-3.10) 94.4 (41.88-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.218 , 0.264 0.217 , 0.262	Depositor DCC
R_{free} test set	3052 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 60418 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19474	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, SO4

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	0.36	0/4813	0.53	2/6504 (0.0%)
1	B	0.35	0/4979	0.51	0/6729
1	C	0.38	0/4997	0.54	1/6755 (0.0%)
1	D	0.37	0/4853	0.53	0/6559
All	All	0.37	0/19642	0.53	3/26547 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	LEU	CA-CB-CG	-7.58	97.86	115.30
1	A	131	GLY	N-CA-C	-6.72	96.29	113.10
1	A	159	LEU	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	C	159	LEU	Peptide

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	4712	0	4518	190	0
1	B	4874	0	4676	191	0
1	C	4891	0	4691	208	0
1	D	4751	0	4562	185	0
2	A	75	0	0	14	0
2	B	65	0	0	8	0
2	C	45	0	0	6	0
2	D	45	0	0	5	0
3	D	16	0	31	7	0
All	All	19474	0	18478	759	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (759) 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:162:HIS:CE1	1:B:164:SER:HB2	1.78	1.18
1:C:160:SER:HB2	1:C:167:ARG:NH1	1.61	1.15
1:C:160:SER:CB	1:C:167:ARG:HH11	1.59	1.14
1:C:159:LEU:HD22	1:C:532:THR:HB	1.23	1.11
1:D:118:PHE:HA	1:D:121:HIS:CE1	1.95	1.01
1:A:106:MET:HE2	1:A:224:GLU:HG2	1.42	1.00
1:A:118:PHE:HA	1:A:121:HIS:CE1	1.99	0.97
1:C:72:PRO:HD3	1:C:94:HIS:CE1	2.00	0.96
1:C:159:LEU:CD2	1:C:532:THR:HB	1.95	0.96
1:C:160:SER:CB	1:C:167:ARG:NH1	2.24	0.95
1:C:160:SER:HB2	1:C:167:ARG:HH11	0.79	0.95
1:C:144:GLU:HB2	1:D:574:GLY:O	1.66	0.95
1:D:164:SER:HB2	1:D:167:ARG:H	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LYS:HE2	2:B:35:SO4:O4	1.73	0.88
1:B:162:HIS:NE2	1:B:164:SER:HB2	1.87	0.88
1:C:116:ASN:ND2	1:C:262:ARG:NH1	2.21	0.88
1:C:116:ASN:ND2	1:C:262:ARG:HH12	1.72	0.88
1:A:118:PHE:HA	1:A:121:HIS:HE1	1.37	0.87
1:D:118:PHE:HA	1:D:121:HIS:HE1	1.35	0.86
1:A:350:GLY:HA2	1:B:138:THR:HG21	1.57	0.85
1:D:162:HIS:HB2	1:D:167:ARG:NE	1.92	0.85
1:B:162:HIS:NE2	1:B:164:SER:CB	2.39	0.84
1:D:580:MET:HB3	1:D:613:THR:HG22	1.57	0.84
1:C:73:ILE:HD12	1:C:74:PRO:HD2	1.59	0.83
1:B:161:GLN:O	1:B:162:HIS:HB2	1.78	0.83
1:C:580:MET:HB3	1:C:613:THR:HG22	1.59	0.83
1:A:580:MET:HB3	1:A:613:THR:HG22	1.60	0.83
1:B:580:MET:HB3	1:B:613:THR:HG22	1.58	0.83
1:D:176:TYR:CD2	3:D:1:LDA:H32	2.15	0.82
1:C:141:PHE:HB2	1:C:148:THR:HG21	1.61	0.81
1:A:574:GLY:O	1:B:144:GLU:HB2	1.81	0.81
1:B:116:ASN:ND2	1:B:262:ARG:NH1	2.28	0.81
1:B:687:THR:HG22	2:B:23:SO4:O2	1.81	0.80
1:B:116:ASN:ND2	1:B:262:ARG:HH12	1.77	0.80
1:C:161:GLN:O	1:C:161:GLN:HG2	1.80	0.80
1:B:162:HIS:CE1	1:B:164:SER:CB	2.62	0.79
1:D:313:ASN:HB2	1:D:540:TYR:CE2	2.18	0.78
1:D:679:SER:HA	2:D:9:SO4:O2	1.84	0.77
1:D:382:LYS:HB2	1:D:385:VAL:HB	1.67	0.77
1:A:382:LYS:HB2	1:A:385:VAL:HB	1.66	0.76
1:C:159:LEU:HD22	1:C:532:THR:CB	2.11	0.76
1:A:126:TYR:HB2	2:A:15:SO4:O2	1.84	0.76
1:C:138:THR:HG21	1:D:350:GLY:HA2	1.68	0.76
1:C:382:LYS:HB2	1:C:385:VAL:HB	1.67	0.76
1:B:382:LYS:HB2	1:B:385:VAL:HB	1.68	0.76
1:C:73:ILE:HG23	1:C:328:GLY:HA3	1.68	0.76
1:D:626:LYS:HD2	1:D:627:VAL:N	2.02	0.74
1:B:233:VAL:HG22	1:B:237:TYR:CE1	2.22	0.74
1:C:313:ASN:HB2	1:C:540:TYR:CE2	2.22	0.74
1:B:530:VAL:HG23	1:B:538:ILE:HD13	1.71	0.73
1:C:233:VAL:HG22	1:C:237:TYR:CE1	2.23	0.73
1:D:159:LEU:HD12	1:D:532:THR:HB	1.70	0.73
1:A:244:LYS:HB2	2:A:17:SO4:O3	1.88	0.72
1:A:116:ASN:ND2	1:A:262:ARG:HH12	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:TYR:CE2	1:B:461:LYS:HE2	2.25	0.72
1:A:567:TYR:CE2	1:A:692:HIS:HB2	2.24	0.72
1:B:92:GLN:O	1:B:93:ARG:HG3	1.90	0.72
1:C:427:TYR:CE2	1:C:461:LYS:HE2	2.25	0.71
1:B:567:TYR:CE2	1:B:692:HIS:HB2	2.26	0.71
1:A:626:LYS:HD2	1:A:627:VAL:N	2.06	0.70
1:C:626:LYS:HD2	1:C:627:VAL:N	2.06	0.70
1:C:73:ILE:HG23	1:C:328:GLY:CA	2.21	0.70
1:A:177:ARG:NH2	2:A:41:SO4:O1	2.24	0.70
1:B:242:HIS:HA	2:B:38:SO4:O4	1.91	0.70
1:B:240:TYR:CD1	1:B:288:ARG:HD3	2.26	0.70
1:B:161:GLN:HE21	1:B:538:ILE:HA	1.57	0.69
1:D:121:HIS:HD2	1:D:125:ASP:HB2	1.57	0.69
1:D:116:ASN:ND2	1:D:262:ARG:HH12	1.90	0.69
1:A:530:VAL:HG23	1:A:538:ILE:HD13	1.74	0.69
1:C:567:TYR:CE2	1:C:692:HIS:HB2	2.27	0.69
1:C:240:TYR:CD1	1:C:288:ARG:HD3	2.27	0.69
1:A:660:GLY:HA3	1:B:255:TYR:CE2	2.28	0.69
1:D:652:MET:O	1:D:656:SER:HB2	1.92	0.69
1:D:164:SER:HB2	1:D:167:ARG:N	2.07	0.69
1:D:530:VAL:HG23	1:D:538:ILE:HD13	1.73	0.69
1:A:240:TYR:CD1	1:A:288:ARG:HD3	2.26	0.69
1:C:679:SER:HA	2:C:4:SO4:O1	1.93	0.69
1:B:217:LYS:HG3	1:B:218:ASP:H	1.59	0.69
1:D:106:MET:HE2	1:D:224:GLU:HG2	1.74	0.68
1:C:474:ALA:HB3	1:C:475:PRO:HD3	1.75	0.68
1:C:106:MET:HE2	1:C:224:GLU:HG2	1.73	0.68
1:A:95:GLU:H	1:A:206:ALA:HB2	1.58	0.68
1:B:626:LYS:HD2	1:B:627:VAL:N	2.08	0.68
1:C:637:GLY:HA2	2:C:31:SO4:O4	1.94	0.68
1:C:652:MET:O	1:C:656:SER:HB2	1.93	0.68
1:C:217:LYS:HG3	1:C:218:ASP:H	1.59	0.68
1:D:233:VAL:HG22	1:D:237:TYR:CE1	2.29	0.68
1:D:427:TYR:CE2	1:D:461:LYS:HE2	2.29	0.68
1:A:233:VAL:HG22	1:A:237:TYR:CE1	2.29	0.68
1:D:457:ILE:HB	1:D:458:PRO:HD3	1.77	0.67
1:A:427:TYR:CE2	1:A:461:LYS:HE2	2.30	0.67
1:A:116:ASN:ND2	1:A:262:ARG:NH1	2.43	0.67
1:A:217:LYS:HG3	1:A:218:ASP:H	1.58	0.67
1:B:665:ARG:NH2	1:B:671:GLY:O	2.28	0.67
1:A:158:PHE:CE1	1:A:159:LEU:HD23	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:MET:O	1:B:656:SER:HB2	1.95	0.67
1:C:530:VAL:HG23	1:C:538:ILE:HD13	1.76	0.67
1:C:389:GLN:HG2	1:C:621:TRP:CZ3	2.30	0.67
1:A:148:THR:HG23	1:A:151:GLN:HB2	1.78	0.66
1:C:71:ASP:HB3	1:C:72:PRO:HD2	1.76	0.66
1:D:116:ASN:ND2	1:D:262:ARG:NH1	2.44	0.66
1:A:389:GLN:HG2	1:A:621:TRP:CZ3	2.30	0.66
1:D:217:LYS:HG3	1:D:218:ASP:H	1.60	0.66
1:D:240:TYR:CD1	1:D:288:ARG:HD3	2.31	0.66
1:A:159:LEU:CD2	1:A:167:ARG:HD3	2.26	0.66
1:B:313:ASN:HB2	1:B:540:TYR:CE2	2.30	0.66
1:A:93:ARG:NH1	1:A:210:TYR:CE2	2.64	0.66
1:D:159:LEU:HD12	1:D:533:ARG:H	1.61	0.66
1:B:116:ASN:C	1:B:116:ASN:HD22	1.99	0.66
1:D:389:GLN:HG2	1:D:621:TRP:CZ3	2.30	0.65
1:B:389:GLN:HG2	1:B:621:TRP:CZ3	2.31	0.65
1:D:567:TYR:CE2	1:D:692:HIS:HB2	2.30	0.65
1:C:72:PRO:CB	1:C:92:GLN:HE22	2.09	0.65
1:A:665:ARG:NH2	1:A:671:GLY:O	2.30	0.65
1:A:652:MET:O	1:A:656:SER:HB2	1.97	0.65
1:A:121:HIS:HD2	1:A:125:ASP:HB2	1.62	0.65
1:D:148:THR:HG23	1:D:151:GLN:HB2	1.79	0.65
1:A:242:HIS:HA	2:A:17:SO4:O4	1.97	0.65
1:A:239:ILE:HD12	1:A:280:LEU:HD22	1.78	0.65
1:D:121:HIS:CD2	1:D:125:ASP:HB2	2.32	0.64
1:B:158:PHE:HZ	1:B:170:GLN:HG2	1.63	0.64
1:C:293:THR:HG22	1:C:294:ASN:H	1.60	0.64
1:A:73:ILE:HD12	1:A:74:PRO:HD2	1.80	0.64
1:B:158:PHE:CZ	1:B:170:GLN:HG2	2.32	0.64
1:A:89:ASP:C	1:A:91:GLY:H	2.02	0.64
1:B:161:GLN:NE2	1:B:538:ILE:HA	2.13	0.63
1:A:177:ARG:NH2	2:A:41:SO4:O4	2.31	0.63
1:C:665:ARG:NH2	1:C:671:GLY:O	2.30	0.63
1:B:162:HIS:CD2	1:B:164:SER:HB2	2.34	0.63
1:D:290:ASN:HB3	1:D:292:ASP:H	1.64	0.63
1:A:201:VAL:HG11	1:A:207:ALA:HA	1.81	0.63
1:B:436:ASN:OD1	1:B:457:ILE:HG12	1.99	0.63
1:C:293:THR:HG22	1:C:294:ASN:N	2.13	0.63
1:D:320:ASN:O	1:D:324:VAL:HG23	2.00	0.62
1:D:665:ARG:NH2	1:D:671:GLY:O	2.32	0.62
1:C:141:PHE:HB2	1:C:148:THR:CG2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD22	1:A:167:ARG:HD3	1.81	0.62
1:D:159:LEU:CD1	1:D:533:ARG:H	2.12	0.62
1:A:95:GLU:N	1:A:206:ALA:HB2	2.13	0.62
1:D:389:GLN:HG3	1:D:394:HIS:CE1	2.35	0.62
1:D:474:ALA:HB3	1:D:475:PRO:HD3	1.81	0.62
1:A:298:GLU:HG3	1:A:341:LYS:HG2	1.81	0.62
1:A:177:ARG:NH2	2:A:41:SO4:S	2.73	0.62
1:C:254:LEU:HD23	1:C:257:MET:HE3	1.82	0.62
1:A:350:GLY:HA2	1:B:138:THR:CG2	2.28	0.61
1:A:457:ILE:HB	1:A:458:PRO:HD3	1.82	0.61
1:D:289:GLN:HB3	1:D:384:VAL:HG21	1.81	0.61
1:C:320:ASN:O	1:C:324:VAL:HG23	2.00	0.61
1:A:196:TYR:CE1	1:A:198:SER:HA	2.35	0.61
1:A:408:PRO:HB2	1:A:466:VAL:HG11	1.82	0.61
1:C:196:TYR:CE1	1:C:198:SER:HA	2.35	0.61
1:B:201:VAL:HG11	1:B:207:ALA:HA	1.81	0.61
1:A:117:ARG:NH2	2:A:15:SO4:O1	2.30	0.61
1:D:538:ILE:H	1:D:538:ILE:HD12	1.66	0.61
1:A:598:ASN:HD22	1:A:629:GLN:HE21	1.47	0.61
1:D:109:ALA:O	1:D:113:THR:HG22	2.01	0.61
1:D:196:TYR:CE1	1:D:198:SER:HA	2.35	0.61
1:C:116:ASN:HD22	1:C:262:ARG:HH12	1.47	0.61
1:A:474:ALA:HB3	1:A:475:PRO:HD3	1.82	0.61
1:D:436:ASN:OD1	1:D:457:ILE:HG12	1.99	0.61
1:B:386:ASN:HA	2:B:25:SO4:O1	2.01	0.61
1:C:201:VAL:HG11	1:C:207:ALA:HA	1.83	0.61
1:D:121:HIS:HD2	1:D:125:ASP:CB	2.13	0.60
1:B:196:TYR:CE1	1:B:198:SER:HA	2.36	0.60
1:B:264:THR:OG1	1:B:267:GLN:HG2	2.01	0.60
1:C:264:THR:OG1	1:C:267:GLN:HG2	2.01	0.60
1:C:436:ASN:OD1	1:C:457:ILE:HG12	2.02	0.60
1:D:295:GLN:O	1:D:296:ASP:HB2	2.00	0.60
1:D:605:LYS:HE2	2:D:7:SO4:O1	2.02	0.60
1:B:474:ALA:HB3	1:B:475:PRO:HD3	1.82	0.60
1:B:389:GLN:HG3	1:B:394:HIS:CE1	2.37	0.60
1:A:264:THR:OG1	1:A:267:GLN:HG2	2.02	0.60
1:C:148:THR:HG23	1:C:151:GLN:HB2	1.84	0.59
1:C:408:PRO:HB2	1:C:466:VAL:HG11	1.83	0.59
1:A:121:HIS:CD2	1:A:125:ASP:HB2	2.36	0.59
1:D:201:VAL:HG11	1:D:207:ALA:HA	1.84	0.59
1:C:457:ILE:HB	1:C:458:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:THR:HG23	1:D:294:ASN:N	2.16	0.59
1:B:148:THR:HG23	1:B:151:GLN:HB2	1.83	0.59
1:A:389:GLN:HG3	1:A:394:HIS:CE1	2.37	0.59
1:A:73:ILE:HG23	1:A:328:GLY:HA3	1.82	0.59
1:A:109:ALA:O	1:A:113:THR:HG22	2.02	0.59
1:B:298:GLU:HG3	1:B:341:LYS:HG2	1.84	0.59
1:C:666:PRO:HG2	1:C:669:VAL:HG22	1.84	0.59
1:D:169:ALA:HB1	3:D:1:LDA:H123	1.84	0.59
1:C:389:GLN:HG3	1:C:394:HIS:CE1	2.37	0.59
1:B:418:ASN:HB3	1:B:674:PRO:O	2.03	0.59
1:B:320:ASN:O	1:B:324:VAL:HG23	2.02	0.59
1:B:183:SER:O	1:B:187:ILE:HG13	2.01	0.59
1:B:538:ILE:H	1:B:538:ILE:HD12	1.68	0.59
1:B:161:GLN:O	1:B:162:HIS:CB	2.51	0.59
1:B:239:ILE:HD12	1:B:280:LEU:HD22	1.84	0.58
1:A:233:VAL:HG23	1:A:233:VAL:O	2.04	0.58
1:A:216:LEU:O	1:A:219:LEU:HD23	2.03	0.58
1:A:73:ILE:HG23	1:A:328:GLY:CA	2.32	0.58
1:D:264:THR:OG1	1:D:267:GLN:HG2	2.03	0.58
1:D:216:LEU:O	1:D:219:LEU:HD23	2.03	0.58
1:C:160:SER:HB3	1:C:167:ARG:NH1	2.16	0.58
1:A:254:LEU:HD23	1:A:257:MET:HE3	1.85	0.58
1:C:233:VAL:O	1:C:233:VAL:HG23	2.02	0.58
1:B:408:PRO:HB2	1:B:466:VAL:HG11	1.86	0.58
1:D:389:GLN:HG2	1:D:621:TRP:HZ3	1.67	0.58
1:C:285:PRO:O	1:C:289:GLN:HG3	2.03	0.58
1:C:109:ALA:O	1:C:113:THR:HG22	2.04	0.57
1:B:162:HIS:CD2	1:B:164:SER:CB	2.88	0.57
1:D:204:ILE:HD11	1:D:227:LEU:HB3	1.87	0.57
1:C:239:ILE:HD12	1:C:280:LEU:HD22	1.86	0.57
1:A:436:ASN:OD1	1:A:457:ILE:HG12	2.03	0.57
1:C:504:SER:OG	1:C:507:GLN:HG3	2.04	0.57
1:C:387:ARG:HG3	1:C:392:ASP:OD2	2.05	0.57
1:A:285:PRO:HB2	1:A:385:VAL:HG13	1.86	0.57
1:B:457:ILE:HB	1:B:458:PRO:HD3	1.86	0.57
1:D:239:ILE:HD12	1:D:280:LEU:HD22	1.87	0.57
1:B:254:LEU:HD23	1:B:257:MET:HE3	1.85	0.57
1:C:204:ILE:HD11	1:C:227:LEU:HB3	1.87	0.57
1:B:73:ILE:CG1	1:B:328:GLY:HA3	2.35	0.57
1:D:387:ARG:HG3	1:D:392:ASP:OD2	2.05	0.57
1:A:320:ASN:O	1:A:324:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:N	2:A:17:SO4:O3	2.38	0.57
1:A:240:TYR:CE2	1:A:280:LEU:HD11	2.40	0.57
1:C:72:PRO:HB2	1:C:92:GLN:HE22	1.69	0.57
1:C:217:LYS:HG3	1:C:218:ASP:N	2.20	0.56
1:C:159:LEU:HD13	1:C:532:THR:HG21	1.87	0.56
1:B:162:HIS:ND1	1:B:164:SER:HB2	2.19	0.56
1:A:217:LYS:HG3	1:A:218:ASP:N	2.21	0.56
1:D:254:LEU:HD23	1:D:257:MET:HE3	1.87	0.56
1:A:158:PHE:CZ	1:A:159:LEU:HD23	2.41	0.56
1:A:313:ASN:HB2	1:A:540:TYR:CE2	2.40	0.56
1:C:72:PRO:CG	1:C:92:GLN:HE22	2.18	0.56
1:B:216:LEU:O	1:B:219:LEU:HD23	2.05	0.56
1:C:230:LEU:HB3	1:C:231:PRO:HD3	1.88	0.56
1:A:355:ASN:HA	1:D:180:GLN:NE2	2.21	0.56
1:B:233:VAL:O	1:B:233:VAL:HG23	2.05	0.56
1:C:302:TYR:CZ	1:C:335:MET:HB2	2.40	0.56
1:D:598:ASN:HD22	1:D:629:GLN:HE21	1.54	0.56
1:C:116:ASN:C	1:C:116:ASN:HD22	2.07	0.56
1:A:538:ILE:H	1:A:538:ILE:HD12	1.69	0.56
1:C:538:ILE:H	1:C:538:ILE:HD12	1.71	0.56
1:D:217:LYS:HG3	1:D:218:ASP:N	2.21	0.56
1:D:544:SER:O	1:D:545:HIS:HB3	2.06	0.56
1:A:660:GLY:CA	1:B:255:TYR:CZ	2.89	0.56
1:A:159:LEU:C	1:A:167:ARG:NH2	2.59	0.56
1:A:93:ARG:NH1	1:A:210:TYR:HE2	2.04	0.56
1:A:418:ASN:HB3	1:A:674:PRO:O	2.07	0.56
1:B:88:LEU:HD12	1:B:325:LEU:HD22	1.89	0.55
1:C:418:ASN:HB3	1:C:674:PRO:O	2.07	0.55
1:B:387:ARG:HG3	1:B:392:ASP:OD2	2.06	0.55
1:C:295:GLN:O	1:C:296:ASP:HB2	2.06	0.55
1:C:216:LEU:O	1:C:219:LEU:HD23	2.07	0.55
1:A:389:GLN:HG2	1:A:621:TRP:HZ3	1.68	0.55
1:D:408:PRO:HB2	1:D:466:VAL:HG11	1.89	0.55
1:B:217:LYS:HG3	1:B:218:ASP:N	2.20	0.55
1:C:106:MET:CE	1:C:224:GLU:HG2	2.36	0.55
1:A:178:LEU:HD23	1:A:182:TYR:HD1	1.71	0.55
1:A:660:GLY:HA3	1:B:255:TYR:CZ	2.41	0.55
1:B:424:GLU:C	1:B:441:SER:HB2	2.27	0.55
1:A:387:ARG:HG3	1:A:392:ASP:OD2	2.07	0.55
1:C:324:VAL:HA	1:C:327:SER:OG	2.07	0.54
1:A:197:TYR:CE2	1:A:231:PRO:HG3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:HD2	1:A:125:ASP:CB	2.20	0.54
1:D:233:VAL:O	1:D:233:VAL:HG23	2.08	0.54
1:D:666:PRO:HG2	1:D:669:VAL:HG22	1.89	0.54
1:A:666:PRO:HG2	1:A:669:VAL:HG22	1.89	0.54
1:D:116:ASN:C	1:D:116:ASN:HD22	2.10	0.54
1:C:544:SER:O	1:C:545:HIS:HB3	2.06	0.54
1:D:196:TYR:OH	1:D:322:GLY:HA3	2.07	0.54
1:C:160:SER:OG	1:C:162:HIS:CD2	2.61	0.54
1:D:290:ASN:O	1:D:291:ILE:HG22	2.07	0.54
1:B:573:HIS:HE1	1:B:646:PHE:CE2	2.25	0.54
1:D:195:ILE:HD12	1:D:231:PRO:HB3	1.90	0.54
1:A:504:SER:OG	1:A:507:GLN:HG3	2.08	0.54
1:C:162:HIS:H	1:C:162:HIS:CD2	2.26	0.54
1:D:427:TYR:HB3	1:D:457:ILE:HD12	1.90	0.54
1:C:389:GLN:HG2	1:C:621:TRP:HZ3	1.71	0.54
1:B:204:ILE:HD11	1:B:227:LEU:HB3	1.90	0.54
1:B:598:ASN:HD22	1:B:629:GLN:HE21	1.55	0.54
1:B:71:ASP:CG	1:B:72:PRO:HD2	2.29	0.54
1:B:544:SER:O	1:B:545:HIS:HB3	2.07	0.53
1:C:427:TYR:HB3	1:C:457:ILE:HD12	1.90	0.53
1:A:389:GLN:HE21	1:A:394:HIS:HE1	1.56	0.53
1:B:141:PHE:HB2	1:B:148:THR:HG21	1.90	0.53
1:A:230:LEU:HB3	1:A:231:PRO:HD3	1.89	0.53
1:D:424:GLU:C	1:D:441:SER:HB2	2.29	0.53
1:C:133:ILE:HD11	1:C:141:PHE:HB3	1.90	0.53
1:A:355:ASN:HA	1:D:180:GLN:HE22	1.72	0.53
1:C:197:TYR:CE2	1:C:231:PRO:HG3	2.43	0.53
1:A:93:ARG:CZ	1:A:210:TYR:HE2	2.21	0.53
1:D:292:ASP:O	1:D:293:THR:HB	2.08	0.53
1:B:133:ILE:HD11	1:B:141:PHE:HB3	1.90	0.53
1:A:637:GLY:HA2	2:A:11:SO4:O3	2.08	0.53
1:B:106:MET:HE1	1:B:224:GLU:HA	1.90	0.53
1:B:453:GLN:OE1	1:B:691:THR:HG21	2.09	0.53
1:C:638:HIS:N	2:C:31:SO4:O4	2.42	0.53
1:B:389:GLN:HG2	1:B:621:TRP:HZ3	1.71	0.53
1:D:197:TYR:CE2	1:D:231:PRO:HG3	2.44	0.53
1:D:230:LEU:HB3	1:D:231:PRO:HD3	1.91	0.53
1:A:424:GLU:C	1:A:441:SER:HB2	2.29	0.53
1:C:424:GLU:C	1:C:441:SER:HB2	2.28	0.53
1:B:666:PRO:HG2	1:B:669:VAL:HG22	1.89	0.53
1:C:194:LYS:NZ	1:C:533:ARG:NH2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:SER:HB3	1:D:401:LYS:HE3	1.89	0.53
1:C:467:LYS:HG2	1:C:472:ASN:HA	1.91	0.53
1:D:106:MET:HE1	1:D:224:GLU:HA	1.91	0.53
1:C:196:TYR:OH	1:C:322:GLY:HA3	2.09	0.53
1:C:95:GLU:H	1:C:206:ALA:HB2	1.74	0.53
1:C:573:HIS:HE1	1:C:646:PHE:CE2	2.27	0.53
1:D:123:ALA:HA	1:D:179:GLU:HG3	1.90	0.53
1:C:196:TYR:CG	1:C:323:ASN:HB2	2.44	0.52
1:C:423:ASP:O	1:C:424:GLU:HG3	2.09	0.52
1:D:607:VAL:HG23	1:D:644:PRO:HG3	1.92	0.52
1:C:289:GLN:HB2	1:C:384:VAL:HG11	1.90	0.52
1:B:91:GLY:HA2	1:B:290:ASN:CG	2.30	0.52
1:A:177:ARG:NH1	2:A:41:SO4:O4	2.42	0.52
1:D:467:LYS:HG2	1:D:472:ASN:HA	1.91	0.52
1:A:427:TYR:HB3	1:A:457:ILE:HD12	1.92	0.52
1:C:389:GLN:HE21	1:C:394:HIS:HE1	1.56	0.52
1:A:448:TYR:HA	1:A:559:MET:CE	2.40	0.52
1:C:165:ILE:O	1:C:165:ILE:HG13	2.10	0.52
1:C:159:LEU:HD11	1:C:534:ASP:OD2	2.09	0.52
1:B:116:ASN:HD21	1:B:262:ARG:NH1	2.08	0.52
1:B:197:TYR:CE2	1:B:231:PRO:HG3	2.44	0.52
1:D:268:TRP:O	1:D:272:LYS:HG2	2.10	0.52
1:B:691:THR:HG22	1:B:692:HIS:CE1	2.44	0.52
1:C:453:GLN:OE1	1:C:691:THR:HG21	2.09	0.52
1:D:538:ILE:N	1:D:538:ILE:HD12	2.24	0.52
1:D:602:ASN:ND2	2:D:5:SO4:O4	2.42	0.52
1:C:598:ASN:HD22	1:C:629:GLN:HE21	1.57	0.52
1:D:389:GLN:HE21	1:D:394:HIS:HE1	1.56	0.52
1:B:165:ILE:HD12	1:D:176:TYR:CE1	2.45	0.52
1:B:196:TYR:OH	1:B:322:GLY:HA3	2.10	0.52
1:B:161:GLN:HG2	1:B:538:ILE:HG13	1.91	0.51
1:D:123:ALA:HB2	1:D:179:GLU:HG3	1.92	0.51
1:B:109:ALA:O	1:B:113:THR:HG22	2.10	0.51
1:A:544:SER:O	1:A:545:HIS:HB3	2.10	0.51
1:C:448:TYR:HA	1:C:559:MET:CE	2.41	0.51
1:B:116:ASN:ND2	1:B:116:ASN:C	2.63	0.51
1:B:131:GLY:HA3	1:D:130:PHE:CZ	2.44	0.51
1:A:467:LYS:HG2	1:A:472:ASN:HA	1.92	0.51
1:C:453:GLN:HG2	1:C:567:TYR:O	2.10	0.51
1:C:93:ARG:NH1	1:C:210:TYR:CE2	2.78	0.51
1:A:573:HIS:HE1	1:A:646:PHE:CE2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:TYR:HA	1:A:559:MET:HE2	1.92	0.51
1:B:438:ASP:O	1:B:439:THR:HG22	2.10	0.51
1:C:233:VAL:HG23	1:C:236:ASN:HB2	1.92	0.51
1:B:240:TYR:CE2	1:B:280:LEU:HD11	2.45	0.51
1:D:226:TYR:CE2	1:D:246:ALA:HB1	2.45	0.51
1:C:293:THR:CG2	1:C:294:ASN:H	2.24	0.51
1:A:93:ARG:HD3	1:A:210:TYR:CD2	2.46	0.51
1:D:453:GLN:OE1	1:D:691:THR:HG21	2.10	0.51
1:B:226:TYR:CE2	1:B:246:ALA:HB1	2.46	0.50
1:D:551:TYR:HD2	1:D:555:MET:CE	2.24	0.50
1:A:244:LYS:CB	2:A:17:SO4:O3	2.59	0.50
1:D:555:MET:O	1:D:559:MET:HG3	2.10	0.50
1:A:691:THR:HG22	1:A:692:HIS:CE1	2.46	0.50
1:D:448:TYR:HA	1:D:559:MET:CE	2.42	0.50
1:D:302:TYR:CZ	1:D:335:MET:HB2	2.46	0.50
1:A:204:ILE:HD11	1:A:227:LEU:HB3	1.93	0.50
1:A:453:GLN:OE1	1:A:691:THR:HG21	2.11	0.50
1:B:241:ASP:OD2	1:B:288:ARG:NH2	2.41	0.50
1:D:178:LEU:HD23	1:D:182:TYR:HD1	1.76	0.50
1:A:551:TYR:HD2	1:A:555:MET:CE	2.25	0.50
1:B:97:VAL:HG12	1:B:193:ASN:OD1	2.11	0.50
1:A:555:MET:O	1:A:559:MET:HG3	2.11	0.50
1:B:244:LYS:N	2:B:38:SO4:O1	2.40	0.50
1:B:230:LEU:HB3	1:B:231:PRO:HD3	1.92	0.50
1:D:289:GLN:HB2	1:D:384:VAL:HG11	1.92	0.50
1:D:418:ASN:HB3	1:D:674:PRO:O	2.12	0.50
1:D:118:PHE:CD2	1:D:149:LEU:HB2	2.47	0.49
1:C:538:ILE:N	1:C:538:ILE:HD12	2.27	0.49
1:D:691:THR:HG22	1:D:692:HIS:CE1	2.47	0.49
1:B:241:ASP:CG	1:B:288:ARG:HH22	2.15	0.49
1:D:214:LYS:HD3	1:D:218:ASP:O	2.12	0.49
1:D:504:SER:OG	1:D:507:GLN:HG3	2.12	0.49
1:C:90:ASN:HB3	1:C:293:THR:OG1	2.12	0.49
1:A:515:ILE:HA	1:A:548:MET:HE3	1.94	0.49
1:B:268:TRP:O	1:B:272:LYS:HG2	2.13	0.49
1:B:427:TYR:HB3	1:B:457:ILE:HD12	1.93	0.49
1:B:423:ASP:O	1:B:424:GLU:HG3	2.12	0.49
1:C:448:TYR:HA	1:C:559:MET:HE2	1.94	0.49
1:B:116:ASN:HD22	1:B:262:ARG:HH12	1.58	0.49
1:A:268:TRP:O	1:A:272:LYS:HG2	2.12	0.49
1:C:268:TRP:O	1:C:272:LYS:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ILE:N	1:A:538:ILE:HD12	2.27	0.49
1:A:241:ASP:CG	1:A:288:ARG:HH22	2.16	0.49
1:A:123:ALA:HA	1:A:179:GLU:HG3	1.94	0.49
1:B:260:HIS:C	1:B:261:LYS:HG2	2.34	0.49
1:B:398:SER:HB3	1:B:401:LYS:HE3	1.94	0.49
1:A:71:ASP:N	1:A:533:ARG:HH22	2.11	0.49
1:B:538:ILE:N	1:B:538:ILE:HD12	2.28	0.49
1:C:164:SER:HB3	1:C:167:ARG:H	1.78	0.49
1:D:573:HIS:HE1	1:D:646:PHE:CE2	2.30	0.49
1:D:310:LEU:HD13	1:D:331:ILE:HD13	1.95	0.49
1:B:448:TYR:HA	1:B:559:MET:CE	2.43	0.49
1:B:129:LEU:HD11	3:D:1:LDA:H111	1.94	0.48
1:C:106:MET:HE1	1:C:224:GLU:HA	1.95	0.48
1:D:277:LYS:HG2	1:D:280:LEU:HD23	1.95	0.48
1:B:106:MET:CE	1:B:224:GLU:HG2	2.43	0.48
1:B:141:PHE:HB2	1:B:148:THR:CG2	2.43	0.48
1:C:195:ILE:HD12	1:C:231:PRO:HB3	1.94	0.48
1:D:106:MET:CE	1:D:224:GLU:HG2	2.41	0.48
1:D:244:LYS:HB2	2:D:39:SO4:O2	2.13	0.48
1:A:398:SER:HB3	1:A:401:LYS:HE3	1.96	0.48
1:C:159:LEU:O	1:C:160:SER:CB	2.61	0.48
1:A:214:LYS:CE	1:A:279:ASN:HD22	2.27	0.48
1:D:448:TYR:HA	1:D:559:MET:HE2	1.95	0.48
1:B:398:SER:O	1:B:583:LYS:HE3	2.14	0.48
1:B:467:LYS:HG2	1:B:472:ASN:HA	1.94	0.48
1:B:360:VAL:HG13	1:B:622:MET:HG2	1.95	0.48
1:B:164:SER:HB3	1:B:166:GLY:H	1.78	0.48
1:A:566:PRO:O	1:A:567:TYR:HB2	2.14	0.48
1:C:72:PRO:HD3	1:C:94:HIS:ND1	2.27	0.48
1:A:148:THR:HG23	1:A:151:GLN:CB	2.42	0.48
1:A:226:TYR:CE2	1:A:246:ALA:HB1	2.48	0.48
1:C:398:SER:O	1:C:583:LYS:HE3	2.13	0.48
1:B:613:THR:HB	1:B:614:PRO:HD2	1.95	0.48
1:A:159:LEU:HD21	1:A:167:ARG:HD3	1.96	0.48
1:A:311:MET:SD	1:A:324:VAL:HG11	2.54	0.48
1:C:219:LEU:HD12	1:C:223:GLU:HB3	1.95	0.48
1:C:194:LYS:HZ2	1:C:533:ARG:NH2	2.12	0.48
1:D:298:GLU:HA	1:D:344:GLN:HG2	1.94	0.48
1:B:389:GLN:HE21	1:B:394:HIS:HE1	1.61	0.48
1:A:423:ASP:O	1:A:424:GLU:HG3	2.14	0.48
1:B:551:TYR:HD2	1:B:555:MET:CE	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:VAL:HG13	1:A:299:TYR:CE1	2.49	0.48
1:C:116:ASN:HD21	1:C:262:ARG:NH1	2.06	0.47
1:C:427:TYR:CB	1:C:457:ILE:HD12	2.43	0.47
1:A:195:ILE:HD12	1:A:231:PRO:HB3	1.96	0.47
1:C:162:HIS:C	1:C:164:SER:H	2.18	0.47
1:C:515:ILE:HA	1:C:548:MET:HE3	1.95	0.47
1:B:161:GLN:HE21	1:B:538:ILE:HG13	1.78	0.47
1:B:242:HIS:CA	2:B:38:SO4:O4	2.61	0.47
1:A:116:ASN:C	1:A:116:ASN:HD22	2.16	0.47
1:C:555:MET:O	1:C:559:MET:HG3	2.13	0.47
1:C:414:LYS:HB3	1:C:678:VAL:HG21	1.97	0.47
1:A:96:HIS:ND1	2:A:3:SO4:O4	2.41	0.47
1:A:567:TYR:CD2	1:A:692:HIS:HB2	2.50	0.47
1:C:691:THR:HG22	1:C:692:HIS:CE1	2.50	0.47
1:C:161:GLN:CG	1:C:161:GLN:O	2.57	0.47
1:D:159:LEU:CD1	1:D:532:THR:HB	2.41	0.47
1:B:93:ARG:NH1	1:B:210:TYR:CE2	2.82	0.47
1:D:109:ALA:O	1:D:113:THR:CG2	2.62	0.47
1:B:638:HIS:O	1:B:642:GLU:HB2	2.14	0.47
1:D:162:HIS:HB2	1:D:167:ARG:CD	2.45	0.47
1:B:214:LYS:CE	1:B:279:ASN:HD22	2.28	0.47
1:D:241:ASP:CG	1:D:288:ARG:HH22	2.17	0.47
1:C:194:LYS:NZ	1:C:533:ARG:HH22	2.13	0.47
1:D:123:ALA:CB	1:D:179:GLU:HG3	2.44	0.47
1:B:95:GLU:H	1:B:206:ALA:HB2	1.79	0.47
1:C:214:LYS:CE	1:C:279:ASN:HD22	2.28	0.47
1:D:438:ASP:O	1:D:439:THR:HG22	2.15	0.47
1:A:97:VAL:HB	1:A:205:LYS:HB2	1.97	0.47
1:C:546:LYS:HE3	1:C:546:LYS:HB3	1.63	0.47
1:A:409:ALA:O	1:A:413:MET:HG2	2.15	0.47
1:C:202:THR:CG2	1:C:326:GLN:OE1	2.62	0.47
1:A:613:THR:HB	1:A:614:PRO:HD2	1.97	0.47
1:C:241:ASP:CG	1:C:288:ARG:HH22	2.19	0.47
1:D:427:TYR:CB	1:D:457:ILE:HD12	2.45	0.47
1:A:427:TYR:CB	1:A:457:ILE:HD12	2.44	0.47
1:D:197:TYR:O	1:D:230:LEU:HD21	2.15	0.47
1:D:398:SER:O	1:D:583:LYS:HE3	2.15	0.47
1:B:402:PRO:O	1:B:407:GLY:HA3	2.14	0.47
1:C:602:ASN:O	1:C:636:VAL:HA	2.15	0.47
1:C:438:ASP:O	1:C:439:THR:HG22	2.15	0.47
1:C:240:TYR:CE2	1:C:280:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ILE:HA	1:B:494:GLU:HG3	1.97	0.46
1:D:613:THR:HB	1:D:614:PRO:HD2	1.96	0.46
1:C:73:ILE:CG2	1:C:328:GLY:HA3	2.44	0.46
1:C:214:LYS:HE3	1:C:279:ASN:HD22	1.80	0.46
1:A:277:LYS:HG2	1:A:280:LEU:HD23	1.97	0.46
1:A:214:LYS:HD3	1:A:218:ASP:O	2.16	0.46
1:A:602:ASN:O	1:A:636:VAL:HA	2.15	0.46
1:C:268:TRP:CE2	1:C:272:LYS:HE2	2.50	0.46
1:C:297:SER:HA	1:C:300:ASN:OD1	2.15	0.46
1:B:515:ILE:HA	1:B:548:MET:HE3	1.96	0.46
1:A:109:ALA:O	1:A:113:THR:CG2	2.63	0.46
1:C:567:TYR:CD2	1:C:692:HIS:HB2	2.50	0.46
1:D:408:PRO:HD3	1:D:478:PHE:CD1	2.51	0.46
1:B:297:SER:HA	1:B:300:ASN:OD1	2.16	0.46
1:B:162:HIS:CG	1:B:164:SER:HB2	2.51	0.46
1:C:457:ILE:O	1:C:461:LYS:HG2	2.15	0.46
1:D:123:ALA:CA	1:D:179:GLU:HG3	2.45	0.46
1:C:551:TYR:HD2	1:C:555:MET:CE	2.28	0.46
1:C:97:VAL:HG12	1:C:193:ASN:OD1	2.16	0.46
1:C:226:TYR:CE2	1:C:246:ALA:HB1	2.50	0.46
1:C:613:THR:HB	1:C:614:PRO:HD2	1.98	0.46
1:D:95:GLU:H	1:D:206:ALA:HB2	1.80	0.46
1:B:302:TYR:CZ	1:B:335:MET:HB2	2.50	0.46
1:C:516:ALA:HB2	1:C:612:PHE:HB2	1.98	0.46
1:D:546:LYS:HB3	1:D:546:LYS:HE3	1.63	0.46
1:C:117:ARG:O	1:C:121:HIS:CD2	2.69	0.46
1:A:398:SER:O	1:A:583:LYS:HE3	2.15	0.46
1:D:297:SER:HA	1:D:300:ASN:OD1	2.15	0.46
1:A:106:MET:HE2	1:A:224:GLU:CG	2.30	0.46
1:A:219:LEU:HD12	1:A:223:GLU:HB3	1.98	0.46
1:A:264:THR:HG23	1:A:267:GLN:OE1	2.16	0.46
1:D:242:HIS:HA	2:D:39:SO4:O3	2.16	0.46
1:C:398:SER:HB3	1:C:401:LYS:HE3	1.98	0.46
1:D:261:LYS:HE2	1:D:261:LYS:HB3	1.65	0.46
1:C:116:ASN:C	1:C:116:ASN:ND2	2.70	0.46
1:A:660:GLY:HA2	1:B:255:TYR:OH	2.16	0.46
1:B:214:LYS:HE3	1:B:279:ASN:HD22	1.81	0.46
1:D:241:ASP:OD2	1:D:288:ARG:NH2	2.45	0.46
1:B:106:MET:HE2	1:B:224:GLU:HG2	1.97	0.46
1:B:210:TYR:HD1	1:B:211:TYR:CD1	2.34	0.45
1:B:277:LYS:HG2	1:B:280:LEU:HD23	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LYS:HG2	1:C:280:LEU:HD23	1.98	0.45
1:D:423:ASP:O	1:D:424:GLU:HG3	2.16	0.45
1:D:516:ALA:HB2	1:D:612:PHE:HB2	1.98	0.45
1:B:566:PRO:O	1:B:567:TYR:HB2	2.16	0.45
1:A:389:GLN:HG3	1:A:394:HIS:HE1	1.80	0.45
1:C:322:GLY:N	2:C:19:SO4:O3	2.44	0.45
1:B:73:ILE:HG13	1:B:328:GLY:CA	2.46	0.45
1:D:360:VAL:HG13	1:D:622:MET:HG2	1.98	0.45
1:C:389:GLN:HG3	1:C:394:HIS:HE1	1.82	0.45
1:C:95:GLU:N	1:C:206:ALA:HB2	2.31	0.45
1:D:389:GLN:HG3	1:D:394:HIS:HE1	1.78	0.45
1:D:414:LYS:HB3	1:D:678:VAL:HG21	1.98	0.45
1:C:194:LYS:HZ1	1:C:533:ARG:HH22	1.63	0.45
1:C:70:GLN:N	1:C:194:LYS:HD2	2.31	0.45
1:B:504:SER:OG	1:B:507:GLN:HG3	2.16	0.45
1:A:490:ILE:HA	1:A:494:GLU:HG3	1.98	0.45
1:B:214:LYS:HD3	1:B:218:ASP:O	2.17	0.45
1:D:240:TYR:CE2	1:D:280:LEU:HD11	2.52	0.45
1:B:148:THR:HG23	1:B:151:GLN:CB	2.47	0.45
1:D:260:HIS:C	1:D:261:LYS:HG2	2.35	0.45
1:D:93:ARG:NH1	1:D:210:TYR:CE2	2.85	0.45
1:A:302:TYR:CZ	1:A:335:MET:HB2	2.52	0.45
1:A:289:GLN:O	1:A:290:ASN:O	2.34	0.45
1:D:429:VAL:O	1:D:430:ASP:HB2	2.17	0.45
1:D:292:ASP:O	1:D:293:THR:CB	2.64	0.45
1:D:417:THR:CG2	1:D:676:ILE:HB	2.47	0.45
1:B:427:TYR:CB	1:B:457:ILE:HD12	2.47	0.45
1:C:691:THR:HB	1:C:692:HIS:H	1.62	0.45
1:C:402:PRO:O	1:C:407:GLY:HA3	2.17	0.45
1:C:486:TYR:CD1	1:C:490:ILE:HD11	2.52	0.45
1:B:250:LYS:HD2	1:B:250:LYS:C	2.38	0.45
1:A:598:ASN:HD22	1:A:629:GLN:NE2	2.14	0.45
1:B:264:THR:HG23	1:B:267:GLN:OE1	2.17	0.44
1:B:457:ILE:O	1:B:461:LYS:HG2	2.17	0.44
1:A:89:ASP:C	1:A:91:GLY:N	2.69	0.44
1:C:254:LEU:HD23	1:C:257:MET:CE	2.46	0.44
1:D:264:THR:HG23	1:D:267:GLN:OE1	2.18	0.44
1:C:260:HIS:C	1:C:261:LYS:HG2	2.37	0.44
1:C:293:THR:CG2	1:C:294:ASN:N	2.79	0.44
1:D:263:ILE:HB	1:D:267:GLN:HG3	1.99	0.44
1:A:444:THR:O	1:A:689:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:648:TYR:CE1	1:D:652:MET:HG3	2.53	0.44
1:D:214:LYS:HD2	1:D:219:LEU:HB2	1.99	0.44
1:B:195:ILE:HD12	1:B:231:PRO:HB3	1.98	0.44
1:D:486:TYR:CD1	1:D:490:ILE:HD11	2.53	0.44
1:B:448:TYR:HA	1:B:559:MET:HE2	2.00	0.44
1:B:555:MET:O	1:B:559:MET:HG3	2.18	0.44
1:B:85:VAL:HG11	1:B:335:MET:HE1	2.00	0.44
1:C:336:ASP:HB2	1:C:373:VAL:HG13	1.99	0.44
1:C:310:LEU:HD13	1:C:331:ILE:HD13	1.99	0.44
1:B:129:LEU:CD1	3:D:1:LDA:H111	2.48	0.44
1:B:242:HIS:CB	2:B:38:SO4:O4	2.66	0.44
1:B:648:TYR:CE1	1:B:652:MET:HG3	2.51	0.44
1:B:261:LYS:HB3	1:B:261:LYS:HE2	1.61	0.44
1:A:297:SER:HA	1:A:300:ASN:OD1	2.18	0.44
1:C:298:GLU:HA	1:C:344:GLN:HG2	1.99	0.44
1:B:233:VAL:HG23	1:B:236:ASN:HB2	2.00	0.44
1:B:567:TYR:CD2	1:B:692:HIS:HB2	2.52	0.44
1:B:244:LYS:HB2	2:B:38:SO4:O1	2.18	0.44
1:A:214:LYS:HE3	1:A:279:ASN:HD22	1.83	0.44
1:D:219:LEU:HD12	1:D:223:GLU:HB3	2.00	0.44
1:D:438:ASP:OD1	1:D:440:LYS:HB2	2.18	0.44
1:B:162:HIS:CD2	1:B:164:SER:HB3	2.53	0.44
1:C:648:TYR:CE1	1:C:652:MET:HG3	2.52	0.44
1:A:438:ASP:O	1:A:439:THR:HG22	2.18	0.44
1:C:429:VAL:O	1:C:430:ASP:HB2	2.18	0.44
1:D:566:PRO:O	1:D:567:TYR:HB2	2.18	0.43
1:B:268:TRP:CD2	1:B:272:LYS:HE2	2.53	0.43
1:C:261:LYS:HB3	1:C:261:LYS:HE2	1.64	0.43
1:C:417:THR:CG2	1:C:676:ILE:HB	2.48	0.43
1:D:163:LYS:HE2	1:D:163:LYS:HB3	1.60	0.43
1:D:116:ASN:C	1:D:116:ASN:ND2	2.72	0.43
1:A:438:ASP:OD1	1:A:440:LYS:HB2	2.18	0.43
1:D:602:ASN:O	1:D:636:VAL:HA	2.18	0.43
1:D:490:ILE:HA	1:D:494:GLU:HG3	1.99	0.43
1:A:556:LEU:HA	1:A:556:LEU:HD12	1.86	0.43
1:B:379:ARG:H	1:B:379:ARG:HG2	1.60	0.43
1:C:387:ARG:NE	1:C:387:ARG:HA	2.33	0.43
1:C:444:THR:O	1:C:689:ARG:HD3	2.18	0.43
1:D:409:ALA:O	1:D:413:MET:HG2	2.18	0.43
1:B:358:GLN:HB2	1:B:624:PHE:CE2	2.54	0.43
1:C:72:PRO:HD3	1:C:94:HIS:NE2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:CG2	1:D:350:GLY:HA2	2.45	0.43
1:A:241:ASP:OD2	1:A:288:ARG:NH2	2.44	0.43
1:C:638:HIS:O	1:C:642:GLU:HB2	2.18	0.43
1:B:389:GLN:HG3	1:B:394:HIS:HE1	1.81	0.43
1:B:263:ILE:HB	1:B:267:GLN:HG3	2.01	0.43
1:A:397:GLY:O	1:A:497:GLY:HA3	2.19	0.43
1:D:567:TYR:CD2	1:D:692:HIS:HB2	2.53	0.43
1:C:263:ILE:HB	1:C:267:GLN:HG3	2.00	0.43
1:A:638:HIS:O	1:A:642:GLU:HB2	2.18	0.43
1:A:360:VAL:HG13	1:A:622:MET:HG2	2.00	0.43
1:D:115:ASP:CG	1:D:118:PHE:HB2	2.39	0.43
1:C:148:THR:HG23	1:C:151:GLN:CB	2.49	0.43
1:A:210:TYR:HD1	1:A:211:TYR:CD1	2.36	0.43
1:A:648:TYR:CE1	1:A:652:MET:HG3	2.54	0.43
1:C:408:PRO:HD3	1:C:478:PHE:CD1	2.53	0.43
1:C:109:ALA:O	1:C:113:THR:CG2	2.66	0.43
1:B:230:LEU:N	1:B:231:PRO:CD	2.82	0.43
1:A:447:ILE:HA	1:A:450:ALA:HB3	2.01	0.43
1:D:638:HIS:O	1:D:642:GLU:HB2	2.17	0.43
1:A:355:ASN:CA	1:D:180:GLN:HE22	2.31	0.43
1:C:159:LEU:O	1:C:160:SER:HB3	2.19	0.43
1:A:260:HIS:C	1:A:261:LYS:HG2	2.38	0.43
1:A:261:LYS:HE2	1:A:261:LYS:HB3	1.65	0.43
1:B:176:TYR:OH	1:D:165:ILE:HD13	2.18	0.43
1:A:691:THR:HB	1:A:692:HIS:H	1.61	0.43
1:C:268:TRP:CD2	1:C:272:LYS:HE2	2.54	0.43
1:D:336:ASP:HB2	1:D:373:VAL:HG13	2.01	0.43
1:B:414:LYS:HB3	1:B:678:VAL:HG21	2.01	0.43
1:D:121:HIS:HD2	1:D:125:ASP:CA	2.31	0.43
1:D:233:VAL:HG23	1:D:236:ASN:HB2	2.00	0.43
1:D:148:THR:HG23	1:D:151:GLN:CB	2.46	0.43
1:C:264:THR:HG23	1:C:267:GLN:OE1	2.19	0.43
1:B:73:ILE:HB	1:B:74:PRO:HD2	2.00	0.43
1:C:117:ARG:HG2	1:C:120:GLU:OE1	2.19	0.43
1:C:186:ASP:O	1:C:190:VAL:HG23	2.19	0.43
1:A:183:SER:O	1:A:187:ILE:HG13	2.19	0.43
1:A:414:LYS:HB3	1:A:678:VAL:HG21	2.00	0.43
1:A:263:ILE:HB	1:A:267:GLN:HG3	2.00	0.42
1:D:298:GLU:HG3	1:D:341:LYS:HG2	2.01	0.42
1:D:523:ASN:O	1:D:525:HIS:HD2	2.01	0.42
1:A:546:LYS:HE3	1:A:546:LYS:HB3	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LYS:HB3	1:B:546:LYS:HE3	1.63	0.42
1:B:214:LYS:HD2	1:B:219:LEU:HB2	2.00	0.42
1:A:298:GLU:OE2	1:A:341:LYS:HE2	2.19	0.42
1:B:602:ASN:O	1:B:636:VAL:HA	2.19	0.42
1:B:516:ALA:HB2	1:B:612:PHE:HB2	2.01	0.42
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.88	0.42
1:A:214:LYS:HD2	1:A:219:LEU:HB2	2.00	0.42
1:D:289:GLN:CB	1:D:384:VAL:HG11	2.48	0.42
1:B:409:ALA:O	1:B:413:MET:HG2	2.19	0.42
1:A:429:VAL:O	1:A:430:ASP:HB2	2.19	0.42
1:C:353:TYR:CZ	1:C:379:ARG:HD2	2.54	0.42
1:D:214:LYS:HE3	1:D:279:ASN:HD22	1.85	0.42
1:C:86:LYS:HE3	1:C:295:GLN:O	2.19	0.42
1:D:230:LEU:N	1:D:231:PRO:CD	2.82	0.42
1:B:438:ASP:OD1	1:B:440:LYS:HB2	2.19	0.42
1:B:117:ARG:NH1	1:B:120:GLU:OE2	2.50	0.42
1:C:241:ASP:OD2	1:C:288:ARG:NH2	2.45	0.42
1:B:219:LEU:HD12	1:B:223:GLU:HB3	2.01	0.42
1:D:214:LYS:CE	1:D:279:ASN:HD22	2.33	0.42
1:C:204:ILE:CD1	1:C:227:LEU:HB3	2.50	0.42
1:B:95:GLU:N	1:B:206:ALA:HB2	2.35	0.42
1:B:417:THR:CG2	1:B:676:ILE:HB	2.49	0.42
1:C:242:HIS:HB3	2:C:18:SO4:O2	2.20	0.42
1:C:566:PRO:O	1:C:567:TYR:HB2	2.20	0.42
1:B:73:ILE:HG13	1:B:328:GLY:HA3	2.00	0.42
1:C:490:ILE:HA	1:C:494:GLU:HG3	2.02	0.42
1:A:643:TYR:N	1:A:644:PRO:HD2	2.35	0.42
1:A:417:THR:CG2	1:A:676:ILE:HB	2.50	0.42
1:C:162:HIS:HB3	1:C:167:ARG:NH1	2.34	0.42
1:C:94:HIS:CD2	1:C:94:HIS:C	2.92	0.42
1:C:292:ASP:O	1:C:293:THR:CB	2.67	0.42
1:C:438:ASP:OD1	1:C:440:LYS:HB2	2.19	0.42
1:A:516:ALA:HB2	1:A:612:PHE:HB2	2.01	0.42
1:C:637:GLY:CA	2:C:31:SO4:O4	2.67	0.42
1:A:230:LEU:N	1:A:231:PRO:CD	2.82	0.42
1:C:93:ARG:CZ	1:C:210:TYR:HE2	2.32	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.89	0.42
1:A:486:TYR:CD1	1:A:490:ILE:HD11	2.55	0.42
1:D:210:TYR:HD1	1:D:211:TYR:CD1	2.37	0.42
1:A:186:ASP:O	1:A:190:VAL:HG23	2.19	0.42
1:D:293:THR:O	1:D:294:ASN:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:ILE:HD13	1:D:674:PRO:HA	2.02	0.42
1:C:117:ARG:O	1:C:121:HIS:CG	2.72	0.42
1:B:496:LEU:HD23	1:B:496:LEU:HA	1.87	0.42
1:C:397:GLY:O	1:C:497:GLY:HA3	2.20	0.42
1:A:302:TYR:CE2	1:A:372:LEU:HG	2.54	0.41
1:A:159:LEU:C	1:A:167:ARG:HH21	2.23	0.41
1:A:336:ASP:HB2	1:A:373:VAL:HG13	2.02	0.41
1:B:447:ILE:HA	1:B:450:ALA:HB3	2.02	0.41
1:A:403:PHE:CD2	1:A:482:LEU:HD13	2.55	0.41
1:A:116:ASN:HD21	1:A:262:ARG:NH1	2.15	0.41
1:B:165:ILE:H	1:B:165:ILE:HG12	1.60	0.41
1:D:237:TYR:O	1:D:246:ALA:HB2	2.20	0.41
1:A:408:PRO:HD3	1:A:478:PHE:CD1	2.55	0.41
1:C:401:LYS:N	1:C:402:PRO:CD	2.83	0.41
1:C:643:TYR:N	1:C:644:PRO:HD2	2.36	0.41
1:B:444:THR:O	1:B:689:ARG:HD3	2.20	0.41
1:D:126:TYR:HE2	3:D:1:LDA:CM1	2.33	0.41
1:B:199:ASP:OD1	1:B:288:ARG:HD2	2.21	0.41
1:C:225:ALA:HB2	1:C:257:MET:HE1	2.03	0.41
1:D:182:TYR:HB3	1:D:186:ASP:HB2	2.03	0.41
1:B:401:LYS:N	1:B:402:PRO:CD	2.83	0.41
1:B:307:LYS:HE2	1:B:307:LYS:HB3	1.71	0.41
1:D:221:LEU:HD23	1:D:221:LEU:HA	1.75	0.41
1:D:250:LYS:HD2	1:D:250:LYS:C	2.40	0.41
3:D:1:LDA:H91	3:D:1:LDA:H122	1.70	0.41
1:A:389:GLN:CG	1:A:621:TRP:CZ3	3.03	0.41
1:C:202:THR:HG23	1:C:326:GLN:OE1	2.21	0.41
1:C:142:GLY:HA3	1:C:147:SER:O	2.20	0.41
1:A:658:ARG:HG2	1:B:256:LEU:HD21	2.03	0.41
1:C:71:ASP:HB3	1:C:72:PRO:CD	2.48	0.41
3:D:1:LDA:HM13	3:D:1:LDA:H22	1.68	0.41
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.92	0.41
1:B:268:TRP:CE2	1:B:272:LYS:HE2	2.55	0.41
1:C:584:THR:HG22	1:C:609:ILE:HG13	2.02	0.41
1:B:336:ASP:HB2	1:B:373:VAL:HG13	2.01	0.41
1:C:496:LEU:HA	1:C:496:LEU:HD23	1.89	0.41
1:C:221:LEU:HA	1:C:221:LEU:HD23	1.78	0.41
1:B:200:GLY:CA	1:B:326:GLN:HE22	2.33	0.41
1:C:292:ASP:O	1:C:293:THR:HB	2.21	0.41
1:A:298:GLU:HG3	1:A:341:LYS:CG	2.49	0.41
1:B:254:LEU:HD23	1:B:257:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.90	0.41
1:D:307:LYS:HE2	1:D:307:LYS:HB3	1.74	0.41
1:D:159:LEU:HD12	1:D:533:ARG:N	2.31	0.41
1:A:233:VAL:HG23	1:A:236:ASN:HB2	2.02	0.41
1:C:324:VAL:HG12	1:C:329:ILE:HD13	2.03	0.41
1:A:392:ASP:HA	1:A:393:PRO:HD3	1.85	0.41
1:B:109:ALA:O	1:B:113:THR:CG2	2.68	0.41
1:A:584:THR:HG22	1:A:609:ILE:HG13	2.02	0.41
1:D:447:ILE:HA	1:D:450:ALA:HB3	2.03	0.41
1:A:114:GLU:O	1:A:128:ARG:NH2	2.54	0.41
1:D:444:THR:O	1:D:689:ARG:HD3	2.21	0.41
1:C:250:LYS:HD2	1:C:250:LYS:C	2.41	0.41
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.86	0.41
1:D:115:ASP:HB3	1:D:149:LEU:HG	2.03	0.41
1:A:457:ILE:O	1:A:461:LYS:HG2	2.21	0.41
1:B:387:ARG:HA	1:B:387:ARG:NE	2.36	0.41
1:C:210:TYR:HD1	1:C:211:TYR:CD1	2.39	0.41
1:A:94:HIS:C	1:A:94:HIS:CD2	2.94	0.41
1:A:177:ARG:CZ	2:A:41:SO4:O4	2.69	0.40
1:D:220:ASN:O	1:D:224:GLU:HG3	2.21	0.40
1:D:457:ILE:O	1:D:461:LYS:HG2	2.21	0.40
1:A:602:ASN:ND2	2:A:11:SO4:O4	2.54	0.40
1:C:118:PHE:HA	1:C:121:HIS:CD2	2.56	0.40
1:D:417:THR:HG23	1:D:676:ILE:HB	2.03	0.40
1:C:403:PHE:CD2	1:C:482:LEU:HD13	2.56	0.40
1:B:294:ASN:OD1	1:B:382:LYS:HD2	2.21	0.40
1:D:563:THR:HG22	1:D:570:ALA:HB3	2.03	0.40
1:A:77:ILE:CD1	1:A:303:VAL:HG22	2.52	0.40
1:D:515:ILE:HA	1:D:548:MET:HE3	2.02	0.40
1:A:379:ARG:H	1:A:379:ARG:HG2	1.61	0.40
1:C:392:ASP:HA	1:C:393:PRO:HD3	1.86	0.40
1:D:387:ARG:NE	1:D:387:ARG:HA	2.37	0.40
1:D:254:LEU:HD23	1:D:257:MET:CE	2.52	0.40
1:A:440:LYS:HE3	1:A:441:SER:H	1.86	0.40
1:D:563:THR:CG2	1:D:570:ALA:HB3	2.51	0.40
1:B:403:PHE:CD2	1:B:482:LEU:HD13	2.55	0.40
1:C:72:PRO:HG3	1:C:92:GLN:HE22	1.87	0.40
1:A:637:GLY:O	1:A:638:HIS:C	2.60	0.40
1:D:403:PHE:CD2	1:D:482:LEU:HD13	2.57	0.40
1:B:643:TYR:N	1:B:644:PRO:HD2	2.36	0.40
1:C:360:VAL:HG13	1:C:622:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:560:LEU:HA	1:D:560:LEU:HD23	1.85	0.40
1:A:402:PRO:O	1:A:407:GLY:HA3	2.21	0.40
1:B:225:ALA:HB2	1:B:257:MET:HE1	2.03	0.40
1:B:197:TYR:O	1:B:230:LEU:HD21	2.21	0.40
1:B:286:GLU:HB3	1:B:291:ILE:HD11	2.02	0.40
1:B:295:GLN:O	1:B:296:ASP:HB2	2.22	0.40
1:C:85:VAL:HG13	1:C:299:TYR:CZ	2.57	0.40
1:A:321:LEU:C	1:A:323:ASN:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	590/625 (94%)	534 (90%)	50 (8%)	6 (1%)	19	58
1	B	617/625 (99%)	565 (92%)	46 (8%)	6 (1%)	19	58
1	C	621/625 (99%)	563 (91%)	50 (8%)	8 (1%)	15	50
1	D	596/625 (95%)	545 (91%)	45 (8%)	6 (1%)	19	58
All	All	2424/2500 (97%)	2207 (91%)	191 (8%)	26 (1%)	17	55

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	SER
1	B	162	HIS
1	B	292	ASP
1	C	143	SER
1	C	160	SER
1	D	290	ASN
1	D	291	ILE

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Mol	Chain	Res	Type
1	D	293	THR
1	C	89	ASP
1	C	293	THR
1	D	294	ASN
1	A	90	ASN
1	C	545	HIS
1	A	545	HIS
1	B	545	HIS
1	D	545	HIS
1	A	165	ILE
1	A	319	GLU
1	C	296	ASP
1	C	535	GLY
1	D	535	GLY
1	A	535	GLY
1	B	133	ILE
1	B	535	GLY
1	C	133	ILE
1	A	322	GLY

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	506/526 (96%)	457 (90%)	49 (10%)	10	36
1	B	522/526 (99%)	472 (90%)	50 (10%)	10	37
1	C	524/526 (100%)	474 (90%)	50 (10%)	11	38
1	D	511/526 (97%)	464 (91%)	47 (9%)	11	40
All	All	2063/2104 (98%)	1867 (90%)	196 (10%)	11	38

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ASP
1	A	87	THR

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Mol	Chain	Res	Type
1	A	113	THR
1	A	116	ASN
1	A	117	ARG
1	A	128	ARG
1	A	147	SER
1	A	148	THR
1	A	159	LEU
1	A	167	ARG
1	A	174	LEU
1	A	177	ARG
1	A	178	LEU
1	A	218	ASP
1	A	219	LEU
1	A	221	LEU
1	A	239	ILE
1	A	244	LYS
1	A	250	LYS
1	A	261	LYS
1	A	265	ASP
1	A	296	ASP
1	A	301	SER
1	A	318	ASP
1	A	346	ASP
1	A	352	PHE
1	A	360	VAL
1	A	379	ARG
1	A	387	ARG
1	A	398	SER
1	A	435	ARG
1	A	439	THR
1	A	454	SER
1	A	494	GLU
1	A	520	THR
1	A	534	ASP
1	A	541	ASP
1	A	556	LEU
1	A	563	THR
1	A	606	ASP
1	A	626	LYS
1	A	627	VAL
1	A	656	SER
1	A	667	SER

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Mol	Chain	Res	Type
1	A	670	SER
1	A	672	SER
1	A	686	THR
1	A	687	THR
1	A	691	THR
1	B	87	THR
1	B	113	THR
1	B	116	ASN
1	B	124	LEU
1	B	138	THR
1	B	148	THR
1	B	160	SER
1	B	161	GLN
1	B	162	HIS
1	B	165	ILE
1	B	167	ARG
1	B	174	LEU
1	B	177	ARG
1	B	178	LEU
1	B	218	ASP
1	B	219	LEU
1	B	221	LEU
1	B	239	ILE
1	B	244	LYS
1	B	250	LYS
1	B	261	LYS
1	B	262	ARG
1	B	265	ASP
1	B	292	ASP
1	B	294	ASN
1	B	301	SER
1	B	346	ASP
1	B	352	PHE
1	B	360	VAL
1	B	379	ARG
1	B	387	ARG
1	B	398	SER
1	B	435	ARG
1	B	439	THR
1	B	454	SER
1	B	494	GLU
1	B	520	THR

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Mol	Chain	Res	Type
1	B	534	ASP
1	B	556	LEU
1	B	563	THR
1	B	606	ASP
1	B	626	LYS
1	B	627	VAL
1	B	656	SER
1	B	667	SER
1	B	670	SER
1	B	672	SER
1	B	686	THR
1	B	687	THR
1	B	691	THR
1	C	70	GLN
1	C	87	THR
1	C	113	THR
1	C	116	ASN
1	C	124	LEU
1	C	138	THR
1	C	148	THR
1	C	158	PHE
1	C	159	LEU
1	C	161	GLN
1	C	164	SER
1	C	165	ILE
1	C	167	ARG
1	C	174	LEU
1	C	177	ARG
1	C	178	LEU
1	C	218	ASP
1	C	219	LEU
1	C	221	LEU
1	C	239	ILE
1	C	244	LYS
1	C	250	LYS
1	C	261	LYS
1	C	265	ASP
1	C	291	ILE
1	C	301	SER
1	C	346	ASP
1	C	352	PHE
1	C	360	VAL

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Mol	Chain	Res	Type
1	C	379	ARG
1	C	387	ARG
1	C	398	SER
1	C	435	ARG
1	C	439	THR
1	C	454	SER
1	C	494	GLU
1	C	520	THR
1	C	534	ASP
1	C	556	LEU
1	C	563	THR
1	C	606	ASP
1	C	626	LYS
1	C	627	VAL
1	C	656	SER
1	C	667	SER
1	C	670	SER
1	C	672	SER
1	C	686	THR
1	C	687	THR
1	C	691	THR
1	D	87	THR
1	D	113	THR
1	D	116	ASN
1	D	128	ARG
1	D	148	THR
1	D	158	PHE
1	D	163	LYS
1	D	164	SER
1	D	167	ARG
1	D	174	LEU
1	D	177	ARG
1	D	178	LEU
1	D	218	ASP
1	D	219	LEU
1	D	221	LEU
1	D	239	ILE
1	D	244	LYS
1	D	250	LYS
1	D	261	LYS
1	D	262	ARG
1	D	265	ASP

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Mol	Chain	Res	Type
1	D	294	ASN
1	D	301	SER
1	D	346	ASP
1	D	352	PHE
1	D	360	VAL
1	D	379	ARG
1	D	387	ARG
1	D	398	SER
1	D	435	ARG
1	D	439	THR
1	D	454	SER
1	D	494	GLU
1	D	520	THR
1	D	534	ASP
1	D	556	LEU
1	D	606	ASP
1	D	610	ASN
1	D	626	LYS
1	D	627	VAL
1	D	656	SER
1	D	667	SER
1	D	670	SER
1	D	672	SER
1	D	686	THR
1	D	687	THR
1	D	691	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	121	HIS
1	A	258	HIS
1	A	279	ASN
1	A	320	ASN
1	A	334	ASN
1	A	389	GLN
1	A	468	GLN
1	A	472	ASN
1	A	525	HIS
1	A	542	HIS
1	A	598	ASN

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Mol	Chain	Res	Type
1	A	692	HIS
1	B	116	ASN
1	B	161	GLN
1	B	258	HIS
1	B	279	ASN
1	B	295	GLN
1	B	326	GLN
1	B	334	ASN
1	B	389	GLN
1	B	468	GLN
1	B	598	ASN
1	B	692	HIS
1	C	90	ASN
1	C	92	GLN
1	C	94	HIS
1	C	116	ASN
1	C	121	HIS
1	C	162	HIS
1	C	258	HIS
1	C	279	ASN
1	C	295	GLN
1	C	323	ASN
1	C	334	ASN
1	C	389	GLN
1	C	468	GLN
1	C	472	ASN
1	C	525	HIS
1	C	542	HIS
1	C	598	ASN
1	C	692	HIS
1	D	94	HIS
1	D	116	ASN
1	D	121	HIS
1	D	180	GLN
1	D	258	HIS
1	D	279	ASN
1	D	334	ASN
1	D	389	GLN
1	D	468	GLN
1	D	472	ASN
1	D	525	HIS
1	D	542	HIS

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Mol	Chain	Res	Type
1	D	598	ASN
1	D	692	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

47 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	SO4	A	11	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SO4	A	12	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	A	15	-	4,4,4	0.24	0	6,6,6	0.29	0
2	SO4	A	16	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	17	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	22	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	A	24	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	A	26	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	A	27	-	4,4,4	0.18	0	6,6,6	0.17	0
2	SO4	A	29	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	41	-	4,4,4	0.14	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	43	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	A	45	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	A	46	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	B	20	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	B	21	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	B	23	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	B	25	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	B	32	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	B	34	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	35	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	B	36	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	B	37	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	B	38	-	4,4,4	0.21	0	6,6,6	0.38	0
2	SO4	B	42	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	B	44	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	B	8	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	C	1	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	C	18	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	C	19	-	4,4,4	0.12	0	6,6,6	0.52	0
2	SO4	C	2	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	28	-	4,4,4	0.20	0	6,6,6	0.27	0
2	SO4	C	31	-	4,4,4	0.19	0	6,6,6	0.35	0
2	SO4	C	33	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	C	4	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	C	6	-	4,4,4	0.12	0	6,6,6	0.18	0
3	LDA	D	1	-	15,15,15	3.92	2 (13%)	16,17,17	0.77	0
2	SO4	D	10	-	4,4,4	0.23	0	6,6,6	0.18	0
2	SO4	D	13	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	D	14	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	D	30	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SO4	D	39	-	4,4,4	0.17	0	6,6,6	0.22	0
2	SO4	D	40	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	D	5	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	D	7	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	D	9	-	4,4,4	0.15	0	6,6,6	0.23	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	SO4	A	11	-	-	0/0/0/0	0/0/0/0
2	SO4	A	12	-	-	0/0/0/0	0/0/0/0
2	SO4	A	15	-	-	0/0/0/0	0/0/0/0
2	SO4	A	16	-	-	0/0/0/0	0/0/0/0
2	SO4	A	17	-	-	0/0/0/0	0/0/0/0
2	SO4	A	22	-	-	0/0/0/0	0/0/0/0
2	SO4	A	24	-	-	0/0/0/0	0/0/0/0
2	SO4	A	26	-	-	0/0/0/0	0/0/0/0
2	SO4	A	27	-	-	0/0/0/0	0/0/0/0
2	SO4	A	29	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	A	41	-	-	0/0/0/0	0/0/0/0
2	SO4	A	43	-	-	0/0/0/0	0/0/0/0
2	SO4	A	45	-	-	0/0/0/0	0/0/0/0
2	SO4	A	46	-	-	0/0/0/0	0/0/0/0
2	SO4	B	20	-	-	0/0/0/0	0/0/0/0
2	SO4	B	21	-	-	0/0/0/0	0/0/0/0
2	SO4	B	23	-	-	0/0/0/0	0/0/0/0
2	SO4	B	25	-	-	0/0/0/0	0/0/0/0
2	SO4	B	32	-	-	0/0/0/0	0/0/0/0
2	SO4	B	34	-	-	0/0/0/0	0/0/0/0
2	SO4	B	35	-	-	0/0/0/0	0/0/0/0
2	SO4	B	36	-	-	0/0/0/0	0/0/0/0
2	SO4	B	37	-	-	0/0/0/0	0/0/0/0
2	SO4	B	38	-	-	0/0/0/0	0/0/0/0
2	SO4	B	42	-	-	0/0/0/0	0/0/0/0
2	SO4	B	44	-	-	0/0/0/0	0/0/0/0
2	SO4	B	8	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1	-	-	0/0/0/0	0/0/0/0
2	SO4	C	18	-	-	0/0/0/0	0/0/0/0
2	SO4	C	19	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2	-	-	0/0/0/0	0/0/0/0
2	SO4	C	28	-	-	0/0/0/0	0/0/0/0
2	SO4	C	31	-	-	0/0/0/0	0/0/0/0
2	SO4	C	33	-	-	0/0/0/0	0/0/0/0
2	SO4	C	4	-	-	0/0/0/0	0/0/0/0
2	SO4	C	6	-	-	0/0/0/0	0/0/0/0
3	LDA	D	1	-	-	0/13/13/13	0/0/0/0
2	SO4	D	10	-	-	0/0/0/0	0/0/0/0
2	SO4	D	13	-	-	0/0/0/0	0/0/0/0
2	SO4	D	14	-	-	0/0/0/0	0/0/0/0
2	SO4	D	30	-	-	0/0/0/0	0/0/0/0
2	SO4	D	39	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	40	-	-	0/0/0/0	0/0/0/0
2	SO4	D	5	-	-	0/0/0/0	0/0/0/0
2	SO4	D	7	-	-	0/0/0/0	0/0/0/0
2	SO4	D	9	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	LDA	O1-N1	-14.72	1.25	1.39
3	D	1	LDA	C1-N1	-3.32	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	11	SO4	2	0
2	A	15	SO4	2	0
2	A	17	SO4	4	0
2	A	3	SO4	1	0
2	A	41	SO4	5	0
2	B	23	SO4	1	0
2	B	25	SO4	1	0
2	B	35	SO4	1	0
2	B	38	SO4	5	0
2	C	18	SO4	1	0
2	C	19	SO4	1	0
2	C	31	SO4	3	0
2	C	4	SO4	1	0
3	D	1	LDA	7	0
2	D	39	SO4	2	0
2	D	5	SO4	1	0
2	D	7	SO4	1	0
2	D	9	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	598/625 (95%)	0.22	14 (2%) 64 40	30, 74, 136, 217	0
1	B	621/625 (99%)	0.11	4 (0%) 90 80	24, 68, 118, 219	0
1	C	623/625 (99%)	0.06	3 (0%) 91 83	14, 60, 112, 317	0
1	D	602/625 (96%)	0.09	3 (0%) 91 83	24, 64, 129, 183	0
All	All	2444/2500 (97%)	0.12	24 (0%) 84 69	14, 66, 125, 317	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	GLY	4.3
1	B	691	THR	3.4
1	B	692	HIS	3.3
1	D	130	PHE	3.1
1	A	326	GLN	3.0
1	A	532	THR	2.9
1	A	322	GLY	2.5
1	D	691	THR	2.3
1	A	427	TYR	2.3
1	A	76	LYS	2.3
1	C	431	GLY	2.3
1	D	211	TYR	2.2
1	C	296	ASP	2.2
1	B	596	GLN	2.2
1	B	127	LYS	2.2
1	A	539	GLU	2.1
1	A	676	ILE	2.1
1	A	534	ASP	2.1
1	A	406	TYR	2.1
1	A	440	LYS	2.1
1	A	325	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	670	SER	2.0
1	A	691	THR	2.0
1	A	533	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	LDA	D	1	16/16	0.97	0.42	3.73	49,49,49,49	0
2	SO4	A	27	5/5	0.88	0.30	2.37	101,101,101,101	0
2	SO4	D	14	5/5	0.93	0.22	0.51	105,105,105,105	0
2	SO4	A	15	5/5	0.98	0.21	-0.34	50,50,50,50	0
2	SO4	C	4	5/5	0.93	0.20	-0.43	79,79,79,79	0
2	SO4	D	9	5/5	0.94	0.18	-0.55	75,75,75,75	0
2	SO4	A	46	5/5	0.90	0.21	-0.65	151,151,151,151	0
2	SO4	C	1	5/5	0.97	0.18	-0.70	82,82,82,82	0
2	SO4	A	26	5/5	0.97	0.17	-0.80	101,101,101,101	0
2	SO4	A	3	5/5	0.97	0.17	-0.94	79,79,79,79	0
2	SO4	A	41	5/5	0.93	0.19	-0.97	91,91,91,91	0
2	SO4	A	45	5/5	0.96	0.15	-1.13	115,115,115,115	0
2	SO4	C	19	5/5	0.97	0.16	-1.13	58,58,58,58	0
2	SO4	D	30	5/5	0.96	0.16	-1.21	112,112,112,112	0
2	SO4	B	8	5/5	0.98	0.16	-1.54	70,70,70,70	0
2	SO4	D	10	5/5	0.98	0.18	-1.68	53,53,53,53	0
2	SO4	B	34	5/5	0.97	0.19	-1.90	69,69,69,69	0
2	SO4	A	24	5/5	0.94	0.18	-1.96	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	D	5	5/5	0.96	0.15	-2.14	85,85,85,85	0
2	SO4	B	42	5/5	0.95	0.15	-2.20	94,94,94,94	0
2	SO4	B	32	5/5	0.92	0.17	-2.25	104,104,104,104	0
2	SO4	B	44	5/5	0.95	0.12	-2.40	118,118,118,118	0
2	SO4	C	33	5/5	0.93	0.16	-2.48	101,101,101,101	0
2	SO4	A	16	5/5	0.90	0.14	-2.62	108,108,108,108	0
2	SO4	A	11	5/5	0.94	0.12	-2.70	90,90,90,90	0
2	SO4	A	43	5/5	0.83	0.18	-2.85	129,129,129,129	0
2	SO4	B	23	5/5	0.97	0.11	-3.22	95,95,95,95	0
2	SO4	C	6	5/5	0.98	0.14	-3.28	77,77,77,77	0
2	SO4	B	35	5/5	0.97	0.12	-3.95	102,102,102,102	0
2	SO4	B	21	5/5	0.96	0.12	-	87,87,87,87	0
2	SO4	B	20	5/5	0.93	0.12	-	119,119,119,119	0
2	SO4	D	13	5/5	0.93	0.16	-	102,102,102,102	0
2	SO4	A	29	5/5	0.97	0.08	-	112,112,112,112	0
2	SO4	A	17	5/5	0.97	0.15	-	88,88,88,88	0
2	SO4	A	12	5/5	0.92	0.20	-	108,108,108,108	0
2	SO4	B	38	5/5	0.96	0.12	-	91,91,91,91	0
2	SO4	C	18	5/5	0.98	0.12	-	75,75,75,75	0
2	SO4	C	2	5/5	0.88	0.18	-	106,106,106,106	0
2	SO4	D	7	5/5	0.99	0.14	-	81,81,81,81	0
2	SO4	B	25	5/5	0.95	0.12	-	100,100,100,100	0
2	SO4	C	28	5/5	0.89	0.17	-	120,120,120,120	0
2	SO4	B	36	5/5	0.93	0.18	-	94,94,94,94	0
2	SO4	D	39	5/5	0.88	0.12	-	123,123,123,123	0
2	SO4	B	37	5/5	0.86	0.17	-	123,123,123,123	0
2	SO4	C	31	5/5	0.93	0.16	-	81,81,81,81	0
2	SO4	D	40	5/5	0.91	0.16	-	104,104,104,104	0
2	SO4	A	22	5/5	0.94	0.14	-	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.