



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:38 AM GMT

PDB ID : 3L24
Title : Crystal Structure of the Nerve Agent Degrading Organophosphate Anhydrolase/Prolidasein Complex with Inhibitors
Authors : Vyas, N.K.; Nichitenko, A.; Rastogi, V.K.; Shah, S.S.; Quioco, F.A.
Deposited on : 2009-12-14
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

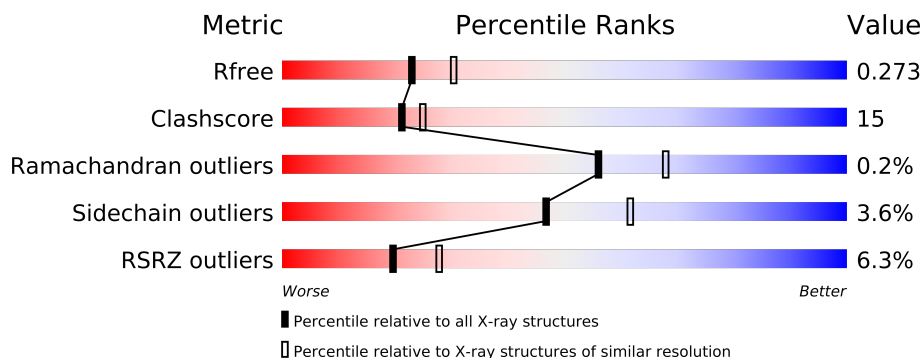
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	517	
1	B	517	
1	C	517	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MN	B	518	-	X
2	MN	B	519	-	X
3	GOA	B	522	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10683 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3443	2208	589	632	14			
1	B	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			
1	C	417	Total	C	N	O	S	0	0	0
			3392	2175	581	624	12			

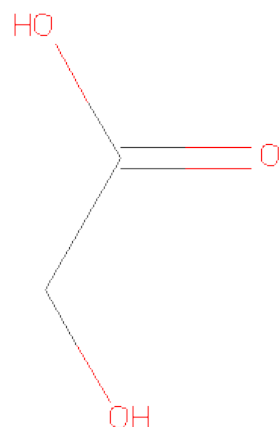
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	PRO	ALA	SEE REMARK 999	UNP Q44238
A	283	MET	CYS	SEE REMARK 999	UNP Q44238
A	439	LEU	ALA	SEE REMARK 999	UNP Q44238
B	211	PRO	ALA	SEE REMARK 999	UNP Q44238
B	283	MET	CYS	SEE REMARK 999	UNP Q44238
B	439	LEU	ALA	SEE REMARK 999	UNP Q44238
C	211	PRO	ALA	SEE REMARK 999	UNP Q44238
C	283	MET	CYS	SEE REMARK 999	UNP Q44238
C	439	LEU	ALA	SEE REMARK 999	UNP Q44238

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Mn	0	0
			4	4		
2	A	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: C₂H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	2	3		
3	B	1	Total	C	O	0	0
			5	2	3		
3	C	1	Total	C	O	0	0
			5	2	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	134	Total	O	0	0
			134	134		
4	C	110	Total	O	0	0
			110	110		

Chain C: 

SER	TYR	H402	I403	D406	K407	V408	A409	E410	L411	K412	P413	F414	G415	G416	E420	D421	H422	I423	V424	H425	H426	S429	L430	E431	N432	M433	T434	R435	F436	L437	R438	L439	R440	LEU	THR	THR	HIS	SER	LEU	VAL	THR	ARG	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N1		
TYR	SER	PRO	SER	GLU	PRO	LEU	SER	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	LEU	THR	THR	HIS	SER	LEU	VAL	THR	ARG	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N2
GLU	PRO	SER	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N3								
LEU	SER	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N4								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N5								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N6								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N7								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N8								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N9								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N10								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N11								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N12								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N13								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N14								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N15								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N16								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N17								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N18								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N19								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N20								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N21								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N22								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N23								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N24								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N25								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N26								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N27								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N28								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N29								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N30								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N31								
GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU	VAL	ARG	ARG	ARG	THR	LEU	PRO	PRO	GLU	GLY	GLN	GLY	ALA	HIS	ASP	GLU	GLN	GLY	GLY	V345	L340	F329	T328	S327	L218	H402	N32								
TYR	GLU	PRO	GLU	PRO	LEU	SER	TYR	TYR	TYR	GLU	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	ILE	VAL	HIS	VAL	ARG	THR	ARG	ARG	ILE	LEU																																			

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.35Å 143.93Å 219.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.30 47.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.10-2.30) 99.9 (47.40-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.273 0.235 , 0.273	Depositor DCC
R_{free} test set	8726 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 99543 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10683	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.39	0/3534	0.62	1/4795 (0.0%)
1	B	0.37	0/3482	0.61	1/4726 (0.0%)
1	C	0.36	1/3482 (0.0%)	0.59	2/4726 (0.0%)
All	All	0.37	1/10498 (0.0%)	0.61	4/14247 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ASP	C-N	-5.47	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ASN	N-CA-CB	-5.69	100.36	110.60
1	C	209	ASP	O-C-N	5.67	131.76	122.70
1	B	210	ASN	N-CA-CB	5.50	120.51	110.60
1	A	210	ASN	N-CA-CB	5.48	120.47	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	0	3318	93	0
1	B	3392	0	3271	98	0
1	C	3392	0	3270	120	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
3	A	5	0	3	0	0
3	B	5	0	3	0	0
3	C	5	0	3	0	0
4	A	187	0	0	6	0
4	B	134	0	0	2	0
4	C	110	0	0	4	0
All	All	10683	0	9868	309	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (309) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:GLN:HG2	1:B:129:ILE:HG21	1.33	1.05
1:A:55:GLN:HG2	1:A:129:ILE:HG21	1.41	1.02
1:A:169:ARG:HA	1:A:433:MET:HE2	1.45	0.97
1:C:3:LYS:HD3	1:C:3:LYS:H	1.30	0.97
1:B:395:ALA:HA	1:B:400:ASN:HD22	1.29	0.97
1:C:315:LEU:HD11	1:C:402:HIS:HB3	1.50	0.93
1:B:210:ASN:HB2	1:B:211:PRO:HD2	1.56	0.87
1:A:71:VAL:HG13	1:A:79:LYS:HB3	1.54	0.86
1:C:71:VAL:HG13	1:C:79:LYS:HB3	1.62	0.82
1:A:79:LYS:HD2	1:A:107:GLU:HG2	1.63	0.81
1:B:381:GLU:HB3	1:B:420:GLU:HB2	1.61	0.81
1:C:169:ARG:HA	1:C:433:MET:HE2	1.61	0.80
1:B:71:VAL:HG13	1:B:79:LYS:HB3	1.62	0.80
1:B:210:ASN:CB	1:B:211:PRO:HD2	2.12	0.79
1:B:169:ARG:CA	1:B:433:MET:HE2	2.13	0.78
1:B:169:ARG:HA	1:B:433:MET:HE2	1.66	0.78
1:A:298:ASP:O	1:A:302:ARG:HG2	1.84	0.78
1:B:298:ASP:O	1:B:302:ARG:HG2	1.85	0.76
1:B:55:GLN:HG2	1:B:129:ILE:CG2	2.14	0.76
1:B:71:VAL:CG1	1:B:79:LYS:HB3	2.15	0.76
1:A:169:ARG:CA	1:A:433:MET:HE2	2.16	0.76
1:C:69:TRP:HB2	1:C:81:ILE:HD12	1.68	0.75
1:C:314:ASP:C	1:C:315:LEU:HD12	2.07	0.75
1:B:395:ALA:CA	1:B:400:ASN:HD22	2.01	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:ASN:CB	1:A:211:PRO:HD2	2.18	0.73
1:A:191:SER:OG	1:A:194:GLU:HG3	1.90	0.71
1:B:210:ASN:CB	1:B:211:PRO:CD	2.69	0.71
1:C:313:VAL:HG12	1:C:315:LEU:HD13	1.72	0.69
1:C:58:ALA:HA	1:C:340:LEU:HD11	1.73	0.69
1:C:276:LYS:HE3	1:C:435:ARG:NH2	2.06	0.69
1:B:183:ARG:HD3	1:B:187:PHE:CE2	2.27	0.69
1:A:3:LYS:HG3	1:A:4:LEU:N	2.07	0.68
1:B:3:LYS:H	1:B:3:LYS:HD2	1.57	0.68
1:C:3:LYS:HG2	1:C:4:LEU:H	1.57	0.68
1:C:210:ASN:ND2	4:C:534:HOH:O	2.26	0.68
1:C:298:ASP:O	1:C:302:ARG:HG2	1.94	0.67
1:A:366:LEU:HD11	1:A:370:ARG:HD3	1.76	0.67
1:A:210:ASN:CB	1:A:211:PRO:CD	2.72	0.67
1:B:119:LEU:HB3	1:B:120:PRO:HD2	1.77	0.67
1:A:71:VAL:CG1	1:A:79:LYS:HB3	2.25	0.67
1:B:169:ARG:N	1:B:433:MET:HE2	2.10	0.66
1:B:3:LYS:H	1:B:3:LYS:CD	2.09	0.66
1:C:3:LYS:CD	1:C:3:LYS:H	2.05	0.65
1:C:2:ASN:HB3	1:C:5:ALA:HB2	1.79	0.65
1:B:14:THR:O	1:B:18:ARG:HG3	1.97	0.65
1:A:14:THR:O	1:A:18:ARG:HG3	1.96	0.64
1:A:79:LYS:HD3	1:A:105:ASP:O	1.97	0.63
1:C:111:LYS:HB2	1:C:114:GLN:NE2	2.14	0.63
1:C:315:LEU:CD1	1:C:402:HIS:HB3	2.26	0.63
1:A:97:ASN:HD22	1:A:97:ASN:H	1.46	0.63
1:A:210:ASN:HB2	1:A:211:PRO:HD2	1.81	0.62
1:B:403:ILE:HD11	1:B:405:TRP:CH2	2.35	0.62
1:B:320:ILE:HG23	1:B:325:ILE:HD11	1.82	0.62
1:B:210:ASN:HB2	1:B:211:PRO:CD	2.21	0.61
1:C:71:VAL:CG1	1:C:79:LYS:HB3	2.29	0.61
1:B:403:ILE:HD11	1:B:405:TRP:CZ2	2.36	0.61
1:A:17:LYS:O	1:A:21:GLU:HG3	2.00	0.61
1:B:17:LYS:O	1:B:21:GLU:HG3	2.01	0.61
1:B:29:ASP:OD2	1:B:125:ARG:HB2	2.00	0.60
1:C:169:ARG:HG3	1:C:433:MET:HE3	1.84	0.60
1:B:183:ARG:HD3	1:B:187:PHE:CD2	2.36	0.60
1:B:421:ASP:OD2	1:B:435:ARG:NH1	2.35	0.59
1:B:395:ALA:HA	1:B:400:ASN:ND2	2.11	0.59
1:C:23:ILE:HD11	4:C:610:HOH:O	2.01	0.59
1:B:33:PHE:HB2	1:B:70:ILE:HB	1.85	0.58
1:B:3:LYS:N	1:B:3:LYS:HD2	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:PHE:CE1	1:A:241:PHE:HB2	2.39	0.58
1:A:55:GLN:HG2	1:A:129:ILE:CG2	2.27	0.58
1:A:169:ARG:HG2	1:A:433:MET:CE	2.34	0.57
1:B:165:LEU:HD22	1:B:424:ILE:HD13	1.85	0.57
1:A:381:GLU:HB3	1:A:420:GLU:HB2	1.84	0.57
1:C:394:LEU:HG	1:C:403:ILE:HD11	1.86	0.57
1:A:315:LEU:HD11	1:A:402:HIS:ND1	2.19	0.57
1:C:14:THR:O	1:C:18:ARG:HG3	2.05	0.57
1:A:412:LYS:HB3	1:A:413:PRO:HD3	1.86	0.57
1:A:183:ARG:HG3	1:A:260:TYR:CE2	2.39	0.57
1:C:3:LYS:HD3	1:C:3:LYS:N	2.13	0.56
1:B:193:PHE:O	1:B:197:GLN:HG2	2.05	0.56
1:C:433:MET:O	1:C:437:LEU:HD22	2.05	0.56
1:A:291:LEU:HD23	1:A:371:LYS:HG2	1.87	0.56
1:C:315:LEU:HD11	1:C:402:HIS:CB	2.31	0.56
1:B:18:ARG:CZ	1:B:156:HIS:HB3	2.35	0.56
1:C:305:GLN:CA	1:C:305:GLN:HE21	2.18	0.56
1:C:320:ILE:HG23	1:C:325:ILE:HG12	1.87	0.56
1:A:3:LYS:O	1:A:6:VAL:HG12	2.06	0.56
1:B:316:SER:O	1:B:320:ILE:HG13	2.05	0.56
1:A:401:GLN:HG3	1:A:402:HIS:CD2	2.40	0.56
1:C:29:ASP:OD2	1:C:125:ARG:HB2	2.04	0.56
1:A:58:ALA:HA	1:A:340:LEU:HD11	1.87	0.55
1:C:183:ARG:HG3	1:C:260:TYR:CE2	2.41	0.55
1:C:211:PRO:HG3	1:C:247:ALA:O	2.06	0.55
1:C:313:VAL:CG1	1:C:315:LEU:HD13	2.36	0.55
1:A:435:ARG:NH2	1:A:440:ARG:O	2.39	0.55
1:B:320:ILE:HG23	1:B:325:ILE:CG1	2.36	0.55
1:B:372:ILE:HG23	1:B:378:PHE:CZ	2.41	0.55
1:B:323:LYS:HE3	1:B:402:HIS:CE1	2.42	0.55
1:C:18:ARG:CZ	1:C:156:HIS:HB3	2.37	0.55
1:A:323:LYS:HE3	1:A:402:HIS:CE1	2.42	0.55
1:B:224:ILE:HB	1:B:227:TYR:HB2	1.89	0.55
1:C:320:ILE:HG23	1:C:325:ILE:CG1	2.37	0.55
1:A:403:ILE:HD11	1:A:405:TRP:CZ2	2.42	0.55
1:A:370:ARG:HD2	4:A:707:HOH:O	2.07	0.54
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.73	0.54
1:A:55:GLN:HE22	1:A:153:TYR:CB	2.20	0.54
1:C:169:ARG:CA	1:C:433:MET:HE2	2.36	0.54
1:B:55:GLN:HE22	1:B:153:TYR:HB3	1.71	0.54
1:C:12:ILE:HG13	1:C:103:TYR:CD2	2.43	0.54
1:C:291:LEU:HB2	1:C:294:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:426:HIS:HB2	1:C:429:SER:O	2.08	0.54
1:A:20:ARG:CD	1:A:75:THR:HG22	2.38	0.54
1:C:169:ARG:HA	1:C:433:MET:CE	2.36	0.54
1:A:403:ILE:HD11	1:A:405:TRP:CE2	2.42	0.54
1:B:299:CYS:O	1:B:303:VAL:HG23	2.07	0.54
1:A:278:HIS:ND1	1:A:302:ARG:HB3	2.23	0.54
1:A:424:ILE:HD11	1:A:433:MET:HE3	1.91	0.53
1:A:169:ARG:HG2	1:A:433:MET:HE3	1.90	0.53
1:A:379:THR:HA	1:A:421:ASP:O	2.09	0.53
1:A:437:LEU:HD22	4:A:628:HOH:O	2.09	0.53
1:C:278:HIS:ND1	1:C:302:ARG:HB3	2.24	0.53
1:A:186:PHE:CD1	1:A:241:PHE:HB2	2.43	0.53
1:A:22:ILE:HD13	1:A:152:PHE:CG	2.44	0.53
1:C:169:ARG:HG3	1:C:433:MET:CE	2.38	0.53
1:A:97:ASN:N	1:A:97:ASN:HD22	2.05	0.53
1:B:303:VAL:HG13	1:B:384:LEU:CD2	2.39	0.53
1:B:398:ASP:O	1:B:401:GLN:HG3	2.08	0.53
1:A:183:ARG:HG3	1:A:260:TYR:CZ	2.44	0.53
1:B:412:LYS:HB3	1:B:413:PRO:HD3	1.90	0.53
1:A:18:ARG:HD3	4:A:560:HOH:O	2.08	0.53
1:A:55:GLN:HE22	1:A:153:TYR:HB3	1.74	0.53
1:A:2:ASN:HB3	1:A:5:ALA:HB3	1.90	0.53
1:C:33:PHE:HB2	1:C:70:ILE:HB	1.89	0.52
1:C:381:GLU:HB3	1:C:420:GLU:HB2	1.90	0.52
1:C:6:VAL:HG13	1:C:7:LEU:N	2.24	0.52
1:C:298:ASP:O	1:C:301:GLN:HB3	2.09	0.52
1:C:6:VAL:HG13	1:C:7:LEU:H	1.75	0.52
1:C:278:HIS:O	1:C:282:LEU:HG	2.09	0.52
1:C:290:LYS:HB3	1:C:372:ILE:HD12	1.91	0.52
1:C:412:LYS:HB3	1:C:413:PRO:HD3	1.91	0.51
1:C:186:PHE:CD1	1:C:241:PHE:HB2	2.45	0.51
1:C:242:LEU:C	1:C:242:LEU:HD23	2.31	0.51
1:B:55:GLN:HE22	1:B:153:TYR:CB	2.23	0.51
1:B:111:LYS:HD2	1:B:114:GLN:NE2	2.26	0.51
1:A:2:ASN:HB3	1:A:5:ALA:CB	2.41	0.51
1:C:186:PHE:CE1	1:C:241:PHE:HB2	2.45	0.51
1:B:69:TRP:HB2	1:B:81:ILE:HD12	1.93	0.51
1:C:372:ILE:HG23	1:C:378:PHE:CZ	2.47	0.50
1:A:395:ALA:CA	1:A:400:ASN:HD22	2.24	0.50
1:C:22:ILE:HB	1:C:152:PHE:CE2	2.46	0.50
1:C:37:GLN:HA	1:C:66:PRO:HB2	1.93	0.50
1:A:329:PHE:HB3	1:A:384:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:GLU:O	1:C:168:MET:HG3	2.11	0.50
1:C:72:ALA:HB1	4:C:549:HOH:O	2.10	0.50
1:B:374:ALA:O	1:B:375:ASN:HB2	2.12	0.50
1:B:314:ASP:O	1:B:315:LEU:HD23	2.12	0.50
1:C:316:SER:OG	1:C:319:GLU:HG3	2.12	0.50
1:B:426:HIS:HB2	1:B:429:SER:O	2.12	0.49
1:C:22:ILE:HD13	1:C:152:PHE:CG	2.47	0.49
1:A:279:GLN:HG3	1:A:419:ILE:HB	1.94	0.49
1:C:323:LYS:HE3	1:C:402:HIS:CE1	2.48	0.49
1:B:164:GLU:O	1:B:168:MET:HG3	2.12	0.49
1:C:22:ILE:HB	1:C:152:PHE:CD2	2.48	0.49
1:B:186:PHE:CE1	1:B:241:PHE:HB2	2.48	0.49
1:C:372:ILE:HG23	1:C:378:PHE:CE1	2.48	0.49
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.78	0.49
1:C:314:ASP:O	1:C:315:LEU:HD12	2.12	0.48
1:B:111:LYS:HB2	1:B:114:GLN:NE2	2.28	0.48
1:A:349:MET:O	1:A:349:MET:HG3	2.12	0.48
1:B:183:ARG:HD3	1:B:187:PHE:HE2	1.73	0.48
1:B:22:ILE:HD13	1:B:152:PHE:CG	2.48	0.48
1:A:432:ASN:ND2	1:A:435:ARG:HG3	2.28	0.48
1:A:210:ASN:ND2	4:A:684:HOH:O	2.36	0.48
1:C:3:LYS:O	1:C:6:VAL:HG12	2.13	0.48
1:C:169:ARG:CG	1:C:433:MET:HE3	2.43	0.48
1:B:79:LYS:HD2	1:B:105:ASP:O	2.13	0.48
1:C:385:TYR:HD1	1:C:416:GLY:HA3	1.79	0.48
1:C:320:ILE:HG22	1:C:326:THR:HG23	1.95	0.48
1:A:111:LYS:HD3	1:A:114:GLN:NE2	2.29	0.48
1:B:320:ILE:HG23	1:B:325:ILE:CD1	2.44	0.48
1:C:291:LEU:HD23	1:C:371:LYS:HG2	1.94	0.48
1:C:160:LYS:HE3	4:C:537:HOH:O	2.13	0.48
1:B:65:ASN:ND2	1:B:68:CYS:SG	2.87	0.48
1:B:440:ARG:NH1	4:B:655:HOH:O	2.31	0.47
1:A:349:MET:HG3	4:A:634:HOH:O	2.14	0.47
1:A:119:LEU:HB3	1:A:120:PRO:CD	2.44	0.47
1:A:164:GLU:HG2	1:A:252:TYR:CZ	2.49	0.47
1:B:279:GLN:OE1	1:B:435:ARG:NH1	2.48	0.47
1:B:440:ARG:N	1:B:440:ARG:HD2	2.30	0.47
1:C:50:PHE:CE1	1:C:66:PRO:HB3	2.50	0.47
1:B:3:LYS:O	1:B:6:VAL:HG12	2.14	0.47
1:B:252:TYR:CE2	1:B:340:LEU:HG	2.50	0.47
1:A:348:PHE:CD2	1:A:349:MET:HG2	2.49	0.47
1:C:437:LEU:O	1:C:438:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:423:ILE:N	1:B:423:ILE:HD12	2.29	0.46
1:B:381:GLU:CB	1:B:420:GLU:HB2	2.39	0.46
1:A:210:ASN:HB2	1:A:211:PRO:CD	2.40	0.46
1:A:210:ASN:HB3	1:A:211:PRO:HD2	1.97	0.46
1:C:305:GLN:NE2	1:C:305:GLN:HA	2.29	0.46
1:A:432:ASN:CG	1:A:435:ARG:HG3	2.36	0.46
1:C:281:ALA:O	1:C:285:GLN:HG3	2.16	0.46
1:C:111:LYS:HD3	1:C:114:GLN:NE2	2.31	0.46
1:C:305:GLN:HA	1:C:305:GLN:HE21	1.81	0.46
1:C:215:ILE:HB	1:C:244:ASP:HB3	1.97	0.46
1:C:3:LYS:HG2	1:C:4:LEU:N	2.29	0.46
1:C:412:LYS:N	1:C:413:PRO:CD	2.79	0.46
1:B:132:TYR:CD1	1:B:132:TYR:N	2.83	0.46
1:C:55:GLN:NE2	1:C:154:HIS:CD2	2.84	0.46
1:C:129:ILE:HA	1:C:145:ASN:OD1	2.16	0.46
1:C:9:ALA:HA	1:C:103:TYR:CE2	2.50	0.46
1:C:315:LEU:HD21	1:C:323:LYS:HD2	1.97	0.45
1:C:8:TYR:CZ	1:C:12:ILE:HD11	2.51	0.45
1:A:132:TYR:N	1:A:132:TYR:CD1	2.84	0.45
1:B:403:ILE:O	1:B:403:ILE:HG13	2.16	0.45
1:C:19:THR:O	1:C:22:ILE:HG22	2.15	0.45
1:A:20:ARG:HD3	1:A:75:THR:HG22	1.99	0.45
1:C:311:ASN:HD22	1:C:311:ASN:N	2.13	0.45
1:C:189:GLY:HA2	1:C:238:HIS:NE2	2.32	0.45
1:B:111:LYS:HD2	1:B:114:GLN:HE21	1.81	0.45
1:A:165:LEU:O	1:A:169:ARG:HG3	2.16	0.45
1:C:114:GLN:HB3	1:C:117:LYS:HE2	1.98	0.45
1:B:3:LYS:H	1:B:3:LYS:CE	2.30	0.45
1:B:323:LYS:HE3	1:B:402:HIS:HE1	1.79	0.45
1:B:97:ASN:HD22	1:B:97:ASN:H	1.64	0.45
1:C:60:LEU:H	1:C:60:LEU:HD23	1.81	0.45
1:A:437:LEU:O	1:A:438:ARG:HB2	2.16	0.45
1:C:86:VAL:O	1:C:87:ASP:HB3	2.17	0.45
1:B:58:ALA:HA	1:B:340:LEU:HD11	2.00	0.44
1:A:398:ASP:O	1:A:401:GLN:HG2	2.17	0.44
1:B:25:ARG:HD2	1:C:426:HIS:NE2	2.31	0.44
1:A:164:GLU:HG2	1:A:252:TYR:OH	2.16	0.44
1:C:7:LEU:HD22	1:C:162:GLN:HB3	1.99	0.44
1:C:14:THR:O	1:C:18:ARG:CG	2.65	0.44
1:A:190:LYS:HB3	1:A:194:GLU:HB2	1.99	0.44
1:B:408:VAL:O	1:B:412:LYS:HB2	2.18	0.44
1:B:283:MET:HG2	1:B:423:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.82	0.44
1:C:113:ASP:OD1	1:C:114:GLN:HG3	2.18	0.43
1:C:379:THR:HA	1:C:421:ASP:O	2.17	0.43
1:A:374:ALA:O	1:A:375:ASN:HB2	2.18	0.43
1:A:3:LYS:CG	1:A:4:LEU:N	2.79	0.43
1:B:403:ILE:HD11	1:B:405:TRP:CE2	2.53	0.43
1:C:124:ALA:O	1:C:125:ARG:HD2	2.19	0.43
1:A:290:LYS:HB3	1:A:372:ILE:HD12	1.99	0.43
1:C:19:THR:HA	1:C:22:ILE:HG22	1.99	0.43
1:C:60:LEU:N	1:C:60:LEU:HD23	2.32	0.43
1:B:1:MET:HG3	1:B:2:ASN:N	2.32	0.43
1:C:144:MET:HA	1:C:144:MET:HE2	2.00	0.43
1:A:98:GLU:HG3	4:A:706:HOH:O	2.19	0.43
1:A:22:ILE:HD13	1:A:152:PHE:CD1	2.54	0.43
1:A:395:ALA:HB1	1:A:400:ASN:ND2	2.33	0.43
1:C:183:ARG:HG3	1:C:260:TYR:CZ	2.54	0.43
1:B:19:THR:O	1:B:22:ILE:HG22	2.18	0.43
1:A:299:CYS:O	1:A:303:VAL:HG23	2.18	0.43
1:B:164:GLU:HG2	1:B:252:TYR:CZ	2.54	0.43
1:B:50:PHE:CE1	1:B:66:PRO:HB3	2.54	0.43
1:C:423:ILE:N	1:C:423:ILE:HD12	2.34	0.43
1:C:374:ALA:HA	1:C:425:VAL:O	2.18	0.43
1:C:315:LEU:CD2	1:C:323:LYS:HD2	2.49	0.43
1:C:311:ASN:ND2	1:C:311:ASN:N	2.67	0.43
1:C:192:GLU:HG3	1:C:218:LEU:HD22	2.01	0.43
1:A:29:ASP:OD2	1:A:125:ARG:HB2	2.18	0.43
1:A:315:LEU:HD11	1:A:402:HIS:CG	2.54	0.42
1:C:210:ASN:ND2	1:C:212:TYR:O	2.51	0.42
1:A:403:ILE:HD11	1:A:405:TRP:CH2	2.54	0.42
1:A:381:GLU:HA	1:A:419:ILE:O	2.19	0.42
1:B:412:LYS:N	1:B:413:PRO:CD	2.82	0.42
1:C:77:LYS:HB3	1:C:105:ASP:OD2	2.18	0.42
1:C:305:GLN:NE2	1:C:305:GLN:CA	2.82	0.42
1:C:239:ARG:HB3	1:C:414:PHE:CE2	2.54	0.42
1:A:440:ARG:HD3	1:A:440:ARG:HA	1.72	0.42
1:B:403:ILE:HD11	1:B:405:TRP:CZ3	2.55	0.42
1:B:25:ARG:HD2	1:C:426:HIS:CE1	2.55	0.42
1:B:229:HIS:CD2	1:B:230:PHE:H	2.37	0.42
1:B:88:PHE:H	1:B:88:PHE:HD1	1.68	0.42
1:C:16:GLN:NE2	1:C:78:PRO:HD3	2.35	0.42
1:C:79:LYS:HD3	1:C:105:ASP:O	2.20	0.42
1:B:169:ARG:HG2	1:B:433:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:424:ILE:HD11	1:B:433:MET:HE3	2.02	0.41
1:A:97:ASN:N	1:A:97:ASN:ND2	2.68	0.41
1:C:88:PHE:CZ	1:C:89:TRP:NE1	2.87	0.41
1:C:210:ASN:HD21	1:C:214:ASN:ND2	2.18	0.41
1:B:113:ASP:OD1	1:B:114:GLN:HG3	2.20	0.41
1:A:184:ASP:O	1:A:188:GLN:HG3	2.20	0.41
1:B:147:GLU:N	1:B:148:PRO:HD2	2.36	0.41
1:B:23:ILE:HD11	4:B:599:HOH:O	2.20	0.41
1:C:432:ASN:CG	1:C:435:ARG:HG3	2.41	0.41
1:A:303:VAL:HG13	1:A:384:LEU:HD23	2.02	0.41
1:C:55:GLN:NE2	1:C:154:HIS:NE2	2.68	0.41
1:A:424:ILE:HD11	1:A:433:MET:CE	2.50	0.41
1:A:241:PHE:CZ	1:A:243:ILE:HB	2.56	0.41
1:C:40:ARG:HG2	1:C:40:ARG:NH1	2.36	0.41
1:A:316:SER:O	1:A:320:ILE:HG13	2.20	0.41
1:B:257:THR:HB	1:B:420:GLU:HB3	2.02	0.41
1:B:298:ASP:OD2	1:B:302:ARG:HD3	2.21	0.41
1:B:32:VAL:HA	1:B:70:ILE:O	2.21	0.41
1:C:164:GLU:HG2	1:C:252:TYR:OH	2.20	0.41
1:B:186:PHE:CD1	1:B:241:PHE:HB2	2.56	0.41
1:B:52:VAL:HG22	1:B:53:ASN:N	2.35	0.41
1:B:310:PHE:O	1:B:407:LYS:HE2	2.21	0.41
1:B:22:ILE:HB	1:B:152:PHE:CE2	2.56	0.40
1:B:437:LEU:HA	1:B:437:LEU:HD12	1.91	0.40
1:C:52:VAL:HG22	1:C:53:ASN:N	2.35	0.40
1:A:3:LYS:O	1:A:6:VAL:CG1	2.69	0.40
1:A:119:LEU:HB3	1:A:120:PRO:HD2	2.03	0.40
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.83	0.40
1:B:210:ASN:ND2	1:B:212:TYR:O	2.49	0.40
1:A:380:ILE:O	1:A:420:GLU:HA	2.21	0.40
1:C:124:ALA:C	1:C:125:ARG:HD2	2.42	0.40
1:C:257:THR:HB	1:C:420:GLU:HB3	2.04	0.40
1:A:60:LEU:N	1:A:60:LEU:HD23	2.36	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	421/517 (81%)	403 (96%)	18 (4%)	0	100	100
1	B	413/517 (80%)	391 (95%)	21 (5%)	1 (0%)	56	68
1	C	413/517 (80%)	389 (94%)	23 (6%)	1 (0%)	56	68
All	All	1247/1551 (80%)	1183 (95%)	62 (5%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	ASP
1	B	96	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	360/443 (81%)	347 (96%)	13 (4%)	47	61
1	B	356/443 (80%)	342 (96%)	14 (4%)	43	57
1	C	356/443 (80%)	344 (97%)	12 (3%)	49	64
All	All	1072/1329 (81%)	1033 (96%)	39 (4%)	47	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	97	ASN
1	A	147	GLU
1	A	172	ASN
1	A	196	GLN
1	A	210	ASN
1	A	218	LEU
1	A	232	ARG
1	A	398	ASP
1	A	406	ASP

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	437	LEU
1	A	440	ARG
1	B	3	LYS
1	B	97	ASN
1	B	121	TYR
1	B	172	ASN
1	B	196	GLN
1	B	210	ASN
1	B	218	LEU
1	B	232	ARG
1	B	302	ARG
1	B	384	LEU
1	B	401	GLN
1	B	406	ASP
1	B	437	LEU
1	B	440	ARG
1	C	3	LYS
1	C	60	LEU
1	C	97	ASN
1	C	137	GLN
1	C	172	ASN
1	C	196	GLN
1	C	232	ARG
1	C	305	GLN
1	C	384	LEU
1	C	406	ASP
1	C	430	LEU
1	C	437	LEU

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	27	ASN
1	A	55	GLN
1	A	97	ASN
1	A	114	GLN
1	A	151	ASN
1	A	177	GLN
1	A	188	GLN
1	A	196	GLN
1	A	208	ASN

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	250	ASN
1	A	284	ASN
1	A	305	GLN
1	A	311	ASN
1	A	375	ASN
1	A	400	ASN
1	A	402	HIS
1	B	41	GLN
1	B	55	GLN
1	B	65	ASN
1	B	67	HIS
1	B	97	ASN
1	B	114	GLN
1	B	151	ASN
1	B	177	GLN
1	B	188	GLN
1	B	196	GLN
1	B	208	ASN
1	B	214	ASN
1	B	229	HIS
1	B	250	ASN
1	B	284	ASN
1	B	296	HIS
1	B	305	GLN
1	B	311	ASN
1	B	375	ASN
1	B	400	ASN
1	B	401	GLN
1	B	402	HIS
1	C	97	ASN
1	C	114	GLN
1	C	151	ASN
1	C	177	GLN
1	C	188	GLN
1	C	196	GLN
1	C	197	GLN
1	C	208	ASN
1	C	210	ASN
1	C	214	ASN
1	C	250	ASN
1	C	284	ASN

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Mol	Chain	Res	Type
1	C	305	GLN
1	C	311	ASN
1	C	375	ASN
1	C	401	GLN
1	C	402	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOA	A	521	2	4,4,4	1.04	0	4,4,4	0.85	0
3	GOA	B	522	2	4,4,4	1.22	0	4,4,4	0.63	0
3	GOA	C	521	2	4,4,4	0.90	0	4,4,4	0.80	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
3	GOA	A	521	2	-	1/2/2/2	0/0/0/0
3	GOA	B	522	2	-	0/2/2/2	0/0/0/0
3	GOA	C	521	2	-	1/2/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	521	GOA	O12-C1-C2-O2
3	A	521	GOA	O12-C1-C2-O2

There are no ring outliers.

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	425/517 (82%)	0.12	21 (4%) 28 39	18, 36, 78, 95	0
1	B	417/517 (80%)	0.27	22 (5%) 25 35	20, 43, 78, 92	0
1	C	417/517 (80%)	0.58	37 (8%) 10 16	28, 51, 88, 98	0
All	All	1259/1551 (81%)	0.32	80 (6%) 19 27	18, 44, 82, 98	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	ILE	4.8
1	A	366	LEU	4.6
1	C	124	ALA	4.6
1	C	394	LEU	4.4
1	B	121	TYR	4.4
1	C	325	ILE	4.2
1	A	398	ASP	3.9
1	C	411	LEU	3.9
1	A	312	ILE	3.7
1	C	369	THR	3.7
1	A	405	TRP	3.6
1	B	369	THR	3.6
1	A	313	VAL	3.6
1	B	403	ILE	3.4
1	C	395	ALA	3.4
1	B	398	ASP	3.3
1	C	313	VAL	3.3
1	C	324	GLY	3.3
1	C	370	ARG	3.2
1	A	322	ALA	3.2
1	C	88	PHE	3.2
1	B	89	TRP	3.2
1	A	401	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	409	ALA	3.1
1	B	88	PHE	3.1
1	C	292	TYR	3.1
1	B	312	ILE	3.1
1	B	117	LYS	3.1
1	C	408	VAL	3.0
1	C	89	TRP	3.0
1	C	398	ASP	3.0
1	C	400	ASN	3.0
1	B	395	ALA	2.9
1	B	402	HIS	2.9
1	C	328	THR	2.9
1	A	325	ILE	2.8
1	A	369	THR	2.8
1	B	394	LEU	2.7
1	C	391	LEU	2.7
1	B	313	VAL	2.7
1	C	120	PRO	2.6
1	A	349	MET	2.6
1	C	322	ALA	2.6
1	C	323	LYS	2.6
1	B	107	GLU	2.6
1	C	121	TYR	2.6
1	A	402	HIS	2.6
1	C	319	GLU	2.5
1	C	226	HIS	2.5
1	B	115	VAL	2.5
1	A	265	GLU	2.5
1	C	396	ALA	2.5
1	C	403	ILE	2.5
1	A	368	CYS	2.4
1	B	320	ILE	2.4
1	A	308	SER	2.4
1	B	405	TRP	2.4
1	C	297	LEU	2.3
1	C	210	ASN	2.3
1	C	386	PHE	2.3
1	B	292	TYR	2.3
1	B	411	LEU	2.3
1	A	403	ILE	2.3
1	C	311	ASN	2.2
1	C	329	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	311	ASN	2.2
1	C	402	HIS	2.2
1	C	237	THR	2.2
1	B	310	PHE	2.1
1	C	378	PHE	2.1
1	A	384	LEU	2.1
1	A	371	LYS	2.1
1	B	386	PHE	2.1
1	C	387	ILE	2.1
1	A	297	LEU	2.0
1	A	400	ASN	2.0
1	C	377	VAL	2.0
1	C	392	GLY	2.0
1	A	329	PHE	2.0
1	B	404	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	B	518	1/1	0.15	3.50	32,32,32,32	0
2	MN	B	519	1/1	0.18	3.50	33,33,33,33	0
3	GOA	B	522	5/5	0.16	2.93	43,48,50,51	0
2	MN	A	518	1/1	0.17	0.61	31,31,31,31	0
2	MN	C	519	1/1	0.14	-0.08	39,39,39,39	0
3	GOA	A	521	5/5	0.14	-0.14	34,34,40,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	C	518	1/1	0.13	-0.46	39,39,39,39	0
2	MN	A	519	1/1	0.13	-0.56	27,27,27,27	0
2	MN	A	520	1/1	0.09	-0.80	36,36,36,36	0
2	MN	B	520	1/1	0.12	-0.88	57,57,57,57	0
3	GOA	C	521	5/5	0.12	-0.96	49,49,51,52	0
2	MN	C	520	1/1	0.07	-4.89	94,94,94,94	0
2	MN	B	521	1/1	0.10	-7.60	75,75,75,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.