



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:17 AM EST

PDB ID : 3L24  
Title : Crystal Structure of the Nerve Agent Degrading Organophosphate Anhydrolase/Prolidase in Complex with Inhibitors  
Authors : Vyas, N.K.; Nichitenko, A.; Rastogi, V.K.; Shah, S.S.; Quiocho, F.A.  
Deposited on : 2009-12-14  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

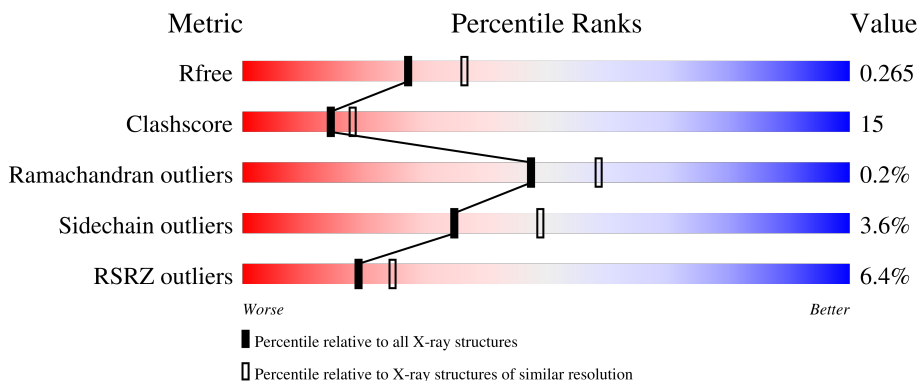
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	517	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">63%      18%      •      18%</p>
1	B	517	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">59%      20%      •      19%</p>
1	C	517	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 40px;">55%      24%      •      19%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10683 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 Xaa-Pro dipeptidase.

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

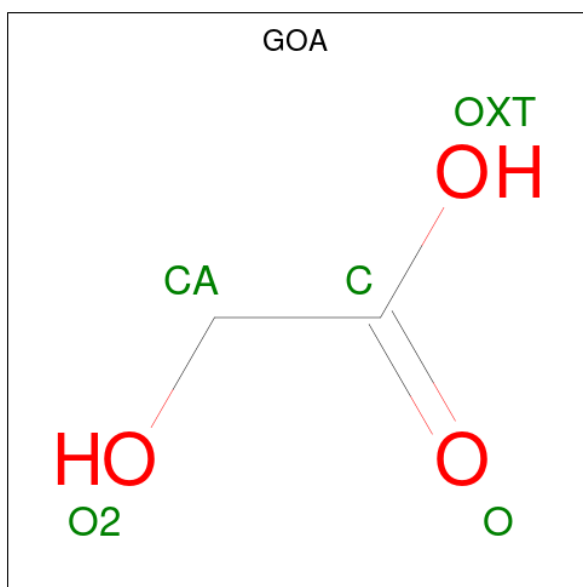
There are 9 discrepancies between the modelled and reference sequences:

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	A	3	Total 3	Mn 3	0	0
2	B	4	Total 4	Mn 4	0	0
2	C	3	Total 3	Mn 3	0	0

- Molecule 3 is GLYCOLIC ACID (three-letter code: GOA) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>).



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

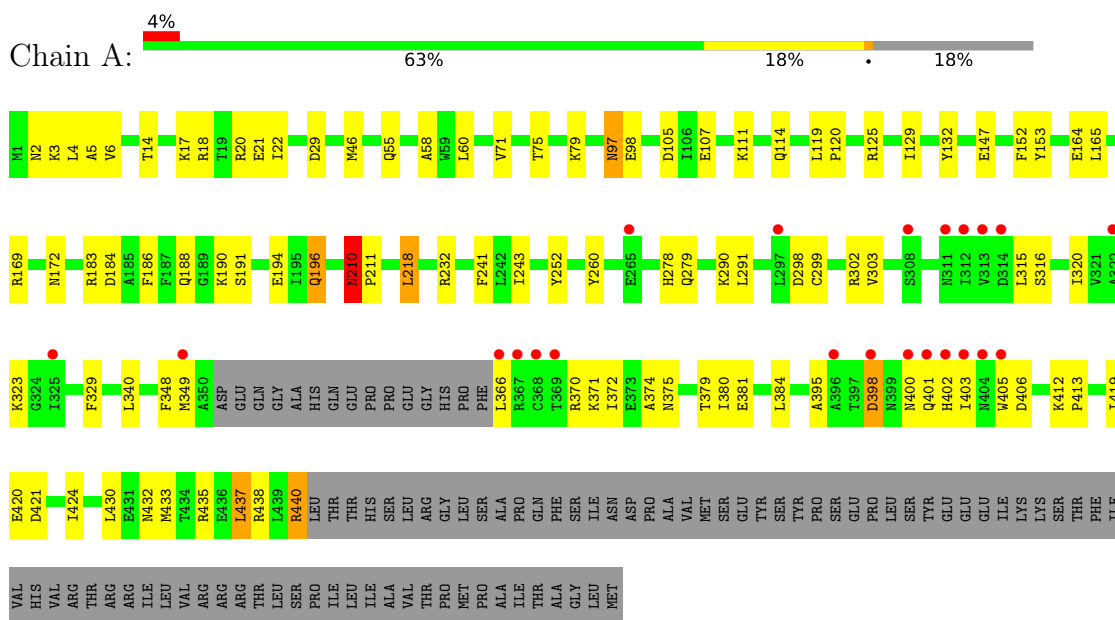
- Molecule 4 is water.

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

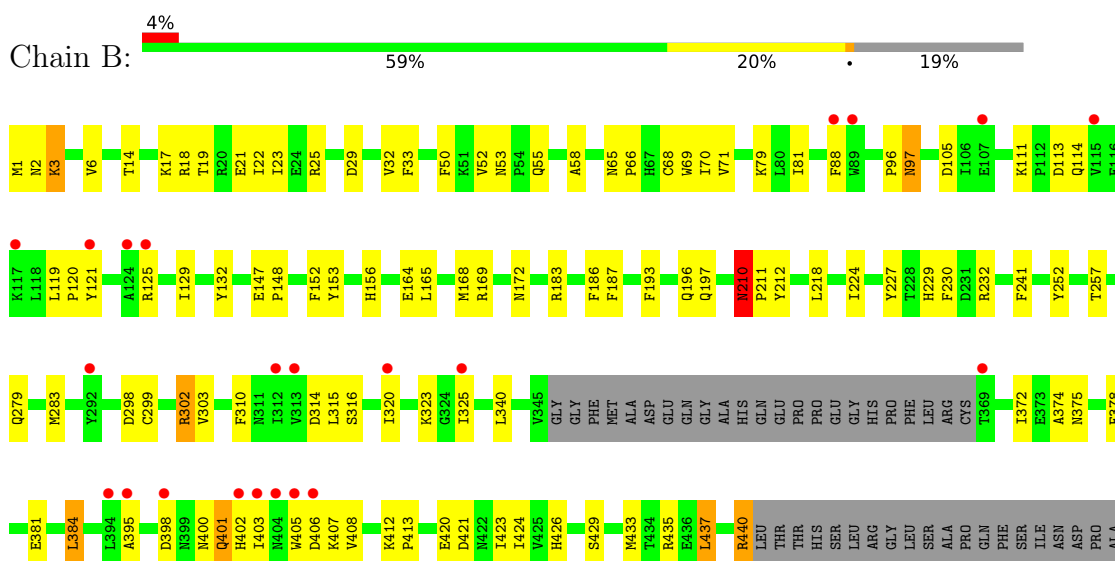
### 3 Residue-property plots i

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

- Molecule 1: Xaa-Pro dipeptidase

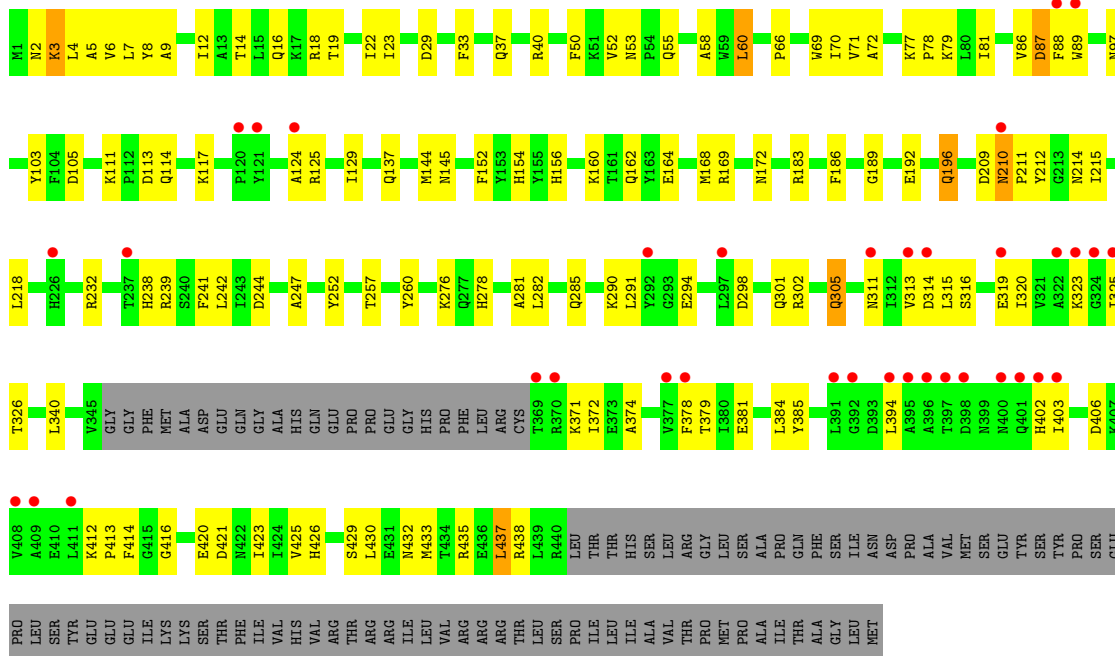


- Molecule 1: Xaa-Pro dipeptidase



VAL	MET	SER	GLU	TYR	SER	TYR	PRO	SER	GLU	PRO	PRO	LEU	SER	TYR	GLU	GLU	ILE	LYS	LYS	SER	THR	PHE	THR	ILE	VAL	HIS	VAL	VAL	ARG	ARG	ILE	LEU	VAL	ARG	ARG	THR	LEU	SER	SER	PRO	PRO	ILE	LEU	ILE	ALA	VAL	THR	THR	PRO	MET	PRO	ALA	ILE	THR	ALA	ALA	GLY	LEU	MET
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● Molecule 1: Xaa-Pro dipeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.273 0.228 , 0.265	Depositor DCC
$R_{free}$ test set	9329 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.485	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	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	9859	309	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 15.

All (309) 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: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:B:71:VAL:HG13	1:B:79:LYS:HB3	1.62	0.80
1:C:169:ARG:HA	1:C:433:MET:HE2	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:58:ALA:HA	1:C:340:LEU:HD11	1.73	0.69
1:C:313:VAL:HG12	1:C:315:LEU:HD13	1.72	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:A:366:LEU:HD11	1:A:370:ARG:HD3	1.76	0.67
1:C:298:ASP:O	1:C:302:ARG:HG2	1.94	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:3:LYS:H	1:B:3:LYS:CD	2.09	0.66
1:B:169:ARG:N	1:B:433:MET:HE2	2.10	0.66
1:C:3:LYS:H	1:C:3:LYS:CD	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:A:97:ASN:HD22	1:A:97:ASN:H	1.46	0.63
1:C:315:LEU:CD1	1:C:402:HIS:HB3	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:B:3:LYS:N	2.18	0.58
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:A:412:LYS:HB3	1:A:413:PRO:HD3	1.86	0.57
1:C:14:THR:O	1:C:18:ARG:HG3	2.05	0.57
1:A:183:ARG:HG3	1:A:260:TYR:CE2	2.39	0.57
1:B:193:PHE:O	1:B:197:GLN:HG2	2.05	0.56
1:C:3:LYS:HD3	1:C:3:LYS:N	2.13	0.56
1:A:291:LEU:HD23	1:A:371:LYS:HG2	1.87	0.56
1:C:433:MET:O	1:C:437:LEU:HD22	2.05	0.56
1:B:18:ARG:CZ	1:B:156:HIS:HB3	2.35	0.56
1:C:315:LEU:HD11	1:C:402:HIS:CB	2.31	0.56
1:C:305:GLN:HE21	1:C:305:GLN:CA	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:A:435:ARG:NH2	1:A:440:ARG:O	2.39	0.55
1:C:313:VAL:CG1	1:C:315:LEU:HD13	2.36	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:A:403:ILE:HD11	1:A:405:TRP:CZ2	2.42	0.55
1:C:320:ILE:HG23	1:C:325:ILE:CG1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:169:ARG:HA	1:C:433:MET:CE	2.36	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:A:22:ILE:HD13	1:A:152:PHE:CG	2.44	0.53
1:A:186:PHE:CD1	1:A:241:PHE:HB2	2.43	0.53
1:C:278:HIS:ND1	1:C:302:ARG:HB3	2.24	0.53
1:A:97:ASN:HD22	1:A:97:ASN:N	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:C:169:ARG:HG3	1:C:433:MET:CE	2.38	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:2:ASN:HB3	1:A:5:ALA:HB3	1.90	0.53
1:A:55:GLN:HE22	1:A:153:TYR:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ALA:CA	1:A:400:ASN:HD22	2.24	0.50
1:C:372:ILE:HG23	1:C:378:PHE:CZ	2.47	0.50
1:C:22:ILE:HB	1:C:152:PHE:CE2	2.46	0.50
1:A:329:PHE:HB3	1:A:384:LEU:HD22	1.92	0.50
1:C:37:GLN:HA	1:C:66:PRO:HB2	1.93	0.50
1:C:72:ALA:HB1	4:C:549:HOH:O	2.10	0.50
1:C:164:GLU:O	1:C:168:MET:HG3	2.11	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:B:186:PHE:CE1	1:B:241:PHE:HB2	2.48	0.49
1:C:22:ILE:HB	1:C:152:PHE:CD2	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:A:349:MET:HG3	1:A:349:MET:O	2.12	0.48
1:B:111:LYS:HB2	1:B:114:GLN:NE2	2.28	0.48
1:C:314:ASP:O	1:C:315:LEU:HD12	2.12	0.48
1:B:22:ILE:HD13	1:B:152:PHE:CG	2.48	0.48
1:B:183:ARG:HD3	1:B:187:PHE:HE2	1.73	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:B:79:LYS:HD2	1:B:105:ASP:O	2.13	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: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:B:65:ASN:ND2	1:B:68:CYS:SG	2.87	0.48
1:C:160:LYS:HE3	4:C:537:HOH:O	2.13	0.48
1:B:440:ARG:NH1	4:B:655:HOH:O	2.31	0.47
1:A:119:LEU:HB3	1:A:120:PRO:CD	2.44	0.47
1:A:349:MET:HG3	4:A:634:HOH:O	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ARG:HD2	1:B:440:ARG:N	2.30	0.47
1:C:50:PHE:CE1	1:C:66:PRO:HB3	2.50	0.47
1:A:348:PHE:CD2	1:A:349:MET:HG2	2.49	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:B:423:ILE:HD12	1:B:423:ILE:N	2.29	0.46
1:C:437:LEU:O	1:C:438:ARG:HB2	2.15	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:A:432:ASN:CG	1:A:435:ARG:HG3	2.36	0.46
1:C:305:GLN:HA	1:C:305:GLN:NE2	2.29	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:HE21	1:C:305:GLN:HA	1.81	0.46
1:C:215:ILE:HB	1:C:244:ASP:HB3	1.97	0.46
1:B:132:TYR:N	1:B:132:TYR:CD1	2.83	0.46
1:C:3:LYS:HG2	1:C:4:LEU:N	2.29	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:412:LYS:N	1:C:413:PRO:CD	2.79	0.46
1:C:9:ALA:HA	1:C:103:TYR:CE2	2.50	0.46
1:A:132:TYR:N	1:A:132:TYR:CD1	2.84	0.45
1:C:8:TYR:CZ	1:C:12:ILE:HD11	2.51	0.45
1:C:315:LEU:HD21	1:C:323:LYS:HD2	1.97	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:189:GLY:HA2	1:C:238:HIS:NE2	2.32	0.45
1:C:311:ASN:N	1:C:311:ASN:HD22	2.13	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:97:ASN:H	1:B:97:ASN:HD22	1.64	0.45
1:B:323:LYS:HE3	1:B:402:HIS:HE1	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:MET:HG2	1:B:423:ILE:HG12	2.00	0.44
1:B:408:VAL:O	1:B:412:LYS:HB2	2.18	0.44
1:C:196:GLN:HE21	1:C:196:GLN:HA	1.82	0.44
1:A:374:ALA:O	1:A:375:ASN:HB2	2.18	0.43
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: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:A:98:GLU:HG3	4:A:706:HOH:O	2.19	0.43
1:B:1:MET:HG3	1:B:2:ASN:N	2.32	0.43
1:C:19:THR:HA	1:C:22:ILE:HG22	1.99	0.43
1:C:60:LEU:HD23	1:C:60:LEU:N	2.32	0.43
1:C:144:MET:HE2	1:C:144:MET:HA	2.00	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:B:19:THR:O	1:B:22:ILE:HG22	2.18	0.43
1:C:183:ARG:HG3	1:C:260:TYR:CZ	2.54	0.43
1:A:299:CYS:O	1:A:303:VAL:HG23	2.18	0.43
1:B:50:PHE:CE1	1:B:66:PRO:HB3	2.54	0.43
1:B:164:GLU:HG2	1:B:252:TYR:CZ	2.54	0.43
1:C:374:ALA:HA	1:C:425:VAL:O	2.18	0.43
1:C:423:ILE:HD12	1:C:423:ILE:N	2.34	0.43
1:C:315:LEU:CD2	1:C:323:LYS:HD2	2.49	0.43
1:C:192:GLU:HG3	1:C:218:LEU:HD22	2.01	0.43
1:C:311:ASN:N	1:C:311:ASN:ND2	2.67	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:A:403:ILE:HD11	1:A:405:TRP:CH2	2.54	0.42
1:C:210:ASN:ND2	1:C:212:TYR:O	2.51	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:CA	1:C:305:GLN:NE2	2.82	0.42
1:C:239:ARG:HB3	1:C:414:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:HA	1:A:440:ARG:HD3	1.72	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:403:ILE:HD11	1:B:405:TRP:CZ3	2.55	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:A:97:ASN:N	1:A:97:ASN:ND2	2.68	0.41
1:B:169:ARG:HG2	1:B:433:MET:HE3	2.02	0.41
1:B:424:ILE:HD11	1:B:433:MET:HE3	2.02	0.41
1:C:88:PHE:CZ	1:C:89:TRP:NE1	2.87	0.41
1:B:113:ASP:OD1	1:B:114:GLN:HG3	2.20	0.41
1:C:210:ASN:HD21	1:C:214:ASN:ND2	2.18	0.41
1:A:184:ASP:O	1:A:188:GLN:HG3	2.20	0.41
1:B:23:ILE:HD11	4:B:599:HOH:O	2.20	0.41
1:B:147:GLU:N	1:B:148:PRO:HD2	2.36	0.41
1:A:303:VAL:HG13	1:A:384:LEU:HD23	2.02	0.41
1:C:432:ASN:CG	1:C:435:ARG:HG3	2.41	0.41
1:C:55:GLN:NE2	1:C:154:HIS:NE2	2.68	0.41
1:A:241:PHE:CZ	1:A:243:ILE:HB	2.56	0.41
1:A:316:SER:O	1:A:320:ILE:HG13	2.20	0.41
1:A:424:ILE:HD11	1:A:433:MET:CE	2.50	0.41
1:C:40:ARG:HG2	1:C:40:ARG:NH1	2.36	0.41
1:B:32:VAL:HA	1:B:70:ILE:O	2.21	0.41
1:B:186:PHE:CD1	1:B:241:PHE:HB2	2.56	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:C:164:GLU:HG2	1:C:252:TYR:OH	2.20	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:HD12	1:B:437:LEU:HA	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:A:60:LEU:HD23	1:A:60:LEU:N	2.36	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



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/517 (81%)	403 (96%)	18 (4%)	0	100	100
1	B	413/517 (80%)	391 (95%)	21 (5%)	1 (0%)	47	58
1	C	413/517 (80%)	389 (94%)	23 (6%)	1 (0%)	47	58
All	All	1247/1551 (80%)	1183 (95%)	62 (5%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	87	ASP
1	B	96	PRO

### 5.3.2 Protein sidechains [i](#)

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%)	35	49
1	B	356/443 (80%)	342 (96%)	14 (4%)	32	46
1	C	356/443 (80%)	344 (97%)	12 (3%)	37	51
All	All	1072/1329 (81%)	1033 (96%)	39 (4%)	35	49

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
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

Sometimes 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
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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	1.15	0	4,4,4	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOA	C	521	2	4,4,4	0.95	0	4,4,4	0.79	0
3	GOA	B	522	2	4,4,4	1.34	0	4,4,4	0.63	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	-	2/2/2/2	-
3	GOA	C	521	2	-	2/2/2/2	-
3	GOA	B	522	2	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	521	GOA	O-C-CA-O2
3	A	521	GOA	OXT-C-CA-O2
3	B	522	GOA	O-C-CA-O2
3	B	522	GOA	OXT-C-CA-O2
3	C	521	GOA	O-C-CA-O2
3	C	521	GOA	OXT-C-CA-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/517 (82%)	0.18	22 (5%) 27 34	18, 36, 78, 95	0
1	B	417/517 (80%)	0.28	22 (5%) 26 33	20, 43, 78, 92	0
1	C	417/517 (80%)	0.61	36 (8%) 10 14	28, 51, 88, 98	0
All	All	1259/1551 (81%)	0.36	80 (6%) 19 25	18, 44, 82, 98	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	TYR	5.1
1	B	325	ILE	4.7
1	C	124	ALA	4.5
1	A	366	LEU	4.4
1	B	369	THR	4.1
1	C	394	LEU	4.1
1	B	395	ALA	4.0
1	C	400	ASN	4.0
1	A	322	ALA	3.7
1	A	398	ASP	3.7
1	C	325	ILE	3.6
1	A	313	VAL	3.6
1	A	308	SER	3.6
1	C	395	ALA	3.5
1	C	396	ALA	3.5
1	C	313	VAL	3.4
1	B	398	ASP	3.4
1	A	401	GLN	3.4
1	C	324	GLY	3.3
1	B	403	ILE	3.3
1	C	292	TYR	3.3
1	A	405	TRP	3.2
1	B	89	TRP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	411	LEU	3.2
1	C	408	VAL	3.1
1	C	398	ASP	3.1
1	C	322	ALA	3.1
1	A	368	CYS	3.0
1	C	323	LYS	3.0
1	C	409	ALA	3.0
1	C	392	GLY	3.0
1	C	369	THR	3.0
1	A	369	THR	2.9
1	A	349	MET	2.9
1	C	311	ASN	2.9
1	C	226	HIS	2.9
1	C	297	LEU	2.8
1	A	402	HIS	2.8
1	A	312	ILE	2.8
1	A	325	ILE	2.8
1	A	403	ILE	2.8
1	C	121	TYR	2.8
1	C	403	ILE	2.8
1	B	402	HIS	2.8
1	B	88	PHE	2.8
1	B	117	LYS	2.7
1	C	391	LEU	2.7
1	C	89	TRP	2.7
1	B	107	GLU	2.7
1	A	311	ASN	2.7
1	B	320	ILE	2.6
1	C	120	PRO	2.6
1	B	394	LEU	2.6
1	C	402	HIS	2.6
1	B	313	VAL	2.5
1	C	370	ARG	2.5
1	A	400	ASN	2.5
1	C	88	PHE	2.4
1	C	319	GLU	2.4
1	A	367	ARG	2.4
1	A	297	LEU	2.4
1	A	265	GLU	2.4
1	B	115	VAL	2.3
1	C	401	GLN	2.3
1	C	378	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	292	TYR	2.2
1	C	377	VAL	2.2
1	C	210	ASN	2.2
1	B	312	ILE	2.2
1	B	404	ASN	2.2
1	A	314	ASP	2.2
1	B	405	TRP	2.1
1	A	404	ASN	2.1
1	B	406	ASP	2.1
1	C	314	ASP	2.1
1	B	124	ALA	2.1
1	C	237	THR	2.0
1	C	397	THR	2.0
1	B	125	ARG	2.0
1	A	396	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	MN	B	521	1/1	0.78	0.10	75,75,75,75	0
3	GOA	B	522	5/5	0.80	0.17	43,48,50,51	0
2	MN	C	520	1/1	0.88	0.08	94,94,94,94	0
3	GOA	C	521	5/5	0.89	0.11	49,49,51,52	0
3	GOA	A	521	5/5	0.94	0.15	34,34,40,41	0
2	MN	B	520	1/1	0.98	0.13	57,57,57,57	0
2	MN	A	518	1/1	0.98	0.17	31,31,31,31	0
2	MN	C	518	1/1	0.98	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	C	519	1/1	0.98	0.13	39,39,39,39	0
2	MN	B	518	1/1	0.99	0.16	32,32,32,32	0
2	MN	A	519	1/1	0.99	0.14	27,27,27,27	0
2	MN	A	520	1/1	0.99	0.09	36,36,36,36	0
2	MN	B	519	1/1	1.00	0.19	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.