



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:09 AM GMT

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
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

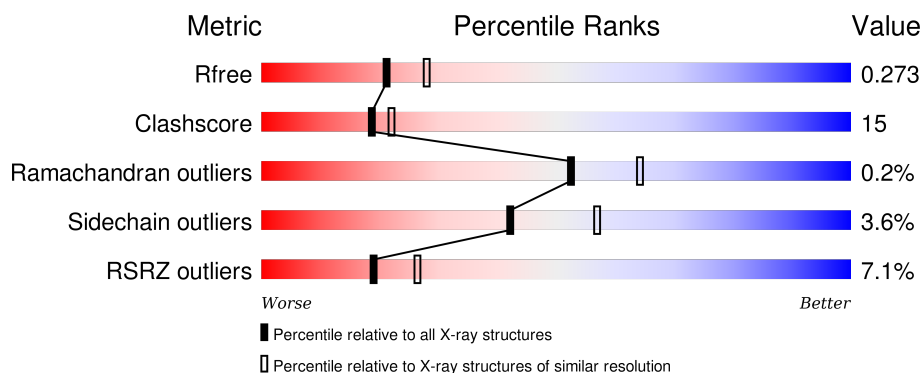
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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> <div>5%</div> <div>63% 18% • 18%</div> </div>
1	B	517	<div> <div>4%</div> <div>59% 20% • 19%</div> </div>
1	C	517	<div> <div>8%</div> <div>55% 24% • 19%</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	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 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
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			

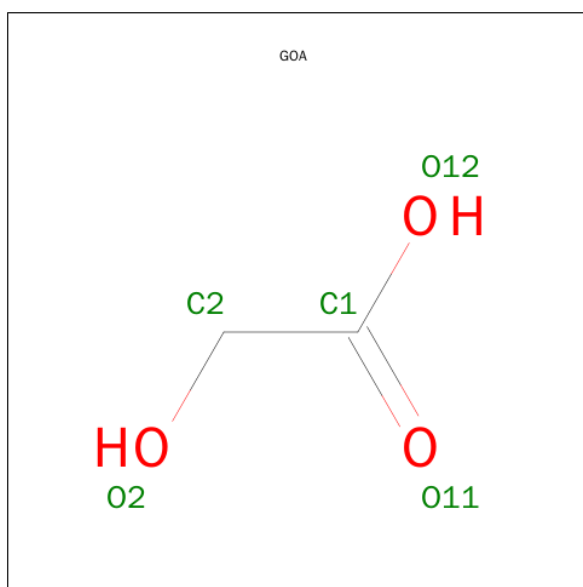
There are 9 discrepancies between the modelled and reference sequences:

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 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

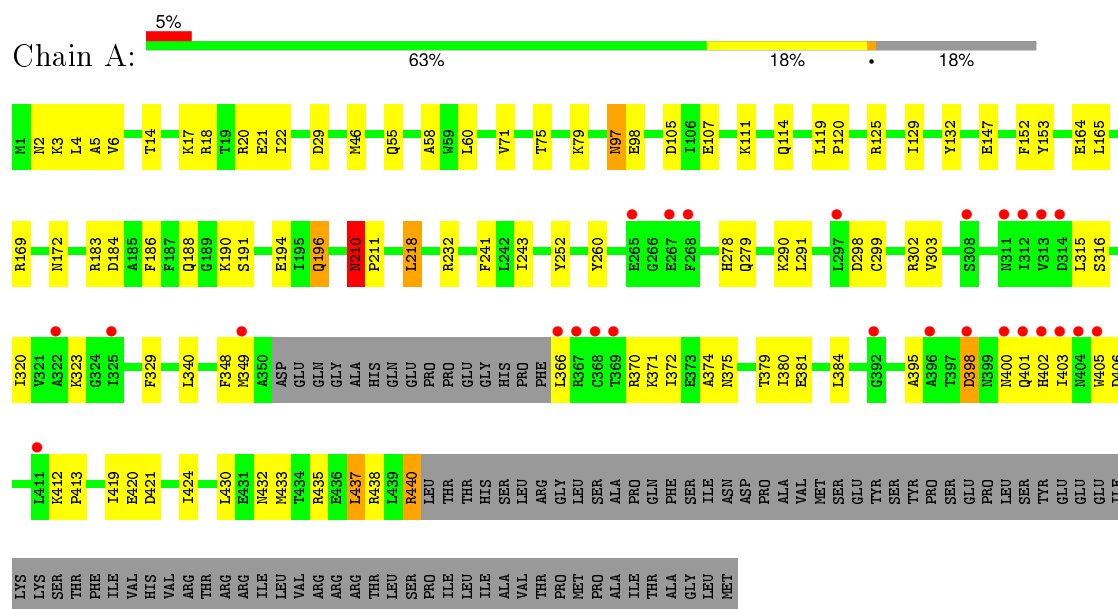
- Molecule 4 is water.

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

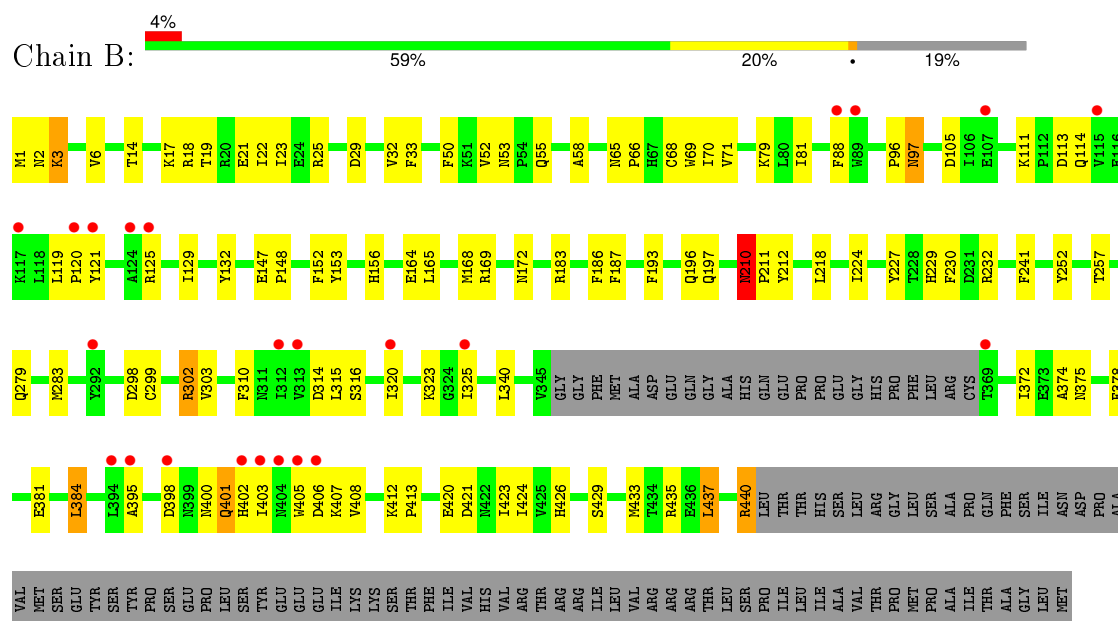
3 Residue-property plots

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.

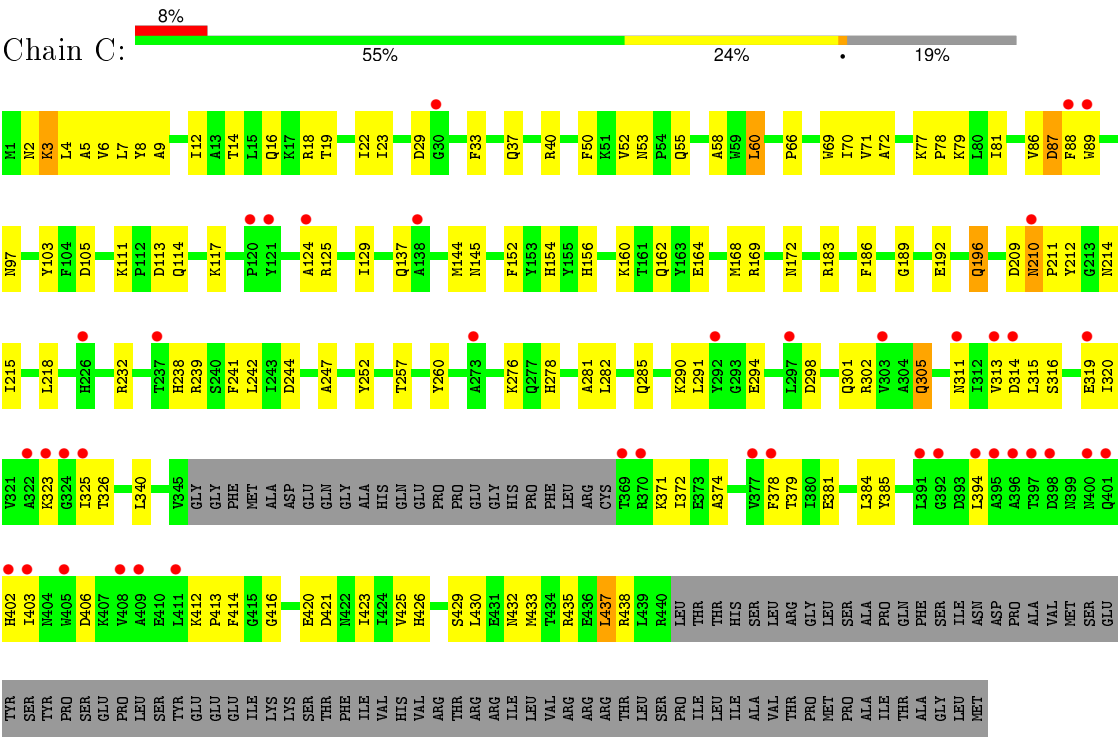
• Molecule 1: Xaa-Pro dipeptidase



• Molecule 1: Xaa-Pro dipeptidase



● 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, 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)	0.33 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.

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 [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	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

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: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

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

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:N	1:B:3:LYS:HD2	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: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

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	52	64
1	C	413/517 (80%)	389 (94%)	23 (6%)	1 (0%)	52	64
All	All	1247/1551 (80%)	1183 (95%)	62 (5%)	2 (0%)	52	64

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%)	42	57
1	B	356/443 (80%)	342 (96%)	14 (4%)	39	53
1	C	356/443 (80%)	344 (97%)	12 (3%)	44	59
All	All	1072/1329 (81%)	1033 (96%)	39 (4%)	42	57

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

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
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

Continued on next page...

Continued from previous page...

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 carbohydrates 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	1,4,4	0.36	0	1,4,4	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOA	B	522	2	1,4,4	0.43	0	1,4,4	0.34	0
3	GOA	C	521	2	1,4,4	0.44	0	1,4,4	0.26	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	-	0/0/2/2	0/0/0/0
3	GOA	B	522	2	-	0/0/2/2	0/0/0/0
3	GOA	C	521	2	-	0/0/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.27	26 (6%) 25 33	18, 36, 78, 95	0
1	B	417/517 (80%)	0.36	23 (5%) 29 37	20, 43, 78, 92	0
1	C	417/517 (80%)	0.71	41 (9%) 10 14	28, 51, 88, 98	0
All	All	1259/1551 (81%)	0.45	90 (7%) 19 26	18, 44, 82, 98	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	121	TYR	5.3
1	B	325	ILE	4.9
1	C	124	ALA	4.8
1	A	366	LEU	4.6
1	B	395	ALA	4.4
1	C	394	LEU	4.2
1	B	369	THR	4.2
1	C	400	ASN	4.2
1	A	322	ALA	4.1
1	C	325	ILE	3.9
1	C	395	ALA	3.8
1	A	313	VAL	3.8
1	A	398	ASP	3.8
1	C	396	ALA	3.8
1	A	308	SER	3.7
1	C	313	VAL	3.7
1	B	398	ASP	3.6
1	C	324	GLY	3.5
1	A	401	GLN	3.5
1	C	292	TYR	3.5
1	A	405	TRP	3.5
1	A	368	CYS	3.4
1	B	89	TRP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	411	LEU	3.3
1	B	403	ILE	3.3
1	C	392	GLY	3.3
1	C	408	VAL	3.3
1	C	322	ALA	3.3
1	C	398	ASP	3.3
1	C	323	LYS	3.2
1	A	369	THR	3.2
1	C	369	THR	3.2
1	C	409	ALA	3.2
1	A	349	MET	3.1
1	C	297	LEU	3.1
1	C	226	HIS	3.1
1	A	325	ILE	3.1
1	A	403	ILE	3.1
1	C	311	ASN	3.1
1	A	402	HIS	3.0
1	B	88	PHE	3.0
1	A	312	ILE	3.0
1	B	402	HIS	3.0
1	B	107	GLU	2.9
1	A	311	ASN	2.9
1	C	121	TYR	2.9
1	C	403	ILE	2.9
1	C	391	LEU	2.9
1	C	120	PRO	2.9
1	C	89	TRP	2.8
1	B	117	LYS	2.8
1	A	400	ASN	2.7
1	B	320	ILE	2.7
1	C	402	HIS	2.7
1	C	88	PHE	2.7
1	B	394	LEU	2.7
1	A	297	LEU	2.5
1	B	313	VAL	2.5
1	C	370	ARG	2.5
1	A	265	GLU	2.5
1	B	115	VAL	2.5
1	C	319	GLU	2.5
1	C	377	VAL	2.4
1	B	312	ILE	2.4
1	C	401	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	292	TYR	2.4
1	C	378	PHE	2.4
1	A	367	ARG	2.4
1	B	404	ASN	2.4
1	C	210	ASN	2.3
1	A	314	ASP	2.3
1	A	404	ASN	2.3
1	B	405	TRP	2.3
1	C	237	THR	2.2
1	B	406	ASP	2.2
1	C	397	THR	2.2
1	A	392	GLY	2.2
1	C	314	ASP	2.2
1	C	30	GLY	2.1
1	C	405	TRP	2.1
1	A	268	PHE	2.1
1	A	267	GLU	2.1
1	C	138	ALA	2.1
1	C	303	VAL	2.1
1	B	125	ARG	2.1
1	B	124	ALA	2.1
1	C	273	ALA	2.0
1	B	120	PRO	2.0
1	A	396	ALA	2.0
1	A	411	LEU	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	B	519	1/1	1.00	0.19	2.98	33,33,33,33	0
3	GOA	B	522	5/5	0.79	0.18	2.90	43,48,50,51	0
2	MN	B	518	1/1	0.99	0.16	2.83	32,32,32,32	0
2	MN	A	518	1/1	0.98	0.17	1.69	31,31,31,31	0
3	GOA	A	521	5/5	0.94	0.15	0.55	34,34,40,41	0
2	MN	A	519	1/1	0.99	0.14	-0.47	27,27,27,27	0
2	MN	C	519	1/1	0.98	0.14	-0.48	39,39,39,39	0
2	MN	C	518	1/1	0.98	0.13	-0.83	39,39,39,39	0
2	MN	A	520	1/1	0.99	0.10	-0.99	36,36,36,36	0
3	GOA	C	521	5/5	0.88	0.11	-1.55	49,49,51,52	0
2	MN	C	520	1/1	0.88	0.09	-	94,94,94,94	0
2	MN	B	520	1/1	0.98	0.13	-	57,57,57,57	0
2	MN	B	521	1/1	0.78	0.10	-	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.