



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:38 AM UTC

PDB ID : 3L24 / pdb_00003L24
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

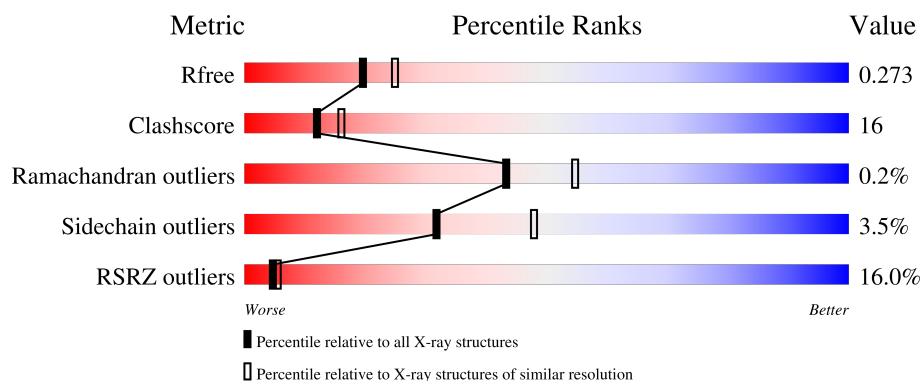
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	9% 60% 20% 18%
1	B	517	11% 57% 21% 19%
1	C	517	19% 54% 25% 19%

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			

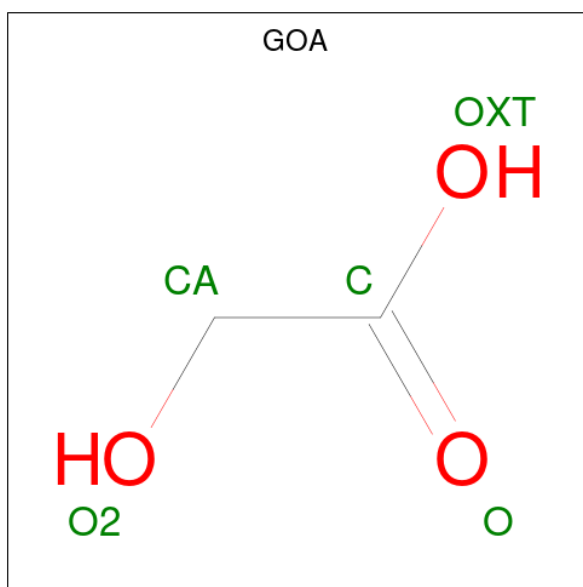
There are 9 discrepancies between the modelled and reference sequences:

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 (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is GLYCOLIC ACID (CCD ID: 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

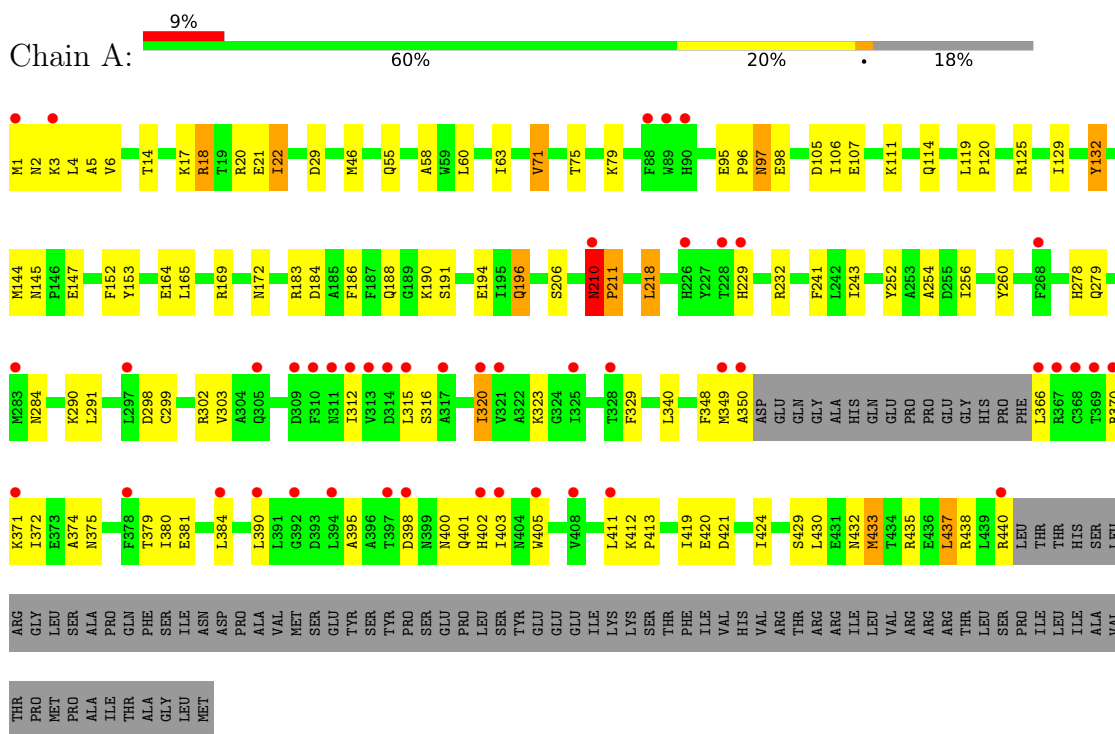
- Molecule 4 is water.

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

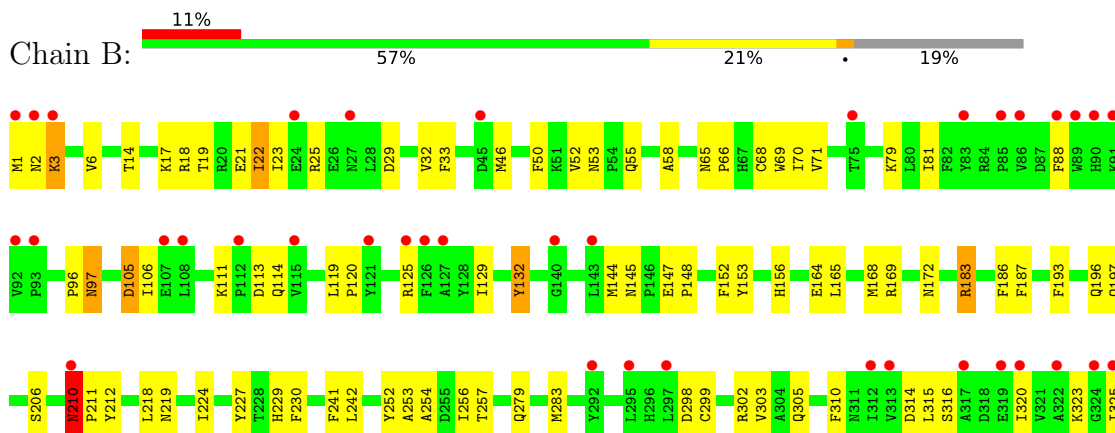
3 Residue-property plots

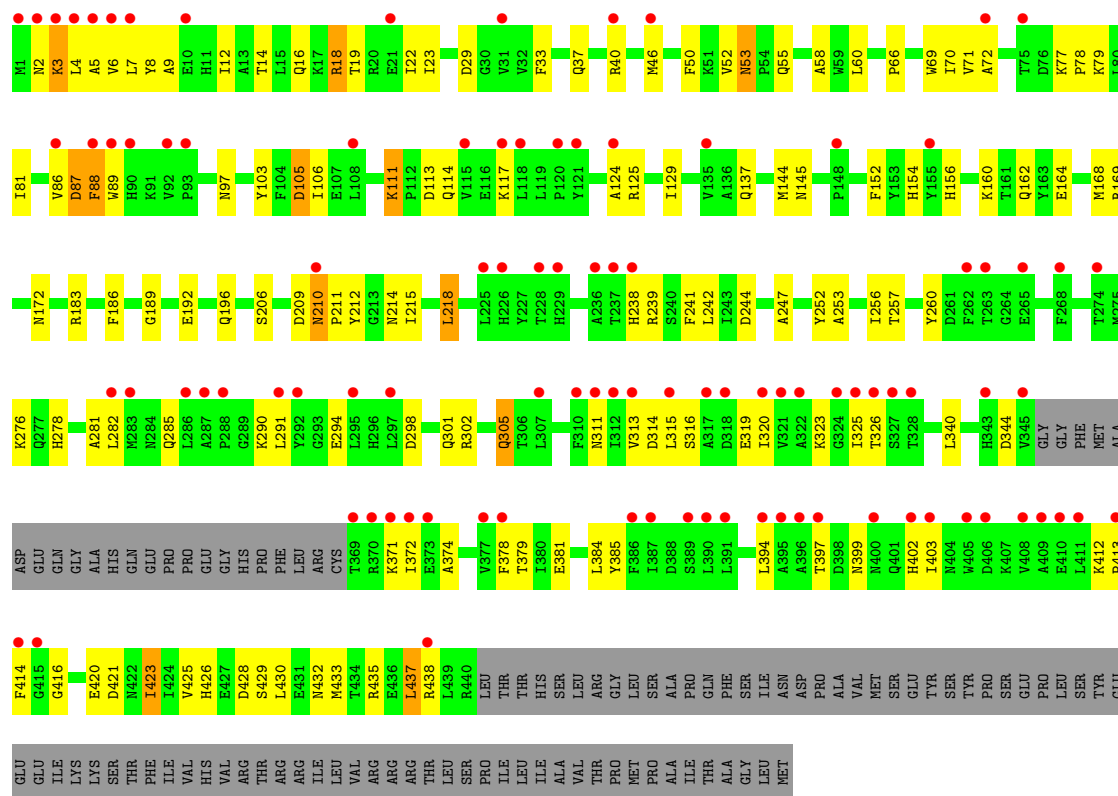
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





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 47.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.10-2.30) 99.9 (47.10-2.30)	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	Depositor
R, R_{free}	0.235 , 0.273 0.235 , 0.273	Depositor DCC
R_{free} test set	9329 reflections (9.37%)	wwPDB-VP
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 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	1/3534 (0.0%)	0.92	13/4795 (0.3%)
1	B	0.43	1/3482 (0.0%)	0.91	14/4726 (0.3%)
1	C	0.41	1/3482 (0.0%)	0.91	16/4726 (0.3%)
All	All	0.43	3/10498 (0.0%)	0.91	43/14247 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ASP	C-N	-7.41	1.21	1.33
1	A	433	MET	SD-CE	-5.78	1.65	1.79
1	B	433	MET	SD-CE	-5.77	1.65	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	SER	N-CA-C	-7.86	99.94	110.55
1	B	210	ASN	N-CA-CB	7.78	120.51	109.78
1	A	210	ASN	N-CA-CB	7.75	120.47	109.78
1	A	106	ILE	N-CA-C	7.67	119.96	108.23
1	C	206	SER	N-CA-C	-7.60	100.28	110.55
1	C	106	ILE	N-CA-C	7.24	118.71	108.36
1	C	253	ALA	N-CA-C	7.05	121.17	109.95
1	A	254	ALA	N-CA-C	-7.04	98.45	109.72
1	B	219	ASN	CB-CA-C	-6.69	108.85	116.54
1	C	209	ASP	O-C-N	6.39	131.76	122.43
1	B	106	ILE	N-CA-C	6.28	117.75	109.21
1	A	206	SER	N-CA-C	-6.16	100.53	110.32
1	C	210	ASN	N-CA-CB	-6.11	100.36	110.02
1	B	253	ALA	N-CA-C	6.07	119.44	109.85
1	C	111	LYS	CA-C-N	5.92	126.06	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	LYS	C-N-CA	5.92	126.06	119.32
1	B	22	ILE	N-CA-C	5.85	116.63	110.72
1	B	105	ASP	N-CA-C	-5.78	99.10	108.41
1	C	256	ILE	N-CA-C	5.71	116.80	108.53
1	C	344	ASP	N-CA-C	5.69	117.89	110.43
1	A	22	ILE	N-CA-C	5.65	116.43	110.72
1	A	132	TYR	N-CA-C	5.63	118.07	109.62
1	B	219	ASN	N-CA-C	5.61	116.83	108.31
1	C	53	ASN	CA-C-N	5.58	125.04	119.24
1	C	53	ASN	C-N-CA	5.58	125.04	119.24
1	A	320	ILE	N-CA-C	-5.45	105.21	110.72
1	B	379	THR	N-CA-C	-5.45	101.01	109.72
1	A	63	ILE	N-CA-C	5.44	118.37	113.10
1	B	254	ALA	N-CA-C	-5.44	101.02	109.72
1	A	256	ILE	N-CA-C	5.40	116.26	108.48
1	C	88	PHE	N-CA-C	5.38	117.14	111.28
1	B	132	TYR	N-CA-C	5.28	117.54	109.62
1	C	105	ASP	N-CA-C	-5.28	98.71	107.99
1	C	209	ASP	CA-C-N	5.24	127.94	120.49
1	C	209	ASP	C-N-CA	5.24	127.94	120.49
1	B	256	ILE	N-CA-C	5.22	116.00	108.48
1	C	423	ILE	N-CA-C	5.16	115.39	108.17
1	A	211	PRO	CB-CA-C	-5.10	104.24	111.68
1	A	429	SER	N-CA-C	5.10	115.07	107.88
1	B	423	ILE	N-CA-C	5.09	115.24	108.11
1	A	229	HIS	N-CA-C	5.05	117.19	110.53
1	B	337	HIS	N-CA-C	-5.02	103.78	110.55
1	A	312	ILE	N-CA-C	-5.01	105.54	112.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	0	3318	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3392	0	3271	101	0
1	C	3392	0	3271	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	7	0
4	B	134	0	0	2	0
4	C	110	0	0	4	0
All	All	10683	0	9860	316	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 16.

All (316) 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: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:A:169:ARG:HA	1:A:433:MET:HE2	1.60	0.83
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:B:424:ILE:HD11	1:B:433:MET:HE3	1.61	0.80
1:C:314:ASP:C	1:C:315:LEU:HD12	2.07	0.80
1:C:169:ARG:HA	1:C:433:MET:HE2	1.64	0.80
1:B:210:ASN:CB	1:B:211:PRO:HD2	2.12	0.79
1:A:298:ASP:O	1:A:302:ARG:HG2	1.84	0.78
1:A:424:ILE:HD11	1:A:433:MET:HE3	1.64	0.77
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: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: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:HA	1:B:433:MET:HE2	1.77	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:C:169:ARG:HG3	1:C:433:MET:HE3	1.78	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:169:ARG:HG2	1:B:433:MET:HE2	1.80	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:169:ARG:CG	1:B:433:MET:HE2	2.31	0.60
1:B:29:ASP:OD2	1:B:125:ARG:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:ARG:CA	1:B:433:MET:HE2	2.33	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:A:169:ARG:CA	1:A:433:MET:HE2	2.34	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:C:169:ARG:HA	1:C:433:MET:CE	2.36	0.56
1:A:401:GLN:HG3	1:A:402:HIS:CD2	2.40	0.56
1:C:242:LEU:C	1:C:242:LEU:HD23	2.31	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:A:169:ARG:HG2	1:A:433:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:278:HIS:ND1	1:A:302:ARG:HB3	2.23	0.54
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:A:432:ASN:CG	1:A:435:ARG:HG3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:168:MET:C	1:C:433:MET:HE1	2.38	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: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:144:MET:HE2	1:C:144:MET:HA	1.95	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:1:MET:N	4:A:698:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:169:ARG:HA	1:A:433:MET:CE	2.40	0.47
1:B:279:GLN:OE1	1:B:435:ARG:NH1	2.48	0.47
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: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:432:ASN:CG	1:C:435:ARG:HG3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ALA:C	1:C:125:ARG:HD2	2.42	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:144:MET:O	1:A:145:ASN:C	2.60	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:A:411:LEU:O	1:A:412:LYS:C	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:242:LEU:HD23	1:B:242:LEU:C	2.44	0.42
1:C:77:LYS:HB3	1:C:105:ASP:OD2	2.18	0.42
1:C:239:ARG:HB3	1:C:414:PHE:CE2	2.54	0.42
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:25:ARG:HH22	1:C:428:ASP:CG	2.28	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: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: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:349:MET:O	1:A:350:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:ND2	1:B:212:TYR:O	2.49	0.40
1:A:95:GLU:O	1:A:96:PRO:C	2.64	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:B:144:MET:O	1:B:145:ASN:C	2.64	0.40
1:C:257:THR:HB	1:C:420:GLU:HB3	2.04	0.40
1:C:397:THR:C	1:C:399:ASN:H	2.29	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%)	43	55
1	C	413/517 (80%)	389 (94%)	23 (6%)	1 (0%)	43	55
All	All	1247/1551 (80%)	1183 (95%)	62 (5%)	2 (0%)	43	55

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%)	346 (96%)	14 (4%)	28	43
1	B	356/443 (80%)	343 (96%)	13 (4%)	30	45
1	C	356/443 (80%)	345 (97%)	11 (3%)	35	52
All	All	1072/1329 (81%)	1034 (96%)	38 (4%)	32	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	46	MET
1	A	71	VAL
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	284	ASN
1	A	390	LEU
1	A	430	LEU
1	A	437	LEU
1	B	3	LYS
1	B	46	MET
1	B	97	ASN
1	B	172	ASN
1	B	183	ARG
1	B	196	GLN
1	B	210	ASN
1	B	218	LEU
1	B	305	GLN
1	B	384	LEU
1	B	401	GLN
1	B	430	LEU
1	B	437	LEU
1	C	3	LYS
1	C	18	ARG
1	C	46	MET
1	C	97	ASN
1	C	137	GLN

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Mol	Chain	Res	Type
1	C	172	ASN
1	C	218	LEU
1	C	305	GLN
1	C	384	LEU
1	C	430	LEU
1	C	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) 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	172	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	296	HIS
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	156	HIS
1	B	177	GLN
1	B	196	GLN
1	B	208	ASN
1	B	214	ASN
1	B	229	HIS

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Mol	Chain	Res	Type
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	C	67	HIS
1	C	97	ASN
1	C	114	GLN
1	C	151	ASN
1	C	172	ASN
1	C	177	GLN
1	C	188	GLN
1	C	196	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	B	522	2	4,4,4	1.40	0	4,4,4	1.59	1 (25%)
3	GOA	C	521	2	4,4,4	0.99	0	4,4,4	1.51	1 (25%)
3	GOA	A	521	2	4,4,4	1.19	0	4,4,4	1.74	1 (25%)

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	B	522	2	-	2/2/2/2	-
3	GOA	C	521	2	-	2/2/2/2	-
3	GOA	A	521	2	-	2/2/2/2	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	521	GOA	OXT-C-CA	2.81	117.00	111.90
3	B	522	GOA	OXT-C-CA	2.77	116.93	111.90
3	C	521	GOA	OXT-C-CA	2.38	116.22	111.90

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

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Mol	Chain	Res	Type	Atoms
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, 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%)	0.53	46 (10%)	11 12	18, 36, 78, 95	0
1	B	417/517 (80%)	0.81	56 (13%)	7 8	20, 43, 78, 92	0
1	C	417/517 (80%)	1.42	99 (23%)	2 2	28, 51, 88, 98	0
All	All	1259/1551 (81%)	0.92	201 (15%)	5 5	18, 44, 82, 98	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	LEU	6.1
1	C	1	MET	5.5
1	C	292	TYR	5.0
1	A	1	MET	4.9
1	C	89	TRP	4.8
1	A	350	ALA	4.5
1	B	325	ILE	4.5
1	A	90	HIS	4.4
1	A	89	TRP	4.4
1	A	349	MET	4.4
1	C	370	ARG	4.3
1	C	313	VAL	4.3
1	B	369	THR	4.2
1	A	367	ARG	4.2
1	C	369	THR	4.2
1	B	89	TRP	4.0
1	B	292	TYR	4.0
1	B	396	ALA	3.9
1	C	121	TYR	3.9
1	A	368	CYS	3.9
1	C	4	LEU	3.8
1	C	237	THR	3.8
1	C	210	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	313	VAL	3.7
1	C	325	ILE	3.6
1	B	1	MET	3.6
1	C	390	LEU	3.5
1	C	324	GLY	3.5
1	A	226	HIS	3.5
1	A	405	TRP	3.5
1	C	394	LEU	3.5
1	C	3	LYS	3.5
1	C	311	ASN	3.5
1	A	403	ILE	3.4
1	C	317	ALA	3.4
1	C	409	ALA	3.3
1	B	370	ARG	3.3
1	B	121	TYR	3.3
1	C	411	LEU	3.2
1	C	378	PHE	3.2
1	C	31	VAL	3.2
1	A	369	THR	3.2
1	C	345	VAL	3.2
1	C	395	ALA	3.2
1	C	225	LEU	3.2
1	C	2	ASN	3.1
1	C	88	PHE	3.1
1	B	210	ASN	3.1
1	C	377	VAL	3.0
1	C	312	ILE	3.0
1	A	210	ASN	3.0
1	B	90	HIS	2.9
1	C	86	VAL	2.9
1	C	328	THR	2.9
1	C	371	LYS	2.8
1	A	312	ILE	2.8
1	C	372	ILE	2.8
1	C	226	HIS	2.8
1	B	395	ALA	2.8
1	C	236	ALA	2.8
1	C	297	LEU	2.8
1	C	262	PHE	2.8
1	B	115	VAL	2.8
1	C	115	VAL	2.8
1	C	400	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	265	GLU	2.7
1	A	371	LYS	2.7
1	B	86	VAL	2.7
1	C	403	ILE	2.7
1	C	321	VAL	2.7
1	B	399	ASN	2.7
1	C	387	ILE	2.7
1	B	75	THR	2.7
1	C	389	SER	2.7
1	A	3	LYS	2.6
1	A	378	PHE	2.6
1	B	88	PHE	2.6
1	C	310	PHE	2.6
1	C	229	HIS	2.6
1	A	317	ALA	2.6
1	C	410	GLU	2.6
1	B	126	PHE	2.6
1	B	328	THR	2.6
1	B	312	ILE	2.6
1	B	2	ASN	2.6
1	C	327	SER	2.6
1	A	297	LEU	2.6
1	C	291	LEU	2.6
1	B	398	ASP	2.6
1	C	75	THR	2.6
1	C	288	PRO	2.6
1	B	143	LEU	2.5
1	B	45	ASP	2.5
1	B	404	ASN	2.5
1	C	92	VAL	2.5
1	B	403	ILE	2.5
1	C	320	ILE	2.5
1	C	155	TYR	2.5
1	C	118	LEU	2.5
1	B	324	GLY	2.5
1	A	402	HIS	2.5
1	C	228	THR	2.5
1	C	6	VAL	2.5
1	B	391	LEU	2.5
1	B	127	ALA	2.5
1	C	386	PHE	2.5
1	C	46	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	283	MET	2.5
1	A	311	ASN	2.5
1	C	120	PRO	2.5
1	B	125	ARG	2.4
1	A	305	GLN	2.4
1	B	85	PRO	2.4
1	B	140	GLY	2.4
1	A	325	ILE	2.4
1	B	108	LEU	2.4
1	B	27	ASN	2.4
1	C	413	PRO	2.4
1	A	228	THR	2.4
1	C	397	THR	2.4
1	B	313	VAL	2.4
1	B	386	PHE	2.4
1	B	295	LEU	2.4
1	C	402	HIS	2.4
1	A	309	ASP	2.4
1	C	287	ALA	2.4
1	A	408	VAL	2.4
1	A	315	LEU	2.4
1	C	391	LEU	2.4
1	C	238	HIS	2.4
1	C	438	ARG	2.4
1	C	318	ASP	2.3
1	A	392	GLY	2.3
1	A	397	THR	2.3
1	B	327	SER	2.3
1	C	295	LEU	2.3
1	B	107	GLU	2.3
1	C	405	TRP	2.3
1	C	396	ALA	2.3
1	C	40	ARG	2.3
1	A	321	VAL	2.3
1	B	345	VAL	2.3
1	C	408	VAL	2.3
1	A	384	LEU	2.3
1	B	91	LYS	2.3
1	C	10	GLU	2.3
1	A	268	PHE	2.3
1	C	414	PHE	2.3
1	A	314	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	21	GLU	2.3
1	C	90	HIS	2.2
1	B	3	LYS	2.2
1	A	320	ILE	2.2
1	B	297	LEU	2.2
1	C	315	LEU	2.2
1	C	268	PHE	2.2
1	A	370	ARG	2.2
1	B	93	PRO	2.2
1	C	93	PRO	2.2
1	A	229	HIS	2.2
1	B	322	ALA	2.2
1	C	307	LEU	2.2
1	B	408	VAL	2.2
1	C	282	LEU	2.2
1	A	310	PHE	2.2
1	B	319	GLU	2.2
1	A	394	LEU	2.1
1	C	286	LEU	2.1
1	B	402	HIS	2.1
1	C	5	ALA	2.1
1	C	7	LEU	2.1
1	A	398	ASP	2.1
1	B	92	VAL	2.1
1	B	405	TRP	2.1
1	C	148	PRO	2.1
1	C	322	ALA	2.1
1	A	411	LEU	2.1
1	C	108	LEU	2.1
1	C	343	HIS	2.1
1	A	88	PHE	2.1
1	A	328	THR	2.1
1	C	263	THR	2.1
1	C	274	THR	2.1
1	C	117	LYS	2.1
1	C	124	ALA	2.1
1	B	24	GLU	2.1
1	B	320	ILE	2.1
1	C	135	VAL	2.1
1	C	415	GLY	2.1
1	A	283	MET	2.0
1	B	317	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	72	ALA	2.0
1	B	394	LEU	2.0
1	C	406	ASP	2.0
1	B	112	PRO	2.0
1	B	83	TYR	2.0
1	B	440	ARG	2.0
1	C	326	THR	2.0
1	C	373	GLU	2.0
1	A	390	LEU	2.0
1	A	440	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	520	1/1	0.76	0.21	94,94,94,94	0
3	GOA	B	522	5/5	0.76	0.20	43,48,50,51	0
2	MN	B	521	1/1	0.78	0.24	75,75,75,75	0
3	GOA	C	521	5/5	0.86	0.15	49,49,51,52	0
3	GOA	A	521	5/5	0.93	0.11	34,34,40,41	0
2	MN	B	520	1/1	0.97	0.20	57,57,57,57	0
2	MN	C	519	1/1	0.97	0.17	39,39,39,39	0
2	MN	B	519	1/1	0.98	0.22	33,33,33,33	0
2	MN	A	518	1/1	0.98	0.20	31,31,31,31	0
2	MN	A	519	1/1	0.98	0.17	27,27,27,27	0
2	MN	A	520	1/1	0.98	0.13	36,36,36,36	0
2	MN	C	518	1/1	0.99	0.17	39,39,39,39	0
2	MN	B	518	1/1	0.99	0.20	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.