



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:53 AM UTC

PDB ID : 1ONP / pdb_00001onp
Title : IspC complex with Mn²⁺ and fosmidomycin
Authors : Steinbacher, S.; Kaiser, J.; Eisenreich, W.; Huber, R.; Bacher, A.; Rohdich, F.
Deposited on : 2003-02-28
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

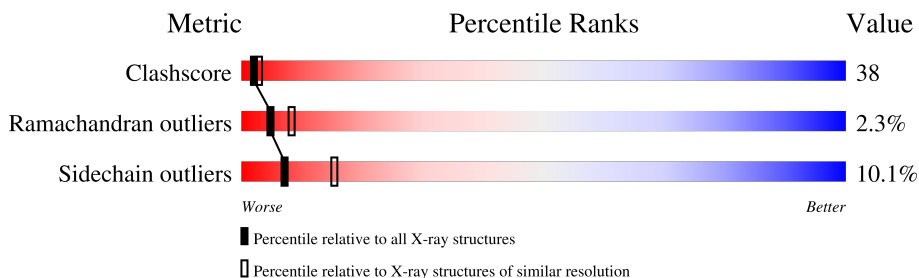
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	45% 43% 10% .
1	B	398	41% 45% 12% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6215 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.

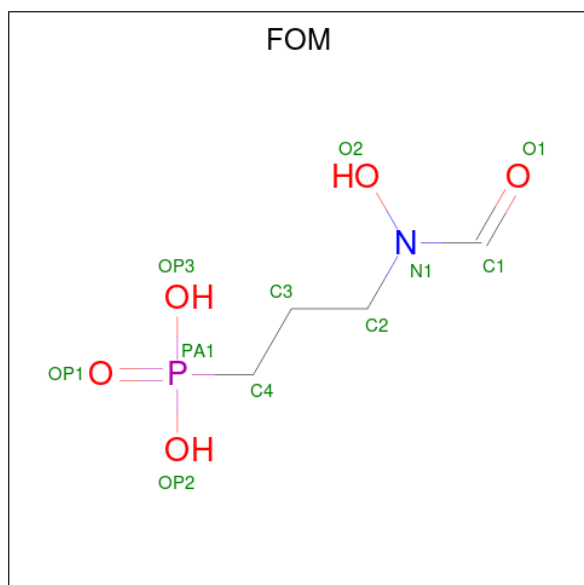
- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3023	1889	533	574	27			
1	B	397	Total	C	N	O	S	0	0	0
			3023	1889	533	574	27			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (CCD ID: FOM) (formula: C₄H₁₀NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

- Molecule 4 is water.

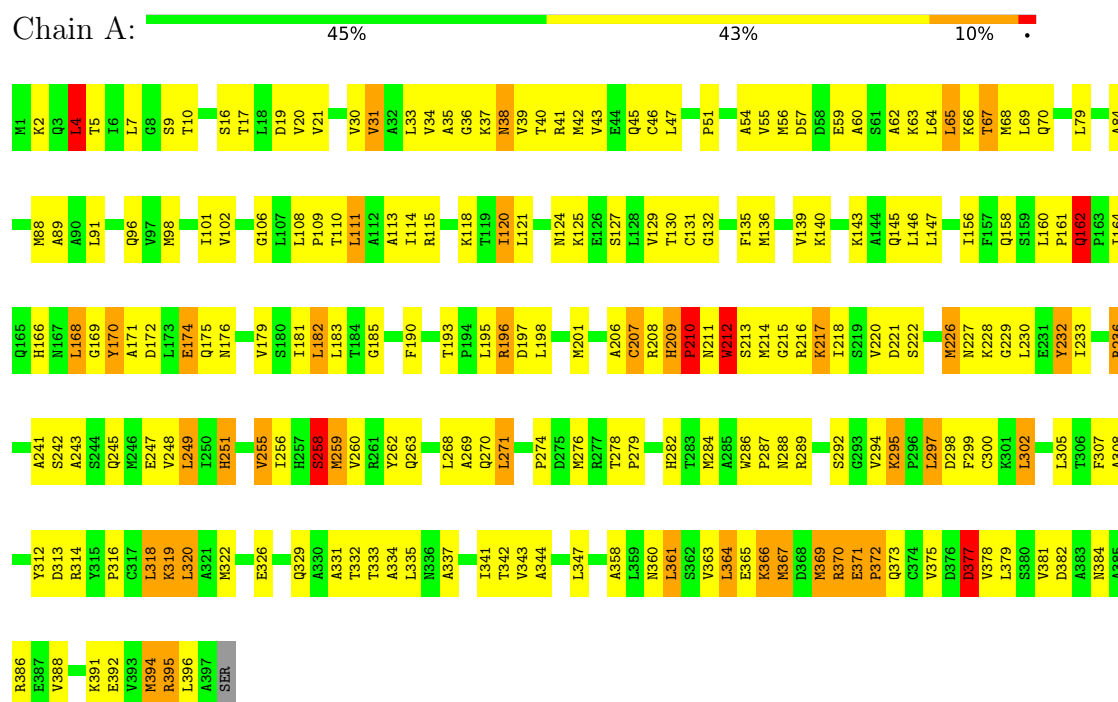
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

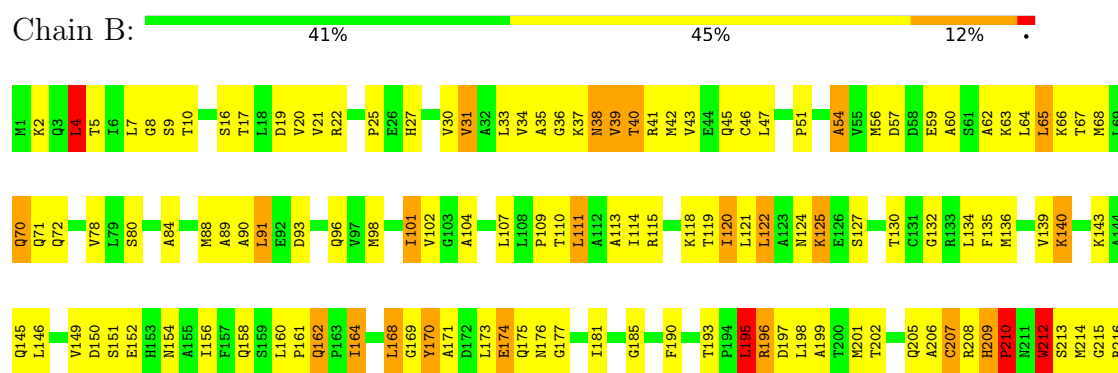
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

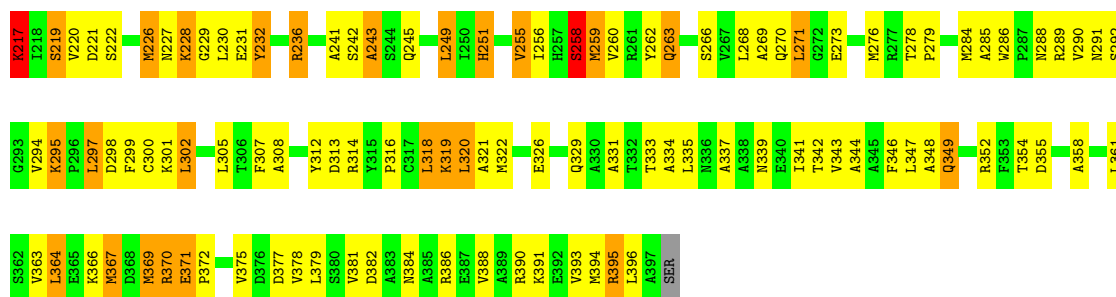
Note EDS was not executed.

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.75Å 52.30Å 107.59Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6215	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.64	0/3071	1.25	33/4163 (0.8%)
1	B	0.67	0/3071	1.26	37/4163 (0.9%)
All	All	0.66	0/6142	1.26	70/8326 (0.8%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	HIS	CA-C-N	11.13	133.75	119.84
1	B	209	HIS	C-N-CA	11.13	133.75	119.84
1	A	209	HIS	CA-C-N	11.11	133.73	119.84
1	A	209	HIS	C-N-CA	11.11	133.73	119.84
1	A	255	VAL	N-CA-C	-9.20	102.89	111.45
1	B	120	ILE	N-CA-C	8.67	119.16	106.85
1	B	255	VAL	N-CA-C	-8.24	103.78	111.45
1	A	226	MET	N-CA-C	-7.80	103.03	112.54
1	B	226	MET	N-CA-C	-7.65	103.21	112.54
1	B	4	LEU	N-CA-C	7.63	120.68	109.69
1	A	232	TYR	N-CA-C	-7.59	102.95	111.14
1	A	120	ILE	N-CA-C	7.58	118.58	107.37
1	B	110	THR	N-CA-C	-7.45	103.24	111.36
1	B	104	ALA	N-CA-C	-7.45	104.19	113.28
1	B	222	SER	N-CA-C	-7.25	102.56	111.40
1	B	251	HIS	CA-C-N	7.07	127.38	119.32
1	B	251	HIS	C-N-CA	7.07	127.38	119.32
1	A	31	VAL	N-CA-C	-7.05	105.17	113.42
1	B	31	VAL	N-CA-C	-6.69	105.59	113.42
1	A	295	LYS	N-CA-C	6.60	119.20	109.50
1	A	251	HIS	CA-C-N	6.59	126.84	119.32
1	A	251	HIS	C-N-CA	6.59	126.84	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	N-CA-C	6.49	119.74	109.81
1	B	393	VAL	N-CA-C	-6.40	104.09	110.62
1	A	263	GLN	N-CA-C	6.30	118.15	111.28
1	B	195	LEU	N-CA-C	6.21	118.56	111.11
1	A	222	SER	N-CA-C	-6.13	104.15	111.69
1	B	259	MET	N-CA-C	6.01	117.71	109.18
1	B	295	LYS	N-CA-C	5.97	118.27	109.50
1	A	19	ASP	N-CA-C	-5.96	104.91	111.82
1	A	313	ASP	N-CA-C	-5.95	103.47	112.04
1	B	78	VAL	N-CA-C	5.93	116.84	108.36
1	A	110	THR	N-CA-C	-5.89	104.94	111.36
1	B	54	ALA	N-CA-C	-5.88	99.07	109.06
1	A	377	ASP	N-CA-C	-5.86	104.90	111.28
1	A	210	PRO	N-CA-C	5.83	124.49	112.47
1	A	106	GLY	N-CA-C	5.82	122.94	115.32
1	A	69	LEU	N-CA-C	-5.75	105.16	111.82
1	A	54	ALA	N-CA-C	-5.68	99.40	109.06
1	A	162	GLN	CA-C-N	-5.62	114.31	119.82
1	A	162	GLN	C-N-CA	-5.62	114.31	119.82
1	B	232	TYR	N-CA-C	-5.58	105.27	111.36
1	A	65	LEU	N-CA-C	-5.56	105.12	111.07
1	B	210	PRO	N-CA-C	5.53	123.86	112.47
1	B	152	GLU	N-CA-C	5.51	117.09	111.14
1	A	295	LYS	CA-C-N	-5.50	113.47	120.23
1	A	295	LYS	C-N-CA	-5.50	113.47	120.23
1	B	256	ILE	N-CA-C	-5.49	101.59	108.84
1	B	70	GLN	N-CA-C	-5.42	105.27	111.07
1	A	394	MET	N-CA-C	5.41	116.86	111.07
1	A	102	VAL	N-CA-C	5.35	116.84	109.46
1	B	219	SER	N-CA-C	-5.33	105.64	111.82
1	B	217	LYS	N-CA-C	5.30	117.13	111.36
1	A	162	GLN	N-CA-C	5.25	119.64	112.55
1	B	39	VAL	N-CA-C	-5.24	105.43	110.72
1	B	140	LYS	N-CA-C	-5.24	105.26	110.97
1	A	360	ASN	N-CA-C	-5.23	105.69	111.71
1	B	164	ILE	N-CA-C	-5.20	107.34	113.42
1	B	263	GLN	N-CA-C	5.16	118.36	111.75
1	A	259	MET	N-CA-C	5.16	116.50	109.18
1	B	313	ASP	N-CA-C	-5.15	105.30	112.45
1	B	319	LYS	N-CA-C	-5.14	105.76	111.36
1	B	291	ASN	N-CA-C	-5.12	103.93	110.53
1	B	93	ASP	N-CA-C	5.09	119.20	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	THR	N-CA-C	5.08	117.59	111.40
1	B	358	ALA	N-CA-C	5.05	116.87	111.36
1	B	154	ASN	N-CA-C	-5.05	105.66	111.07
1	A	319	LYS	N-CA-C	-5.05	105.86	111.36
1	B	40	THR	N-CA-C	5.02	117.14	111.11
1	B	65	LEU	N-CA-C	-5.02	105.89	111.36

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	3023	0	3050	230	0
1	B	3023	0	3050	236	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	11	0	7	0	0
3	B	11	0	7	0	0
4	A	83	0	0	6	0
4	B	62	0	0	6	1
All	All	6215	0	6114	461	1

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 38.

All (461) 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:132:GLY:H	1:B:329:GLN:HE21	1.04	1.00
1:A:162:GLN:HG3	1:B:162:GLN:HG3	1.52	0.92
1:A:132:GLY:H	1:A:329:GLN:HE21	1.16	0.91
1:B:262:TYR:CE1	1:B:268:LEU:HD12	2.05	0.91
1:B:395:ARG:NH1	1:B:395:ARG:HB3	1.88	0.89
1:A:4:LEU:HD11	1:A:284:MET:HE3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:O	1:B:379:LEU:HG	1.77	0.84
1:A:369:MET:HE3	1:A:369:MET:H	1.44	0.83
1:B:220:VAL:HG21	1:B:347:LEU:HD21	1.62	0.82
1:A:375:VAL:O	1:A:379:LEU:HG	1.79	0.82
1:A:395:ARG:HB3	1:A:395:ARG:NH1	1.94	0.81
1:A:220:VAL:HG21	1:A:347:LEU:HD21	1.63	0.81
1:A:391:LYS:HD3	1:A:394:MET:HE3	1.60	0.81
1:A:7:LEU:C	1:A:101:ILE:HG13	2.05	0.81
1:A:190:PHE:CD2	1:A:201:MET:HE3	2.15	0.80
1:A:262:TYR:CE1	1:A:268:LEU:HD12	2.15	0.80
1:A:132:GLY:H	1:A:329:GLN:NE2	1.80	0.80
1:B:130:THR:HB	1:B:378:VAL:CG1	2.12	0.79
1:B:391:LYS:HD3	1:B:394:MET:CE	2.13	0.79
1:B:391:LYS:HD3	1:B:394:MET:HE3	1.64	0.78
1:B:228:LYS:HE3	1:B:228:LYS:HA	1.64	0.78
1:A:39:VAL:HG11	1:A:64:LEU:HD22	1.66	0.78
1:A:38:ASN:ND2	1:A:41:ARG:HB3	1.99	0.78
1:A:391:LYS:HD3	1:A:394:MET:CE	2.15	0.77
1:B:39:VAL:HG13	1:B:65:LEU:HB2	1.66	0.76
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.51	0.76
1:B:132:GLY:H	1:B:329:GLN:NE2	1.81	0.76
1:A:363:VAL:HG13	1:A:388:VAL:HB	1.66	0.76
1:B:38:ASN:ND2	1:B:41:ARG:HB3	1.99	0.76
1:A:118:LYS:O	1:A:120:ILE:HG13	1.87	0.75
1:B:384:ASN:O	1:B:388:VAL:HG23	1.87	0.74
1:A:249:LEU:HD21	1:A:307:PHE:HB3	1.67	0.74
1:A:369:MET:H	1:A:369:MET:CE	2.00	0.74
1:A:164:ILE:HG23	1:A:171:ALA:HB3	1.68	0.74
1:B:39:VAL:HG11	1:B:64:LEU:HD22	1.70	0.73
1:B:208:ARG:HG2	1:B:215:GLY:N	2.04	0.73
1:B:395:ARG:HB3	1:B:395:ARG:HH11	1.51	0.73
1:B:363:VAL:HG13	1:B:388:VAL:HB	1.71	0.72
1:A:190:PHE:CZ	1:A:206:ALA:HB2	2.24	0.72
1:B:226:MET:HE2	1:B:230:LEU:HG	1.72	0.72
1:B:249:LEU:HD21	1:B:307:PHE:HB3	1.71	0.72
1:A:384:ASN:O	1:A:388:VAL:HG23	1.89	0.72
1:A:251:HIS:HE1	1:A:255:VAL:H	1.38	0.71
1:B:146:LEU:O	1:B:168:LEU:HD12	1.89	0.71
1:A:130:THR:HB	1:A:378:VAL:CG1	2.21	0.71
1:A:132:GLY:N	1:A:329:GLN:HE21	1.87	0.71
1:A:185:GLY:HA3	1:A:228:LYS:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ALA:CB	1:B:42:MET:HE2	2.20	0.71
1:B:251:HIS:HE1	1:B:255:VAL:H	1.36	0.71
1:A:208:ARG:HG2	1:A:215:GLY:N	2.07	0.70
1:A:146:LEU:O	1:A:168:LEU:HD12	1.91	0.69
1:A:298:ASP:O	1:A:302:LEU:HD13	1.92	0.69
1:B:41:ARG:O	1:B:45:GLN:HG3	1.92	0.69
1:A:208:ARG:HH11	1:A:208:ARG:HB2	1.58	0.69
1:B:228:LYS:HA	1:B:228:LYS:CE	2.22	0.69
1:B:259:MET:HG2	1:B:269:ALA:HB2	1.73	0.69
1:B:320:LEU:HD13	1:B:335:LEU:HD21	1.74	0.69
1:A:226:MET:HE1	1:A:335:LEU:HD11	1.74	0.69
1:B:236:ARG:NH2	1:B:326:GLU:OE2	2.26	0.68
1:A:196:ARG:CZ	1:A:196:ARG:HA	2.23	0.68
1:B:217:LYS:NZ	1:B:217:LYS:HB3	2.08	0.67
1:B:190:PHE:CZ	1:B:206:ALA:HB2	2.29	0.67
1:A:320:LEU:HD13	1:A:335:LEU:HD21	1.75	0.67
1:B:132:GLY:N	1:B:329:GLN:HE21	1.87	0.67
1:A:39:VAL:HG13	1:A:65:LEU:HB2	1.76	0.67
1:B:164:ILE:HA	1:B:171:ALA:CB	2.25	0.67
1:A:221:ASP:HB3	1:A:227:ASN:HB2	1.77	0.67
1:A:249:LEU:CD2	1:A:307:PHE:HB3	2.24	0.67
1:B:190:PHE:CD2	1:B:201:MET:HE3	2.30	0.66
1:B:16:SER:O	1:B:20:VAL:HG23	1.94	0.66
1:B:62:ALA:O	1:B:66:LYS:HB2	1.95	0.66
1:B:64:LEU:HD23	1:B:64:LEU:O	1.95	0.66
1:B:118:LYS:O	1:B:120:ILE:HG13	1.95	0.66
1:A:62:ALA:O	1:A:66:LYS:HB2	1.95	0.66
1:A:16:SER:O	1:A:20:VAL:HG23	1.95	0.66
1:B:298:ASP:O	1:B:302:LEU:HD13	1.95	0.65
1:B:377:ASP:O	1:B:381:VAL:HG23	1.97	0.65
1:B:115:ARG:HG3	1:B:115:ARG:NH1	2.09	0.64
1:B:193:THR:HG21	1:B:201:MET:HE2	1.79	0.64
1:B:130:THR:HG22	1:B:333:THR:HA	1.80	0.64
1:A:114:ILE:HA	1:A:120:ILE:HD11	1.80	0.63
1:A:35:ALA:HB3	1:A:42:MET:HE2	1.79	0.63
1:A:251:HIS:CE1	1:A:255:VAL:H	2.16	0.63
1:A:156:ILE:O	1:A:160:LEU:HG	1.98	0.63
1:A:212:TRP:CH2	1:A:276:MET:HE2	2.33	0.63
1:B:208:ARG:HH11	1:B:208:ARG:HB2	1.62	0.63
1:A:395:ARG:HB3	1:A:395:ARG:HH11	1.61	0.63
1:A:174:GLU:HB3	1:A:245:GLN:HE22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:O	1:B:367:MET:HB2	1.98	0.63
1:B:30:VAL:HG12	1:B:51:PRO:HB3	1.80	0.62
1:B:251:HIS:CE1	1:B:255:VAL:H	2.17	0.62
1:A:236:ARG:HH21	1:A:243:ALA:HB2	1.64	0.62
1:B:35:ALA:HB3	1:B:42:MET:HE2	1.81	0.62
1:B:114:ILE:HA	1:B:120:ILE:HD11	1.81	0.62
1:B:216:ARG:HB3	1:B:216:ARG:NH1	2.15	0.62
1:A:7:LEU:O	1:A:101:ILE:HG13	1.99	0.61
1:A:89:ALA:HB1	1:A:113:ALA:HB2	1.82	0.60
1:B:130:THR:HB	1:B:378:VAL:HG11	1.83	0.60
1:A:115:ARG:NH1	1:A:115:ARG:HG3	2.17	0.60
1:B:68:MET:O	1:B:71:GLN:HB2	2.02	0.60
1:B:217:LYS:HB3	1:B:217:LYS:HZ2	1.65	0.59
1:A:164:ILE:HA	1:A:171:ALA:CB	2.32	0.59
1:A:217:LYS:NZ	1:A:217:LYS:HB3	2.17	0.59
1:A:386:ARG:HH11	1:A:386:ARG:HG2	1.67	0.59
1:B:64:LEU:HD23	1:B:64:LEU:C	2.27	0.59
1:B:170:TYR:N	1:B:170:TYR:CD2	2.70	0.59
1:A:2:LYS:HD2	1:A:96:GLN:NE2	2.16	0.59
1:A:193:THR:HG21	1:A:201:MET:HE2	1.82	0.59
1:A:64:LEU:O	1:A:64:LEU:HD23	2.02	0.59
1:A:226:MET:HE1	1:A:335:LEU:CD1	2.33	0.59
1:A:10:THR:HG22	1:A:41:ARG:HG2	1.84	0.59
1:B:107:LEU:O	1:B:111:LEU:HB2	2.02	0.59
1:B:19:ASP:OD1	1:B:22:ARG:NH1	2.36	0.59
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.68	0.59
1:A:67:THR:O	1:A:70:GLN:HB3	2.03	0.58
1:A:170:TYR:N	1:A:170:TYR:CD2	2.71	0.58
1:B:369:MET:CE	1:B:369:MET:H	2.16	0.58
1:A:366:LYS:O	1:A:367:MET:HB2	2.03	0.58
1:A:164:ILE:HG23	1:A:171:ALA:CB	2.33	0.58
1:B:33:LEU:HD12	1:B:51:PRO:HG3	1.85	0.58
1:A:130:THR:HG22	1:A:333:THR:HA	1.85	0.58
1:B:135:PHE:O	1:B:139:VAL:HG23	2.04	0.58
1:A:255:VAL:HG21	1:A:305:LEU:HD21	1.85	0.57
1:A:7:LEU:O	1:A:101:ILE:N	2.37	0.57
1:A:208:ARG:NH1	1:A:208:ARG:CB	2.68	0.57
1:B:196:ARG:HA	1:B:196:ARG:CZ	2.34	0.57
1:A:259:MET:HG2	1:A:269:ALA:HB2	1.87	0.57
1:A:35:ALA:CB	1:A:42:MET:HE2	2.35	0.57
1:B:59:GLU:O	1:B:60:ALA:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH1	1:B:208:ARG:CB	2.68	0.57
1:A:158:GLN:OE1	1:A:289:ARG:NH2	2.31	0.57
1:A:229:GLY:O	1:A:232:TYR:HB3	2.03	0.57
1:B:22:ARG:O	1:B:25:PRO:HD3	2.04	0.57
1:A:115:ARG:HG3	1:A:115:ARG:HH11	1.67	0.57
1:A:161:PRO:HD3	1:A:262:TYR:OH	2.04	0.57
1:B:7:LEU:C	1:B:101:ILE:HG13	2.30	0.57
1:A:216:ARG:NH1	1:A:216:ARG:HB3	2.19	0.57
1:A:341:ILE:O	1:A:344:ALA:HB3	2.05	0.57
1:B:25:PRO:HB3	4:B:1044:HOH:O	2.04	0.56
1:B:164:ILE:HG23	1:B:171:ALA:HB3	1.86	0.56
1:B:208:ARG:HH11	1:B:208:ARG:CB	2.18	0.56
1:A:375:VAL:O	1:A:375:VAL:HG12	2.05	0.56
1:A:84:ALA:O	1:A:88:MET:HG2	2.06	0.56
1:A:98:MET:HA	1:A:121:LEU:HB2	1.88	0.56
1:A:98:MET:HE2	1:A:121:LEU:HD12	1.88	0.56
1:B:111:LEU:HD22	1:B:135:PHE:CE1	2.41	0.56
1:B:212:TRP:CH2	1:B:276:MET:HE2	2.40	0.56
1:A:64:LEU:O	1:A:67:THR:HB	2.05	0.56
1:A:249:LEU:HD23	1:A:308:ALA:O	2.05	0.56
1:A:262:TYR:CZ	1:A:268:LEU:HD12	2.41	0.56
1:A:164:ILE:HA	1:A:171:ALA:HB1	1.88	0.56
1:A:295:LYS:NZ	1:A:298:ASP:HB2	2.21	0.56
1:A:391:LYS:HA	1:A:394:MET:HE3	1.87	0.56
1:B:35:ALA:HB2	1:B:42:MET:HE2	1.87	0.56
1:B:124:ASN:ND2	1:B:127:SER:H	2.04	0.56
1:B:146:LEU:HB2	1:B:168:LEU:HD13	1.88	0.56
1:B:228:LYS:HE3	1:B:228:LYS:CA	2.29	0.56
1:B:299:PHE:HA	1:B:302:LEU:HD22	1.88	0.56
1:A:108:LEU:HG	1:A:375:VAL:HG11	1.87	0.55
1:B:249:LEU:CD2	1:B:307:PHE:HB3	2.33	0.55
1:A:2:LYS:HD2	1:A:96:GLN:HE21	1.70	0.55
1:A:98:MET:HE2	1:A:121:LEU:CD1	2.37	0.55
1:B:386:ARG:HG2	1:B:386:ARG:HH11	1.71	0.55
1:A:64:LEU:HD23	1:A:64:LEU:C	2.32	0.55
1:B:270:GLN:C	1:B:271:LEU:HD23	2.31	0.55
1:A:335:LEU:HB2	1:A:364:LEU:HD21	1.88	0.55
1:B:67:THR:O	1:B:70:GLN:HB3	2.07	0.55
1:B:111:LEU:HD23	1:B:375:VAL:CG2	2.37	0.55
1:B:136:MET:O	1:B:140:LYS:HG3	2.06	0.55
1:B:43:VAL:HG12	1:B:47:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASP:HB3	1:B:227:ASN:HB2	1.87	0.54
1:A:164:ILE:HG22	1:A:164:ILE:O	2.06	0.54
1:B:130:THR:CG2	1:B:333:THR:HG23	2.37	0.54
1:B:212:TRP:HA	1:B:212:TRP:CE3	2.42	0.54
1:A:46:CYS:HA	1:A:51:PRO:HD2	1.90	0.54
1:A:377:ASP:O	1:A:381:VAL:HG23	2.08	0.54
1:A:30:VAL:HG12	1:A:51:PRO:HB3	1.89	0.54
1:A:208:ARG:NH2	1:A:214:MET:SD	2.81	0.54
1:A:226:MET:CE	1:A:230:LEU:HG	2.38	0.54
1:B:158:GLN:OE1	1:B:289:ARG:NH2	2.33	0.53
1:B:209:HIS:O	1:B:213:SER:HB3	2.08	0.53
1:B:215:GLY:O	1:B:219:SER:HB2	2.09	0.53
1:A:9:SER:CB	1:A:33:LEU:HD22	2.39	0.53
1:A:226:MET:HE2	1:A:230:LEU:HG	1.89	0.53
1:A:297:LEU:HD22	1:A:302:LEU:HD11	1.91	0.53
1:B:207:CYS:N	1:B:209:HIS:NE2	2.49	0.53
1:B:216:ARG:HG3	4:B:1050:HOH:O	2.08	0.53
1:B:375:VAL:O	1:B:375:VAL:HG12	2.08	0.53
1:A:218:ILE:HA	1:A:221:ASP:HB2	1.91	0.53
1:A:365:GLU:O	1:A:367:MET:N	2.42	0.53
1:A:226:MET:CE	1:A:335:LEU:HD11	2.39	0.53
1:B:342:THR:O	1:B:343:VAL:C	2.52	0.53
1:B:391:LYS:O	1:B:394:MET:HB2	2.09	0.52
1:A:208:ARG:HH11	1:A:208:ARG:CB	2.23	0.52
1:B:124:ASN:HD21	1:B:127:SER:CB	2.21	0.52
1:B:34:VAL:HG12	1:B:101:ILE:HD11	1.90	0.52
1:B:278:THR:HB	1:B:279:PRO:CD	2.39	0.52
1:B:331:ALA:HB1	1:B:364:LEU:HD11	1.89	0.52
1:A:369:MET:HE3	1:A:369:MET:N	2.20	0.52
1:B:136:MET:HE2	1:B:169:GLY:HA3	1.92	0.52
1:A:64:LEU:O	1:A:68:MET:HG3	2.10	0.52
1:B:98:MET:HE2	1:B:121:LEU:HD12	1.92	0.52
1:B:10:THR:HG22	1:B:41:ARG:HG2	1.91	0.52
1:B:334:ALA:HB2	1:B:367:MET:HE1	1.92	0.52
1:A:140:LYS:HE3	4:A:1061:HOH:O	2.10	0.51
1:A:195:LEU:HD21	1:A:314:ARG:HB2	1.92	0.51
1:A:334:ALA:HB2	1:A:367:MET:HE1	1.91	0.51
1:B:64:LEU:O	1:B:68:MET:HG3	2.10	0.51
1:B:226:MET:CE	1:B:230:LEU:HG	2.39	0.51
1:B:259:MET:HG2	1:B:269:ALA:CB	2.40	0.51
1:B:273:GLU:OE2	1:B:297:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASP:OD1	1:B:300:CYS:HB2	2.09	0.51
1:A:382:ASP:O	1:A:386:ARG:HG3	2.10	0.51
1:B:164:ILE:HG12	1:B:171:ALA:HB1	1.92	0.51
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.45	0.51
1:B:236:ARG:HH21	1:B:243:ALA:HB2	1.75	0.51
1:B:391:LYS:HD3	1:B:394:MET:HE1	1.91	0.51
1:A:372:PRO:HB3	1:A:377:ASP:HB3	1.92	0.51
1:B:2:LYS:HD2	1:B:96:GLN:NE2	2.26	0.51
1:B:164:ILE:HA	1:B:171:ALA:HB1	1.92	0.51
1:A:33:LEU:HD12	1:A:51:PRO:HG3	1.92	0.51
1:A:9:SER:HB2	1:A:33:LEU:HD22	1.93	0.51
1:B:174:GLU:HG3	1:B:175:GLN:N	2.26	0.51
1:A:270:GLN:C	1:A:271:LEU:HD23	2.36	0.51
1:A:262:TYR:CE1	1:A:268:LEU:CD1	2.92	0.50
1:A:337:ALA:HB2	1:A:382:ASP:OD1	2.10	0.50
1:B:212:TRP:HA	1:B:212:TRP:HE3	1.75	0.50
1:B:278:THR:HG21	4:B:1031:HOH:O	2.11	0.50
1:B:391:LYS:HA	1:B:394:MET:HE3	1.93	0.50
1:B:395:ARG:HB3	1:B:395:ARG:CZ	2.40	0.50
1:A:160:LEU:HD23	1:A:260:VAL:HG11	1.94	0.50
1:A:236:ARG:HD3	1:A:241:ALA:O	2.11	0.50
1:B:56:MET:SD	1:B:65:LEU:HD22	2.52	0.50
1:A:305:LEU:HB2	1:B:305:LEU:HB2	1.93	0.50
1:B:9:SER:HB2	1:B:33:LEU:HD22	1.94	0.50
1:A:270:GLN:NE2	1:B:266:SER:OG	2.38	0.50
1:B:102:VAL:HG22	4:B:1055:HOH:O	2.11	0.49
1:B:334:ALA:CB	1:B:367:MET:HE1	2.42	0.49
1:B:367:MET:O	1:B:369:MET:HG3	2.11	0.49
1:A:395:ARG:HB3	1:A:395:ARG:CZ	2.43	0.49
1:B:216:ARG:CB	1:B:216:ARG:HH11	2.26	0.49
1:A:17:THR:O	1:A:21:VAL:HG23	2.13	0.49
1:B:208:ARG:NH1	1:B:208:ARG:HB3	2.28	0.49
1:B:30:VAL:CG1	1:B:51:PRO:HB3	2.42	0.49
1:B:208:ARG:NH2	1:B:214:MET:CG	2.76	0.49
1:A:59:GLU:O	1:A:60:ALA:C	2.53	0.49
1:A:129:VAL:HG11	1:A:230:LEU:HD22	1.93	0.49
1:A:236:ARG:NH1	4:A:1064:HOH:O	2.45	0.49
1:B:9:SER:CB	1:B:33:LEU:HD22	2.42	0.49
1:B:228:LYS:HE2	1:B:231:GLU:OE2	2.12	0.49
1:B:41:ARG:O	1:B:41:ARG:HG3	2.12	0.49
1:B:216:ARG:NH1	1:B:216:ARG:CB	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG12	1:A:101:ILE:HD11	1.94	0.49
1:A:162:GLN:CG	1:B:162:GLN:HG3	2.34	0.49
1:A:329:GLN:HB2	1:A:371:GLU:OE2	2.13	0.49
1:A:367:MET:O	1:A:369:MET:HE2	2.12	0.49
1:A:316:PRO:HD2	4:A:1009:HOH:O	2.13	0.49
1:A:130:THR:HB	1:A:378:VAL:HG11	1.92	0.48
1:A:130:THR:HB	1:A:378:VAL:HG13	1.92	0.48
1:A:172:ASP:OD2	1:A:175:GLN:HB2	2.13	0.48
1:A:212:TRP:HH2	1:A:276:MET:HE2	1.76	0.48
1:B:329:GLN:HA	1:B:329:GLN:OE1	2.12	0.48
1:A:334:ALA:CB	1:A:367:MET:HE1	2.43	0.48
1:B:329:GLN:HB2	1:B:371:GLU:OE2	2.13	0.48
1:B:367:MET:HE2	1:B:369:MET:HG2	1.95	0.48
1:A:131:CYS:HB3	1:A:135:PHE:CD1	2.48	0.48
1:A:318:LEU:O	1:A:322:MET:HG3	2.13	0.48
1:A:329:GLN:HA	1:A:329:GLN:OE1	2.12	0.48
1:B:295:LYS:NZ	1:B:298:ASP:HB2	2.29	0.48
1:B:156:ILE:HD13	1:B:181:ILE:CG2	2.44	0.48
1:B:156:ILE:O	1:B:160:LEU:HG	2.14	0.48
1:B:226:MET:HE1	1:B:335:LEU:HD11	1.95	0.48
1:A:292:SER:OG	1:A:294:VAL:HG23	2.13	0.48
1:A:295:LYS:HZ1	1:A:298:ASP:HB2	1.76	0.48
1:A:319:LYS:HD2	1:A:319:LYS:HA	1.64	0.48
1:A:146:LEU:O	1:A:147:LEU:HD23	2.12	0.48
1:B:89:ALA:HB1	1:B:113:ALA:HB2	1.96	0.48
1:B:382:ASP:O	1:B:386:ARG:HG3	2.14	0.47
1:B:202:THR:OG1	1:B:205:GLN:HG3	2.13	0.47
1:A:135:PHE:O	1:A:139:VAL:HG23	2.14	0.47
1:B:17:THR:HG23	1:B:284:MET:SD	2.54	0.47
1:B:161:PRO:HD3	1:B:262:TYR:OH	2.15	0.47
1:B:206:ALA:HA	1:B:209:HIS:NE2	2.29	0.47
1:B:300:CYS:O	1:B:302:LEU:N	2.48	0.47
1:A:64:LEU:HD21	1:A:68:MET:SD	2.55	0.47
1:A:208:ARG:HB2	1:A:208:ARG:NH1	2.23	0.47
1:A:208:ARG:CZ	1:A:214:MET:HG3	2.44	0.47
1:A:278:THR:HB	1:A:279:PRO:CD	2.45	0.47
1:A:63:LYS:HE2	1:A:63:LYS:HB3	1.68	0.47
1:A:207:CYS:H	1:A:209:HIS:CD2	2.33	0.47
1:A:391:LYS:HD3	1:A:394:MET:HE1	1.96	0.47
1:B:226:MET:HE2	1:B:230:LEU:CG	2.43	0.47
1:B:341:ILE:O	1:B:344:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH2	1:A:214:MET:CG	2.78	0.47
1:B:255:VAL:HG21	1:B:305:LEU:HD21	1.95	0.47
1:B:348:ALA:O	1:B:349:GLN:HB2	2.15	0.46
1:A:125:LYS:NZ	1:A:125:LYS:HB3	2.30	0.46
1:B:2:LYS:HD2	1:B:96:GLN:HE21	1.79	0.46
1:A:166:HIS:HB3	4:A:1075:HOH:O	2.16	0.46
1:B:36:GLY:HA2	1:B:57:ASP:CG	2.40	0.46
1:B:297:LEU:HD22	1:B:302:LEU:HD11	1.98	0.46
1:B:335:LEU:HB2	1:B:364:LEU:HD21	1.97	0.46
1:B:226:MET:HE1	1:B:321:ALA:HB2	1.97	0.46
1:B:212:TRP:HH2	1:B:276:MET:HE2	1.80	0.46
1:B:262:TYR:CZ	1:B:268:LEU:HD12	2.49	0.46
1:B:312:TYR:HD2	1:B:319:LYS:HB2	1.79	0.46
1:B:84:ALA:O	1:B:88:MET:HG2	2.16	0.46
1:B:136:MET:CE	1:B:169:GLY:HA3	2.45	0.46
1:B:249:LEU:HD23	1:B:308:ALA:O	2.16	0.46
1:A:38:ASN:HD21	1:A:41:ARG:HB3	1.79	0.46
1:A:55:VAL:HG22	1:A:79:LEU:HB2	1.98	0.46
1:B:111:LEU:HD23	1:B:375:VAL:HG21	1.97	0.46
1:B:260:VAL:HG12	1:B:262:TYR:CE1	2.50	0.46
1:B:318:LEU:O	1:B:322:MET:HG3	2.15	0.46
1:A:88:MET:HA	1:A:91:LEU:HD13	1.96	0.46
1:A:212:TRP:HA	1:A:212:TRP:HE3	1.80	0.46
1:A:226:MET:CE	1:A:335:LEU:CD1	2.94	0.46
1:A:372:PRO:HA	1:A:377:ASP:HB3	1.97	0.46
1:B:130:THR:HB	1:B:378:VAL:HG13	1.92	0.46
1:A:212:TRP:CG	1:A:274:PRO:HB3	2.51	0.45
1:A:236:ARG:NH2	1:A:243:ALA:HB2	2.30	0.45
1:B:143:LYS:HE3	1:B:170:TYR:HE1	1.82	0.45
1:B:343:VAL:O	1:B:346:PHE:HB3	2.17	0.45
1:A:156:ILE:HD13	1:A:181:ILE:CG2	2.45	0.45
1:A:174:GLU:HB3	1:A:245:GLN:NE2	2.29	0.45
1:A:217:LYS:HD2	1:A:343:VAL:CG1	2.46	0.45
1:B:119:THR:HA	1:B:145:GLN:HB3	1.98	0.45
1:B:208:ARG:CZ	1:B:214:MET:HG3	2.46	0.45
1:A:37:LYS:O	1:A:39:VAL:N	2.49	0.45
1:B:8:GLY:N	1:B:101:ILE:HG13	2.32	0.45
1:A:216:ARG:CB	1:A:216:ARG:HH11	2.30	0.45
1:B:199:ALA:HA	1:B:354:THR:HG22	1.99	0.45
1:A:41:ARG:O	1:A:45:GLN:HG3	2.17	0.45
1:A:299:PHE:O	1:B:307:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:O	1:B:43:VAL:HG23	2.17	0.45
1:A:156:ILE:HG13	1:A:258:SER:HB3	1.99	0.44
1:A:220:VAL:CG2	1:A:347:LEU:HD21	2.40	0.44
1:A:136:MET:HE2	1:A:169:GLY:HA3	1.99	0.44
1:B:38:ASN:HD21	1:B:41:ARG:HB3	1.79	0.44
1:B:185:GLY:HA3	1:B:228:LYS:HD2	1.99	0.44
1:A:56:MET:SD	1:A:65:LEU:HD22	2.58	0.44
1:A:36:GLY:HA2	1:A:57:ASP:OD2	2.17	0.44
1:A:369:MET:HE1	4:A:1084:HOH:O	2.17	0.44
1:B:46:CYS:SG	1:B:54:ALA:HB2	2.57	0.44
1:B:232:TYR:CZ	1:B:322:MET:HE3	2.52	0.44
1:A:161:PRO:CG	1:A:164:ILE:HD12	2.47	0.44
1:B:285:ALA:HB2	1:B:290:VAL:HG13	2.00	0.44
1:B:292:SER:OG	1:B:294:VAL:HG23	2.17	0.44
1:A:394:MET:C	1:A:396:LEU:N	2.76	0.44
1:B:27:HIS:HB3	4:B:1043:HOH:O	2.18	0.44
1:B:208:ARG:NH2	1:B:214:MET:SD	2.91	0.44
1:A:158:GLN:HG2	1:A:282:HIS:NE2	2.33	0.44
1:B:7:LEU:O	1:B:101:ILE:N	2.51	0.44
1:A:299:PHE:HA	1:A:302:LEU:HD22	2.00	0.44
1:B:164:ILE:O	1:B:164:ILE:HG22	2.17	0.44
1:A:217:LYS:HB3	1:A:217:LYS:HZ2	1.82	0.43
1:A:64:LEU:CD2	1:A:68:MET:SD	3.06	0.43
1:A:111:LEU:HD12	1:A:111:LEU:O	2.17	0.43
1:A:370:ARG:O	1:A:371:GLU:C	2.61	0.43
1:B:7:LEU:HD13	1:B:109:PRO:HB2	2.00	0.43
1:B:276:MET:HB2	4:B:1051:HOH:O	2.18	0.43
1:A:160:LEU:HB3	1:A:161:PRO:HD2	1.99	0.43
1:A:37:LYS:O	1:A:39:VAL:HG23	2.18	0.43
1:A:209:HIS:O	1:A:213:SER:HB3	2.18	0.43
1:A:236:ARG:NH2	1:A:326:GLU:OE2	2.51	0.43
1:B:9:SER:O	1:B:45:GLN:NE2	2.50	0.43
1:B:4:LEU:HD11	1:B:284:MET:HE3	1.99	0.43
1:A:30:VAL:CG1	1:A:51:PRO:HB3	2.49	0.43
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.91	0.43
1:A:209:HIS:HA	1:A:210:PRO:HD2	1.66	0.43
1:A:216:ARG:NH1	1:A:216:ARG:CB	2.81	0.43
1:B:242:SER:O	1:B:245:GLN:N	2.50	0.43
1:B:319:LYS:HA	1:B:319:LYS:HD2	1.78	0.43
1:A:111:LEU:O	1:A:115:ARG:HG2	2.19	0.43
1:B:195:LEU:HD23	1:B:195:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:MET:HB2	4:A:1033:HOH:O	2.18	0.42
1:B:31:VAL:CG1	1:B:91:LEU:HD23	2.49	0.42
1:B:156:ILE:HG13	1:B:258:SER:HB3	2.01	0.42
1:B:331:ALA:O	1:B:335:LEU:HB2	2.19	0.42
1:A:124:ASN:ND2	1:A:127:SER:H	2.17	0.42
1:A:286:TRP:CG	1:A:287:PRO:HA	2.54	0.42
1:B:174:GLU:HB3	1:B:245:GLN:HE22	1.83	0.42
1:B:314:ARG:O	1:B:316:PRO:HD3	2.19	0.42
1:A:21:VAL:HG23	1:A:284:MET:HE1	2.01	0.42
1:A:259:MET:HG2	1:A:269:ALA:CB	2.48	0.42
1:A:358:ALA:O	1:A:361:LEU:HB3	2.19	0.42
1:A:179:VAL:HG23	1:A:262:TYR:C	2.43	0.42
1:A:392:GLU:OE1	1:A:392:GLU:HA	2.19	0.42
1:B:17:THR:O	1:B:21:VAL:HG23	2.19	0.42
1:B:80:SER:O	1:B:84:ALA:HB2	2.20	0.42
1:B:369:MET:H	1:B:369:MET:HE2	1.84	0.42
1:A:31:VAL:CG1	1:A:91:LEU:HD23	2.50	0.42
1:A:212:TRP:CE3	1:A:212:TRP:CA	3.02	0.42
1:B:372:PRO:HA	1:B:377:ASP:HB3	2.00	0.42
1:A:198:LEU:HA	1:A:201:MET:HG2	2.01	0.42
1:A:375:VAL:O	1:A:375:VAL:CG1	2.66	0.42
1:B:160:LEU:HD23	1:B:260:VAL:HG11	2.01	0.42
1:A:312:TYR:HD2	1:A:319:LYS:HB2	1.84	0.42
1:B:4:LEU:N	1:B:4:LEU:HD23	2.35	0.42
1:B:226:MET:HE1	1:B:335:LEU:CD1	2.49	0.42
1:B:162:GLN:HE21	1:B:162:GLN:HB3	1.61	0.42
1:B:177:GLY:HA2	1:B:263:GLN:NE2	2.35	0.42
1:B:236:ARG:NH2	1:B:243:ALA:HB2	2.34	0.42
1:A:183:LEU:O	1:A:248:VAL:HA	2.19	0.42
1:A:190:PHE:CE2	1:A:201:MET:HE3	2.51	0.42
1:A:331:ALA:HB1	1:A:364:LEU:HD11	2.01	0.42
1:B:90:ALA:O	1:B:91:LEU:C	2.61	0.42
1:B:198:LEU:HA	1:B:201:MET:HG2	2.01	0.42
1:B:207:CYS:H	1:B:209:HIS:CD2	2.37	0.42
1:B:278:THR:HB	1:B:279:PRO:HD3	2.02	0.42
1:A:182:LEU:HD12	1:A:247:GLU:HB2	2.01	0.41
1:A:207:CYS:N	1:A:209:HIS:NE2	2.59	0.41
1:B:196:ARG:HH11	1:B:196:ARG:HG3	1.84	0.41
1:B:212:TRP:CE3	1:B:212:TRP:CA	3.03	0.41
1:B:255:VAL:HG21	1:B:305:LEU:CD2	2.50	0.41
1:A:145:GLN:HE22	1:A:166:HIS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:HG2	1:A:386:ARG:NH1	2.33	0.41
1:B:375:VAL:O	1:B:375:VAL:CG1	2.69	0.41
1:A:228:LYS:HD3	1:A:228:LYS:HA	1.92	0.41
1:A:361:LEU:HD22	1:A:365:GLU:CD	2.45	0.41
1:B:130:THR:HG22	1:B:333:THR:HG23	2.01	0.41
1:B:209:HIS:HA	1:B:210:PRO:HD2	1.61	0.41
1:A:43:VAL:HG12	1:A:47:LEU:CD1	2.50	0.41
1:B:37:LYS:O	1:B:39:VAL:N	2.53	0.41
1:B:341:ILE:HD12	1:B:390:ARG:HG3	2.01	0.41
1:A:7:LEU:HD13	1:A:109:PRO:HB2	2.03	0.41
1:A:70:GLN:HA	1:A:70:GLN:NE2	2.34	0.41
1:A:298:ASP:OD1	1:A:300:CYS:HB2	2.20	0.41
1:B:150:ASP:O	1:B:151:SER:C	2.64	0.41
1:B:352:ARG:O	1:B:355:ASP:HB2	2.20	0.41
1:A:394:MET:C	1:A:396:LEU:H	2.28	0.41
1:B:130:THR:CB	1:B:378:VAL:HG11	2.51	0.41
1:B:149:VAL:HG12	1:B:149:VAL:O	2.21	0.41
1:B:173:LEU:HD11	1:B:241:ALA:HB2	2.03	0.41
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.36	0.41
1:B:285:ALA:O	1:B:286:TRP:C	2.63	0.41
1:A:233:ILE:HD13	1:A:332:THR:HB	2.02	0.41
1:B:229:GLY:O	1:B:232:TYR:HB3	2.20	0.41
1:B:337:ALA:HB2	1:B:382:ASP:OD1	2.21	0.41
1:B:348:ALA:O	1:B:349:GLN:CB	2.69	0.41
1:A:64:LEU:C	1:A:64:LEU:CD2	2.94	0.41
1:A:208:ARG:NH1	1:A:208:ARG:HB3	2.36	0.41
1:A:331:ALA:O	1:A:335:LEU:HB2	2.21	0.41
1:B:63:LYS:HB3	1:B:63:LYS:HE2	1.66	0.40
1:A:342:THR:O	1:A:343:VAL:C	2.64	0.40
1:B:161:PRO:CG	1:B:164:ILE:HD12	2.51	0.40
1:A:164:ILE:O	1:A:164:ILE:CG2	2.70	0.40
1:A:236:ARG:NH1	1:A:242:SER:HA	2.37	0.40
1:A:363:VAL:HG13	1:A:388:VAL:CB	2.46	0.40
1:A:372:PRO:HB3	1:A:377:ASP:CB	2.51	0.40
1:B:33:LEU:CD1	1:B:51:PRO:HG3	2.49	0.40
1:A:251:HIS:CE1	1:A:256:ILE:H	2.39	0.40
1:A:139:VAL:O	1:A:143:LYS:N	2.54	0.40
1:A:211:ASN:O	1:A:212:TRP:CB	2.70	0.40
1:A:255:VAL:HG21	1:A:305:LEU:CD2	2.49	0.40
1:B:122:LEU:HD12	1:B:122:LEU:C	2.46	0.40
1:B:156:ILE:HD13	1:B:181:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.82	0.40
1:B:226:MET:HG2	1:B:339:ASN:CG	2.46	0.40
1:B:262:TYR:HE1	1:B:268:LEU:HD12	1.75	0.40
1:B:394:MET:C	1:B:396:LEU:H	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:NH2	4:B:1045:HOH:O[1_565]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/398 (99%)	344 (87%)	42 (11%)	9 (2%)	5	8
1	B	395/398 (99%)	340 (86%)	46 (12%)	9 (2%)	5	8
All	All	790/796 (99%)	684 (87%)	88 (11%)	18 (2%)	5	8

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
1	A	367	MET
1	B	210	PRO
1	B	367	MET
1	A	197	ASP
1	A	212	TRP
1	A	258	SER
1	A	366	LYS
1	B	38	ASN

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Mol	Chain	Res	Type
1	B	197	ASP
1	B	258	SER
1	A	38	ASN
1	B	212	TRP
1	A	373	GLN
1	B	301	LYS
1	B	349	GLN
1	B	243	ALA
1	A	372	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/328 (100%)	297 (91%)	30 (9%)	8	19
1	B	327/328 (100%)	291 (89%)	36 (11%)	6	13
All	All	654/656 (100%)	588 (90%)	66 (10%)	7	15

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	THR
1	A	40	THR
1	A	111	LEU
1	A	162	GLN
1	A	168	LEU
1	A	170	TYR
1	A	174	GLU
1	A	176	ASN
1	A	182	LEU
1	A	196	ARG
1	A	207	CYS
1	A	212	TRP
1	A	217	LYS

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Mol	Chain	Res	Type
1	A	236	ARG
1	A	249	LEU
1	A	258	SER
1	A	271	LEU
1	A	288	ASN
1	A	297	LEU
1	A	302	LEU
1	A	318	LEU
1	A	320	LEU
1	A	361	LEU
1	A	364	LEU
1	A	369	MET
1	A	370	ARG
1	A	371	GLU
1	A	377	ASP
1	A	395	ARG
1	B	4	LEU
1	B	5	THR
1	B	40	THR
1	B	72	GLN
1	B	91	LEU
1	B	101	ILE
1	B	111	LEU
1	B	122	LEU
1	B	125	LYS
1	B	134	LEU
1	B	162	GLN
1	B	168	LEU
1	B	170	TYR
1	B	174	GLU
1	B	176	ASN
1	B	195	LEU
1	B	196	ARG
1	B	207	CYS
1	B	212	TRP
1	B	217	LYS
1	B	228	LYS
1	B	236	ARG
1	B	249	LEU
1	B	258	SER
1	B	271	LEU
1	B	288	ASN

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Mol	Chain	Res	Type
1	B	297	LEU
1	B	302	LEU
1	B	318	LEU
1	B	320	LEU
1	B	361	LEU
1	B	364	LEU
1	B	369	MET
1	B	370	ARG
1	B	371	GLU
1	B	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	45	GLN
1	A	70	GLN
1	A	71	GLN
1	A	72	GLN
1	A	124	ASN
1	A	145	GLN
1	A	162	GLN
1	A	175	GLN
1	A	176	ASN
1	A	245	GLN
1	A	251	HIS
1	A	257	HIS
1	A	263	GLN
1	A	329	GLN
1	B	3	GLN
1	B	45	GLN
1	B	70	GLN
1	B	71	GLN
1	B	72	GLN
1	B	96	GLN
1	B	124	ASN
1	B	162	GLN
1	B	165	GLN
1	B	175	GLN
1	B	176	ASN
1	B	227	ASN
1	B	245	GLN

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Mol	Chain	Res	Type
1	B	251	HIS
1	B	257	HIS
1	B	263	GLN
1	B	288	ASN
1	B	329	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	FOM	B	1001	2	10,10,10	3.48	3 (30%)	11,13,13	2.07	2 (18%)
3	FOM	A	1001	2	10,10,10	3.28	3 (30%)	11,13,13	2.08	3 (27%)

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	FOM	B	1001	2	-	1/7/9/9	-
3	FOM	A	1001	2	-	1/7/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	FOM	O2-N1	-9.49	1.28	1.39
3	A	1001	FOM	O2-N1	-8.48	1.29	1.39
3	A	1001	FOM	PA1-OP1	5.05	1.60	1.50
3	B	1001	FOM	PA1-OP1	4.63	1.59	1.50
3	B	1001	FOM	PA1-OP2	2.21	1.59	1.55
3	A	1001	FOM	PA1-OP2	2.13	1.59	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FOM	OP3-PA1-C4	4.72	118.19	106.91
3	B	1001	FOM	OP3-PA1-C4	4.65	118.02	106.91
3	B	1001	FOM	OP2-PA1-OP1	-3.77	102.64	112.39
3	A	1001	FOM	OP2-PA1-OP1	-3.55	103.19	112.39
3	A	1001	FOM	O2-N1-C2	2.03	118.50	113.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FOM	C3-C2-N1-O2
3	B	1001	FOM	C3-C2-N1-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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.