



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:22 PM UTC

PDB ID : 1G0I / pdb_00001g0i
Title : CRYSTAL STRUCTURE OF MJ0109 GENE PRODUCT INOSITOL MONOPHOSPHATASE-FRUCTOSE 1,6 BISPHTHATASE
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Deposited on : 2000-10-06
Resolution : 2.40 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

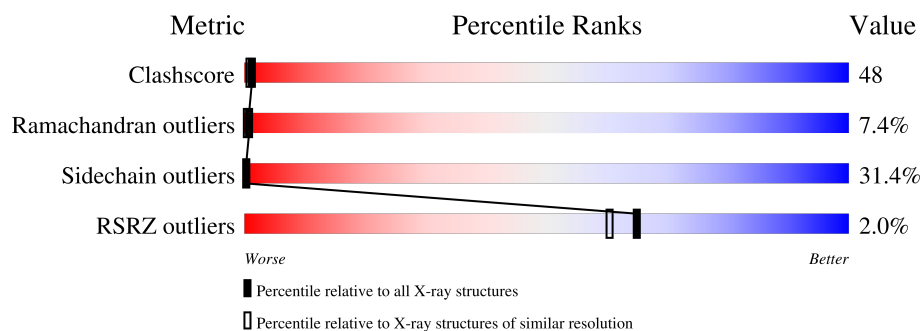
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	252	3% 25% 49% 23% .
1	B	252	% 23% 50% 26% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4124 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 INOSITOL MONOPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2018	1309	321	382	6			
1	B	252	Total	C	N	O	S	0	0	0
			2018	1309	321	382	6			

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

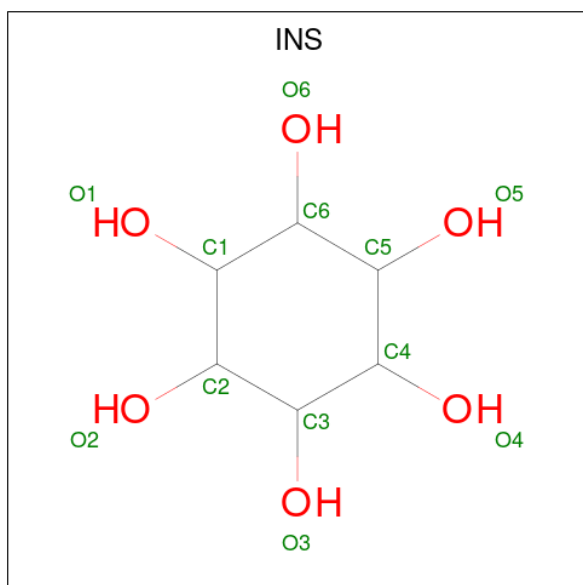
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (CCD ID: INS) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

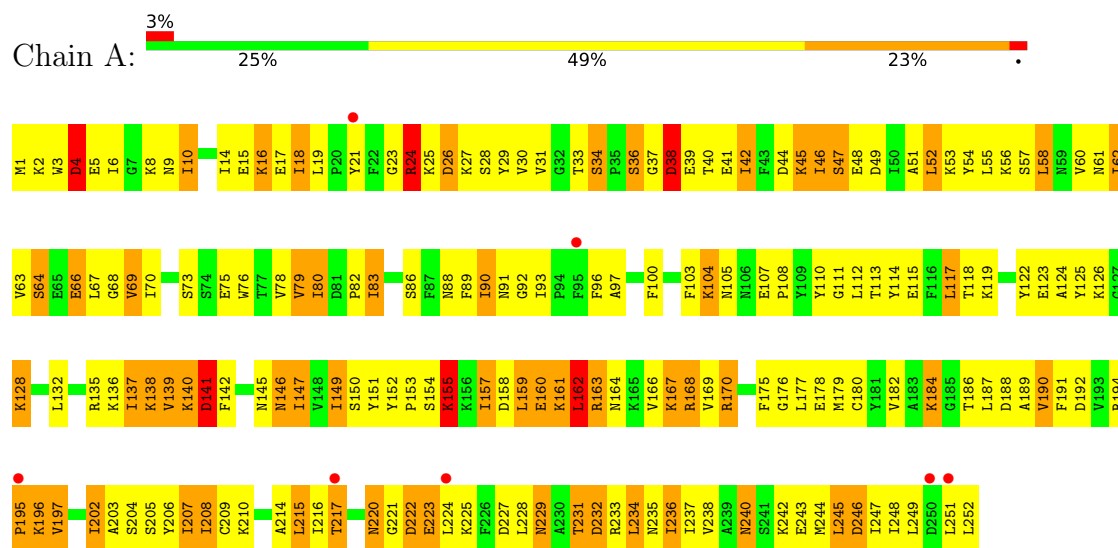
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	27	Total	O	0	0
			27	27		

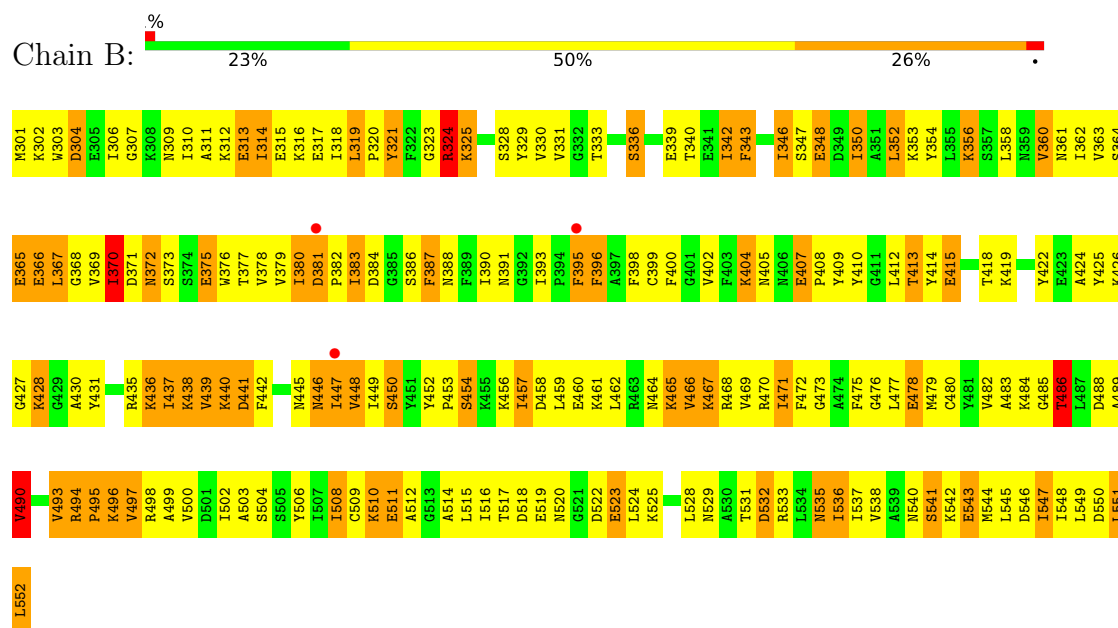
3 Residue-property plots

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: INOSITOL MONOPHOSPHATASE



• Molecule 1: INOSITOL MONOPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.02Å 78.45Å 130.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40 12.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (12.00-2.40) 93.7 (12.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.24Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.339 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4124	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: INS, PO4, MN

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	0.40	0/2058	1.32	14/2774 (0.5%)
1	B	0.36	0/2058	1.32	17/2774 (0.6%)
All	All	0.38	0/4116	1.32	31/5548 (0.6%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	O-C-N	-13.52	105.12	122.70
1	A	46	ILE	CA-C-N	7.09	130.08	120.44
1	A	46	ILE	C-N-CA	7.09	130.08	120.44
1	A	80	ILE	CA-C-N	6.74	131.91	122.74
1	A	80	ILE	C-N-CA	6.74	131.91	122.74
1	B	506	TYR	CA-C-N	6.68	131.02	120.47
1	B	506	TYR	C-N-CA	6.68	131.02	120.47
1	B	381	ASP	O-C-N	6.64	127.56	120.85
1	B	494	ARG	CA-C-N	6.48	127.94	119.84
1	B	494	ARG	C-N-CA	6.48	127.94	119.84
1	A	137	ILE	CA-C-N	6.46	132.67	122.21
1	A	137	ILE	C-N-CA	6.46	132.67	122.21
1	B	469	VAL	CA-C-N	6.02	132.05	122.59
1	B	469	VAL	C-N-CA	6.02	132.05	122.59
1	B	448	VAL	CA-C-N	-6.02	115.83	122.27
1	B	448	VAL	C-N-CA	-6.02	115.83	122.27
1	A	64	SER	CA-C-N	5.95	130.66	121.19
1	A	64	SER	C-N-CA	5.95	130.66	121.19
1	A	141	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	324	ARG	CD-NE-CZ	5.88	132.63	124.40
1	B	396	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	518	ASP	CA-CB-CG	5.57	118.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	GLY	CA-C-N	5.49	129.01	121.33
1	B	473	GLY	C-N-CA	5.49	129.01	121.33
1	B	324	ARG	CA-C-N	5.35	129.16	120.60
1	B	324	ARG	C-N-CA	5.35	129.16	120.60
1	B	343	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	222	ASP	CA-C-N	5.28	131.62	121.54
1	A	222	ASP	C-N-CA	5.28	131.62	121.54
1	A	4	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	24	ARG	CD-NE-CZ	5.05	131.47	124.40

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	2018	0	2035	196	0
1	B	2018	0	2032	195	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	12	0	12	1	0
4	B	12	0	12	3	0
5	A	21	0	0	1	0
5	B	27	0	0	2	0
All	All	4124	0	4091	389	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 48.

All (389) 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:A:217:THR:HG21	1:A:245:LEU:HD21	1.35	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:SER:H	1:B:457:ILE:HG13	1.28	0.97
1:A:55:LEU:HD22	1:A:78:VAL:HG21	1.47	0.95
1:B:452:TYR:HB3	1:B:494:ARG:HE	1.33	0.93
1:A:63:VAL:HG22	1:A:69:VAL:HG22	1.49	0.92
1:A:168:ARG:HG2	4:A:594:INS:H6	1.50	0.91
1:A:217:THR:HG21	1:A:245:LEU:CD2	2.07	0.83
1:A:88:ASN:HB3	1:A:93:ILE:HB	1.65	0.79
1:B:375:GLU:HB3	1:B:405:ASN:OD1	1.83	0.78
1:B:400:PHE:HB3	1:B:412:LEU:HB3	1.66	0.78
1:A:227:ASP:O	1:A:228:LEU:HD23	1.83	0.78
1:A:179:MET:SD	1:A:202:ILE:HG22	2.24	0.78
1:A:55:LEU:HD11	1:A:100:PHE:HE1	1.49	0.78
1:A:162:LEU:O	1:A:166:VAL:HG23	1.84	0.77
1:A:186:THR:HG22	1:A:187:LEU:HD23	1.67	0.77
1:B:529:ASN:HD21	1:B:532:ASP:HB2	1.49	0.77
1:B:454:SER:HB2	1:B:493:VAL:HG23	1.67	0.77
1:B:517:THR:HG21	1:B:545:LEU:CD2	2.15	0.76
1:B:352:LEU:O	1:B:356:LYS:HB2	1.85	0.76
1:B:479:MET:SD	1:B:502:ILE:HG22	2.26	0.76
1:B:524:LEU:HD22	1:B:536:ILE:HD12	1.67	0.75
1:B:439:VAL:HG13	1:B:512:ALA:O	1.86	0.75
1:A:243:GLU:O	1:A:247:ILE:HG13	1.87	0.75
1:B:415:GLU:OE2	1:B:477:LEU:HD21	1.86	0.75
1:B:488:ASP:O	1:B:540:ASN:HB2	1.87	0.74
1:A:202:ILE:HG21	1:A:236:ILE:HD13	1.68	0.74
1:A:204:SER:O	1:A:208:ILE:HD12	1.88	0.73
1:A:192:ASP:OD1	1:A:194:ARG:HG3	1.89	0.73
1:B:447:ILE:HD13	1:B:447:ILE:H	1.50	0.73
1:A:18:ILE:HD13	1:A:83:ILE:HD11	1.69	0.73
1:A:28:SER:HB3	1:A:90:ILE:HD11	1.71	0.72
1:A:188:ASP:O	1:A:240:ASN:HB2	1.88	0.72
1:B:407:GLU:HG3	1:B:408:PRO:HD2	1.71	0.72
1:B:468:ARG:HG2	4:B:294:INS:H4	1.69	0.72
1:A:125:TYR:H	1:A:128:LYS:HG2	1.55	0.72
1:B:382:PRO:O	1:B:383:ILE:HD12	1.90	0.72
1:A:1:MET:HE3	1:A:6:ILE:HG12	1.71	0.71
1:A:150:SER:HB2	1:A:170:ARG:O	1.90	0.71
1:A:97:ALA:HB2	1:A:177:LEU:HD13	1.72	0.70
1:B:457:ILE:HD11	1:B:493:VAL:HG21	1.72	0.70
1:A:62:ILE:HG23	1:A:70:ILE:HB	1.74	0.70
1:A:115:GLU:OE2	1:A:177:LEU:HD21	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLU:HG2	1:B:350:ILE:HG21	1.73	0.69
1:B:462:LEU:O	1:B:466:VAL:HG23	1.93	0.69
1:A:153:PRO:HB2	1:A:157:ILE:HG13	1.74	0.68
1:B:494:ARG:HH12	1:B:496:LYS:HG2	1.58	0.68
1:B:378:VAL:HG22	1:B:402:VAL:HG12	1.76	0.68
1:B:531:THR:HG22	1:B:532:ASP:H	1.57	0.68
1:A:104:LYS:O	1:A:107:GLU:HB3	1.93	0.68
1:B:402:VAL:HG22	1:B:410:TYR:O	1.94	0.68
1:A:30:VAL:HG21	1:A:39:GLU:OE1	1.94	0.67
1:A:139:VAL:HG22	1:A:140:LYS:H	1.58	0.67
1:B:517:THR:HG21	1:B:545:LEU:HD22	1.75	0.67
1:B:304:ASP:HB3	1:B:410:TYR:OH	1.96	0.66
1:A:34:SER:HA	5:A:612:HOH:O	1.96	0.66
1:A:196:LYS:HG3	1:A:233:ARG:NH2	2.11	0.66
1:B:509:CYS:HB3	1:B:514:ALA:HB3	1.78	0.66
1:B:435:ARG:HH21	1:B:437:ILE:HG22	1.61	0.65
1:A:147:ILE:HG22	1:A:149:ILE:HG22	1.77	0.65
1:A:206:TYR:CD1	1:A:216:ILE:HD13	2.30	0.65
1:B:424:ALA:HB2	1:B:430:ALA:HA	1.77	0.65
1:B:336:SER:HB2	1:B:533:ARG:NH2	2.12	0.65
1:B:497:VAL:HG11	1:B:536:ILE:HG22	1.78	0.65
1:B:340:THR:HG23	1:B:366:GLU:HG3	1.78	0.65
1:B:447:ILE:HD11	1:B:465:LYS:O	1.96	0.65
1:A:125:TYR:HD2	1:A:128:LYS:HD2	1.62	0.64
1:B:499:ALA:HB3	1:B:529:ASN:O	1.97	0.64
1:A:205:SER:O	1:A:209:CYS:HB2	1.98	0.64
1:A:86:SER:O	1:A:89:PHE:HB3	1.97	0.63
1:B:445:ASN:O	1:B:447:ILE:HD13	1.99	0.63
1:B:454:SER:N	1:B:457:ILE:HG13	2.07	0.63
1:A:48:GLU:HB2	1:A:82:PRO:HG2	1.80	0.63
1:A:243:GLU:O	1:A:246:ASP:HB2	1.99	0.62
1:B:365:GLU:H	1:B:500:VAL:HG21	1.65	0.62
1:B:495:PRO:HG3	1:B:535:ASN:HD21	1.65	0.62
1:A:75:GLU:HB3	1:A:105:ASN:ND2	2.15	0.61
1:B:410:TYR:HB2	1:B:425:TYR:CD1	2.34	0.61
1:B:380:ILE:HA	1:B:399:CYS:O	2.00	0.61
1:B:447:ILE:HA	1:B:488:ASP:OD1	2.00	0.61
1:B:447:ILE:HG12	1:B:467:LYS:H	1.65	0.61
1:A:149:ILE:HD11	1:A:191:PHE:HE1	1.65	0.60
1:A:111:GLY:O	1:A:123:GLU:HA	2.01	0.60
1:A:179:MET:HA	1:A:182:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LYS:HG2	1:B:439:VAL:N	2.16	0.60
1:B:388:ASN:HA	1:B:393:ILE:HD12	1.84	0.60
1:B:462:LEU:HD12	1:B:551:LEU:HD13	1.84	0.59
1:B:517:THR:HG21	1:B:545:LEU:HD21	1.84	0.59
1:A:206:TYR:CD1	1:A:224:LEU:HD23	2.37	0.59
1:B:452:TYR:HB3	1:B:494:ARG:NE	2.12	0.59
1:A:229:ASN:HD22	1:A:229:ASN:H	1.47	0.59
1:A:122:TYR:CD2	1:A:180:CYS:HB3	2.38	0.59
1:A:140:LYS:HD3	1:A:188:ASP:OD1	2.02	0.59
1:A:42:ILE:O	1:A:46:ILE:HG12	2.02	0.59
1:B:445:ASN:O	1:B:467:LYS:HB2	2.03	0.59
1:B:509:CYS:HB2	1:B:516:ILE:HD11	1.85	0.59
1:B:552:LEU:HD12	1:B:552:LEU:O	2.03	0.58
1:B:544:MET:O	1:B:547:ILE:HB	2.02	0.58
1:A:55:LEU:CD1	1:A:80:ILE:HD11	2.33	0.58
1:B:462:LEU:HD12	1:B:551:LEU:CD1	2.33	0.58
1:A:125:TYR:HB2	1:A:128:LYS:HB3	1.85	0.58
1:B:312:LYS:O	1:B:315:GLU:HB3	2.03	0.58
1:B:343:PHE:CE2	1:B:390:ILE:HD13	2.38	0.58
1:B:364:SER:HB2	1:B:380:ILE:HD11	1.85	0.58
1:A:45:LYS:O	1:A:45:LYS:HG2	2.04	0.58
1:A:25:LYS:O	1:A:25:LYS:HG2	2.03	0.57
1:B:516:ILE:O	1:B:524:LEU:HB3	2.03	0.57
1:B:440:LYS:HD3	1:B:485:GLY:O	2.04	0.57
1:B:536:ILE:HG13	1:B:537:ILE:N	2.18	0.57
1:A:169:VAL:O	1:A:170:ARG:HG2	2.05	0.57
1:A:192:ASP:OD2	1:A:197:VAL:HG12	2.05	0.57
1:B:313:GLU:HG2	1:B:350:ILE:CG2	2.34	0.57
1:A:88:ASN:HA	1:A:93:ILE:HD12	1.87	0.56
1:B:395:PHE:CE1	1:B:477:LEU:HD23	2.39	0.56
1:B:435:ARG:NH2	1:B:437:ILE:HG22	2.20	0.56
1:B:364:SER:HB2	1:B:380:ILE:CD1	2.36	0.56
1:B:480:CYS:O	1:B:483:ALA:HB3	2.05	0.56
1:A:4:ASP:HB3	1:A:125:TYR:OH	2.05	0.56
1:B:447:ILE:O	1:B:467:LYS:HB3	2.05	0.56
1:A:14:ILE:HD12	1:A:47:SER:OG	2.05	0.56
1:B:504:SER:O	1:B:508:ILE:HG13	2.05	0.56
1:A:58:LEU:HB3	1:A:60:VAL:HG13	1.87	0.56
1:B:376:TRP:CD2	1:B:404:LYS:HG2	2.40	0.56
1:B:453:PRO:HA	1:B:493:VAL:HG22	1.87	0.56
1:B:497:VAL:HG11	1:B:536:ILE:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ASN:N	1:B:535:ASN:HD22	2.04	0.56
1:B:402:VAL:HG23	1:B:409:TYR:HB3	1.86	0.55
1:A:110:TYR:O	1:A:207:ILE:HD13	2.07	0.55
1:A:224:LEU:HD22	1:A:236:ILE:HD12	1.88	0.55
1:B:454:SER:O	1:B:457:ILE:HB	2.07	0.55
1:A:112:LEU:HD12	1:A:113:THR:N	2.22	0.55
1:B:346:ILE:O	1:B:350:ILE:HD12	2.06	0.55
1:B:412:LEU:HD12	1:B:413:THR:H	1.71	0.55
1:A:186:THR:HG22	1:A:187:LEU:CD2	2.34	0.55
1:A:210:LYS:HG2	1:A:216:ILE:HD12	1.88	0.55
1:B:336:SER:CB	1:B:498:ARG:HD3	2.36	0.54
1:A:3:TRP:HA	1:A:6:ILE:HD12	1.89	0.54
1:A:191:PHE:HB2	1:A:237:ILE:HG12	1.89	0.54
1:B:412:LEU:HD12	1:B:413:THR:N	2.23	0.54
1:B:468:ARG:HG2	4:B:294:INS:H6	1.90	0.54
1:A:62:ILE:CG2	1:A:70:ILE:HB	2.38	0.54
1:A:229:ASN:HD22	1:A:229:ASN:N	2.04	0.54
1:B:361:ASN:HB2	1:B:377:THR:HB	1.89	0.54
1:B:495:PRO:CG	1:B:535:ASN:HD21	2.19	0.54
1:A:24:ARG:CB	1:A:24:ARG:HH11	2.21	0.54
1:A:159:LEU:CD2	1:A:163:ARG:HH21	2.20	0.54
1:B:376:TRP:CE3	1:B:404:LYS:HG2	2.44	0.53
1:B:452:TYR:O	1:B:494:ARG:HG2	2.08	0.53
1:A:48:GLU:CD	1:A:66:GLU:HB2	2.34	0.53
1:A:246:ASP:O	1:A:249:LEU:HB2	2.08	0.53
1:A:2:LYS:HB2	1:A:5:GLU:OE1	2.07	0.53
1:B:303:TRP:HB2	5:B:627:HOH:O	2.07	0.53
1:A:96:PHE:CE2	1:A:117:LEU:HD23	2.43	0.53
1:B:390:ILE:HG23	1:B:391:ASN:OD1	2.09	0.53
1:B:415:GLU:HG2	1:B:418:THR:HB	1.90	0.53
1:A:16:LYS:NZ	1:A:17:GLU:HG2	2.23	0.53
1:A:147:ILE:HD13	1:A:244:MET:SD	2.49	0.53
1:B:340:THR:CG2	1:B:366:GLU:HG3	2.38	0.53
1:A:100:PHE:HB3	1:A:112:LEU:HB3	1.91	0.52
1:A:162:LEU:HA	1:A:251:LEU:HD21	1.91	0.52
1:A:176:GLY:O	1:A:179:MET:HB2	2.09	0.52
1:A:48:GLU:OE2	1:A:66:GLU:HB2	2.10	0.52
1:A:231:THR:HG22	1:A:232:ASP:H	1.75	0.52
1:B:413:THR:HG21	1:B:480:CYS:SG	2.50	0.52
1:B:422:TYR:CD2	1:B:480:CYS:HB3	2.44	0.52
1:B:454:SER:HB2	1:B:493:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ILE:O	1:B:321:TYR:HB2	2.10	0.52
1:B:458:ASP:CG	1:B:461:LYS:HB2	2.35	0.52
1:B:468:ARG:CG	4:B:294:INS:H4	2.36	0.52
1:B:475:PHE:CE2	1:B:490:VAL:HG22	2.45	0.52
1:A:47:SER:HB3	1:A:82:PRO:HB3	1.90	0.51
1:A:76:TRP:CH2	1:A:104:LYS:HD2	2.45	0.51
1:A:179:MET:HG2	1:A:238:VAL:HG21	1.92	0.51
1:A:61:ASN:HB2	1:A:76:TRP:O	2.10	0.51
1:A:149:ILE:HG23	1:A:166:VAL:HG11	1.92	0.51
1:B:306:ILE:O	1:B:310:ILE:HG13	2.10	0.51
1:B:381:ASP:OD1	1:B:384:ASP:HA	2.09	0.51
1:A:125:TYR:N	1:A:128:LYS:HG2	2.24	0.51
1:B:342:ILE:O	1:B:342:ILE:HG13	2.10	0.51
1:A:190:VAL:HG13	1:A:190:VAL:O	2.11	0.51
1:A:41:GLU:O	1:A:44:ASP:HB2	2.11	0.51
1:A:45:LYS:O	1:A:49:ASP:HB2	2.10	0.51
1:A:69:VAL:HG12	1:A:69:VAL:O	2.11	0.51
1:B:447:ILE:CG1	1:B:466:VAL:HA	2.40	0.50
1:A:175:PHE:CE2	1:A:190:VAL:HG22	2.46	0.50
1:A:182:VAL:HG22	1:A:182:VAL:O	2.11	0.50
1:A:197:VAL:HG13	1:A:234:LEU:O	2.11	0.50
1:A:237:ILE:HG22	1:A:237:ILE:O	2.10	0.50
1:B:304:ASP:HB3	1:B:410:TYR:CZ	2.45	0.50
1:B:476:GLY:O	1:B:479:MET:HB2	2.12	0.50
1:A:124:ALA:CB	1:A:208:ILE:HA	2.40	0.50
1:B:314:ILE:O	1:B:318:ILE:HG13	2.11	0.50
1:B:449:ILE:HG22	1:B:489:ALA:N	2.26	0.50
1:A:6:ILE:O	1:A:10:ILE:HD12	2.12	0.50
1:A:18:ILE:O	1:A:21:TYR:HB2	2.12	0.50
1:A:222:ASP:O	1:A:223:GLU:O	2.30	0.50
1:B:395:PHE:CD1	1:B:477:LEU:HD23	2.47	0.50
1:B:524:LEU:CD2	1:B:536:ILE:HD12	2.38	0.50
1:A:194:ARG:NH1	1:A:196:LYS:HB2	2.27	0.49
1:A:152:TYR:OH	1:A:178:GLU:OE2	2.30	0.49
1:B:520:ASN:O	1:B:522:ASP:OD2	2.30	0.49
1:A:55:LEU:HD11	1:A:100:PHE:CE1	2.38	0.49
1:A:53:LYS:HE2	1:A:54:TYR:CE1	2.47	0.49
1:A:125:TYR:HB2	1:A:128:LYS:CG	2.42	0.49
1:B:468:ARG:HG3	1:B:468:ARG:HH11	1.78	0.49
1:B:311:ALA:HB1	1:B:414:TYR:CD1	2.48	0.49
1:B:360:VAL:HG12	1:B:376:TRP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ILE:O	1:B:551:LEU:HG	2.12	0.49
1:A:58:LEU:CB	1:A:60:VAL:HG13	2.43	0.49
1:A:179:MET:O	1:A:182:VAL:HG12	2.13	0.49
1:B:328:SER:HB3	1:B:390:ILE:HD11	1.95	0.49
1:A:4:ASP:O	1:A:8:LYS:HG3	2.13	0.48
1:B:410:TYR:HB2	1:B:425:TYR:CE1	2.48	0.48
1:A:63:VAL:HB	1:A:79:VAL:HG12	1.95	0.48
1:A:103:PHE:CE2	1:A:108:PRO:HD3	2.48	0.48
1:B:408:PRO:O	1:B:426:LYS:HG3	2.13	0.48
1:A:149:ILE:HD11	1:A:191:PHE:CE1	2.45	0.48
1:A:24:ARG:HH11	1:A:24:ARG:HA	1.78	0.48
1:B:516:ILE:O	1:B:516:ILE:HG22	2.13	0.48
1:A:152:TYR:HB3	1:A:194:ARG:NE	2.28	0.48
1:B:496:LYS:HA	1:B:496:LYS:HD3	1.45	0.48
1:B:343:PHE:CD2	1:B:390:ILE:HD13	2.48	0.48
1:A:125:TYR:HB2	1:A:128:LYS:CB	2.44	0.48
1:A:154:SER:N	1:A:157:ILE:HG13	2.28	0.48
1:A:186:THR:C	1:A:187:LEU:HD23	2.39	0.48
1:B:361:ASN:HB2	1:B:377:THR:CB	2.44	0.48
1:B:482:VAL:HG21	1:B:490:VAL:HG12	1.96	0.48
1:A:48:GLU:HB2	1:A:82:PRO:CG	2.43	0.47
1:A:125:TYR:CD2	1:A:128:LYS:HD2	2.46	0.47
1:A:202:ILE:HG21	1:A:236:ILE:CD1	2.39	0.47
1:B:440:LYS:HB2	1:B:485:GLY:HA2	1.95	0.47
1:A:248:ILE:O	1:A:252:LEU:HG	2.14	0.47
1:B:448:VAL:HG22	1:B:468:ARG:HB2	1.96	0.47
1:A:113:THR:HB	1:A:122:TYR:HB2	1.96	0.47
1:B:343:PHE:CZ	1:B:386:SER:HB3	2.50	0.47
1:A:37:GLY:O	1:A:38:ASP:O	2.32	0.47
1:B:370:ILE:O	1:B:370:ILE:HG22	2.15	0.47
1:B:457:ILE:CD1	1:B:493:VAL:HG21	2.42	0.47
1:A:159:LEU:HB3	1:B:459:LEU:CD1	2.45	0.47
1:A:214:ALA:C	1:A:215:LEU:HD23	2.41	0.46
1:B:375:GLU:O	1:B:404:LYS:HA	2.15	0.46
1:A:63:VAL:HG13	1:A:69:VAL:CG2	2.46	0.46
1:B:383:ILE:HG22	1:B:383:ILE:O	2.15	0.46
1:B:449:ILE:HG13	1:B:466:VAL:CG1	2.46	0.46
1:A:184:LYS:O	1:A:184:LYS:HG3	2.15	0.46
1:A:60:VAL:HG21	1:A:78:VAL:HG23	1.97	0.46
1:A:160:GLU:O	1:A:164:ASN:HB2	2.15	0.46
1:B:447:ILE:HG12	1:B:466:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LEU:HD12	1:B:549:LEU:HG	1.98	0.46
1:B:510:LYS:HD2	1:B:510:LYS:HA	1.53	0.46
1:A:224:LEU:HD22	1:A:236:ILE:CD1	2.46	0.45
1:A:51:ALA:HB1	1:A:80:ILE:HD13	1.98	0.45
1:B:529:ASN:ND2	1:B:532:ASP:HB2	2.26	0.45
1:A:16:LYS:HZ3	1:A:17:GLU:HG2	1.80	0.45
1:A:24:ARG:NH1	1:A:26:ASP:OD2	2.50	0.45
1:A:147:ILE:HD12	1:A:244:MET:HE1	1.97	0.45
1:A:216:ILE:HG22	1:A:224:LEU:CB	2.46	0.45
1:A:151:TYR:OH	1:A:163:ARG:NH2	2.50	0.45
1:A:194:ARG:O	1:A:196:LYS:N	2.50	0.45
1:A:235:ASN:O	1:A:236:ILE:HB	2.16	0.45
1:B:316:LYS:NZ	1:B:317:GLU:OE2	2.50	0.45
1:B:348:GLU:OE2	1:B:366:GLU:HB2	2.16	0.45
1:B:440:LYS:HE3	1:B:440:LYS:HB3	1.51	0.45
1:A:23:GLY:O	1:A:25:LYS:N	2.50	0.45
1:A:62:ILE:HD11	1:A:80:ILE:HD12	1.99	0.45
1:B:450:SER:OG	1:B:478:GLU:OE1	2.30	0.45
1:A:216:ILE:HG22	1:A:224:LEU:HB3	1.99	0.45
1:B:312:LYS:HB3	1:B:312:LYS:HE3	1.68	0.45
1:B:542:LYS:O	1:B:545:LEU:HB3	2.17	0.45
1:B:352:LEU:HD21	1:B:367:LEU:HD13	1.99	0.45
1:A:55:LEU:HD12	1:A:80:ILE:HD11	1.99	0.44
1:A:202:ILE:HD13	1:A:224:LEU:HD21	1.98	0.44
1:A:24:ARG:HH11	1:A:24:ARG:CA	2.29	0.44
1:A:147:ILE:CG2	1:A:149:ILE:HG22	2.46	0.44
1:A:166:VAL:HG12	1:A:167:LYS:N	2.32	0.44
1:A:182:VAL:HG21	1:A:189:ALA:HA	1.99	0.44
1:A:246:ASP:O	1:A:249:LEU:N	2.50	0.44
1:B:361:ASN:HB2	1:B:377:THR:CG2	2.47	0.44
1:A:45:LYS:NZ	1:A:49:ASP:OD2	2.50	0.44
1:A:91:ASN:HB3	1:B:486:THR:HG23	1.98	0.44
1:A:167:LYS:O	1:A:168:ARG:HG3	2.17	0.44
1:B:303:TRP:HA	1:B:306:ILE:HD12	2.00	0.44
1:B:519:GLU:HG3	1:B:520:ASN:H	1.83	0.44
1:A:40:THR:HG23	1:A:66:GLU:HG3	1.98	0.44
1:A:90:ILE:HG23	1:A:91:ASN:OD1	2.18	0.44
1:A:112:LEU:HD12	1:A:113:THR:H	1.81	0.44
1:B:319:LEU:N	1:B:320:PRO:HD2	2.32	0.44
1:A:28:SER:OG	1:A:29:TYR:N	2.51	0.44
1:A:63:VAL:HG13	1:A:69:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:O	1:A:189:ALA:HB2	2.17	0.44
1:B:311:ALA:HB2	1:B:398:PHE:CD2	2.52	0.44
1:B:383:ILE:N	5:B:644:HOH:O	2.50	0.44
1:A:196:LYS:HG3	1:A:233:ARG:HH21	1.80	0.44
1:B:342:ILE:HG13	1:B:346:ILE:HD12	2.00	0.44
1:B:470:ARG:HD2	1:B:472:PHE:CZ	2.53	0.44
1:A:154:SER:OG	1:A:155:LYS:N	2.50	0.44
1:A:207:ILE:O	1:A:210:LYS:N	2.49	0.44
1:B:448:VAL:N	1:B:488:ASP:OD1	2.50	0.44
1:A:28:SER:CB	1:A:90:ILE:HD11	2.45	0.44
1:B:324:ARG:HG2	1:B:324:ARG:HH11	1.83	0.44
1:B:479:MET:HE3	1:B:538:VAL:HG21	1.99	0.44
1:B:531:THR:O	1:B:532:ASP:O	2.35	0.44
1:A:136:LYS:HG2	1:A:138:LYS:HE3	2.00	0.44
1:A:179:MET:HA	1:A:182:VAL:CG1	2.48	0.44
1:A:244:MET:HG3	1:A:248:ILE:CD1	2.47	0.44
1:A:30:VAL:HA	1:A:41:GLU:HG2	2.00	0.43
1:B:303:TRP:CE3	1:B:306:ILE:HD13	2.53	0.43
1:B:448:VAL:HG12	1:B:448:VAL:O	2.17	0.43
1:B:537:ILE:O	1:B:537:ILE:HG22	2.17	0.43
1:A:30:VAL:HG11	1:A:39:GLU:OE1	2.18	0.43
1:A:216:ILE:C	1:A:217:THR:CG2	2.91	0.43
1:B:367:LEU:HD23	1:B:368:GLY:O	2.18	0.43
1:B:441:ASP:OD2	1:B:441:ASP:N	2.49	0.43
1:A:55:LEU:HD13	1:A:78:VAL:HG11	2.01	0.43
1:A:68:GLY:O	1:A:69:VAL:HG23	2.19	0.43
1:A:139:VAL:HG13	1:A:140:LYS:N	2.33	0.43
1:B:372:ASN:HD22	1:B:372:ASN:HA	1.65	0.43
1:A:41:GLU:O	1:A:44:ASP:N	2.49	0.43
1:B:446:ASN:O	1:B:448:VAL:HG23	2.19	0.43
1:A:52:LEU:HD23	1:A:52:LEU:N	2.33	0.43
1:A:145:ASN:O	1:A:146:ASN:HB2	2.19	0.43
1:A:47:SER:HB3	1:A:82:PRO:CB	2.49	0.43
1:A:125:TYR:HB2	1:A:128:LYS:HD2	2.00	0.43
1:B:306:ILE:HG22	1:B:307:GLY:N	2.33	0.43
1:B:544:MET:O	1:B:548:ILE:HD12	2.19	0.43
1:A:245:LEU:HD12	1:A:249:LEU:HG	2.01	0.43
1:B:460:GLU:O	1:B:464:ASN:ND2	2.52	0.43
1:B:480:CYS:HA	1:B:483:ALA:CB	2.49	0.43
1:B:361:ASN:ND2	1:B:377:THR:HG22	2.34	0.42
1:B:402:VAL:CG2	1:B:410:TYR:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:HA	1:B:533:ARG:HD3	2.00	0.42
1:A:161:LYS:HB3	1:A:251:LEU:HG	2.01	0.42
1:B:498:ARG:NH2	3:B:593:PO4:O1	2.52	0.42
1:A:64:SER:HA	1:A:80:ILE:O	2.19	0.42
1:A:159:LEU:HD23	1:A:163:ARG:HH21	1.83	0.42
1:B:323:GLY:O	1:B:325:LYS:N	2.49	0.42
1:B:495:PRO:HD3	1:B:535:ASN:HD21	1.83	0.42
1:A:58:LEU:N	1:A:58:LEU:HD23	2.34	0.42
1:A:118:THR:HG22	1:A:118:THR:O	2.20	0.42
1:A:141:ASP:OD2	1:A:141:ASP:N	2.50	0.42
1:A:215:LEU:HD23	1:A:215:LEU:N	2.34	0.42
1:B:447:ILE:HG13	1:B:466:VAL:HA	2.00	0.42
1:B:449:ILE:CG2	1:B:489:ALA:HB3	2.49	0.42
1:B:361:ASN:HB2	1:B:377:THR:HG22	2.01	0.42
1:A:97:ALA:HB2	1:A:177:LEU:CD1	2.45	0.42
1:B:303:TRP:O	1:B:306:ILE:HB	2.20	0.42
1:B:319:LEU:O	1:B:321:TYR:N	2.50	0.42
1:B:543:GLU:O	1:B:546:ASP:HB2	2.19	0.42
1:A:3:TRP:CH2	1:A:58:LEU:HD12	2.55	0.42
1:A:97:ALA:HB1	1:A:114:TYR:O	2.19	0.42
1:A:36:SER:OG	1:A:233:ARG:NH1	2.53	0.42
1:A:132:LEU:HB2	1:A:137:ILE:HG21	2.01	0.42
1:A:244:MET:O	1:A:248:ILE:HD12	2.20	0.42
1:B:431:TYR:HD1	1:B:436:LYS:HA	1.85	0.42
1:B:439:VAL:HG11	1:B:514:ALA:N	2.34	0.42
1:A:170:ARG:HG2	1:A:170:ARG:HH11	1.85	0.41
1:B:353:LYS:HE2	1:B:354:TYR:HE1	1.84	0.41
1:B:471:ILE:HD13	1:B:471:ILE:HG21	1.88	0.41
1:B:425:TYR:O	1:B:511:GLU:HG3	2.20	0.41
1:B:364:SER:HB3	1:B:367:LEU:HD22	2.02	0.41
1:B:509:CYS:HB3	1:B:514:ALA:CB	2.49	0.41
1:B:388:ASN:O	1:B:393:ILE:N	2.50	0.41
1:A:207:ILE:HG22	1:A:208:ILE:N	2.36	0.41
1:B:496:LYS:O	1:B:533:ARG:HD3	2.21	0.41
1:A:52:LEU:HD11	1:A:67:LEU:HD23	2.03	0.41
1:B:387:PHE:O	1:B:390:ILE:HG22	2.20	0.41
1:A:220:ASN:ND2	1:A:220:ASN:H	2.16	0.41
1:A:14:ILE:HG23	1:A:47:SER:OG	2.20	0.41
1:A:30:VAL:HG21	1:A:39:GLU:CD	2.45	0.41
1:A:160:GLU:OE2	1:A:161:LYS:HG3	2.21	0.41
1:A:195:PRO:HD3	1:A:235:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ARG:NH1	1:B:324:ARG:HA	2.36	0.41
1:B:379:VAL:CG1	1:B:500:VAL:HA	2.51	0.41
1:B:468:ARG:HG3	1:B:468:ARG:NH1	2.36	0.41
1:A:124:ALA:HB3	1:A:208:ILE:HA	2.03	0.41
1:A:149:ILE:HG23	1:A:166:VAL:CG1	2.50	0.41
1:B:380:ILE:HG22	1:B:400:PHE:HD1	1.86	0.40
1:B:435:ARG:HH21	1:B:437:ILE:CG2	2.31	0.40
1:B:476:GLY:O	1:B:479:MET:N	2.51	0.40
1:B:479:MET:HG2	1:B:538:VAL:HG21	2.03	0.40
1:B:517:THR:CG2	1:B:545:LEU:HD22	2.48	0.40
1:B:523:GLU:O	1:B:525:LYS:HG2	2.20	0.40
1:B:541:SER:OG	1:B:542:LYS:N	2.50	0.40
1:B:367:LEU:HD11	1:B:370:ILE:HD11	2.03	0.40
1:A:4:ASP:HB2	1:A:110:TYR:OH	2.22	0.40
1:B:366:GLU:HA	1:B:366:GLU:OE2	2.22	0.40
1:B:378:VAL:HG12	1:B:380:ILE:HG23	2.03	0.40
1:B:431:TYR:CE1	1:B:436:LYS:HG3	2.57	0.40
1:A:113:THR:N	1:A:122:TYR:O	2.52	0.40
1:B:495:PRO:CD	1:B:535:ASN:HD21	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/252 (99%)	185 (74%)	44 (18%)	21 (8%)	0	0
1	B	250/252 (99%)	191 (76%)	43 (17%)	16 (6%)	1	0
All	All	500/504 (99%)	376 (75%)	87 (17%)	37 (7%)	1	0

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	38	ASP
1	A	146	ASN
1	A	203	ALA
1	A	223	GLU
1	B	428	LYS
1	B	532	ASP
1	A	42	ILE
1	A	142	PHE
1	A	195	PRO
1	A	207	ILE
1	A	208	ILE
1	B	365	GLU
1	B	471	ILE
1	B	495	PRO
1	A	139	VAL
1	A	190	VAL
1	A	236	ILE
1	B	321	TYR
1	B	324	ARG
1	B	387	PHE
1	B	446	ASN
1	B	503	ALA
1	B	511	GLU
1	B	442	PHE
1	A	162	LEU
1	A	168	ARG
1	A	240	ASN
1	B	370	ILE
1	A	155	LYS
1	A	158	ASP
1	A	246	ASP
1	B	427	GLY
1	B	486	THR
1	B	490	VAL
1	A	92	GLY
1	A	18	ILE

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	221/221 (100%)	160 (72%)	61 (28%)	0	0
1	B	221/221 (100%)	143 (65%)	78 (35%)	0	0
All	All	442/442 (100%)	303 (69%)	139 (31%)	0	0

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	9	ASN
1	A	10	ILE
1	A	15	GLU
1	A	16	LYS
1	A	19	LEU
1	A	24	ARG
1	A	26	ASP
1	A	27	LYS
1	A	31	VAL
1	A	33	THR
1	A	34	SER
1	A	36	SER
1	A	38	ASP
1	A	45	LYS
1	A	47	SER
1	A	52	LEU
1	A	56	LYS
1	A	57	SER
1	A	58	LEU
1	A	62	ILE
1	A	66	GLU
1	A	69	VAL
1	A	73	SER
1	A	79	VAL
1	A	83	ILE
1	A	90	ILE
1	A	104	LYS
1	A	117	LEU
1	A	119	LYS
1	A	126	LYS
1	A	128	LYS
1	A	135	ARG

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Mol	Chain	Res	Type
1	A	138	LYS
1	A	140	LYS
1	A	141	ASP
1	A	147	ILE
1	A	149	ILE
1	A	155	LYS
1	A	157	ILE
1	A	159	LEU
1	A	160	GLU
1	A	161	LYS
1	A	162	LEU
1	A	163	ARG
1	A	167	LYS
1	A	170	ARG
1	A	184	LYS
1	A	196	LYS
1	A	197	VAL
1	A	202	ILE
1	A	215	LEU
1	A	217	THR
1	A	220	ASN
1	A	225	LYS
1	A	229	ASN
1	A	231	THR
1	A	232	ASP
1	A	234	LEU
1	A	242	LYS
1	A	245	LEU
1	B	301	MET
1	B	302	LYS
1	B	304	ASP
1	B	309	ASN
1	B	313	GLU
1	B	314	ILE
1	B	319	LEU
1	B	324	ARG
1	B	325	LYS
1	B	329	TYR
1	B	330	VAL
1	B	331	VAL
1	B	333	THR
1	B	336	SER

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Mol	Chain	Res	Type
1	B	339	GLU
1	B	342	ILE
1	B	346	ILE
1	B	347	SER
1	B	348	GLU
1	B	350	ILE
1	B	352	LEU
1	B	356	LYS
1	B	358	LEU
1	B	360	VAL
1	B	362	ILE
1	B	363	VAL
1	B	366	GLU
1	B	367	LEU
1	B	369	VAL
1	B	370	ILE
1	B	371	ASP
1	B	372	ASN
1	B	373	SER
1	B	375	GLU
1	B	380	ILE
1	B	383	ILE
1	B	395	PHE
1	B	396	PHE
1	B	404	LYS
1	B	407	GLU
1	B	413	THR
1	B	415	GLU
1	B	419	LYS
1	B	428	LYS
1	B	436	LYS
1	B	437	ILE
1	B	438	LYS
1	B	439	VAL
1	B	440	LYS
1	B	441	ASP
1	B	447	ILE
1	B	450	SER
1	B	454	SER
1	B	456	LYS
1	B	457	ILE
1	B	465	LYS

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Mol	Chain	Res	Type
1	B	466	VAL
1	B	467	LYS
1	B	478	GLU
1	B	484	LYS
1	B	486	THR
1	B	490	VAL
1	B	493	VAL
1	B	496	LYS
1	B	497	VAL
1	B	508	ILE
1	B	510	LYS
1	B	515	LEU
1	B	523	GLU
1	B	528	LEU
1	B	535	ASN
1	B	536	ILE
1	B	541	SER
1	B	543	GLU
1	B	547	ILE
1	B	550	ASP
1	B	551	LEU
1	B	552	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	145	ASN
1	A	220	ASN
1	A	229	ASN
1	A	240	ASN
1	B	359	ASN
1	B	372	ASN
1	B	443	ASN
1	B	445	ASN
1	B	464	ASN
1	B	520	ASN
1	B	535	ASN

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	PO4	A	293	2	4,4,4	1.36	0	6,6,6	0.49	0
3	PO4	B	593	2	4,4,4	1.34	0	6,6,6	0.47	0
4	INS	B	294	-	12,12,12	1.29	1 (8%)	18,18,18	1.41	3 (16%)
4	INS	A	594	-	12,12,12	1.35	3 (25%)	18,18,18	0.97	2 (11%)

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
4	INS	B	294	-	-	-	0/1/1/1
4	INS	A	594	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	294	INS	O1-C1	3.00	1.50	1.43
4	A	594	INS	O1-C1	2.88	1.50	1.43
4	A	594	INS	C2-C1	2.08	1.57	1.52
4	A	594	INS	C6-C1	2.05	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	294	INS	O2-C2-C1	3.01	117.47	110.38
4	B	294	INS	C4-C3-C2	3.01	116.11	110.83
4	B	294	INS	C3-C2-C1	2.58	115.37	110.83
4	A	594	INS	O2-C2-C1	2.47	116.20	110.38
4	A	594	INS	C4-C3-C2	2.03	114.39	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	593	PO4	1	0
4	B	294	INS	3	0
4	A	594	INS	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	252/252 (100%)	0.37	7 (2%) 55 51	6, 48, 87, 120	0
1	B	252/252 (100%)	0.29	3 (1%) 76 73	12, 46, 85, 118	0
All	All	504/504 (100%)	0.33	10 (1%) 65 60	6, 47, 86, 120	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	PHE	3.3
1	A	224	LEU	2.9
1	A	251	LEU	2.6
1	A	21	TYR	2.6
1	A	217	THR	2.5
1	B	381	ASP	2.5
1	A	195	PRO	2.2
1	A	250	ASP	2.2
1	B	447	ILE	2.1
1	B	395	PHE	2.1

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(Å ²)	Q<0.9
4	INS	A	594	12/12	0.64	0.15	50,82,94,101	12
4	INS	B	294	12/12	0.64	0.18	53,71,83,93	12
2	MN	B	591	1/1	0.91	0.05	38,38,38,38	0
2	MN	B	590	1/1	0.92	0.09	19,19,19,19	0
2	MN	A	292	1/1	0.92	0.06	60,60,60,60	0
3	PO4	A	293	5/5	0.94	0.07	29,40,49,67	0
3	PO4	B	593	5/5	0.94	0.08	18,25,34,58	0
2	MN	B	592	1/1	0.95	0.05	45,45,45,45	0
2	MN	A	290	1/1	0.98	0.04	39,39,39,39	0
2	MN	A	291	1/1	0.99	0.01	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.