



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:11 PM UTC

PDB ID : 5C3M / pdb_00005c3m
Title : Crystal structure of Gan4C, a GH4 6-phospho-glucosidase from *Geobacillus stearothermophilus*
Authors : Cohen, T.; Lansky, S.; Zehavi, A.; Shoham, Y.; Shoham, G.
Deposited on : 2015-06-17
Resolution : 3.06 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
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

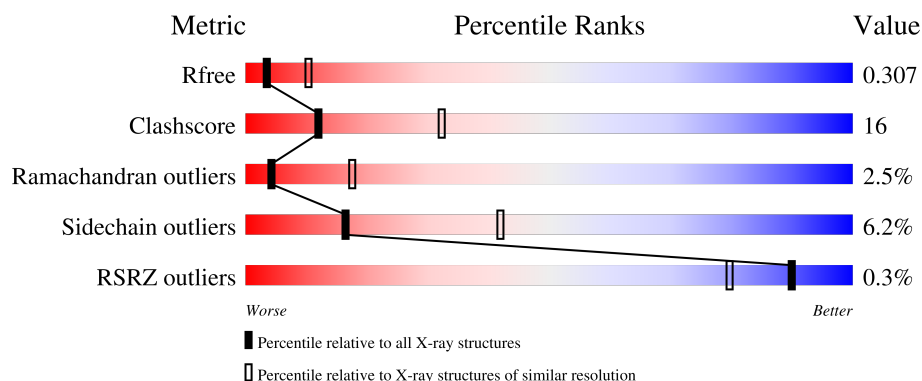
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	447	55% 33% • 8%
1	B	447	61% 28% • 8%
1	C	447	56% 31% • 8%
1	D	447	58% 29% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	A	501	-	-	X	-
2	MN	C	501	-	-	X	-
2	MN	D	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12494 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 Putative 6-phospho-beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3080	1966	514	584	16			
1	B	411	Total	C	N	O	S	0	0	0
			3069	1964	516	573	16			
1	C	410	Total	C	N	O	S	0	0	0
			3114	1996	522	580	16			
1	D	409	Total	C	N	O	S	0	0	1
			3136	2006	528	586	16			

- 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		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

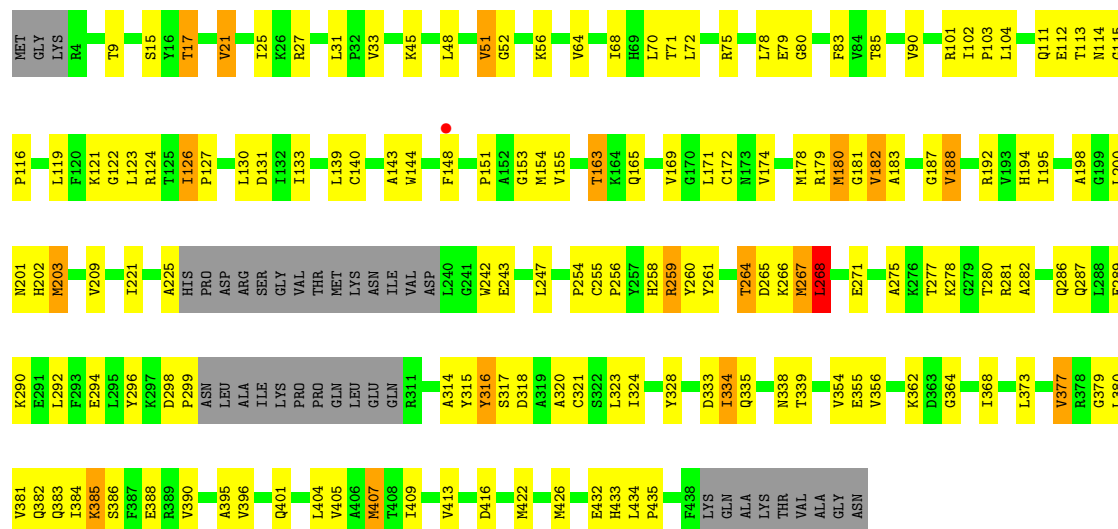
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	27	Total	O	0	0
			27	27		
3	C	19	Total	O	0	0
			19	19		
3	D	24	Total	O	0	0
			24	24		



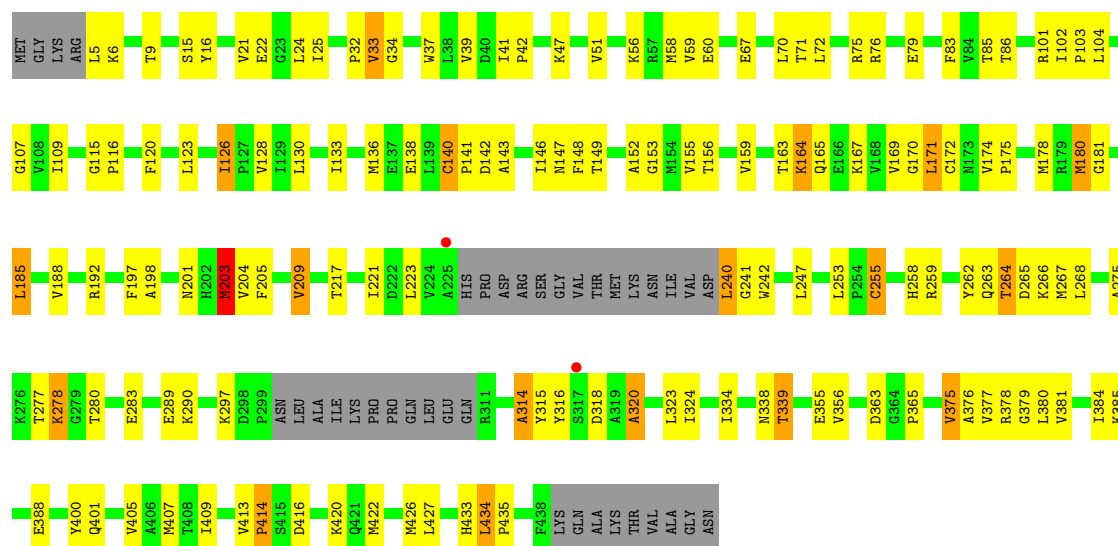
• Molecule 1: Putative 6-phospho-beta-glucosidase

Chain C: 56% 31% 8%



• Molecule 1: Putative 6-phospho-beta-glucosidase

Chain D: 58% 29% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.32Å 83.20Å 151.37Å 90.00° 113.61° 90.00°	Depositor
Resolution (Å)	46.60 – 3.06 46.60 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.60-3.06) 99.0 (46.60-3.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.306 0.234 , 0.307	Depositor DCC
R_{free} test set	1970 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12494	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5664e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.69	1/3141 (0.0%)	0.94	11/4275 (0.3%)
1	B	0.69	0/3130	0.96	11/4260 (0.3%)
1	C	0.75	0/3173	0.98	12/4314 (0.3%)
1	D	0.78	1/3195 (0.0%)	0.94	10/4338 (0.2%)
All	All	0.73	2/12639 (0.0%)	0.95	44/17187 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	HIS	CE1-NE2	7.69	1.40	1.32
1	D	320	ALA	CA-CB	-5.44	1.45	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	MET	N-CA-C	11.11	128.74	114.75
1	D	115	GLY	CA-C-N	8.24	127.81	119.24
1	D	115	GLY	C-N-CA	8.24	127.81	119.24
1	C	180	MET	N-CA-C	8.14	121.07	111.71
1	B	126	ILE	CA-C-N	-8.14	110.32	119.28
1	B	126	ILE	C-N-CA	-8.14	110.32	119.28
1	D	180	MET	N-CA-C	7.46	119.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	MET	CA-C-N	7.42	135.05	121.70
1	C	267	MET	C-N-CA	7.42	135.05	121.70
1	C	115	GLY	CA-C-N	7.25	126.78	119.24
1	C	115	GLY	C-N-CA	7.25	126.78	119.24
1	B	136	MET	N-CA-C	7.20	121.36	111.71
1	D	126	ILE	CA-C-N	-6.92	111.37	119.05
1	D	126	ILE	C-N-CA	-6.92	111.37	119.05
1	C	318	ASP	N-CA-C	-6.45	105.23	113.23
1	B	253	LEU	CA-C-N	6.29	126.62	119.83
1	B	253	LEU	C-N-CA	6.29	126.62	119.83
1	A	371	GLY	N-CA-C	-5.89	104.28	111.35
1	C	17	THR	CA-C-N	-5.87	112.97	119.19
1	C	17	THR	C-N-CA	-5.87	112.97	119.19
1	A	147	ASN	N-CA-C	5.71	118.78	109.24
1	A	174	VAL	CB-CA-C	-5.67	108.34	114.35
1	A	432	GLU	CA-C-N	-5.61	113.77	123.25
1	A	432	GLU	C-N-CA	-5.61	113.77	123.25
1	D	334	ILE	N-CA-C	5.42	114.54	106.85
1	A	253	LEU	CA-C-N	5.40	125.34	119.78
1	A	253	LEU	C-N-CA	5.40	125.34	119.78
1	B	325	SER	N-CA-C	-5.37	105.12	110.97
1	A	337	VAL	N-CA-C	5.37	115.08	108.53
1	C	334	ILE	N-CA-C	5.34	115.27	107.37
1	C	126	ILE	CA-C-N	-5.30	113.17	119.05
1	C	126	ILE	C-N-CA	-5.30	113.17	119.05
1	A	115	GLY	CA-C-N	5.26	125.31	119.32
1	A	115	GLY	C-N-CA	5.26	125.31	119.32
1	D	314	ALA	N-CA-C	5.23	115.44	108.38
1	B	297	LYS	N-CA-C	5.23	119.75	113.17
1	D	363	ASP	N-CA-C	-5.22	106.76	113.23
1	D	41	ILE	CA-C-N	5.15	126.28	119.84
1	D	41	ILE	C-N-CA	5.15	126.28	119.84
1	A	136	MET	N-CA-C	-5.14	105.75	112.23
1	B	147	ASN	N-CA-C	5.11	117.29	109.07
1	B	334	ILE	N-CA-C	5.09	114.94	107.15
1	B	136	MET	CA-C-N	5.03	130.75	121.70
1	B	136	MET	C-N-CA	5.03	130.75	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	136	MET	Peptide

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	3080	0	2981	112	0
1	B	3069	0	2968	93	0
1	C	3114	0	3094	103	1
1	D	3136	0	3145	86	1
2	A	1	0	0	2	0
2	B	1	0	0	1	0
2	C	1	0	0	3	0
2	D	1	0	0	2	0
3	A	21	0	0	2	0
3	B	27	0	0	2	0
3	C	19	0	0	3	0
3	D	24	0	0	0	0
All	All	12494	0	12188	385	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 16.

All (385) 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:C:52:GLY:HA3	1:C:70:LEU:HD21	1.52	0.92
1:C:27:ARG:HH21	1:C:321:CYS:HB2	1.36	0.90
1:D:140:CYS:O	1:D:142:ASP:N	2.03	0.90
1:A:136:MET:HE1	1:A:145:LEU:HB2	1.63	0.80
1:B:203:MET:HE1	1:B:380:LEU:HG	1.63	0.79
1:C:172:CYS:SG	2:C:501:MN:MN	1.83	0.77
1:A:265:ASP:OD1	1:A:266:LYS:N	2.17	0.76
1:A:174:VAL:HG12	1:A:178:MET:HE2	1.66	0.75
1:A:96:ARG:HH22	1:A:281:ARG:HH11	1.31	0.75
1:C:172:CYS:HG	2:C:501:MN:MN	1.11	0.74
1:C:265:ASP:HA	1:C:268:LEU:HD23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:CYS:SG	2:A:501:MN:MN	1.83	0.74
1:C:119:LEU:HD23	1:C:407:MET:HE2	1.70	0.74
1:A:172:CYS:HG	2:A:501:MN:MN	1.10	0.73
1:A:159:VAL:O	1:A:163:THR:OG1	2.07	0.73
1:D:172:CYS:SG	2:D:501:MN:MN	1.88	0.71
1:B:56:LYS:O	1:B:59:VAL:N	2.23	0.71
1:B:119:LEU:HB2	1:B:387:PHE:HZ	1.56	0.70
1:B:416:ASP:OD1	1:B:416:ASP:N	2.18	0.70
1:C:126:ILE:HG22	1:C:155:VAL:HG22	1.72	0.70
1:A:98:LYS:NZ	1:A:429:ALA:O	2.23	0.70
1:C:198:ALA:HA	1:C:356:VAL:HG12	1.73	0.70
1:A:372:ASP:OD2	1:A:378:ARG:NH1	2.24	0.69
1:A:255:CYS:HB3	1:A:258:HIS:ND1	2.07	0.69
1:C:112:GLU:HG3	1:C:113:THR:HG23	1.75	0.69
1:A:171:LEU:HG	1:A:320:ALA:HB2	1.74	0.68
1:B:50:ILE:HG22	1:B:297:LYS:HE2	1.73	0.68
1:B:296:TYR:C	1:B:297:LYS:HD2	2.17	0.68
1:C:200:LEU:HD22	1:C:385:LYS:HZ3	1.59	0.68
1:A:317:SER:HA	1:A:320:ALA:HB3	1.76	0.68
1:C:316:TYR:OH	2:C:501:MN:MN	1.53	0.67
1:B:297:LYS:HD2	1:B:297:LYS:N	2.10	0.67
1:A:416:ASP:N	1:A:416:ASP:OD1	2.28	0.67
1:B:40:ASP:OD1	1:B:41:ILE:N	2.28	0.67
1:B:172:CYS:SG	2:B:501:MN:MN	1.93	0.67
1:D:277:THR:OG1	1:D:278:LYS:N	2.28	0.66
1:D:171:LEU:HD11	1:D:323:LEU:HD22	1.76	0.66
1:C:102:ILE:HD12	1:C:426:MET:HG2	1.78	0.66
1:C:407:MET:HG2	1:C:413:VAL:HG21	1.77	0.66
1:B:50:ILE:O	1:B:297:LYS:NZ	2.27	0.66
1:B:89:ARG:NH1	1:B:96:ARG:HD2	2.10	0.66
1:D:56:LYS:O	1:D:60:GLU:HG2	1.96	0.66
1:B:389:ARG:NH1	3:B:602:HOH:O	2.25	0.65
1:C:101:ARG:HH12	1:C:275:ALA:HB1	1.60	0.65
1:B:209:VAL:N	1:B:217:THR:OG1	2.25	0.65
1:B:401:GLN:O	1:B:405:VAL:HG23	1.97	0.65
1:D:178:MET:HE3	1:D:197:PHE:HE1	1.62	0.64
1:D:240:LEU:HG	1:D:259:ARG:HD3	1.79	0.64
1:A:165:GLN:HE21	1:A:167:LYS:HB2	1.63	0.63
1:C:111:GLN:OE1	1:C:112:GLU:N	2.31	0.63
1:A:315:TYR:O	1:A:317:SER:N	2.31	0.63
1:C:328:TYR:O	1:C:362:LYS:NZ	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:MET:O	1:A:271:GLU:HG3	1.99	0.63
1:C:9:THR:OG1	1:C:85:THR:OG1	2.15	0.62
1:B:209:VAL:HG11	1:B:220:VAL:HG21	1.81	0.62
1:C:385:LYS:NZ	1:C:388:GLU:OE1	2.33	0.62
1:D:75:ARG:NH2	1:D:138:GLU:OE1	2.33	0.61
1:B:159:VAL:O	1:B:163:THR:OG1	2.16	0.61
1:B:288:LEU:HA	1:B:291:GLU:HG2	1.83	0.61
1:C:171:LEU:HD21	1:C:323:LEU:HD23	1.83	0.61
1:B:174:VAL:HG13	1:B:256:PRO:HD2	1.81	0.61
1:C:56:LYS:HE2	1:C:68:ILE:HB	1.83	0.61
1:D:198:ALA:HA	1:D:356:VAL:HG12	1.81	0.61
1:B:75:ARG:NH2	1:B:138:GLU:OE1	2.34	0.60
1:A:382:GLN:HG3	1:C:379:GLY:HA2	1.84	0.60
1:B:27:ARG:NH1	1:B:321:CYS:SG	2.75	0.60
1:A:172:CYS:SG	1:A:174:VAL:HG23	2.42	0.60
1:C:401:GLN:O	1:C:405:VAL:HG23	2.02	0.60
1:A:111:GLN:OE1	1:A:112:GLU:N	2.34	0.59
1:A:291:GLU:O	1:A:294:GLU:HB2	2.02	0.59
1:A:174:VAL:HG13	1:A:256:PRO:HD2	1.83	0.59
1:C:265:ASP:O	1:C:268:LEU:HB3	2.03	0.59
1:A:401:GLN:O	1:A:405:VAL:HG23	2.03	0.59
1:C:9:THR:HG1	1:C:85:THR:HG1	1.45	0.58
1:D:101:ARG:HH12	1:D:275:ALA:HB1	1.69	0.58
1:D:163:THR:HG22	1:D:165:GLN:H	1.67	0.58
1:C:133:ILE:HG21	1:C:163:THR:HG21	1.85	0.58
1:A:196:ASP:OD2	1:A:210:TYR:OH	2.15	0.58
1:A:255:CYS:HB3	1:A:258:HIS:CE1	2.39	0.58
1:B:46:GLU:O	1:B:50:ILE:HG13	2.04	0.58
1:D:15:SER:OG	1:D:289:GLU:OE1	2.22	0.57
1:B:192:ARG:HG2	1:B:212:ASP:OD1	2.04	0.57
1:C:15:SER:OG	1:C:289:GLU:OE2	2.22	0.57
1:A:96:ARG:HH22	1:A:281:ARG:NH1	2.02	0.57
1:B:265:ASP:OD1	1:B:266:LYS:N	2.37	0.57
1:A:83:PHE:CE2	1:A:324:ILE:HG23	2.40	0.57
1:C:334:ILE:HD12	1:C:368:ILE:HD11	1.86	0.57
1:A:383:GLN:OE1	1:C:383:GLN:HG3	2.04	0.56
1:D:24:LEU:HD13	1:D:33:VAL:HG21	1.86	0.56
1:B:286:GLN:HA	1:B:289:GLU:HB3	1.87	0.56
1:C:188:VAL:HG13	1:C:192:ARG:HD3	1.88	0.56
1:A:413:VAL:HG11	1:A:419:ALA:HB2	1.85	0.56
1:C:333:ASP:OD2	1:C:335:GLN:NE2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:LYS:NZ	1:B:424:ASP:OD2	2.37	0.55
1:C:298:ASP:OD1	1:C:299:PRO:HD2	2.06	0.55
1:B:116:PRO:HB3	1:B:407:MET:SD	2.47	0.55
1:A:432:GLU:HB3	1:A:433:HIS:ND1	2.22	0.55
1:D:39:VAL:HG22	1:D:71:THR:HG23	1.89	0.55
1:D:405:VAL:O	1:D:409:ILE:HG12	2.07	0.55
1:C:123:LEU:HD23	1:C:395:ALA:HB2	1.88	0.55
1:C:247:LEU:HD11	1:C:254:PRO:HD3	1.89	0.55
1:A:78:LEU:O	1:A:139:LEU:HB3	2.07	0.54
1:B:338:ASN:ND2	1:B:355:GLU:OE1	2.40	0.54
1:D:255:CYS:HB3	1:D:258:HIS:CE1	2.43	0.54
1:A:171:LEU:HG	1:A:320:ALA:CB	2.37	0.54
1:A:260:TYR:CE1	1:A:267:MET:HE2	2.43	0.54
1:D:172:CYS:HG	2:D:501:MN:MN	1.28	0.54
1:A:111:GLN:HG3	1:A:260:TYR:CE2	2.43	0.53
1:A:157:GLU:OE1	1:A:385:LYS:NZ	2.40	0.53
1:B:83:PHE:CE2	1:B:324:ILE:HG23	2.43	0.53
1:D:242:TRP:HZ3	1:D:262:TYR:HB2	1.72	0.53
1:B:59:VAL:O	1:B:63:GLY:N	2.41	0.53
1:A:174:VAL:HG11	1:A:255:CYS:SG	2.49	0.53
1:D:116:PRO:HG3	1:D:407:MET:HE1	1.89	0.53
1:D:203:MET:HE1	1:D:380:LEU:HG	1.90	0.53
1:B:289:GLU:O	1:B:293:PHE:HB2	2.08	0.53
1:C:151:PRO:HG2	1:C:154:MET:HE2	1.88	0.53
1:C:180:MET:N	1:C:181:GLY:HA3	2.24	0.53
1:D:203:MET:CE	1:D:380:LEU:HG	2.39	0.53
1:C:255:CYS:HB3	1:C:258:HIS:ND1	2.23	0.53
1:A:281:ARG:HG2	1:A:285:VAL:HG23	1.90	0.53
1:A:428:GLU:O	1:A:431:LYS:HG3	2.09	0.53
1:A:121:LYS:HG2	1:A:151:PRO:HD3	1.90	0.53
1:B:255:CYS:HB3	1:B:258:HIS:CE1	2.43	0.53
1:A:297:LYS:O	1:A:298:ASP:HB2	2.09	0.52
1:C:384:ILE:O	1:C:388:GLU:HG3	2.09	0.52
1:A:57:ARG:NH1	3:A:602:HOH:O	2.22	0.52
1:B:46:GLU:O	1:B:48:LEU:N	2.42	0.52
1:B:293:PHE:O	1:B:297:LYS:HD3	2.09	0.52
1:B:407:MET:HG3	1:B:413:VAL:HG21	1.91	0.52
1:D:209:VAL:HG23	1:D:217:THR:HG23	1.91	0.52
1:B:283:GLU:HA	1:B:286:GLN:HG3	1.92	0.52
1:C:169:VAL:HG11	1:C:323:LEU:HD21	1.91	0.52
1:C:267:MET:H	1:C:268:LEU:HB3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLN:CD	1:A:112:GLU:H	2.17	0.52
1:A:152:ALA:HB3	1:A:201:ASN:CG	2.34	0.52
1:C:255:CYS:HB3	1:C:258:HIS:CE1	2.45	0.52
1:A:64:VAL:HG12	1:A:66:ILE:HG13	1.92	0.52
1:A:135:ASP:O	1:A:138:GLU:HB3	2.10	0.52
1:D:180:MET:N	1:D:181:GLY:HA3	2.25	0.52
1:D:400:TYR:OH	1:D:420:LYS:NZ	2.43	0.52
1:C:380:LEU:N	3:C:601:HOH:O	2.29	0.52
1:A:180:MET:HA	1:A:183:ALA:HB3	1.91	0.51
1:C:119:LEU:O	1:C:123:LEU:HG	2.10	0.51
1:D:133:ILE:HG21	1:D:163:THR:HG21	1.91	0.51
1:D:148:PHE:CE1	1:D:320:ALA:HB2	2.45	0.51
1:B:56:LYS:O	1:B:58:MET:N	2.44	0.51
1:D:101:ARG:NH2	1:D:283:GLU:OE2	2.44	0.51
1:B:36:LEU:HD12	1:B:37:TRP:H	1.76	0.51
1:B:109:ILE:HG12	3:B:607:HOH:O	2.09	0.51
1:C:83:PHE:CD2	1:C:324:ILE:HG23	2.45	0.51
1:C:203:MET:HE3	1:C:258:HIS:HE2	1.76	0.51
1:D:86:THR:OG1	1:D:147:ASN:OD1	2.25	0.51
1:C:282:ALA:O	1:C:286:GLN:HG3	2.11	0.51
1:C:373:LEU:HD13	1:C:381:VAL:HG21	1.93	0.51
1:D:47:LYS:O	1:D:51:VAL:HG22	2.10	0.51
1:C:27:ARG:O	1:C:31:LEU:HB2	2.11	0.50
1:C:126:ILE:HD11	1:C:395:ALA:HB3	1.94	0.50
1:D:148:PHE:HE1	1:D:320:ALA:HB2	1.76	0.50
1:A:195:ILE:HG23	1:A:209:VAL:HG22	1.93	0.50
1:B:50:ILE:HG22	1:B:297:LYS:CE	2.41	0.50
1:C:433:HIS:C	1:C:435:PRO:HD3	2.36	0.50
1:D:401:GLN:O	1:D:405:VAL:HG23	2.11	0.50
1:B:50:ILE:CG2	1:B:297:LYS:HE2	2.38	0.50
1:B:277:THR:OG1	1:B:278:LYS:N	2.25	0.50
1:C:386:SER:O	1:C:390:VAL:HG23	2.11	0.50
1:D:339:THR:HG21	1:D:365:PRO:HB2	1.94	0.50
1:D:83:PHE:CD2	1:D:324:ILE:HG23	2.46	0.50
1:C:25:ILE:HG12	1:C:64:VAL:HG21	1.92	0.50
1:A:81:ALA:HB3	1:A:140:CYS:SG	2.52	0.50
1:B:184:LYS:O	1:B:187:GLY:N	2.32	0.50
1:B:203:MET:HE2	1:B:384:ILE:CG1	2.41	0.50
1:B:53:ALA:HA	1:B:56:LYS:HG3	1.94	0.49
1:C:144:TRP:CH2	1:C:364:GLY:HA2	2.47	0.49
1:A:119:LEU:HB2	1:A:387:PHE:HZ	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLN:HG3	1:C:260:TYR:CZ	2.47	0.49
1:A:433:HIS:O	1:A:434:LEU:HD23	2.12	0.49
1:C:315:TYR:O	1:C:317:SER:N	2.45	0.49
1:B:93:LEU:HD23	1:B:93:LEU:O	2.12	0.49
1:B:386:SER:O	1:B:390:VAL:HG23	2.13	0.49
1:A:277:THR:OG1	1:A:278:LYS:N	2.44	0.49
1:D:126:ILE:O	1:D:130:LEU:HG	2.13	0.49
1:D:140:CYS:HB3	1:D:143:ALA:HB2	1.93	0.49
1:B:340:ARG:NH1	1:B:342:ASN:OD1	2.46	0.49
1:A:93:LEU:HD21	1:A:285:VAL:HG12	1.94	0.49
1:C:267:MET:O	1:C:271:GLU:HG3	2.13	0.49
1:C:195:ILE:HG12	1:C:209:VAL:HG22	1.95	0.49
1:D:101:ARG:O	1:D:104:LEU:HB3	2.13	0.48
1:A:93:LEU:HG	1:A:286:GLN:HG3	1.95	0.48
1:C:338:ASN:ND2	1:C:355:GLU:OE1	2.41	0.48
1:A:22:GLU:O	1:A:25:ILE:HG13	2.13	0.48
1:D:16:TYR:CE1	1:D:314:ALA:HB3	2.49	0.48
1:D:56:LYS:C	1:D:58:MET:H	2.22	0.48
1:D:265:ASP:OD1	1:D:266:LYS:N	2.44	0.48
1:A:203:MET:HE1	1:A:380:LEU:HG	1.96	0.48
1:C:280:THR:HG22	1:C:281:ARG:N	2.28	0.48
1:A:259:ARG:HG2	1:A:263:GLN:NE2	2.28	0.48
1:A:54:LEU:HD13	1:A:57:ARG:NH1	2.29	0.47
1:B:203:MET:HE1	1:B:380:LEU:CG	2.38	0.47
1:C:405:VAL:O	1:C:409:ILE:HG12	2.14	0.47
1:D:152:ALA:O	1:D:156:THR:OG1	2.31	0.47
1:A:349:PRO:HD3	3:C:604:HOH:O	2.13	0.47
1:D:159:VAL:O	1:D:163:THR:HB	2.15	0.47
1:D:203:MET:HE3	1:D:381:VAL:HA	1.96	0.47
1:D:242:TRP:HB2	1:D:247:LEU:HD22	1.96	0.47
1:D:384:ILE:O	1:D:388:GLU:HG3	2.15	0.47
1:A:341:ASN:ND2	1:A:348:ILE:HB	2.30	0.47
1:B:56:LYS:O	1:B:59:VAL:HG22	2.14	0.47
1:B:102:ILE:HB	1:B:103:PRO:HD3	1.96	0.47
1:B:112:GLU:HG3	1:B:113:THR:HG23	1.97	0.47
1:D:71:THR:OG1	1:D:72:LEU:N	2.48	0.47
1:B:383:GLN:NE2	1:B:409:ILE:O	2.48	0.47
1:A:294:GLU:O	1:A:297:LYS:HD2	2.15	0.46
1:B:16:TYR:CE1	1:B:314:ALA:HB3	2.50	0.46
1:D:188:VAL:HG13	1:D:192:ARG:HD3	1.97	0.46
1:B:255:CYS:SG	1:B:257:TYR:HB2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HG3	1:A:212:ASP:OD1	2.15	0.46
1:D:375:VAL:O	1:D:378:ARG:N	2.34	0.46
1:A:379:GLY:HA2	1:C:382:GLN:HG3	1.97	0.46
1:D:126:ILE:HG22	1:D:155:VAL:HG22	1.98	0.46
1:B:172:CYS:SG	1:B:174:VAL:HG23	2.55	0.46
1:D:266:LYS:HE2	1:D:267:MET:CE	2.45	0.46
1:D:153:GLY:HA3	1:D:201:ASN:HB3	1.98	0.46
1:A:172:CYS:SG	1:A:202:HIS:NE2	2.89	0.46
1:B:153:GLY:HA3	1:B:201:ASN:HB3	1.97	0.46
1:B:71:THR:OG1	1:B:72:LEU:N	2.49	0.46
1:B:119:LEU:HB2	1:B:387:PHE:CZ	2.45	0.45
1:D:120:PHE:HA	1:D:123:LEU:HD12	1.96	0.45
1:D:338:ASN:ND2	1:D:355:GLU:OE1	2.49	0.45
1:A:200:LEU:HD21	1:A:385:LYS:HD2	1.97	0.45
1:B:18:PRO:HG2	1:B:296:TYR:CZ	2.52	0.45
1:C:266:LYS:O	1:C:266:LYS:HG2	2.17	0.45
1:D:5:LEU:HD23	1:D:5:LEU:HA	1.80	0.45
1:A:361:THR:HG22	1:A:363:ASP:H	1.81	0.45
1:A:395:ALA:O	1:A:436:GLN:NE2	2.49	0.45
1:B:78:LEU:O	1:B:80:GLY:N	2.49	0.45
1:C:126:ILE:O	1:C:130:LEU:HG	2.16	0.45
1:C:256:PRO:O	1:C:259:ARG:HG2	2.17	0.45
1:D:203:MET:SD	1:D:258:HIS:NE2	2.89	0.45
1:C:48:LEU:HG	1:C:70:LEU:HD23	1.98	0.45
1:A:119:LEU:HB2	1:A:387:PHE:CZ	2.51	0.45
1:C:153:GLY:HA3	1:C:201:ASN:HB3	1.99	0.45
1:A:54:LEU:O	1:A:58:MET:HE2	2.17	0.45
1:D:240:LEU:CD2	1:D:241:GLY:H	2.30	0.45
1:B:293:PHE:O	1:B:296:TYR:HB2	2.16	0.45
1:C:140:CYS:HB2	1:C:143:ALA:HB2	1.99	0.45
1:C:201:ASN:ND2	1:C:202:HIS:HD2	2.14	0.45
1:D:185:LEU:HD22	1:D:223:LEU:HB2	1.99	0.45
1:D:385:LYS:HD2	1:D:385:LYS:HA	1.49	0.45
1:A:57:ARG:NH1	1:A:299:PRO:HD3	2.32	0.44
1:C:71:THR:OG1	1:C:72:LEU:N	2.50	0.44
1:C:432:GLU:H	1:C:432:GLU:HG3	1.51	0.44
1:B:151:PRO:O	1:B:155:VAL:HG23	2.16	0.44
1:C:78:LEU:O	1:C:80:GLY:N	2.50	0.44
1:A:111:GLN:HG3	1:A:260:TYR:CZ	2.52	0.44
1:B:330:ASP:HB2	1:B:362:LYS:HG3	2.00	0.44
1:B:416:ASP:OD1	1:D:263:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:O	1:C:33:VAL:HG23	2.17	0.44
1:C:179:ARG:C	1:C:181:GLY:HA3	2.43	0.44
1:B:31:LEU:O	1:B:33:VAL:N	2.48	0.44
1:B:203:MET:HE2	1:B:384:ILE:HG13	2.00	0.44
1:B:278:LYS:H	1:B:278:LYS:HG3	1.61	0.44
1:C:51:VAL:HG12	1:C:296:TYR:HD2	1.83	0.44
1:C:114:ASN:ND2	1:C:261:TYR:OH	2.49	0.44
1:C:338:ASN:HA	1:C:354:VAL:O	2.17	0.44
1:D:240:LEU:HD21	1:D:259:ARG:HG2	2.00	0.44
1:A:379:GLY:N	3:A:606:HOH:O	2.49	0.44
1:C:183:ALA:O	1:C:187:GLY:N	2.51	0.44
1:D:148:PHE:O	1:D:149:THR:C	2.61	0.44
1:B:334:ILE:HD12	1:B:368:ILE:HD11	2.00	0.44
1:A:96:ARG:NH2	1:A:281:ARG:HD3	2.33	0.43
1:A:211:LEU:O	1:A:212:ASP:HB2	2.18	0.43
1:A:253:LEU:HA	1:A:254:PRO:HD2	1.84	0.43
1:B:347:SER:HB3	1:B:372:ASP:OD1	2.18	0.43
1:A:151:PRO:O	1:A:155:VAL:HG23	2.17	0.43
1:B:111:GLN:O	1:B:117:GLY:HA3	2.18	0.43
1:A:155:VAL:O	1:A:159:VAL:HG23	2.18	0.43
1:A:179:ARG:O	1:A:182:VAL:HG12	2.18	0.43
1:B:10:ILE:HA	1:B:39:VAL:HG13	1.98	0.43
1:C:83:PHE:CE2	1:C:324:ILE:HG23	2.52	0.43
1:A:413:VAL:HA	1:A:414:PRO:HD3	1.80	0.43
1:C:416:ASP:OD1	1:C:416:ASP:N	2.50	0.43
1:A:294:GLU:OE2	1:A:297:LYS:NZ	2.50	0.43
1:B:211:LEU:HB2	1:B:216:VAL:HG21	2.01	0.43
1:A:245:ASP:HB2	1:C:404:LEU:HD23	2.01	0.43
1:D:277:THR:OG1	1:D:278:LYS:HG3	2.19	0.43
1:B:208:HIS:ND1	1:B:215:GLU:OE2	2.49	0.43
1:C:242:TRP:NE1	1:C:259:ARG:HH21	2.17	0.43
1:C:320:ALA:O	1:C:324:ILE:HG13	2.19	0.43
1:D:102:ILE:HB	1:D:103:PRO:HD3	2.01	0.43
1:A:180:MET:HB3	1:A:180:MET:HE2	1.78	0.43
1:B:148:PHE:HE1	1:B:320:ALA:HB2	1.83	0.43
1:C:122:GLY:HA3	1:C:154:MET:HE3	2.01	0.43
1:D:164:LYS:H	1:D:164:LYS:HG3	1.62	0.43
1:A:338:ASN:HA	1:A:354:VAL:O	2.19	0.42
1:B:417:THR:O	1:B:421:GLN:HG3	2.18	0.42
1:C:194:HIS:CD2	1:C:195:ILE:N	2.87	0.42
1:D:136:MET:C	1:D:138:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ASP:OD1	1:D:416:ASP:N	2.51	0.42
1:A:113:THR:HG21	1:A:150:ASN:HB3	2.01	0.42
1:C:277:THR:HG22	1:C:278:LYS:N	2.33	0.42
1:D:433:HIS:C	1:D:435:PRO:HD3	2.44	0.42
1:A:361:THR:HB	1:A:364:GLY:O	2.19	0.42
1:B:111:GLN:HG3	1:B:260:TYR:CZ	2.55	0.42
1:C:377:VAL:O	1:C:381:VAL:HG23	2.19	0.42
1:D:205:PHE:CE1	1:D:377:VAL:HG13	2.54	0.42
1:B:203:MET:HE2	1:B:384:ILE:HG12	2.00	0.42
1:B:422:MET:HB3	1:B:422:MET:HE2	1.66	0.42
1:C:56:LYS:HE3	1:C:56:LYS:HB2	1.84	0.42
1:A:422:MET:O	1:A:426:MET:HG3	2.19	0.42
1:B:14:SER:C	1:B:16:TYR:H	2.28	0.42
1:C:174:VAL:HG13	1:C:256:PRO:HD2	2.01	0.42
1:B:418:ILE:O	1:B:422:MET:HG3	2.20	0.42
1:D:278:LYS:HG3	1:D:278:LYS:H	1.53	0.42
1:A:314:ALA:HB1	1:A:316:TYR:H	1.83	0.42
1:C:264:THR:O	1:C:267:MET:HB2	2.20	0.42
1:D:9:THR:OG1	1:D:85:THR:OG1	2.33	0.42
1:A:159:VAL:HG11	1:A:168:VAL:HG21	2.02	0.42
1:C:45:LYS:HD2	1:C:72:LEU:HD11	2.01	0.42
1:B:291:GLU:HG3	1:B:292:LEU:N	2.35	0.42
1:B:382:GLN:HG3	1:D:379:GLY:HA2	2.02	0.42
1:A:119:LEU:O	1:A:123:LEU:HG	2.20	0.42
1:A:416:ASP:HB2	1:C:243:GLU:HG3	2.01	0.42
1:C:17:THR:O	1:C:21:VAL:HG13	2.20	0.42
1:D:170:GLY:O	1:D:338:ASN:HB2	2.19	0.42
1:D:422:MET:O	1:D:426:MET:HG3	2.19	0.42
1:B:414:PRO:O	1:D:264:THR:OG1	2.37	0.41
1:C:116:PRO:HB3	1:C:426:MET:HE1	2.01	0.41
1:D:107:GLY:O	1:D:268:LEU:HD11	2.20	0.41
1:D:413:VAL:HA	1:D:414:PRO:HD3	1.76	0.41
1:A:36:LEU:HD12	1:A:37:TRP:H	1.84	0.41
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.84	0.41
1:B:112:GLU:O	1:B:121:LYS:HD2	2.20	0.41
1:C:287:GLN:O	1:C:290:LYS:N	2.52	0.41
1:D:126:ILE:HD13	1:D:126:ILE:HG21	1.77	0.41
1:B:253:LEU:HA	1:B:254:PRO:HD2	1.76	0.41
1:C:225:ALA:HB1	3:C:616:HOH:O	2.19	0.41
1:D:174:VAL:N	1:D:175:PRO:HD2	2.35	0.41
1:A:203:MET:CE	1:A:380:LEU:HG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:HB3	1:A:437:PHE:HD2	1.85	0.41
1:B:413:VAL:HA	1:B:414:PRO:HD3	1.85	0.41
1:C:31:LEU:O	1:C:33:VAL:N	2.52	0.41
1:C:85:THR:HB	1:C:148:PHE:HE2	1.85	0.41
1:C:124:ARG:HG2	1:C:434:LEU:CD1	2.51	0.41
1:A:36:LEU:HD12	1:A:37:TRP:N	2.35	0.41
1:C:127:PRO:O	1:C:131:ASP:HB2	2.20	0.41
1:A:338:ASN:ND2	1:A:355:GLU:OE1	2.50	0.41
1:C:103:PRO:HA	1:C:422:MET:HE3	2.03	0.41
1:D:6:LYS:HE3	1:D:37:TRP:NE1	2.36	0.41
1:A:9:THR:O	1:A:39:VAL:HG22	2.21	0.41
1:A:346:ALA:HB3	1:A:372:ASP:CG	2.46	0.41
1:B:17:THR:O	1:B:21:VAL:HG22	2.21	0.41
1:B:178:MET:HE2	1:B:178:MET:HB3	1.86	0.41
1:C:314:ALA:HB1	1:C:316:TYR:HD1	1.85	0.41
1:B:31:LEU:O	1:B:33:VAL:HG23	2.21	0.41
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.93	0.41
1:B:89:ARG:HH12	1:B:96:ARG:HD2	1.83	0.41
1:D:247:LEU:HA	1:D:247:LEU:HD12	1.85	0.41
1:D:427:LEU:HD23	1:D:434:LEU:HD23	2.03	0.41
1:A:5:LEU:HB3	1:A:32:PRO:O	2.21	0.41
1:A:100:GLU:OE2	1:A:280:THR:HB	2.21	0.41
1:A:119:LEU:HD23	1:A:407:MET:HE2	2.03	0.41
1:A:148:PHE:O	1:A:150:ASN:N	2.54	0.41
1:B:48:LEU:C	1:B:50:ILE:N	2.78	0.41
1:D:22:GLU:O	1:D:25:ILE:HB	2.21	0.41
1:A:9:THR:HG23	1:A:85:THR:HG23	2.03	0.40
1:A:47:LYS:O	1:A:293:PHE:HE2	2.04	0.40
1:A:179:ARG:O	1:A:183:ALA:N	2.47	0.40
1:B:48:LEU:O	1:B:50:ILE:N	2.54	0.40
1:D:385:LYS:NZ	1:D:388:GLU:OE1	2.54	0.40
1:A:43:GLU:O	1:A:43:GLU:HG3	2.20	0.40
1:A:431:LYS:HA	1:A:438:PHE:CE2	2.56	0.40
1:D:85:THR:HA	1:D:146:ILE:O	2.20	0.40
1:D:280:THR:HG23	1:D:283:GLU:OE2	2.21	0.40
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.77	0.40
1:A:319:ALA:O	1:A:322:SER:OG	2.40	0.40
1:A:377:VAL:O	1:A:381:VAL:HG13	2.20	0.40
1:C:178:MET:O	1:C:182:VAL:HG13	2.21	0.40
1:A:433:HIS:ND1	1:A:433:HIS:N	2.69	0.40
1:A:75:ARG:HH12	1:A:138:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:O	1:A:130:LEU:HG	2.21	0.40
1:A:379:GLY:HA3	1:C:383:GLN:HA	2.04	0.40
1:C:267:MET:H	1:C:268:LEU:CB	2.34	0.40
1:D:5:LEU:HB2	1:D:32:PRO:O	2.21	0.40
1:D:56:LYS:HA	1:D:59:VAL:HG22	2.03	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:C:131:ASP:OD1	1:D:76:ARG:NH2[3_556]	2.13	0.07

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	404/447 (90%)	361 (89%)	34 (8%)	9 (2%)	5	20
1	B	405/447 (91%)	353 (87%)	37 (9%)	15 (4%)	2	12
1	C	404/447 (90%)	360 (89%)	39 (10%)	5 (1%)	10	32
1	D	403/447 (90%)	356 (88%)	35 (9%)	12 (3%)	3	15
All	All	1616/1788 (90%)	1430 (88%)	145 (9%)	41 (2%)	4	17

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	149	THR
1	A	277	THR
1	B	46	GLU
1	B	57	ARG

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Mol	Chain	Res	Type
1	B	79	GLU
1	C	79	GLU
1	C	203	MET
1	D	141	PRO
1	A	316	TYR
1	B	47	LYS
1	B	244	PRO
1	C	316	TYR
1	D	79	GLU
1	D	140	CYS
1	D	315	TYR
1	D	376	ALA
1	A	123	LEU
1	A	251	LYS
1	B	203	MET
1	B	212	ASP
1	C	165	GLN
1	D	109	ILE
1	D	414	PRO
1	A	185	LEU
1	A	244	PRO
1	B	34	GLY
1	B	56	LYS
1	D	203	MET
1	B	48	LEU
1	B	245	ASP
1	B	298	ASP
1	B	340	ARG
1	C	268	LEU
1	A	203	MET
1	D	316	TYR
1	D	42	PRO
1	B	32	PRO
1	B	414	PRO
1	D	34	GLY
1	D	375	VAL

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	308/371 (83%)	290 (94%)	18 (6%)	18	44
1	B	302/371 (81%)	287 (95%)	15 (5%)	22	49
1	C	319/371 (86%)	298 (93%)	21 (7%)	15	40
1	D	329/371 (89%)	305 (93%)	24 (7%)	13	36
All	All	1258/1484 (85%)	1180 (94%)	78 (6%)	16	42

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	27	ARG
1	A	30	GLU
1	A	35	GLU
1	A	41	ILE
1	A	75	ARG
1	A	89	ARG
1	A	128	VAL
1	A	226	HIS
1	A	264	THR
1	A	286	GLN
1	A	291	GLU
1	A	317	SER
1	A	339	THR
1	A	381	VAL
1	A	389	ARG
1	A	416	ASP
1	A	433	HIS
1	B	30	GLU
1	B	41	ILE
1	B	51	VAL
1	B	60	GLU
1	B	169	VAL
1	B	195	ILE
1	B	280	THR
1	B	286	GLN
1	B	295	LEU
1	B	297	LYS
1	B	311	ARG
1	B	321	CYS

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Mol	Chain	Res	Type
1	B	377	VAL
1	B	383	GLN
1	B	416	ASP
1	C	21	VAL
1	C	51	VAL
1	C	75	ARG
1	C	90	VAL
1	C	104	LEU
1	C	121	LYS
1	C	139	LEU
1	C	163	THR
1	C	182	VAL
1	C	188	VAL
1	C	221	ILE
1	C	259	ARG
1	C	264	THR
1	C	268	LEU
1	C	292	LEU
1	C	294	GLU
1	C	339	THR
1	C	377	VAL
1	C	385	LYS
1	C	396	VAL
1	C	407	MET
1	D	21	VAL
1	D	33	VAL
1	D	67	GLU
1	D	70	LEU
1	D	128	VAL
1	D	164	LYS
1	D	167	LYS
1	D	169	VAL
1	D	171	LEU
1	D	185	LEU
1	D	203	MET
1	D	204	VAL
1	D	209	VAL
1	D	221	ILE
1	D	240	LEU
1	D	253	LEU
1	D	255	CYS
1	D	264	THR

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Mol	Chain	Res	Type
1	D	278	LYS
1	D	290	LYS
1	D	297	LYS
1	D	318	ASP
1	D	339	THR
1	D	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	382	GLN
1	B	430	HIS
1	C	150	ASN
1	D	114	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	410/447 (91%)	-0.15	1 (0%) 91 83	33, 61, 82, 97	0
1	B	411/447 (91%)	-0.25	1 (0%) 91 83	36, 56, 77, 87	0
1	C	410/447 (91%)	-0.41	1 (0%) 91 83	27, 50, 66, 79	0
1	D	409/447 (91%)	-0.44	2 (0%) 87 72	28, 49, 65, 91	0
All	All	1640/1788 (91%)	-0.31	5 (0%) 90 80	27, 52, 77, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	GLY	3.0
1	B	87	GLN	2.8
1	D	225	ALA	2.6
1	C	148	PHE	2.3
1	D	317	SER	2.3

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
2	MN	A	501	1/1	0.99	0.04	58,58,58,58	0
2	MN	B	501	1/1	0.99	0.04	50,50,50,50	0
2	MN	C	501	1/1	0.99	0.03	51,51,51,51	0
2	MN	D	501	1/1	0.99	0.03	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.