



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 9QQO / pdb_00009qqo
Title : Crystal structure of a beta-glycosidase from Prevotella sp.
Authors : Schwartz, M.; Neiers, F.
Deposited on : 2025-04-01
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)	:	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

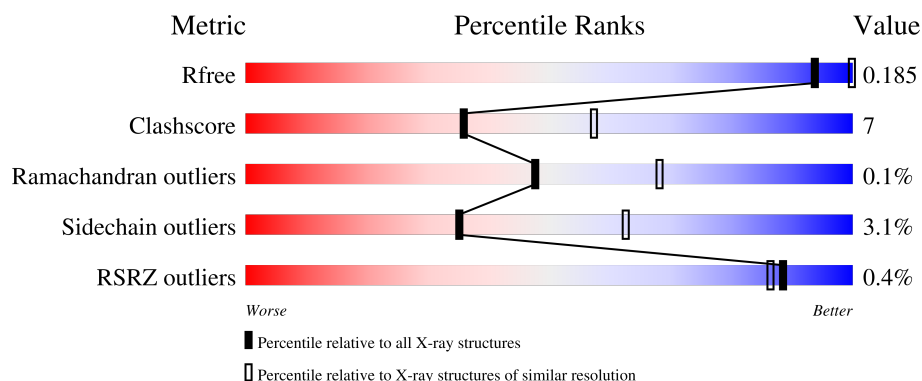
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



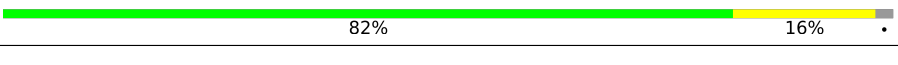
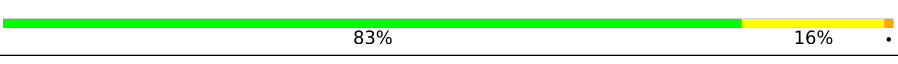
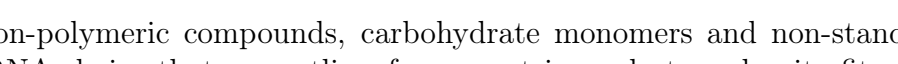
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	449	85%15%
1	B	449	86%13%
1	C	449	80%18%
1	D	449	78%19%
1	E	449	82%17%

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Mol	Chain	Length	Quality of chain
1	F	449	 83% 16% .
1	G	449	 82% 16% .
1	H	449	 84% 13% . .
1	I	449	 78% 19% . .
1	J	449	 77% 20% . .
1	K	449	 83% 16% .
1	L	449	 83% 15% .

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	GOL	F	501	-	-	X	-
2	GOL	K	501	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46238 atoms, of which 96 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 Beta-glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3631	2324	621	669	17			
1	B	447	Total	C	N	O	S	0	0	0
			3618	2316	619	667	16			
1	C	443	Total	C	N	O	S	0	0	0
			3578	2292	607	663	16			
1	D	442	Total	C	N	O	S	0	0	0
			3567	2286	603	662	16			
1	E	447	Total	C	N	O	S	0	0	0
			3618	2316	619	667	16			
1	F	447	Total	C	N	O	S	0	0	0
			3618	2316	619	667	16			
1	G	442	Total	C	N	O	S	0	0	0
			3568	2286	604	662	16			
1	H	441	Total	C	N	O	S	0	0	0
			3557	2280	600	661	16			
1	I	442	Total	C	N	O	S	0	0	0
			3567	2286	603	662	16			
1	J	442	Total	C	N	O	S	0	0	0
			3567	2286	603	662	16			
1	K	447	Total	C	N	O	S	0	0	0
			3618	2316	619	667	16			
1	L	447	Total	C	N	O	S	0	0	0
			3618	2316	619	667	16			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	H	1	Total	C	H	O	0	0
			14	3	8	3		
2	I	1	Total	C	H	O	0	0
			14	3	8	3		
2	J	1	Total	C	H	O	0	0
			14	3	8	3		
2	K	1	Total	C	H	O	0	0
			14	3	8	3		
2	L	1	Total	C	H	O	0	0
			14	3	8	3		

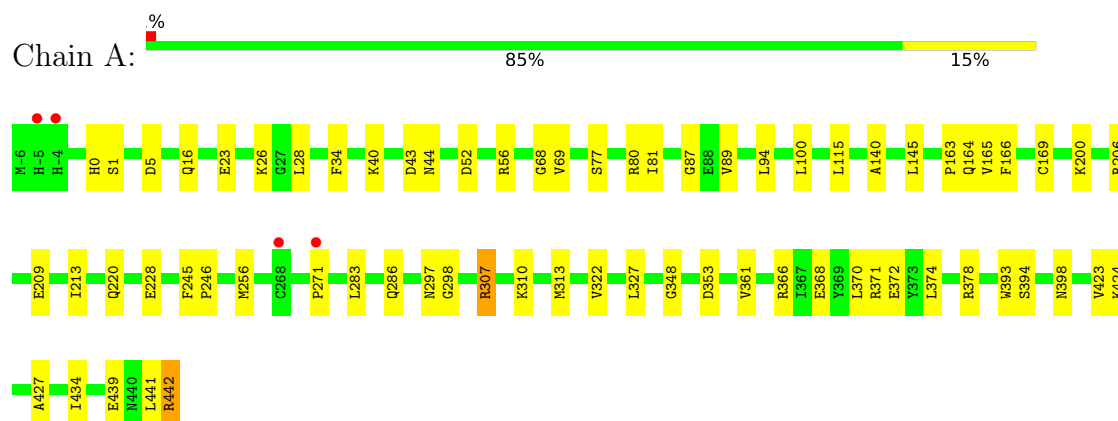
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total 265	O 265	0	0
3	B	288	Total 288	O 288	0	0
3	C	220	Total 220	O 220	0	0
3	D	191	Total 191	O 191	0	0
3	E	251	Total 251	O 251	0	0
3	F	253	Total 253	O 253	0	0
3	G	226	Total 226	O 226	0	0
3	H	265	Total 265	O 265	0	0
3	I	215	Total 215	O 215	0	0
3	J	224	Total 224	O 224	0	0
3	K	272	Total 272	O 272	0	0
3	L	275	Total 275	O 275	0	0

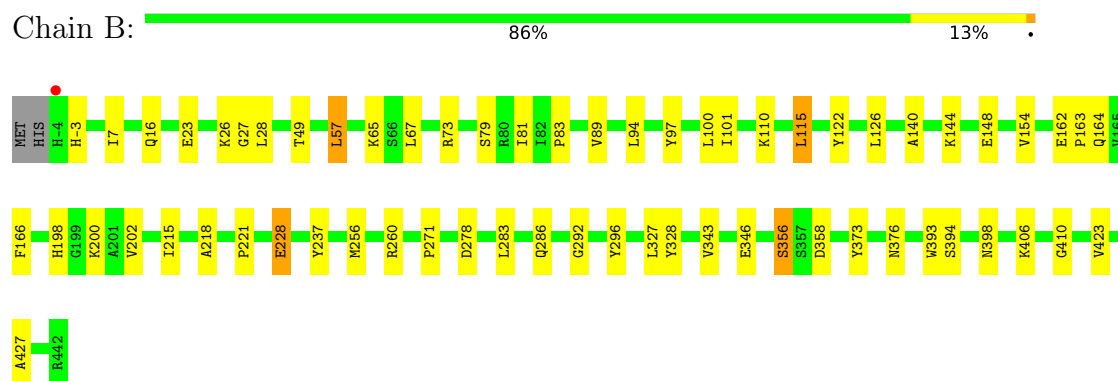
3 Residue-property plots [i](#)

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.

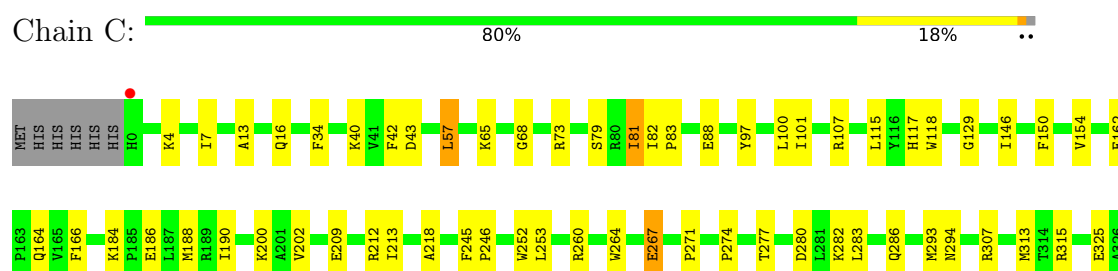
• Molecule 1: Beta-glycosidase



• Molecule 1: Beta-glycosidase

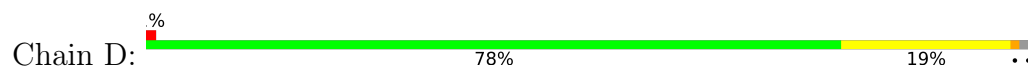


• Molecule 1: Beta-glycosidase

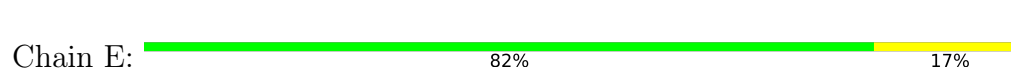




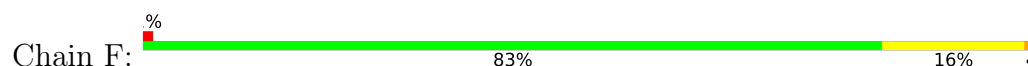
● Molecule 1: Beta-glycosidase



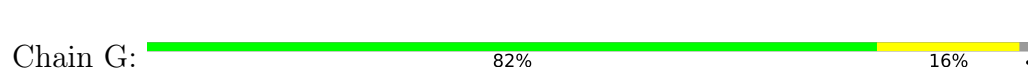
● Molecule 1: Beta-glycosidase

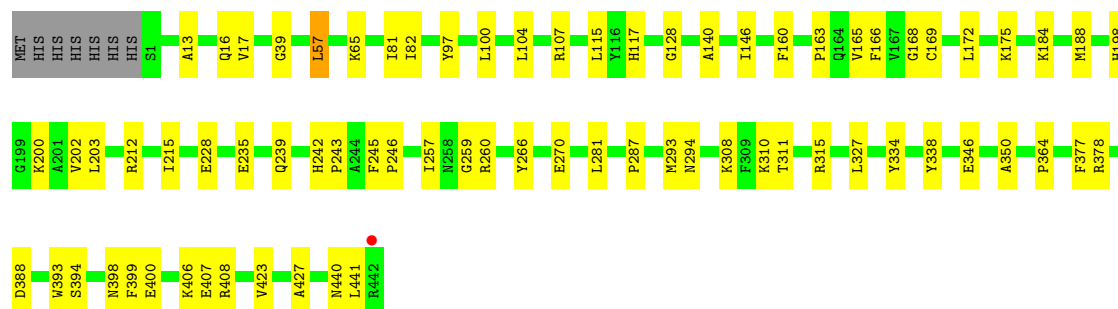


● Molecule 1: Beta-glycosidase



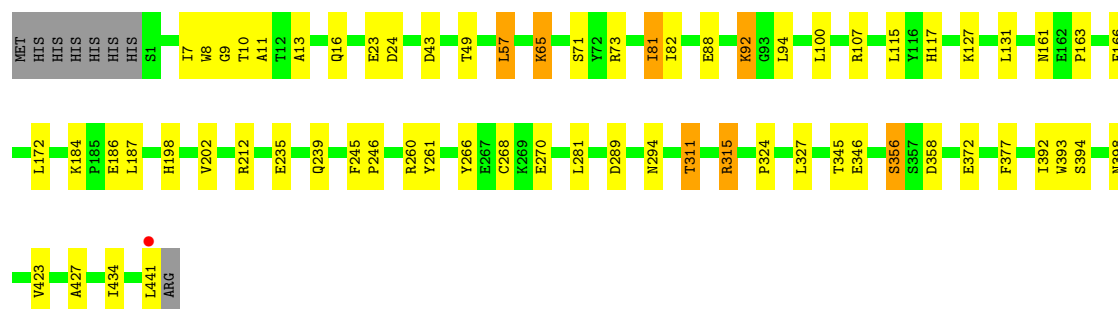
● Molecule 1: Beta-glycosidase





• Molecule 1: Beta-glycosidase

Chain H: 84% 13% ..



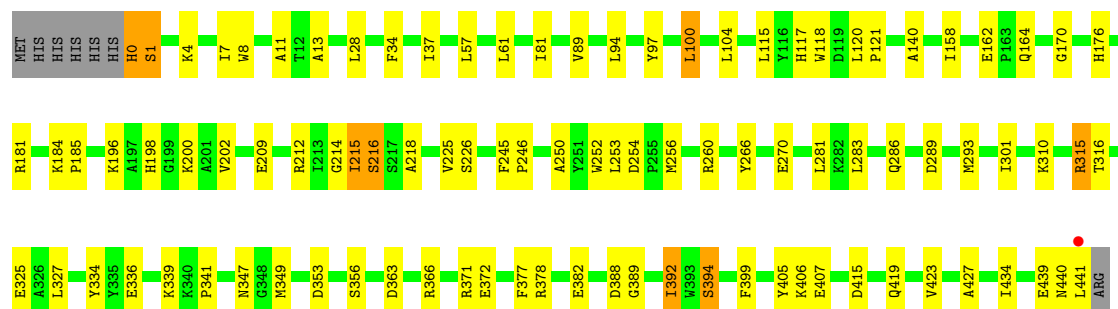
• Molecule 1: Beta-glycosidase

Chain I: 78% 19% ..



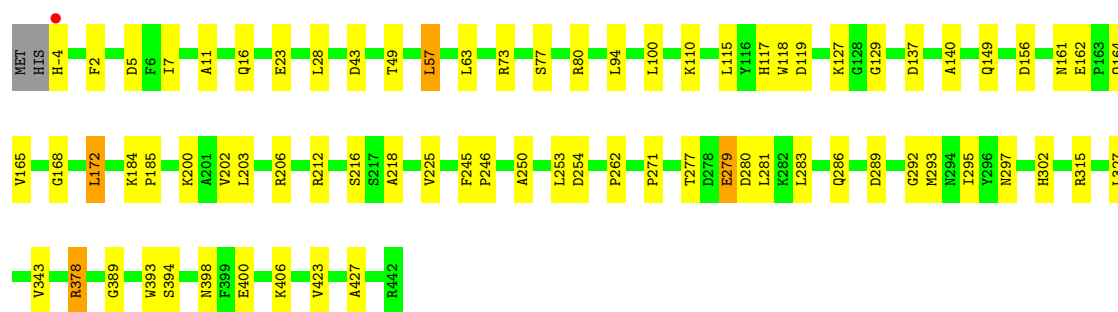
• Molecule 1: Beta-glycosidase

Chain J: 77% 20% ..



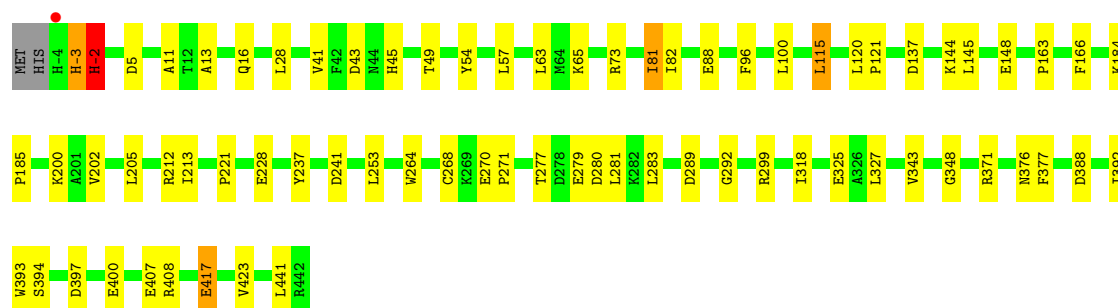
- Molecule 1: Beta-glycosidase

Chain K:  83% 16%



- Molecule 1: Beta-glycosidase

Chain L:  83% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.18Å 139.49Å 172.66Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	114.28 – 2.50 114.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (114.28-2.50) 96.9 (114.28-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.169 , 0.182 0.173 , 0.185	Depositor DCC
R_{free} test set	10744 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	46238	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/3745	0.55	0/5078
1	B	0.36	0/3732	0.54	0/5061
1	C	0.32	0/3688	0.51	0/5001
1	D	0.31	0/3677	0.49	0/4987
1	E	0.33	0/3732	0.52	0/5061
1	F	0.35	0/3732	0.53	0/5061
1	G	0.33	0/3677	0.52	0/4986
1	H	0.35	0/3666	0.54	0/4972
1	I	0.33	0/3677	0.51	0/4987
1	J	0.32	0/3677	0.51	0/4987
1	K	0.35	0/3732	0.55	0/5061
1	L	0.34	0/3732	0.53	0/5061
All	All	0.34	0/44467	0.53	0/60303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3631	0	3431	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3618	0	3420	46	0
1	C	3578	0	3392	52	0
1	D	3567	0	3379	65	0
1	E	3618	0	3420	51	0
1	F	3618	0	3420	49	0
1	G	3568	0	3385	48	0
1	H	3557	0	3372	46	0
1	I	3567	0	3379	67	0
1	J	3567	0	3379	70	0
1	K	3618	0	3420	46	0
1	L	3618	0	3420	44	0
2	A	6	8	8	0	0
2	B	6	8	7	0	0
2	C	6	8	8	0	0
2	D	6	8	7	0	0
2	E	6	8	8	1	0
2	F	6	8	8	4	0
2	G	6	8	8	1	0
2	H	6	8	8	0	0
2	I	6	8	8	0	0
2	J	6	8	7	1	0
2	K	6	8	7	1	0
2	L	6	8	8	0	0
3	A	265	0	0	7	0
3	B	288	0	0	6	0
3	C	220	0	0	5	0
3	D	191	0	0	4	0
3	E	251	0	0	8	0
3	F	253	0	0	2	0
3	G	226	0	0	9	0
3	H	265	0	0	3	0
3	I	215	0	0	2	0
3	J	224	0	0	6	0
3	K	272	0	0	7	0
3	L	275	0	0	3	0
All	All	46142	96	40909	612	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 7.

All (612) 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:J:215:ILE:HD13	1:J:256:MET:HE1	1.15	1.13
1:I:81:ILE:HD12	1:I:94:LEU:HD23	1.43	0.99
1:J:162:GLU:HG2	1:J:218:ALA:HB2	1.48	0.94
1:C:162:GLU:HG2	1:C:218:ALA:HB2	1.51	0.93
1:I:162:GLU:HG2	1:I:218:ALA:HB2	1.49	0.92
1:E:81:ILE:HD12	1:E:94:LEU:HD23	1.55	0.87
1:C:264:TRP:O	1:C:267:GLU:HG3	1.78	0.83
1:A:307:ARG:HD3	3:A:630:HOH:O	1.81	0.81
1:D:120:LEU:HD12	1:D:121:PRO:HD2	1.63	0.81
1:B:144:LYS:HE3	1:B:148:GLU:OE2	1.83	0.79
1:A:441:LEU:O	1:A:442:ARG:HB2	1.82	0.78
1:E:266:TYR:OH	1:E:281:LEU:HD11	1.83	0.78
1:D:81:ILE:HG22	1:D:82:ILE:HG13	1.65	0.76
1:J:120:LEU:HD12	1:J:121:PRO:HD2	1.67	0.76
1:L:-3:HIS:O	1:L:-2:HIS:HB2	1.86	0.75
1:D:356:SER:HB2	1:D:358:ASP:OD1	1.88	0.74
1:D:433:VAL:HG22	1:D:441:LEU:HD23	1.70	0.74
1:C:370:LEU:HD21	1:C:392:ILE:HD12	1.69	0.74
1:I:310:LYS:NZ	1:L:417:GLU:HG3	2.03	0.74
1:G:259:GLY:O	1:G:281:LEU:HD13	1.87	0.73
1:H:81:ILE:HD12	1:H:94:LEU:HG	1.70	0.73
1:F:417:GLU:HG3	1:G:310:LYS:HE3	1.71	0.72
1:I:81:ILE:HD12	1:I:94:LEU:CD2	2.18	0.71
1:E:318:ILE:HD12	1:E:407:GLU:HG3	1.71	0.71
1:J:371:ARG:HG3	1:J:441:LEU:HD22	1.74	0.70
1:A:353:ASP:OD2	1:A:366:ARG:NH2	2.22	0.70
1:H:81:ILE:HG22	1:H:82:ILE:HG13	1.73	0.68
1:E:311:THR:HB	3:E:692:HOH:O	1.93	0.67
1:F:360:LYS:HE3	3:F:823:HOH:O	1.93	0.67
1:D:436:SER:HB2	1:D:439:GLU:HB3	1.76	0.67
1:A:209:GLU:HG3	3:A:775:HOH:O	1.96	0.66
1:D:293:MET:HE2	1:D:295:ILE:HD11	1.76	0.66
1:E:371:ARG:HG3	1:E:441:LEU:HD22	1.76	0.66
1:B:162:GLU:HG2	1:B:218:ALA:HB2	1.76	0.66
1:F:10:THR:OG1	1:F:395:PHE:HB2	1.97	0.64
1:I:100:LEU:HD23	1:I:100:LEU:C	2.23	0.64
1:E:10:THR:HG22	1:E:392:ILE:CG2	2.27	0.64
1:L:81:ILE:HG22	1:L:82:ILE:HG13	1.79	0.64
1:H:24:ASP:CA	1:H:92:LYS:HE3	2.27	0.64
1:D:57:LEU:HB2	3:D:636:HOH:O	1.97	0.64
1:G:440:ASN:O	1:G:441:LEU:HD23	1.97	0.64
1:G:364:PRO:HD3	3:G:707:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LYS:HE2	1:E:148:GLU:OE2	1.98	0.63
1:I:215:ILE:CD1	1:I:256:MET:HE1	2.27	0.63
1:D:440:ASN:CG	1:D:441:LEU:H	2.05	0.63
1:I:209:GLU:HG3	3:I:766:HOH:O	1.96	0.63
1:H:10:THR:HG22	1:H:392:ILE:CG2	2.28	0.63
1:I:392:ILE:HD12	1:I:430:TYR:CE2	2.32	0.63
1:K:271:PRO:HB2	1:L:28:LEU:HD11	1.79	0.63
1:L:241:ASP:HB2	1:L:264:TRP:CD1	2.33	0.62
1:E:327:LEU:HD22	1:E:373:TYR:HB3	1.81	0.62
1:A:374:LEU:HB3	1:A:441:LEU:CD1	2.30	0.62
1:C:423:VAL:HG13	1:C:427:ALA:HB3	1.81	0.62
1:C:81:ILE:HG22	1:C:82:ILE:HG13	1.81	0.62
1:K:77:SER:HB3	1:K:80:ARG:HB2	1.80	0.62
1:H:23:GLU:HG3	3:H:744:HOH:O	2.00	0.61
1:G:378:ARG:NH2	1:G:441:LEU:O	2.31	0.61
1:J:353:ASP:OD2	1:J:366:ARG:NH2	2.33	0.61
1:J:378:ARG:O	1:J:382:GLU:HG3	2.01	0.61
1:C:209:GLU:HG3	3:C:633:HOH:O	2.01	0.61
1:E:308:LYS:NZ	1:H:43:ASP:HB3	2.16	0.61
1:J:89:VAL:CG1	1:J:94:LEU:HD11	2.30	0.61
1:L:212:ARG:HA	1:L:289:ASP:OD2	2.00	0.61
1:E:423:VAL:HG13	1:E:427:ALA:HB3	1.82	0.61
1:I:162:GLU:CG	1:I:218:ALA:HB2	2.29	0.61
1:I:34:PHE:CE1	1:I:40:LYS:HD2	2.35	0.60
1:E:162:GLU:HG2	1:E:218:ALA:HB2	1.83	0.60
1:I:310:LYS:HZ3	1:L:417:GLU:HG3	1.66	0.60
1:H:356:SER:HB3	1:H:358:ASP:OD1	2.01	0.60
1:I:0:HIS:O	1:I:1:SER:HB2	2.00	0.60
1:L:120:LEU:HD12	1:L:121:PRO:HD2	1.82	0.60
1:A:374:LEU:HB3	1:A:441:LEU:HD11	1.84	0.60
1:E:245:PHE:CG	1:E:246:PRO:HD3	2.36	0.59
1:J:89:VAL:HG11	1:J:94:LEU:HD11	1.82	0.59
1:D:436:SER:O	1:D:439:GLU:HB2	2.01	0.59
1:K:162:GLU:HG2	1:K:218:ALA:HB2	1.83	0.59
1:D:370:LEU:CD2	1:D:392:ILE:HD12	2.33	0.59
1:J:81:ILE:HD11	1:J:97:TYR:HD2	1.67	0.59
1:B:423:VAL:HG13	1:B:427:ALA:HB3	1.84	0.59
1:E:181:ARG:HD3	3:E:665:HOH:O	2.03	0.59
1:D:436:SER:HB2	1:D:439:GLU:CB	2.32	0.59
1:E:110:LYS:HE2	1:E:156:ASP:OD1	2.03	0.59
1:F:371:ARG:HG3	1:F:441:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:ILE:HD11	1:H:94:LEU:HA	1.85	0.59
1:I:266:TYR:OH	1:I:281:LEU:HD11	2.03	0.58
1:F:267:GLU:O	1:F:269:LYS:HE2	2.04	0.58
1:I:215:ILE:HG12	1:I:256:MET:HE1	1.85	0.58
1:K:212:ARG:HA	1:K:289:ASP:OD2	2.04	0.58
1:G:293:MET:HE3	1:G:334:TYR:CE2	2.39	0.58
1:H:24:ASP:C	1:H:92:LYS:HE3	2.29	0.58
1:H:9:GLY:O	1:H:392:ILE:HG22	2.04	0.57
1:H:266:TYR:OH	1:H:281:LEU:HD11	2.04	0.57
1:K:293:MET:HE2	1:K:295:ILE:HD11	1.84	0.57
1:C:327:LEU:HD23	1:C:377:PHE:HB2	1.86	0.57
1:J:266:TYR:OH	1:J:281:LEU:HD11	2.05	0.57
1:L:268:CYS:SG	1:L:270:GLU:OE1	2.62	0.57
1:I:89:VAL:HG11	1:I:94:LEU:HD11	1.87	0.57
1:E:163:PRO:HA	1:E:166:PHE:CE2	2.39	0.57
1:F:423:VAL:CG1	1:F:427:ALA:HB3	2.35	0.57
1:B:67:LEU:HD22	1:B:427:ALA:HB1	1.86	0.57
1:F:65:LYS:HD2	1:F:107:ARG:HB3	1.86	0.57
3:B:669:HOH:O	1:L:88:GLU:HG3	2.05	0.56
1:J:81:ILE:HD11	1:J:97:TYR:CD2	2.40	0.56
1:B:215:ILE:HD13	1:B:256:MET:HE1	1.86	0.56
1:B:140:ALA:HB2	1:B:200:LYS:HB3	1.86	0.56
1:D:378:ARG:O	1:D:382:GLU:HG3	2.05	0.56
1:K:28:LEU:HD11	1:L:271:PRO:HB2	1.86	0.56
1:F:16:GLN:O	1:F:398:ASN:HB2	2.06	0.56
1:L:137:ASP:OD1	1:L:200:LYS:NZ	2.32	0.56
1:A:16:GLN:O	1:A:398:ASN:HB2	2.06	0.56
1:I:423:VAL:HG13	1:I:427:ALA:HB3	1.88	0.56
1:A:26:LYS:HD2	1:A:80:ARG:HG3	1.88	0.56
1:A:52:ASP:O	1:A:56:ARG:HG3	2.05	0.56
1:I:357:SER:HB3	1:L:371:ARG:NH2	2.21	0.56
1:A:372:GLU:CD	1:D:354:ARG:HH22	2.14	0.56
1:J:140:ALA:HB2	1:J:200:LYS:HB3	1.87	0.56
1:A:245:PHE:CG	1:A:246:PRO:HD3	2.40	0.55
1:D:120:LEU:HD12	1:D:121:PRO:CD	2.33	0.55
1:E:271:PRO:HB2	1:F:28:LEU:HD11	1.88	0.55
1:J:196:LYS:NZ	3:J:606:HOH:O	2.39	0.55
1:I:271:PRO:HB2	1:J:28:LEU:HD11	1.88	0.55
1:C:294:ASN:CG	1:C:346:GLU:HB2	2.31	0.55
1:C:403:ASP:O	1:C:406:LYS:HG2	2.05	0.55
1:F:296:TYR:OH	1:F:346:GLU:OE1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:TYR:HB2	1:H:311:THR:HG22	1.88	0.55
1:E:423:VAL:CG1	1:E:427:ALA:HB3	2.37	0.55
1:C:16:GLN:O	1:C:398:ASN:HB2	2.06	0.55
1:E:245:PHE:CD2	1:E:246:PRO:HD3	2.41	0.55
1:B:65:LYS:NZ	3:B:605:HOH:O	2.36	0.55
1:C:65:LYS:HE3	1:C:107:ARG:O	2.07	0.55
1:I:371:ARG:O	1:I:375:GLN:HG3	2.07	0.55
1:J:11:ALA:O	1:J:394:SER:HB2	2.06	0.55
1:K:127:LYS:HE3	3:K:780:HOH:O	2.06	0.55
2:J:501:GOL:H31	3:J:689:HOH:O	2.07	0.55
1:K:117:HIS:O	1:K:118:TRP:HB2	2.07	0.55
1:B:393:TRP:CE2	1:B:394:SER:HB2	2.41	0.54
1:C:212:ARG:NH2	1:C:388:ASP:OD2	2.39	0.54
1:I:292:GLY:HA2	1:I:343:VAL:O	2.08	0.54
1:K:277:THR:O	1:K:280:ASP:HB2	2.08	0.54
1:L:200:LYS:HG3	1:L:283:LEU:HD21	1.88	0.54
1:C:186:GLU:O	1:C:190:ILE:HG13	2.08	0.54
1:F:209:GLU:HG3	3:F:704:HOH:O	2.08	0.54
1:E:308:LYS:HZ1	1:H:43:ASP:HB3	1.72	0.54
1:B:23:GLU:HG3	3:B:732:HOH:O	2.08	0.54
1:E:26:LYS:HE3	3:E:722:HOH:O	2.08	0.54
1:G:260:ARG:HA	1:G:281:LEU:HD13	1.90	0.54
1:I:215:ILE:HD13	1:I:256:MET:HE1	1.89	0.54
1:G:203:LEU:HD23	3:G:748:HOH:O	2.08	0.54
1:H:172:LEU:HD13	1:H:187:LEU:HD11	1.89	0.54
1:C:162:GLU:CG	1:C:218:ALA:HB2	2.33	0.54
1:I:168:GLY:O	1:I:172:LEU:HB3	2.08	0.54
1:I:294:ASN:CG	1:I:346:GLU:HB2	2.33	0.54
1:D:10:THR:OG1	1:D:395:PHE:HB2	2.08	0.54
1:L:65:LYS:HG3	3:L:613:HOH:O	2.07	0.53
1:F:13:ALA:HB2	1:F:117:HIS:CE1	2.42	0.53
1:I:253:LEU:HD13	1:I:334:TYR:CE2	2.42	0.53
1:F:184:LYS:HB3	1:F:185:PRO:HD3	1.89	0.53
1:F:5:ASP:OD1	1:F:5:ASP:N	2.38	0.53
1:A:68:GLY:HA3	3:A:729:HOH:O	2.07	0.53
1:L:144:LYS:O	1:L:148:GLU:HG3	2.08	0.53
1:B:110:LYS:HG2	3:B:695:HOH:O	2.09	0.53
1:C:117:HIS:O	1:C:118:TRP:HB2	2.09	0.53
1:A:442:ARG:HD3	3:A:762:HOH:O	2.09	0.53
1:D:250:ALA:O	1:D:254:ASP:HB2	2.08	0.53
1:D:268:CYS:SG	1:D:270:GLU:OE1	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:LYS:HZ2	1:L:417:GLU:HG3	1.71	0.53
1:L:81:ILE:CG2	1:L:145:LEU:HD23	2.38	0.53
1:H:24:ASP:CB	1:H:92:LYS:HE3	2.38	0.53
1:D:245:PHE:CG	1:D:246:PRO:HD3	2.43	0.53
1:L:371:ARG:HG3	1:L:441:LEU:HD22	1.91	0.53
1:D:370:LEU:HD21	1:D:392:ILE:HD12	1.89	0.52
1:G:327:LEU:HD23	1:G:377:PHE:HB2	1.90	0.52
1:I:215:ILE:CG1	1:I:256:MET:HE1	2.39	0.52
1:I:81:ILE:HG22	1:I:82:ILE:HG13	1.92	0.52
1:J:245:PHE:CD1	1:J:246:PRO:HD3	2.45	0.52
1:D:16:GLN:O	1:D:398:ASN:HB2	2.10	0.52
1:G:293:MET:HE3	1:G:334:TYR:CD2	2.45	0.52
1:E:315:ARG:NE	3:E:615:HOH:O	2.42	0.52
1:I:81:ILE:CD1	1:I:94:LEU:HD23	2.30	0.52
1:K:140:ALA:HB2	1:K:200:LYS:HB3	1.92	0.52
1:A:81:ILE:HD12	1:A:94:LEU:HD23	1.92	0.52
1:H:24:ASP:HB3	1:H:92:LYS:HE3	1.91	0.52
1:K:7:ILE:HB	1:K:389:GLY:HA3	1.92	0.52
1:K:279:GLU:H	1:K:279:GLU:CD	2.17	0.52
1:C:7:ILE:HB	1:C:389:GLY:HA3	1.91	0.52
1:J:245:PHE:CG	1:J:246:PRO:HD3	2.45	0.51
1:B:260:ARG:CZ	1:K:279:GLU:HG2	2.41	0.51
1:H:88:GLU:OE2	1:K:262:PRO:HA	2.10	0.51
1:H:327:LEU:HD23	1:H:377:PHE:HB2	1.92	0.51
1:C:441:LEU:O	1:C:442:ARG:HD3	2.09	0.51
1:G:266:TYR:OH	1:G:281:LEU:HD11	2.09	0.51
1:I:100:LEU:HD23	1:I:100:LEU:O	2.11	0.51
1:I:392:ILE:HD12	1:I:430:TYR:CD2	2.45	0.51
1:J:336:GLU:O	1:J:339:LYS:HE2	2.11	0.51
1:E:212:ARG:HA	1:E:289:ASP:OD2	2.10	0.51
1:C:81:ILE:HD11	1:C:97:TYR:CD2	2.46	0.51
1:C:313:MET:O	1:C:315:ARG:HG3	2.11	0.51
1:A:140:ALA:HB2	1:A:200:LYS:HB3	1.92	0.51
1:G:39:GLY:HA2	3:G:715:HOH:O	2.11	0.51
1:G:423:VAL:CG1	1:G:427:ALA:HB3	2.40	0.51
1:H:73:ARG:NH2	1:H:161:ASN:OD1	2.36	0.51
1:D:188:MET:CE	1:D:265:VAL:HG13	2.41	0.51
1:I:289:ASP:O	1:I:341:PRO:HD2	2.11	0.51
1:K:423:VAL:HG12	1:K:427:ALA:HB3	1.93	0.51
1:A:23:GLU:HG3	3:A:751:HOH:O	2.10	0.50
1:J:0:HIS:O	1:J:1:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PHE:CE2	1:A:40:LYS:HB3	2.46	0.50
1:D:198:HIS:O	1:D:202:VAL:HG23	2.11	0.50
1:E:131:LEU:HD21	1:E:186:GLU:HB3	1.93	0.50
1:F:140:ALA:HB2	1:F:200:LYS:HB3	1.92	0.50
1:J:198:HIS:CD2	1:J:256:MET:HE2	2.47	0.50
1:F:403:ASP:O	1:F:406:LYS:HG2	2.11	0.50
1:K:94:LEU:HD22	1:K:149:GLN:HG3	1.94	0.50
1:C:202:VAL:HG22	1:C:213:ILE:HG21	1.94	0.49
1:K:168:GLY:O	1:K:172:LEU:HB3	2.12	0.49
1:H:24:ASP:CG	1:H:92:LYS:HD2	2.36	0.49
1:J:440:ASN:O	1:J:441:LEU:HG	2.13	0.49
1:A:87:GLY:HA3	3:A:746:HOH:O	2.12	0.49
1:E:370:LEU:HD21	1:E:392:ILE:HD12	1.93	0.49
1:J:0:HIS:O	1:J:1:SER:CB	2.60	0.49
1:K:5:ASP:OD1	1:K:5:ASP:N	2.45	0.49
1:A:163:PRO:HA	1:A:166:PHE:CE2	2.48	0.49
1:E:430:TYR:O	1:E:434:ILE:HG13	2.13	0.49
1:G:260:ARG:HA	1:G:281:LEU:CD1	2.42	0.49
1:J:293:MET:HE3	1:J:334:TYR:CE2	2.47	0.49
1:C:73:ARG:NH1	1:C:346:GLU:HG3	2.27	0.49
1:A:283:LEU:O	1:A:286:GLN:HG2	2.12	0.49
1:D:288:ILE:O	1:D:340:LYS:NZ	2.35	0.49
1:G:400:GLU:OE2	2:G:501:GOL:H31	2.12	0.49
1:J:162:GLU:CG	1:J:218:ALA:HB2	2.32	0.49
1:C:57:LEU:HB2	3:C:735:HOH:O	2.11	0.49
1:F:81:ILE:HG22	1:F:145:LEU:CD2	2.43	0.49
1:K:203:LEU:HG	1:K:286:GLN:HG3	1.94	0.49
1:E:140:ALA:HB2	1:E:200:LYS:HB3	1.95	0.49
1:G:57:LEU:HB2	3:G:635:HOH:O	2.12	0.49
1:J:61:LEU:HD22	1:J:104:LEU:HD23	1.94	0.49
1:J:198:HIS:CG	1:J:256:MET:HE2	2.48	0.49
1:G:115:LEU:HD21	1:G:146:ILE:HG21	1.95	0.48
1:C:277:THR:O	1:C:280:ASP:HB2	2.13	0.48
1:E:429:TRP:O	1:E:433:VAL:HG23	2.14	0.48
1:J:8:TRP:HB3	1:J:434:ILE:HG12	1.94	0.48
1:E:162:GLU:OE1	2:E:501:GOL:H11	2.13	0.48
1:L:13:ALA:HB3	1:L:16:GLN:HG3	1.95	0.48
1:A:313:MET:HE3	1:A:322:VAL:O	2.14	0.48
1:C:378:ARG:NH1	1:C:441:LEU:HB2	2.28	0.48
1:I:268:CYS:HB3	1:I:270:GLU:OE1	2.14	0.48
1:B:122:TYR:CE2	1:B:126:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:ILE:O	1:F:392:ILE:HG22	2.12	0.48
1:K:162:GLU:CG	1:K:218:ALA:HB2	2.44	0.48
1:B:215:ILE:CD1	1:B:256:MET:HE1	2.42	0.48
1:D:440:ASN:OD1	1:D:441:LEU:N	2.41	0.48
1:D:147:LYS:NZ	3:D:606:HOH:O	2.46	0.48
1:H:57:LEU:HD11	1:H:100:LEU:HD12	1.95	0.48
1:L:348:GLY:HA3	1:L:393:TRP:O	2.14	0.48
1:B:283:LEU:O	1:B:286:GLN:HG2	2.14	0.48
1:C:283:LEU:O	1:C:286:GLN:HG2	2.13	0.48
1:B:97:TYR:O	1:B:101:ILE:HG13	2.13	0.48
1:G:310:LYS:HG2	1:G:311:THR:O	2.14	0.48
1:J:349:MET:O	1:J:366:ARG:NH1	2.46	0.48
1:H:423:VAL:CG1	1:H:427:ALA:HB3	2.44	0.47
1:A:393:TRP:HA	1:A:394:SER:HA	1.68	0.47
1:C:200:LYS:HG2	1:C:283:LEU:HD11	1.96	0.47
1:C:419:GLN:OE1	1:C:419:GLN:HA	2.14	0.47
1:C:166:PHE:HA	3:C:692:HOH:O	2.14	0.47
1:A:310:LYS:HD2	1:D:417:GLU:OE2	2.14	0.47
1:E:348:GLY:HA3	1:E:393:TRP:O	2.14	0.47
1:F:81:ILE:CG2	1:F:145:LEU:HD21	2.44	0.47
1:H:7:ILE:HG23	1:H:71:SER:HB2	1.95	0.47
1:J:164:GLN:HG3	1:J:252:TRP:CD1	2.49	0.47
1:K:118:TRP:CH2	1:K:165:VAL:HG11	2.49	0.47
1:K:212:ARG:NH2	3:K:617:HOH:O	2.47	0.47
1:H:268:CYS:SG	1:H:270:GLU:OE1	2.72	0.47
1:K:16:GLN:O	1:K:398:ASN:HB2	2.14	0.47
1:A:1:SER:HB2	1:A:378:ARG:HG2	1.96	0.47
1:F:370:LEU:HD13	1:F:392:ILE:HD11	1.97	0.47
1:B:423:VAL:CG1	1:B:427:ALA:HB3	2.45	0.47
1:B:115:LEU:N	1:B:115:LEU:HD23	2.30	0.47
1:A:327:LEU:HD12	1:A:327:LEU:HA	1.65	0.47
1:B:356:SER:HB3	1:B:358:ASP:OD1	2.14	0.47
1:F:400:GLU:OE1	2:F:501:GOL:O1	2.32	0.47
1:G:350:ALA:HA	1:G:408:ARG:O	2.15	0.47
1:L:81:ILE:N	1:L:81:ILE:HD13	2.30	0.47
1:L:277:THR:O	1:L:280:ASP:HB2	2.15	0.47
1:A:206:ARG:CZ	1:A:213:ILE:HD12	2.45	0.47
1:H:324:PRO:HB3	1:H:372:GLU:HB3	1.96	0.47
1:I:202:VAL:HG22	1:I:213:ILE:HG21	1.97	0.47
1:A:348:GLY:HA3	1:A:393:TRP:O	2.14	0.46
1:B:16:GLN:O	1:B:398:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:HIS:O	1:D:118:TRP:HB2	2.15	0.46
1:E:73:ARG:NH1	1:E:346:GLU:HG3	2.30	0.46
1:F:215:ILE:HG13	1:F:216:SER:N	2.30	0.46
1:G:140:ALA:HB2	1:G:200:LYS:HB3	1.96	0.46
1:J:120:LEU:HD12	1:J:121:PRO:CD	2.41	0.46
1:C:162:GLU:CD	1:C:294:ASN:HD22	2.23	0.46
1:I:423:VAL:CG1	1:I:427:ALA:HB3	2.45	0.46
1:L:318:ILE:HD12	1:L:407:GLU:HG3	1.97	0.46
1:A:69:VAL:HA	1:A:434:ILE:HD13	1.96	0.46
1:B:89:VAL:HG11	1:B:94:LEU:HD11	1.97	0.46
1:B:163:PRO:HA	1:B:166:PHE:CE2	2.51	0.46
1:E:397:ASP:OD2	1:E:413:TYR:HA	2.15	0.46
1:I:313:MET:O	1:I:315:ARG:HG3	2.14	0.46
1:J:293:MET:HE3	1:J:334:TYR:CD2	2.50	0.46
1:B:292:GLY:HA2	1:B:343:VAL:O	2.15	0.46
1:G:13:ALA:HB2	1:G:117:HIS:CE1	2.50	0.46
1:J:198:HIS:O	1:J:202:VAL:HG23	2.16	0.46
1:E:2:PHE:CZ	1:E:378:ARG:HG2	2.50	0.46
1:G:81:ILE:HD11	1:G:97:TYR:HD2	1.81	0.46
1:H:16:GLN:O	1:H:398:ASN:HB2	2.16	0.46
1:J:100:LEU:C	1:J:100:LEU:HD23	2.40	0.46
1:C:271:PRO:HB2	1:D:28:LEU:HD11	1.98	0.46
1:E:338:TYR:HB2	3:E:727:HOH:O	2.15	0.46
1:F:401:TRP:HE1	2:F:501:GOL:H12	1.80	0.46
1:A:245:PHE:CD2	1:A:246:PRO:HD3	2.50	0.46
1:I:23:GLU:HG3	3:I:718:HOH:O	2.15	0.46
1:J:100:LEU:HD23	1:J:100:LEU:O	2.16	0.46
1:F:3:LYS:NZ	1:F:386:ASP:OD1	2.35	0.46
1:F:81:ILE:HG22	1:F:145:LEU:HD21	1.97	0.46
1:H:131:LEU:HD21	1:H:186:GLU:HB3	1.98	0.46
1:H:423:VAL:HG13	1:H:427:ALA:HB3	1.97	0.46
1:K:406:LYS:HD3	3:K:646:HOH:O	2.15	0.46
1:I:327:LEU:HD22	1:I:373:TYR:HB3	1.98	0.46
1:E:81:ILE:HD12	1:E:94:LEU:CD2	2.37	0.46
1:I:242:HIS:CE1	1:I:244:ALA:HB3	2.51	0.46
1:I:393:TRP:CD2	1:I:394:SER:HB2	2.51	0.46
1:J:347:ASN:O	1:J:392:ILE:HA	2.16	0.46
1:K:202:VAL:O	1:K:206:ARG:HG2	2.16	0.46
1:I:393:TRP:HA	1:I:394:SER:HA	1.61	0.45
1:I:410:GLY:O	1:I:424:LYS:HD2	2.17	0.45
1:I:414:ASN:OD1	1:I:421:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:LYS:HD3	1:J:270:GLU:OE2	2.16	0.45
1:L:202:VAL:HG22	1:L:213:ILE:HG21	1.98	0.45
1:H:24:ASP:O	1:H:92:LYS:HE3	2.15	0.45
1:I:162:GLU:HG2	1:I:218:ALA:CB	2.36	0.45
1:A:423:VAL:HG13	1:A:427:ALA:HB3	1.96	0.45
1:E:313:MET:HE1	3:E:770:HOH:O	2.15	0.45
1:F:294:ASN:CG	1:F:346:GLU:HB2	2.41	0.45
1:G:168:GLY:O	1:G:172:LEU:HB3	2.16	0.45
1:G:294:ASN:CG	1:G:346:GLU:HB2	2.40	0.45
1:I:393:TRP:CE2	1:I:394:SER:HB2	2.51	0.45
1:J:407:GLU:OE2	1:K:315:ARG:NH1	2.43	0.45
1:G:128:GLY:HA2	3:H:741:HOH:O	2.16	0.45
1:G:165:VAL:O	1:G:169:CYS:HB2	2.17	0.45
1:G:242:HIS:HB2	1:G:243:PRO:CD	2.46	0.45
1:J:440:ASN:O	1:J:440:ASN:CG	2.59	0.45
1:L:41:VAL:HG11	1:L:45:HIS:O	2.16	0.45
1:F:292:GLY:HA2	1:F:343:VAL:O	2.17	0.45
1:F:401:TRP:NE1	2:F:501:GOL:H12	2.31	0.45
1:F:401:TRP:CD1	2:F:501:GOL:H12	2.51	0.45
1:K:164:GLN:HA	1:K:246:PRO:O	2.16	0.45
1:L:-3:HIS:O	1:L:-2:HIS:CB	2.63	0.45
1:A:361:VAL:HG11	1:A:424:LYS:HG2	1.99	0.45
1:B:101:ILE:HD13	1:B:154:VAL:CG2	2.46	0.45
1:H:260:ARG:HG2	1:H:261:TYR:O	2.15	0.45
1:L:184:LYS:HB3	1:L:185:PRO:CD	2.46	0.45
1:C:325:GLU:HA	1:C:376:ASN:OD1	2.17	0.45
1:C:393:TRP:HA	1:C:394:SER:HA	1.70	0.45
1:D:166:PHE:HA	3:D:747:HOH:O	2.15	0.45
1:D:423:VAL:CG1	1:D:427:ALA:HB3	2.47	0.45
1:H:212:ARG:HA	1:H:289:ASP:OD2	2.17	0.45
1:L:397:ASP:CG	1:L:408:ARG:HB3	2.42	0.45
1:B:198:HIS:CG	1:B:256:MET:HE2	2.52	0.45
1:B:393:TRP:HA	1:B:394:SER:HA	1.70	0.45
1:G:212:ARG:NH2	1:G:388:ASP:OD2	2.50	0.45
1:I:73:ARG:HA	1:I:112:CYS:O	2.17	0.45
1:I:366:ARG:O	1:I:370:LEU:HG	2.17	0.45
1:J:423:VAL:HG13	1:J:427:ALA:HB3	1.99	0.45
1:B:110:LYS:NZ	3:B:622:HOH:O	2.49	0.45
1:D:393:TRP:HA	1:D:394:SER:HA	1.60	0.45
1:D:394:SER:O	1:D:410:GLY:HA2	2.16	0.45
1:F:26:LYS:HD2	1:F:80:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:LEU:HD23	1:F:67:LEU:HA	1.77	0.45
1:G:407:GLU:HA	3:G:646:HOH:O	2.16	0.45
1:J:226:SER:HB2	3:J:681:HOH:O	2.17	0.45
1:A:89:VAL:HG11	1:A:94:LEU:HD11	1.98	0.45
1:A:256:MET:HE3	1:A:256:MET:HB2	1.89	0.45
1:B:81:ILE:HD11	1:B:97:TYR:HD2	1.82	0.45
1:D:23:GLU:HG3	3:D:713:HOH:O	2.17	0.45
1:D:245:PHE:CD2	1:D:246:PRO:HD3	2.52	0.45
1:E:24:ASP:OD2	1:E:54:TYR:OH	2.33	0.45
1:L:325:GLU:HA	1:L:376:ASN:OD1	2.17	0.45
1:D:440:ASN:CG	1:D:441:LEU:N	2.73	0.44
1:F:430:TYR:CE2	1:F:434:ILE:HD11	2.53	0.44
1:J:117:HIS:O	1:J:118:TRP:HB2	2.17	0.44
1:F:162:GLU:HG2	1:F:218:ALA:HB2	1.98	0.44
1:B:198:HIS:O	1:B:202:VAL:HG23	2.17	0.44
1:D:294:ASN:CG	1:D:346:GLU:HB2	2.42	0.44
1:J:372:GLU:HG3	3:J:601:HOH:O	2.17	0.44
1:K:2:PHE:CE2	1:K:378:ARG:HG3	2.53	0.44
1:B:296:TYR:OH	1:B:346:GLU:OE1	2.32	0.44
1:F:61:LEU:HD22	1:F:104:LEU:HD23	1.99	0.44
1:H:393:TRP:HA	1:H:394:SER:HA	1.72	0.44
1:I:8:TRP:CB	1:I:434:ILE:HG12	2.48	0.44
1:L:212:ARG:NH2	1:L:388:ASP:OD2	2.51	0.44
1:B:228:GLU:H	1:B:228:GLU:HG3	1.42	0.44
1:C:407:GLU:HA	1:C:407:GLU:OE1	2.17	0.44
1:G:198:HIS:O	1:G:202:VAL:HG23	2.17	0.44
1:H:8:TRP:HB3	1:H:434:ILE:HG12	1.99	0.44
1:J:13:ALA:HB2	1:J:117:HIS:CE1	2.53	0.44
1:J:415:ASP:O	1:J:419:GLN:N	2.51	0.44
1:L:221:PRO:HA	1:L:237:TYR:CE1	2.52	0.44
1:C:42:PHE:CE1	1:C:406:LYS:HE3	2.53	0.44
1:D:41:VAL:O	1:D:42:PHE:C	2.61	0.44
1:D:162:GLU:CD	1:D:294:ASN:HD22	2.25	0.44
1:E:245:PHE:N	1:E:246:PRO:CD	2.80	0.44
1:J:8:TRP:CG	1:J:434:ILE:HG12	2.52	0.44
1:C:42:PHE:CG	1:C:406:LYS:HD2	2.52	0.44
1:C:370:LEU:CD2	1:C:392:ILE:HD12	2.45	0.44
1:D:64:MET:O	1:D:67:LEU:HB2	2.17	0.44
1:I:361:VAL:HG11	1:I:424:LYS:HG2	1.99	0.44
1:L:163:PRO:HA	1:L:166:PHE:CE2	2.53	0.44
1:D:170:GLY:HA2	1:D:176:HIS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:PHE:CG	1:F:246:PRO:HD3	2.53	0.44
1:K:250:ALA:O	1:K:254:ASP:HB2	2.18	0.44
1:G:184:LYS:O	1:G:188:MET:HG3	2.18	0.44
1:J:215:ILE:HG13	1:J:216:SER:N	2.33	0.44
1:J:253:LEU:HD13	1:J:334:TYR:CE2	2.52	0.44
1:L:11:ALA:HA	1:L:73:ARG:O	2.18	0.44
1:L:81:ILE:HG22	1:L:145:LEU:HD23	1.99	0.44
1:I:8:TRP:HB3	1:I:434:ILE:HG12	1.99	0.43
1:E:73:ARG:NH2	1:E:161:ASN:OD1	2.42	0.43
1:E:393:TRP:HA	1:E:394:SER:HA	1.64	0.43
1:F:81:ILE:CG2	1:F:145:LEU:CD2	2.96	0.43
1:H:13:ALA:HB2	1:H:117:HIS:CE1	2.54	0.43
1:H:65:LYS:HD3	1:H:107:ARG:HB3	2.00	0.43
1:L:115:LEU:N	1:L:115:LEU:HD23	2.33	0.43
1:D:81:ILE:CG2	1:D:145:LEU:HD23	2.49	0.43
1:E:120:LEU:HD12	1:E:121:PRO:HD2	2.00	0.43
1:G:245:PHE:CG	1:G:246:PRO:HD3	2.53	0.43
1:H:11:ALA:HA	1:H:73:ARG:O	2.18	0.43
1:J:158:ILE:HA	1:J:214:GLY:O	2.17	0.43
1:J:281:LEU:HD23	1:J:281:LEU:HA	1.89	0.43
1:D:293:MET:CE	1:D:295:ILE:HD11	2.43	0.43
1:G:16:GLN:O	1:G:398:ASN:HB2	2.18	0.43
1:H:198:HIS:O	1:H:202:VAL:HG23	2.18	0.43
1:J:170:GLY:HA2	1:J:176:HIS:O	2.18	0.43
1:D:162:GLU:HG2	1:D:218:ALA:HB2	2.00	0.43
1:E:54:TYR:HA	1:E:96:PHE:CE1	2.53	0.43
1:F:423:VAL:HG12	1:F:427:ALA:HB3	1.99	0.43
1:I:281:LEU:HA	1:I:281:LEU:HD23	1.82	0.43
1:I:397:ASP:OD2	1:I:413:TYR:HA	2.19	0.43
1:A:165:VAL:O	1:A:169:CYS:HB2	2.18	0.43
1:B:164:GLN:HB2	1:B:218:ALA:HB3	1.99	0.43
1:B:328:TYR:HB2	1:B:376:ASN:HB3	2.01	0.43
1:C:245:PHE:N	1:C:246:PRO:CD	2.81	0.43
1:F:8:TRP:HB3	1:F:434:ILE:HG12	1.99	0.43
1:F:423:VAL:HG13	1:F:427:ALA:HB3	2.00	0.43
1:G:212:ARG:CZ	3:G:607:HOH:O	2.66	0.43
1:J:327:LEU:HD23	1:J:377:PHE:HB2	2.00	0.43
1:J:363:ASP:OD1	1:J:363:ASP:N	2.52	0.43
1:A:271:PRO:HB2	1:B:28:LEU:HD11	1.99	0.43
1:A:200:LYS:HG2	1:A:283:LEU:HD11	2.00	0.43
1:A:368:GLU:OE2	1:A:371:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:SER:O	1:C:83:PRO:HA	2.18	0.43
1:C:101:ILE:HD13	1:C:154:VAL:CG2	2.48	0.43
1:F:417:GLU:HG2	3:G:731:HOH:O	2.18	0.43
1:J:283:LEU:O	1:J:286:GLN:HG2	2.19	0.43
1:J:440:ASN:O	1:J:440:ASN:OD1	2.36	0.43
1:A:0:HIS:CD2	1:A:439:GLU:HG3	2.54	0.43
1:D:400:GLU:HG3	1:D:400:GLU:O	2.19	0.43
1:H:81:ILE:HD13	1:H:81:ILE:HA	1.65	0.43
1:I:337:ARG:HD3	1:I:338:TYR:CZ	2.53	0.43
1:K:245:PHE:CG	1:K:246:PRO:HD3	2.54	0.43
1:L:400:GLU:O	1:L:400:GLU:HG3	2.19	0.43
1:F:407:GLU:OE1	1:F:407:GLU:HA	2.19	0.43
1:J:184:LYS:HB3	1:J:185:PRO:HD3	2.00	0.43
1:J:325:GLU:CD	1:J:325:GLU:H	2.27	0.43
1:B:221:PRO:HA	1:B:237:TYR:CE1	2.54	0.42
1:C:325:GLU:CD	1:C:325:GLU:H	2.27	0.42
1:D:10:THR:HG1	1:D:395:PHE:HB2	1.84	0.42
1:F:264:TRP:O	1:F:267:GLU:HB2	2.18	0.42
1:I:100:LEU:C	1:I:100:LEU:CD2	2.91	0.42
1:K:11:ALA:HA	1:K:73:ARG:O	2.19	0.42
1:K:161:ASN:HA	1:K:216:SER:HB2	2.01	0.42
1:A:77:SER:HB3	1:A:80:ARG:HB2	2.01	0.42
1:G:287:PRO:HB2	3:G:803:HOH:O	2.19	0.42
1:I:440:ASN:OD1	1:I:440:ASN:C	2.62	0.42
1:K:184:LYS:HB3	1:K:185:PRO:HD3	2.01	0.42
1:B:26:LYS:HG2	1:B:27:GLY:O	2.19	0.42
1:I:261:TYR:CD1	1:I:265:VAL:HG21	2.53	0.42
1:D:370:LEU:HD22	1:D:392:ILE:HD12	2.01	0.42
1:F:245:PHE:N	1:F:246:PRO:CD	2.82	0.42
1:G:81:ILE:HG22	1:G:82:ILE:HG13	2.00	0.42
1:G:163:PRO:HA	1:G:166:PHE:CE2	2.54	0.42
1:I:24:ASP:OD2	1:I:54:TYR:OH	2.27	0.42
1:I:221:PRO:HA	1:I:237:TYR:CE1	2.54	0.42
1:I:261:TYR:HB3	1:I:265:VAL:HG21	2.00	0.42
1:J:7:ILE:HB	1:J:389:GLY:HA3	2.01	0.42
1:L:65:LYS:HE3	3:L:613:HOH:O	2.18	0.42
1:A:368:GLU:HG2	1:D:354:ARG:CZ	2.50	0.42
1:C:293:MET:HE3	1:C:334:TYR:CE2	2.54	0.42
1:D:121:PRO:HD2	1:D:124:LEU:HD12	2.01	0.42
1:E:129:GLY:HA3	3:E:634:HOH:O	2.20	0.42
1:E:215:ILE:O	1:E:292:GLY:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASP:O	1:E:419:GLN:N	2.48	0.42
1:J:399:PHE:HB2	1:J:405:TYR:CE1	2.55	0.42
1:B:81:ILE:HD11	1:B:97:TYR:CD2	2.54	0.42
1:J:8:TRP:CB	1:J:434:ILE:HG12	2.50	0.42
1:K:129:GLY:HA3	3:K:653:HOH:O	2.19	0.42
1:K:172:LEU:C	1:K:172:LEU:HD12	2.44	0.42
1:K:327:LEU:HA	1:K:327:LEU:HD12	1.80	0.42
1:A:44:ASN:HA	3:A:754:HOH:O	2.20	0.42
1:E:294:ASN:CG	1:E:346:GLU:HB2	2.45	0.42
1:F:393:TRP:CE2	1:F:394:SER:HB2	2.55	0.42
1:I:13:ALA:O	1:I:17:VAL:HG22	2.19	0.42
1:J:181:ARG:NE	3:J:618:HOH:O	2.53	0.42
1:J:225:VAL:HG23	1:J:301:ILE:O	2.19	0.42
1:L:327:LEU:HD23	1:L:377:PHE:HB2	2.02	0.42
1:B:7:ILE:HD11	3:B:668:HOH:O	2.18	0.42
1:J:4:LYS:HE3	1:J:4:LYS:HB2	1.87	0.42
1:D:292:GLY:HA2	1:D:343:VAL:O	2.19	0.42
1:G:257:ILE:HG21	1:G:338:TYR:HB3	2.01	0.42
1:I:28:LEU:HD23	1:I:28:LEU:HA	1.86	0.42
1:I:85:GLY:HA3	1:I:124:LEU:HG	2.02	0.42
1:D:13:ALA:O	1:D:17:VAL:HG22	2.20	0.42
1:D:184:LYS:O	1:D:188:MET:HG3	2.20	0.42
1:A:34:PHE:CZ	1:A:40:LYS:HB3	2.55	0.41
1:A:164:GLN:HA	1:A:246:PRO:O	2.20	0.41
1:B:393:TRP:CD2	1:B:394:SER:HB2	2.54	0.41
1:D:105:ILE:HD11	1:D:153:ARG:HB3	2.02	0.41
1:F:43:ASP:O	1:G:308:LYS:NZ	2.23	0.41
1:H:184:LYS:NZ	3:H:613:HOH:O	2.49	0.41
1:I:34:PHE:CB	1:I:177:ALA:HB2	2.50	0.41
1:I:390:TYR:CE2	1:I:392:ILE:HG13	2.55	0.41
1:L:423:VAL:HG23	3:L:724:HOH:O	2.19	0.41
1:A:366:ARG:O	1:A:370:LEU:HG	2.20	0.41
1:B:57:LEU:HA	1:B:57:LEU:HD12	1.74	0.41
1:D:57:LEU:HD12	1:D:57:LEU:HA	1.93	0.41
3:E:745:HOH:O	1:H:315:ARG:HD2	2.20	0.41
1:F:393:TRP:HA	1:F:394:SER:HA	1.70	0.41
1:J:209:GLU:HG3	3:J:656:HOH:O	2.20	0.41
1:J:245:PHE:N	1:J:246:PRO:CD	2.83	0.41
1:K:23:GLU:HG3	3:K:702:HOH:O	2.19	0.41
1:A:28:LEU:HD11	1:B:271:PRO:HB2	2.00	0.41
1:A:81:ILE:CG2	1:A:145:LEU:HD23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:HD12	1:C:150:PHE:CD1	2.55	0.41
1:D:144:LYS:O	1:D:148:GLU:HG3	2.21	0.41
1:D:253:LEU:CD1	1:D:334:TYR:CE2	3.03	0.41
1:D:415:ASP:O	1:D:419:GLN:N	2.48	0.41
1:E:13:ALA:HB2	1:E:117:HIS:CE1	2.55	0.41
1:F:144:LYS:O	1:F:148:GLU:HG3	2.20	0.41
1:F:253:LEU:HD13	1:F:334:TYR:CE2	2.55	0.41
1:G:160:PHE:HB2	1:G:215:ILE:HD11	2.03	0.41
1:L:292:GLY:HA2	1:L:343:VAL:O	2.20	0.41
1:B:327:LEU:HD22	1:B:373:TYR:HB3	2.01	0.41
1:D:13:ALA:HB2	1:D:117:HIS:CE1	2.56	0.41
1:G:65:LYS:HD2	1:G:107:ARG:HB3	2.02	0.41
1:K:292:GLY:HA2	1:K:343:VAL:O	2.20	0.41
1:C:188:MET:CE	1:C:274:PRO:HD2	2.51	0.41
1:D:440:ASN:O	1:D:441:LEU:HB2	2.21	0.41
1:J:250:ALA:O	1:J:254:ASP:HB2	2.21	0.41
1:J:289:ASP:O	1:J:341:PRO:HD2	2.20	0.41
1:K:57:LEU:HB2	3:K:684:HOH:O	2.20	0.41
1:L:54:TYR:HA	1:L:96:PHE:CE1	2.55	0.41
1:B:278:ASP:HB2	1:K:137:ASP:OD2	2.20	0.41
1:C:34:PHE:CE1	1:C:40:LYS:HD2	2.56	0.41
1:D:133:ASP:O	1:D:136:PRO:HD2	2.20	0.41
1:D:242:HIS:CE1	1:D:244:ALA:HB3	2.55	0.41
1:E:162:GLU:CG	1:E:218:ALA:HB2	2.50	0.41
1:E:378:ARG:NH2	1:E:442:ARG:HA	2.36	0.41
1:D:100:LEU:CD2	1:D:104:LEU:HD11	2.50	0.41
1:G:245:PHE:N	1:G:246:PRO:CD	2.84	0.41
1:J:315:ARG:HE	1:J:315:ARG:HB2	1.69	0.41
1:E:253:LEU:HD13	1:E:334:TYR:CE2	2.56	0.41
1:L:393:TRP:HA	1:L:394:SER:HA	1.68	0.41
1:B:79:SER:O	1:B:83:PRO:HA	2.21	0.41
1:B:423:VAL:HG13	1:B:427:ALA:CB	2.51	0.41
1:C:184:LYS:O	1:C:188:MET:HG3	2.21	0.41
1:C:423:VAL:CG1	1:C:427:ALA:HB3	2.50	0.41
1:D:95:ASP:O	1:D:99:ARG:HG3	2.21	0.41
1:G:235:GLU:O	1:G:239:GLN:HG3	2.21	0.41
1:G:393:TRP:HA	1:G:394:SER:HA	1.72	0.41
1:H:235:GLU:O	1:H:239:GLN:HG3	2.21	0.41
1:H:245:PHE:N	1:H:246:PRO:CD	2.84	0.41
1:H:345:THR:O	1:H:346:GLU:HG3	2.21	0.41
1:J:164:GLN:HA	1:J:246:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:VAL:HG21	1:K:302:HIS:HB2	2.03	0.41
1:K:423:VAL:CG1	1:K:427:ALA:HB3	2.51	0.41
1:A:1:SER:CB	1:A:378:ARG:HG2	2.51	0.41
1:B:394:SER:O	1:B:410:GLY:HA2	2.21	0.41
1:C:13:ALA:HB2	1:C:117:HIS:CE1	2.56	0.41
1:G:100:LEU:HD23	1:G:100:LEU:C	2.46	0.41
1:J:34:PHE:HA	1:J:37:ILE:HD12	2.03	0.41
1:D:172:LEU:HD13	1:D:187:LEU:HD11	2.03	0.40
1:I:165:VAL:O	1:I:169:CYS:HB2	2.21	0.40
1:K:200:LYS:HG2	1:K:283:LEU:HD11	2.03	0.40
1:L:205:LEU:HD23	1:L:205:LEU:HA	1.94	0.40
1:B:73:ARG:NH1	1:B:346:GLU:HG3	2.35	0.40
1:C:164:GLN:HG3	1:C:252:TRP:CD1	2.57	0.40
1:C:253:LEU:HD13	1:C:334:TYR:CE2	2.56	0.40
1:D:64:MET:HE3	1:D:64:MET:HB2	1.92	0.40
1:G:16:GLN:HG2	1:G:399:PHE:O	2.21	0.40
1:H:163:PRO:HA	1:H:166:PHE:CE2	2.56	0.40
1:I:25:GLY:O	1:I:90:ASN:ND2	2.55	0.40
1:I:327:LEU:HD12	1:I:327:LEU:HA	1.90	0.40
1:K:110:LYS:HE2	1:K:156:ASP:OD1	2.21	0.40
2:K:501:GOL:H31	3:K:749:HOH:O	2.21	0.40
1:A:374:LEU:HB3	1:A:441:LEU:HD13	2.04	0.40
1:C:68:GLY:HA3	3:C:729:HOH:O	2.21	0.40
1:D:26:LYS:HD2	1:D:80:ARG:HG3	2.04	0.40
1:E:370:LEU:CD2	1:E:392:ILE:HD12	2.51	0.40
1:F:120:LEU:HD12	1:F:121:PRO:HD2	2.02	0.40
1:G:13:ALA:O	1:G:17:VAL:HG22	2.21	0.40
1:G:100:LEU:HD21	1:G:104:LEU:HD11	2.03	0.40
1:J:212:ARG:NH2	1:J:388:ASP:OD2	2.55	0.40
1:C:129:GLY:HA3	3:C:647:HOH:O	2.22	0.40
3:G:618:HOH:O	1:H:127:LYS:NZ	2.53	0.40
1:H:294:ASN:CG	1:H:346:GLU:HB2	2.47	0.40
1:K:119:ASP:OD1	1:K:119:ASP:N	2.54	0.40
1:A:220:GLN:HG2	1:A:298:GLY:HA2	2.04	0.40
1:C:293:MET:HE3	1:C:334:TYR:CZ	2.56	0.40
1:I:163:PRO:HA	1:I:166:PHE:CE2	2.56	0.40
1:K:393:TRP:HA	1:K:394:SER:HA	1.68	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	447/449 (100%)	438 (98%)	9 (2%)	0	100	100
1	B	445/449 (99%)	433 (97%)	12 (3%)	0	100	100
1	C	441/449 (98%)	429 (97%)	12 (3%)	0	100	100
1	D	440/449 (98%)	428 (97%)	12 (3%)	0	100	100
1	E	445/449 (99%)	431 (97%)	14 (3%)	0	100	100
1	F	445/449 (99%)	433 (97%)	12 (3%)	0	100	100
1	G	440/449 (98%)	431 (98%)	9 (2%)	0	100	100
1	H	439/449 (98%)	428 (98%)	11 (2%)	0	100	100
1	I	440/449 (98%)	427 (97%)	12 (3%)	1 (0%)	43	63
1	J	440/449 (98%)	430 (98%)	9 (2%)	1 (0%)	43	63
1	K	445/449 (99%)	436 (98%)	9 (2%)	0	100	100
1	L	445/449 (99%)	429 (96%)	15 (3%)	1 (0%)	43	63
All	All	5312/5388 (99%)	5173 (97%)	136 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	1	SER
1	L	-2	HIS
1	I	1	SER

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	378/379 (100%)	370 (98%)	8 (2%)	47	74
1	B	377/379 (100%)	369 (98%)	8 (2%)	47	74
1	C	373/379 (98%)	359 (96%)	14 (4%)	29	56
1	D	372/379 (98%)	364 (98%)	8 (2%)	45	73
1	E	377/379 (100%)	365 (97%)	12 (3%)	34	62
1	F	377/379 (100%)	359 (95%)	18 (5%)	23	46
1	G	372/379 (98%)	366 (98%)	6 (2%)	55	79
1	H	371/379 (98%)	361 (97%)	10 (3%)	39	67
1	I	372/379 (98%)	361 (97%)	11 (3%)	36	64
1	J	372/379 (98%)	357 (96%)	15 (4%)	28	54
1	K	377/379 (100%)	363 (96%)	14 (4%)	30	57
1	L	377/379 (100%)	360 (96%)	17 (4%)	24	49
All	All	4495/4548 (99%)	4354 (97%)	141 (3%)	35	62

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	43	ASP
1	A	100	LEU
1	A	115	LEU
1	A	228	GLU
1	A	297	ASN
1	A	307	ARG
1	A	442	ARG
1	B	-3	HIS
1	B	49	THR
1	B	57	LEU
1	B	100	LEU
1	B	115	LEU
1	B	228	GLU
1	B	356	SER
1	B	406	LYS
1	C	4	LYS
1	C	43	ASP
1	C	57	LEU
1	C	81	ILE
1	C	88	GLU
1	C	100	LEU

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Mol	Chain	Res	Type
1	C	115	LEU
1	C	146	ILE
1	C	260	ARG
1	C	267	GLU
1	C	282	LYS
1	C	307	ARG
1	C	356	SER
1	C	392	ILE
1	D	10	THR
1	D	43	ASP
1	D	57	LEU
1	D	81	ILE
1	D	115	LEU
1	D	175	LYS
1	D	215	ILE
1	D	239	GLN
1	E	38	ASP
1	E	57	LEU
1	E	79	SER
1	E	100	LEU
1	E	115	LEU
1	E	270	GLU
1	E	297	ASN
1	E	307	ARG
1	E	311	THR
1	E	356	SER
1	E	392	ILE
1	E	400	GLU
1	F	-4	HIS
1	F	-1	HIS
1	F	5	ASP
1	F	10	THR
1	F	57	LEU
1	F	88	GLU
1	F	98	SER
1	F	100	LEU
1	F	115	LEU
1	F	215	ILE
1	F	281	LEU
1	F	297	ASN
1	F	307	ARG
1	F	311	THR

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Mol	Chain	Res	Type
1	F	356	SER
1	F	392	ILE
1	F	417	GLU
1	F	432	ASP
1	G	57	LEU
1	G	175	LYS
1	G	228	GLU
1	G	270	GLU
1	G	315	ARG
1	G	406	LYS
1	H	49	THR
1	H	57	LEU
1	H	65	LYS
1	H	81	ILE
1	H	92	LYS
1	H	115	LEU
1	H	311	THR
1	H	315	ARG
1	H	356	SER
1	H	441	LEU
1	I	0	HIS
1	I	1	SER
1	I	57	LEU
1	I	115	LEU
1	I	175	LYS
1	I	256	MET
1	I	310	LYS
1	I	356	SER
1	I	400	GLU
1	I	406	LYS
1	I	441	LEU
1	J	0	HIS
1	J	57	LEU
1	J	100	LEU
1	J	115	LEU
1	J	215	ILE
1	J	216	SER
1	J	260	ARG
1	J	310	LYS
1	J	315	ARG
1	J	316	THR
1	J	356	SER

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Mol	Chain	Res	Type
1	J	392	ILE
1	J	394	SER
1	J	406	LYS
1	J	439	GLU
1	K	-4	HIS
1	K	43	ASP
1	K	49	THR
1	K	57	LEU
1	K	63	LEU
1	K	100	LEU
1	K	115	LEU
1	K	172	LEU
1	K	253	LEU
1	K	279	GLU
1	K	281	LEU
1	K	297	ASN
1	K	378	ARG
1	K	400	GLU
1	L	-3	HIS
1	L	-2	HIS
1	L	5	ASP
1	L	43	ASP
1	L	49	THR
1	L	57	LEU
1	L	63	LEU
1	L	81	ILE
1	L	100	LEU
1	L	115	LEU
1	L	228	GLU
1	L	253	LEU
1	L	279	GLU
1	L	281	LEU
1	L	299	ARG
1	L	392	ILE
1	L	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-4	HIS
1	B	-1	HIS
1	B	149	GLN

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Mol	Chain	Res	Type
1	B	220	GLN
1	B	239	GLN
1	B	414	ASN
1	C	294	ASN
1	D	161	ASN
1	D	286	GLN
1	D	294	ASN
1	D	302	HIS
1	E	258	ASN
1	F	220	GLN
1	F	347	ASN
1	G	297	ASN
1	I	149	GLN
1	I	239	GLN
1	I	286	GLN
1	I	297	ASN
1	J	297	ASN
1	J	302	HIS
1	L	-4	HIS
1	L	294	ASN
1	L	375	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](#)

12 ligands are modelled in this entry.

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
2	GOL	B	501	-	5,5,5	1.49	1 (20%)	5,5,5	1.78	1 (20%)
2	GOL	F	501	-	5,5,5	0.93	0	5,5,5	1.21	1 (20%)
2	GOL	A	501	-	5,5,5	0.98	0	5,5,5	1.33	1 (20%)
2	GOL	D	501	-	5,5,5	1.31	1 (20%)	5,5,5	1.63	1 (20%)
2	GOL	K	501	-	5,5,5	2.19	3 (60%)	5,5,5	2.72	2 (40%)
2	GOL	C	501	-	5,5,5	0.68	0	5,5,5	1.08	0
2	GOL	G	501	-	5,5,5	0.88	0	5,5,5	1.04	0
2	GOL	E	501	-	5,5,5	0.94	0	5,5,5	1.55	1 (20%)
2	GOL	H	501	-	5,5,5	1.01	0	5,5,5	1.44	1 (20%)
2	GOL	I	501	-	5,5,5	1.08	0	5,5,5	1.60	1 (20%)
2	GOL	J	501	-	5,5,5	1.27	0	5,5,5	1.92	1 (20%)
2	GOL	L	501	-	5,5,5	1.08	0	5,5,5	1.52	1 (20%)

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
2	GOL	B	501	-	-	1/4/4/4	-
2	GOL	F	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	4/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	K	501	-	-	1/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
2	GOL	G	501	-	-	3/4/4/4	-
2	GOL	E	501	-	-	2/4/4/4	-
2	GOL	H	501	-	-	2/4/4/4	-
2	GOL	I	501	-	-	2/4/4/4	-
2	GOL	J	501	-	-	2/4/4/4	-
2	GOL	L	501	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	GOL	O2-C2	-3.17	1.34	1.43
2	B	501	GOL	O2-C2	-2.67	1.35	1.43
2	K	501	GOL	C1-C2	2.61	1.61	1.51
2	D	501	GOL	O2-C2	-2.28	1.36	1.43
2	K	501	GOL	C3-C2	2.18	1.60	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	GOL	C3-C2-C1	-5.30	92.35	111.80
2	J	501	GOL	C3-C2-C1	-3.56	98.75	111.80
2	I	501	GOL	C3-C2-C1	-3.20	100.06	111.80
2	D	501	GOL	C3-C2-C1	-3.03	100.68	111.80
2	B	501	GOL	C3-C2-C1	-2.95	100.97	111.80
2	E	501	GOL	C3-C2-C1	-2.86	101.31	111.80
2	L	501	GOL	C3-C2-C1	-2.86	101.33	111.80
2	H	501	GOL	C3-C2-C1	-2.75	101.71	111.80
2	K	501	GOL	O2-C2-C3	2.49	119.50	109.18
2	F	501	GOL	C3-C2-C1	-2.24	103.58	111.80
2	A	501	GOL	C3-C2-C1	-2.18	103.82	111.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	501	GOL	C1-C2-C3-O3
2	C	501	GOL	C1-C2-C3-O3
2	F	501	GOL	O1-C1-C2-C3
2	H	501	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	E	501	GOL	O1-C1-C2-C3
2	G	501	GOL	C1-C2-C3-O3
2	L	501	GOL	O1-C1-C2-C3
2	C	501	GOL	O2-C2-C3-O3
2	F	501	GOL	O1-C1-C2-O2
2	A	501	GOL	O2-C2-C3-O3
2	E	501	GOL	O1-C1-C2-O2
2	H	501	GOL	O1-C1-C2-O2
2	L	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O1-C1-C2-O2
2	G	501	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	J	501	GOL	O1-C1-C2-O2
2	K	501	GOL	O1-C1-C2-O2
2	G	501	GOL	O1-C1-C2-C3
2	I	501	GOL	O1-C1-C2-O2
2	I	501	GOL	O1-C1-C2-C3
2	J	501	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	GOL	4	0
2	K	501	GOL	1	0
2	G	501	GOL	1	0
2	E	501	GOL	1	0
2	J	501	GOL	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	449/449 (100%)	-0.37	4 (0%) 81 78	20, 29, 41, 87	0
1	B	447/449 (99%)	-0.48	1 (0%) 91 89	21, 26, 37, 61	0
1	C	443/449 (98%)	-0.33	1 (0%) 91 89	22, 30, 45, 70	0
1	D	442/449 (98%)	-0.20	3 (0%) 84 81	26, 34, 48, 78	0
1	E	447/449 (99%)	-0.44	1 (0%) 91 89	21, 28, 40, 58	0
1	F	447/449 (99%)	-0.39	4 (0%) 81 78	22, 29, 39, 57	0
1	G	442/449 (98%)	-0.38	1 (0%) 91 89	22, 30, 42, 80	0
1	H	441/449 (98%)	-0.45	1 (0%) 91 89	21, 28, 40, 57	0
1	I	442/449 (98%)	-0.32	1 (0%) 91 89	23, 30, 43, 71	0
1	J	442/449 (98%)	-0.31	1 (0%) 91 89	23, 31, 43, 72	0
1	K	447/449 (99%)	-0.41	1 (0%) 91 89	22, 28, 39, 65	0
1	L	447/449 (99%)	-0.43	1 (0%) 91 89	21, 29, 40, 59	0
All	All	5336/5388 (99%)	-0.37	20 (0%) 88 86	20, 29, 42, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	-4	HIS	3.8
1	B	-4	HIS	3.3
1	F	-4	HIS	3.1
1	A	-4	HIS	3.0
1	G	442	ARG	2.8
1	D	0	HIS	2.8
1	A	-5	HIS	2.7
1	L	-4	HIS	2.7
1	J	441	LEU	2.6
1	C	0	HIS	2.6
1	A	271	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	441	LEU	2.4
1	F	267	GLU	2.2
1	I	0	HIS	2.2
1	A	268	CYS	2.1
1	D	440	ASN	2.1
1	D	271	PRO	2.1
1	F	81	ILE	2.0
1	E	-4	HIS	2.0
1	F	268	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	H	501	6/6	0.82	0.17	36,46,54,55	0
2	GOL	D	501	6/6	0.83	0.12	36,43,52,54	0
2	GOL	J	501	6/6	0.85	0.12	33,41,52,55	0
2	GOL	G	501	6/6	0.87	0.12	30,40,51,51	0
2	GOL	E	501	6/6	0.87	0.12	29,39,51,61	0
2	GOL	F	501	6/6	0.87	0.10	32,44,50,53	0
2	GOL	A	501	6/6	0.88	0.11	35,42,49,50	0
2	GOL	B	501	6/6	0.88	0.11	31,37,41,47	0
2	GOL	I	501	6/6	0.89	0.10	28,40,44,48	0
2	GOL	K	501	6/6	0.89	0.10	28,35,42,47	0
2	GOL	C	501	6/6	0.90	0.11	28,40,48,54	0
2	GOL	L	501	6/6	0.91	0.11	29,35,47,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.