Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 07:50 PM EDT

PDB ID	:	4HU8
Title	:	Crystal Structure of a Bacterial Ig-like Domain Containing GH10 Xylanase from Termite Gut
Authors	:	Han, Q.; Liu, N.; Robinson, H.; Cao, L.; Qian, C.; Wang, Q.; Xie, L.; Ding, H.; Wang, Q.; Huang, Y.; Li, J.; Zhou, Z.
Deposited on	:	2012-11-02
Resolution	:	2.00 Å(reported)

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

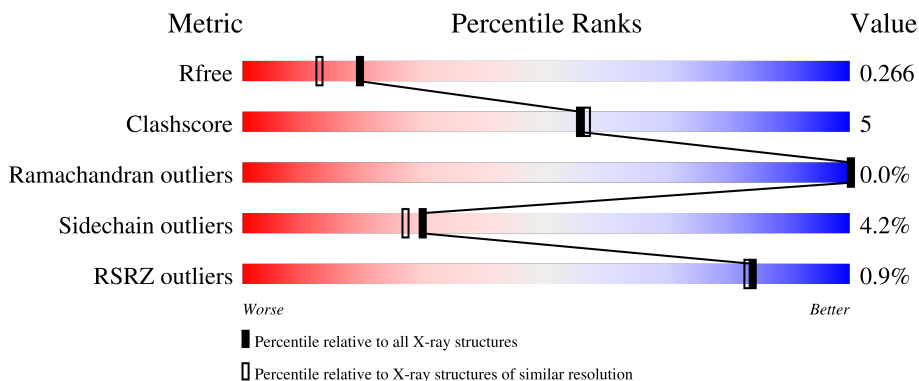|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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.
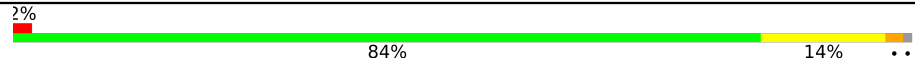
Metric	Percentile Ranks	Value
Rfree		0.266
Clashscore		5
Ramachandran outliers		0.0%
Sidechain outliers		4.2%
RSRZ outliers		0.9%

Worse ————————————————— *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	456	84% 14% ··
1	B	456	86% 12% ··
1	C	456	87% 11% ··
1	D	456	89% 9% ·
1	E	456	86% 12% ··

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	456	2% 84% 14% ··
1	G	456	2% 81% 18% ··
1	H	456	.% 89% 10% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 30836 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 GH10 Xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3558	2248	613	679	18			
1	B	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	C	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	D	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	E	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	F	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	G	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			
1	H	452	Total	C	N	O	S	0	0	0
			3572	2257	616	681	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total 248	O 248	0	0

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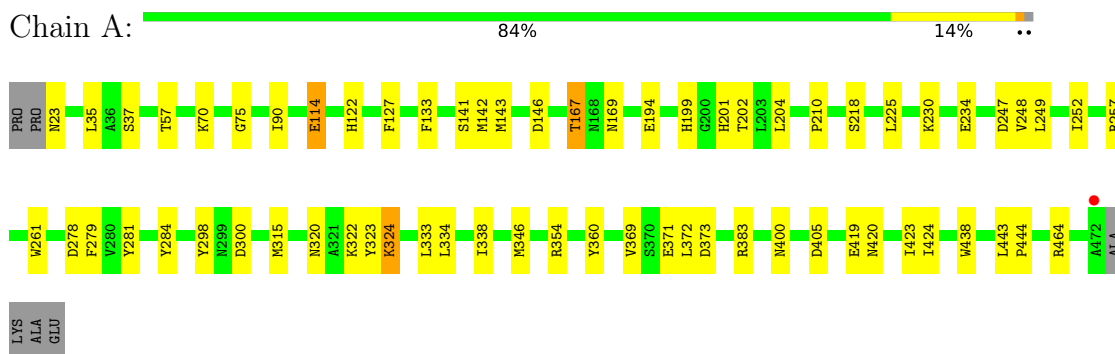*Continued from previous page...*

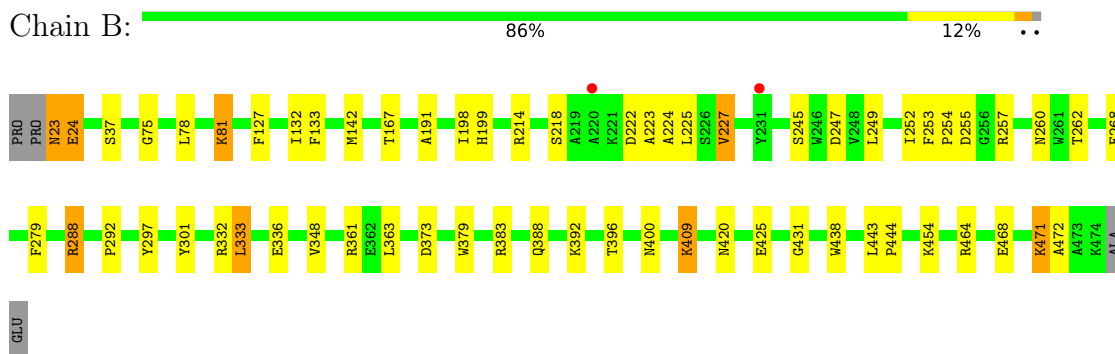| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	216	Total 216	O 216	0	0
4	C	457	Total 457	O 457	0	0
4	D	412	Total 412	O 412	0	0
4	E	207	Total 207	O 207	0	0
4	F	177	Total 177	O 177	0	0
4	G	134	Total 134	O 134	0	0
4	H	297	Total 297	O 297	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
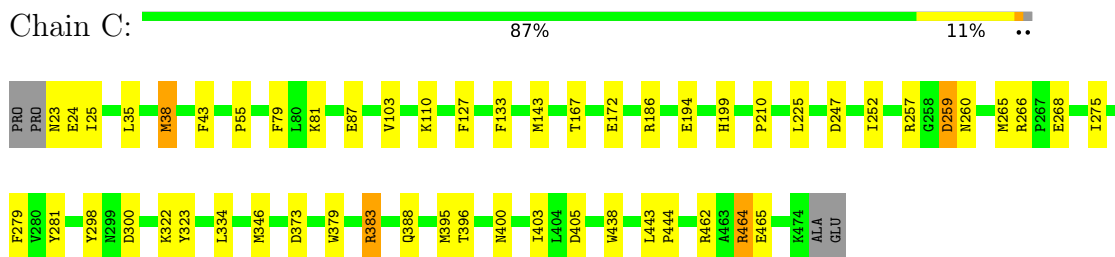
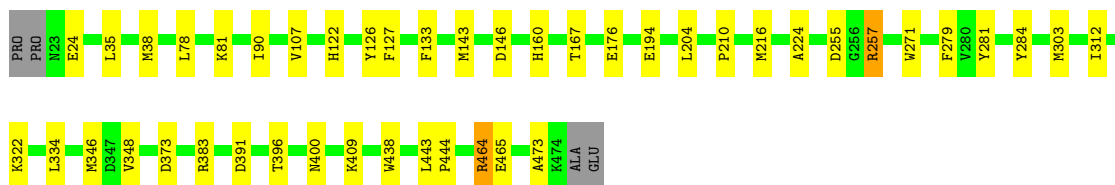- Molecule 1: GH10 Xylanase

- Molecule 1: GH10 Xylanase

- Molecule 1: GH10 Xylanase

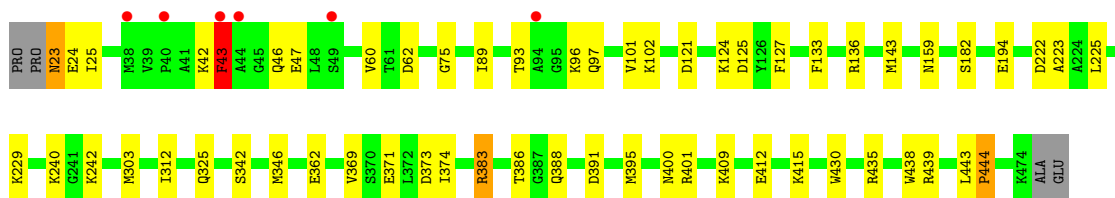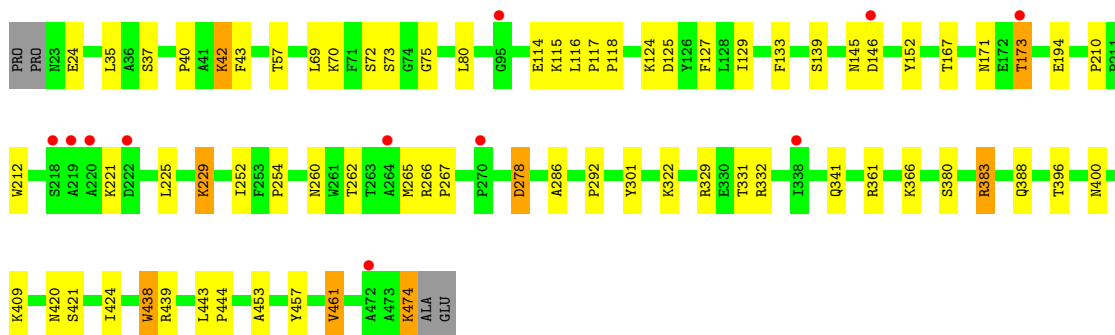
- Molecule 1: GH10 Xylanase

Chain D: 89% 9%

PRO PRO N23 E24 L35 M38 L78 K81 I90 V107 H122 Y126 F127 F133 M143 D146 H160 T167 E176 E194 L204 P210 M216 A224 D255 G256 R257 W271 F279 V280 Y281 Y284 M303 I312

K322 L334 M346 D347 V348 D373 R383 D391 T396 N400 K409 W438 L443 P444 R464 E465 A473 K474 ALA GLU

• Molecule 1: GH10 Xylanase

%

Chain E: 86% 12%

PRO PRO N23 E24 I25 M38 V39 P40 A41 K42 F43 A44 G45 Q46 E47 L48 S49 V60 T61 D62 G75 I89 T93 A94 G95 K96 Q97 V101 K102 D121 K124 D125 Y126 F127 F133 R136 M143 N159 S182 E194 D222 A223 A224 L225

K229 K240 G241 K242 M303 I312 Q325 S342 M346 E362 V369 S370 E371 L372 D373 I374 R383 T386 G387 Q388 D391 M395 N400 R401 K409 E412 K415 W430 R435 W438 R439 L443 P444 K474 ALA GLU

• Molecule 1: GH10 Xylanase

2%

Chain F: 84% 14%

PRO PRO N23 E24 L35 A36 S37 P40 A41 K42 F43 T57 L69 K70 F71 S72 S73 G74 G75 L80 G95 E114 K115 L116 P117 P118 K124 D125 Y126 F127 L128 I129 F133 S139 N145 D146 Y152 T167 N171 E172 T173 E194 P210 P211

W212 S218 A219 A220 K221 D222 L225 K229 I252 F253 P254 N260 W261 T262 T263 A264 M265 R266 P267 P270 D278 A286 P292 Y301 K322 R329 E330 T331 R332 I338 Q341 R361 K366 S380 R383 Q388 T396 N400

K409 N420 S421 I424 W438 R439 L443 P444 A453 Y457 V461 A472 A473 K474 ALA GLU

• Molecule 1: GH10 Xylanase

2%

Chain G: 81% 18%

PRO PRO N23 E24 I25 Q32 K33 V39 P40 A41 K42 F43 A44 G45 Q46 S49 V66 T67 S73 G74 N77 T93 A94 G95 S98 K102 V103 I104 V107 K115 K120 F127 F133 H150 T167 N168 N169 P210 Q213 R214 S215 M216

E217 K229 L249 N250 E251 I252 W261 T262 T263 A264 M265 R266 P267 E268 S274 D278 A286 A287 R288 P292 Y298 Y299 D300 M303 D304 I312 D318 V319 N320 A321 K322 Q325 T331 R332 L333 M340 H344 N345 M346 R354 R361 E362 L363

I367 S368 R383 D391 D394 M395 T396 N400 E419 N420 S421 D422 I423 I424 F425 R426 W438 L443 K452 R464 E465 K474 ALA GLU

• Molecule 1: GH10 Xylanase

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.69Å 86.96Å 246.43Å 92.96° 90.86° 108.56°	Depositor
Resolution (Å)	49.08 – 2.00 49.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.08-2.00) 92.8 (49.08-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.266 0.218 , 0.266	Depositor DCC
R_{free} test set	14505 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.0	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.129 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30836	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	0.46	0/3640	0.59	0/4932
1	B	0.41	0/3654	0.57	0/4950
1	C	0.52	0/3654	0.63	0/4950
1	D	0.51	0/3654	0.62	0/4950
1	E	0.45	0/3654	0.58	0/4950
1	F	0.40	0/3654	0.54	0/4950
1	G	0.41	0/3654	0.57	1/4950 (0.0%)
1	H	0.43	0/3654	0.59	1/4950 (0.0%)
All	All	0.45	0/29218	0.59	2/39582 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	1
1	H	0	2
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	225	LEU	CA-CB-CG	5.91	128.88	115.30
1	G	45	GLY	N-CA-C	-5.89	98.39	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	43	PHE	Peptide
1	D	473	ALA	Peptide
1	E	46	GLN	Peptide
1	H	220	ALA	Peptide
1	H	473	ALA	Peptide

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	3558	0	3474	40	0
1	B	3572	0	3492	38	0
1	C	3572	0	3492	34	0
1	D	3572	0	3492	23	0
1	E	3572	0	3492	38	0
1	F	3572	0	3492	41	0
1	G	3572	0	3492	64	0
1	H	3572	0	3492	16	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	1	0
2	E	5	0	0	1	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	18	0	24	3	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	G	12	0	16	0	0
3	H	12	0	16	2	0
4	A	248	0	0	4	0
4	B	216	0	0	3	0
4	C	457	0	0	6	0
4	D	412	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	207	0	0	4	0
4	F	177	0	0	5	0
4	G	134	0	0	4	0
4	H	297	0	0	0	0
All	All	30836	0	28006	291	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 5.

All (291) 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:G:24:GLU:CG	1:G:102:LYS:HE2	1.77	1.14
1:G:24:GLU:CG	1:G:102:LYS:CE	2.26	1.13
1:G:24:GLU:HG3	1:G:102:LYS:HE2	1.20	1.10
1:G:24:GLU:HG2	1:G:102:LYS:HE3	1.40	1.03
1:F:75:GLY:HA2	1:F:400:ASN:HB2	1.43	1.00
1:B:75:GLY:HA2	1:B:400:ASN:HB2	1.44	0.98
1:C:395:MET:SD	4:C:1040:HOH:O	2.22	0.97
1:G:24:GLU:HG2	1:G:102:LYS:CE	1.93	0.94
1:A:75:GLY:HA2	1:A:400:ASN:HB2	1.49	0.93
1:H:167:THR:HG23	1:H:210:PRO:HG3	1.50	0.91
1:E:42:LYS:HG3	1:E:43:PHE:CD2	2.05	0.91
1:B:471:LYS:HG2	1:B:472:ALA:N	1.84	0.90
1:F:474:LYS:HE3	1:F:474:LYS:H	1.38	0.89
1:G:24:GLU:CG	1:G:102:LYS:HE3	1.98	0.89
1:C:464:ARG:NH1	1:C:465:GLU:OE2	2.06	0.88
1:F:361:ARG:HH21	1:F:420:ASN:HD22	1.22	0.87
1:E:75:GLY:HA2	1:E:400:ASN:HB2	1.56	0.85
1:A:324:LYS:HE2	1:A:324:LYS:HA	1.59	0.84
1:E:42:LYS:HG3	1:E:43:PHE:HD2	1.46	0.78
1:G:24:GLU:HG3	1:G:102:LYS:CE	2.00	0.78
1:B:223:ALA:O	1:B:227:VAL:HG12	1.85	0.77
1:C:464:ARG:HH11	1:C:464:ARG:HG2	1.51	0.76
1:F:260:ASN:ND2	1:F:262:THR:OG1	2.20	0.75
1:A:202:THR:HG22	1:A:247:ASP:HB2	1.67	0.74
1:G:251:GLU:O	1:G:266:ARG:NH1	2.21	0.73
1:F:388:GLN:NE2	4:F:627:HOH:O	2.21	0.73
1:G:229:LYS:HG3	1:G:286:ALA:CB	2.20	0.71
3:C:504:GOL:C1	4:C:940:HOH:O	2.38	0.71
3:C:504:GOL:H12	4:C:940:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:NH1	4:D:672:HOH:O	2.24	0.70
1:B:199:HIS:NE2	1:B:247:ASP:OD1	2.24	0.70
1:G:229:LYS:HG3	1:G:286:ALA:HB2	1.74	0.69
1:B:361:ARG:HH21	1:B:420:ASN:HD22	1.41	0.69
1:E:42:LYS:HG3	1:E:43:PHE:CE2	2.27	0.69
1:G:93:THR:HG22	1:G:98:SER:HB3	1.75	0.68
1:G:288:ARG:NH2	1:G:333:LEU:O	2.27	0.67
1:G:320:ASN:HB3	1:G:333:LEU:HD11	1.76	0.67
1:C:464:ARG:NH1	1:C:464:ARG:HG2	2.08	0.67
1:E:371:GLU:HG2	1:E:430:TRP:CE3	2.31	0.66
1:H:143:MET:HG3	1:H:194:GLU:HG3	1.78	0.66
1:B:23:ASN:OD1	1:B:23:ASN:C	2.33	0.66
1:D:464:ARG:HG3	1:D:465:GLU:N	2.09	0.66
1:A:143:MET:HG3	1:A:194:GLU:HG3	1.78	0.66
1:B:333:LEU:H	1:B:333:LEU:HD12	1.59	0.65
1:A:324:LYS:HA	1:A:324:LYS:CE	2.25	0.65
1:D:78:LEU:HB2	1:D:81:LYS:HD3	1.77	0.65
1:C:395:MET:HE2	4:C:942:HOH:O	1.95	0.65
1:C:464:ARG:HH11	1:C:464:ARG:CG	2.09	0.65
1:E:23:ASN:ND2	1:E:23:ASN:O	2.30	0.65
1:D:346:MET:SD	4:D:946:HOH:O	2.54	0.64
1:F:396:THR:HG21	1:F:443:LEU:HD11	1.78	0.64
1:A:324:LYS:HE2	1:A:324:LYS:CA	2.21	0.63
1:D:143:MET:HG3	1:D:194:GLU:HG3	1.80	0.63
1:F:221:LYS:NZ	1:F:278:ASP:OD2	2.32	0.62
1:B:75:GLY:CA	1:B:400:ASN:HB2	2.26	0.62
1:F:383:ARG:NH2	4:F:627:HOH:O	2.31	0.62
1:G:367:ILE:HB	1:G:424:ILE:HG12	1.82	0.62
1:A:383:ARG:NH2	4:A:750:HOH:O	2.32	0.61
1:A:423:ILE:HD12	1:A:424:ILE:HG13	1.83	0.60
1:B:292:PRO:O	1:B:332:ARG:NH1	2.23	0.60
1:B:23:ASN:ND2	4:B:732:HOH:O	2.34	0.60
1:F:457:TYR:O	1:F:461:VAL:HG12	2.00	0.60
1:H:214:ARG:NH2	1:H:268:GLU:O	2.29	0.60
1:B:78:LEU:HB2	1:B:81:LYS:HD3	1.83	0.60
1:B:191:ALA:HB3	1:B:198:ILE:HD11	1.84	0.60
1:F:329:ARG:HG2	1:F:329:ARG:HH11	1.66	0.60
1:A:141:SER:HB3	4:A:837:HOH:O	2.01	0.60
1:B:224:ALA:HA	1:B:227:VAL:CG1	2.32	0.60
1:E:401:ARG:NH2	2:E:501:SO4:O3	2.33	0.60
1:G:261:TRP:HZ3	1:G:318:ASP:OD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASP:OD2	1:C:259:ASP:N	2.32	0.59
1:D:122:HIS:NE2	1:D:464:ARG:HG2	2.17	0.59
1:B:348:VAL:O	1:B:409:LYS:NZ	2.28	0.58
1:F:388:GLN:OE1	1:F:439:ARG:NH1	2.36	0.58
1:A:249:LEU:HD11	1:A:252:ILE:HD12	1.84	0.58
1:C:143:MET:HG3	1:C:194:GLU:HG3	1.85	0.58
1:B:443:LEU:N	1:B:444:PRO:HD3	2.18	0.58
1:C:388:GLN:HG3	3:C:502:GOL:H2	1.85	0.58
1:F:438:TRP:CD1	1:F:439:ARG:HG2	2.39	0.57
1:F:361:ARG:HH21	1:F:420:ASN:ND2	2.00	0.57
1:G:24:GLU:CD	1:G:102:LYS:CE	2.72	0.57
1:F:114:GLU:OE1	1:F:146:ASP:HB2	2.05	0.57
1:D:303:MET:HE2	1:D:312:ILE:HD13	1.87	0.57
1:B:255:ASP:OD2	1:B:257:ARG:NE	2.36	0.57
1:B:468:GLU:HA	1:B:471:LYS:HD3	1.86	0.57
1:A:354:ARG:NH2	1:A:419:GLU:OE1	2.38	0.56
1:H:252:ILE:HG13	1:H:265:MET:HG2	1.86	0.56
1:G:452:LYS:NZ	4:G:675:HOH:O	2.38	0.56
1:A:278:ASP:OD1	1:A:322:LYS:NZ	2.38	0.56
1:A:354:ARG:NH1	4:A:606:HOH:O	2.37	0.56
1:F:443:LEU:N	1:F:444:PRO:HD3	2.21	0.56
1:C:167:THR:HG23	1:C:210:PRO:HG3	1.87	0.55
1:A:320:ASN:HB3	1:A:333:LEU:HD11	1.89	0.55
1:A:323:TYR:CD1	1:A:334:LEU:HD22	2.42	0.55
1:B:249:LEU:HD11	1:B:252:ILE:HD13	1.88	0.55
1:B:388:GLN:O	1:B:392:LYS:NZ	2.31	0.55
1:E:342:SER:OG	1:E:369:VAL:HG13	2.07	0.55
1:A:201:HIS:ND1	1:A:202:THR:HG23	2.21	0.54
1:G:261:TRP:CD1	1:G:261:TRP:C	2.79	0.54
1:E:443:LEU:N	1:E:444:PRO:HD3	2.22	0.54
1:F:278:ASP:N	1:F:278:ASP:OD1	2.41	0.54
1:G:304:ASP:N	4:G:601:HOH:O	2.40	0.54
1:D:348:VAL:O	1:D:409:LYS:NZ	2.40	0.54
1:F:474:LYS:HE3	1:F:474:LYS:N	2.17	0.54
1:E:42:LYS:C	1:E:43:PHE:CD2	2.81	0.53
1:H:437:SER:HB2	1:H:445:LEU:HD11	1.91	0.53
1:G:249:LEU:HD11	1:G:252:ILE:HD13	1.90	0.53
1:H:233:THR:O	1:H:237:THR:OG1	2.24	0.53
1:B:199:HIS:ND1	1:B:245:SER:OG	2.30	0.52
1:C:186:ARG:NE	3:H:503:GOL:O1	2.34	0.52
1:A:298:TYR:OH	1:A:300:ASP:OD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:LYS:NZ	2:D:501:SO4:O3	2.31	0.52
1:G:25:ILE:HD11	1:G:33:LYS:HE3	1.91	0.52
1:A:373:ASP:HB2	1:A:444:PRO:HB2	1.91	0.52
1:E:346:MET:O	1:E:409:LYS:NZ	2.42	0.52
1:F:72:SER:OG	1:F:73:SER:N	2.43	0.52
1:A:114:GLU:OE1	1:A:146:ASP:HB2	2.10	0.51
1:F:145:ASN:ND2	4:F:766:HOH:O	2.32	0.51
1:F:116:LEU:HD11	1:F:453:ALA:HB2	1.93	0.51
1:H:443:LEU:N	1:H:444:PRO:HD3	2.25	0.51
1:B:255:ASP:OD1	1:B:255:ASP:N	2.43	0.51
1:F:254:PRO:HG3	1:F:266:ARG:HG2	1.93	0.51
1:G:24:GLU:CD	1:G:102:LYS:HE3	2.32	0.51
1:A:57:THR:HA	1:A:70:LYS:HG2	1.93	0.50
1:A:167:THR:HG23	1:A:210:PRO:HG3	1.92	0.50
1:A:122:HIS:CE1	1:A:464:ARG:HE	2.29	0.50
1:C:79:PHE:HB2	1:C:403:ILE:HD11	1.93	0.50
1:H:379:TRP:HE1	1:H:383:ARG:NH2	2.09	0.50
1:E:42:LYS:O	1:E:43:PHE:CD2	2.64	0.50
1:B:199:HIS:CE1	1:B:245:SER:HG	2.26	0.50
1:C:55:PRO:HG2	1:E:182:SER:HB2	1.94	0.49
1:G:368:SER:OG	1:G:426:ARG:HB3	2.12	0.49
1:F:420:ASN:O	1:F:424:ILE:HG22	2.13	0.49
1:A:443:LEU:N	1:A:444:PRO:HD3	2.27	0.49
1:C:87:GLU:OE2	1:G:73:SER:HB2	2.11	0.49
1:G:229:LYS:HG3	1:G:286:ALA:HB1	1.92	0.49
1:B:23:ASN:OD1	1:B:23:ASN:O	2.30	0.49
1:G:278:ASP:OD1	1:G:278:ASP:N	2.46	0.49
1:F:229:LYS:HE2	1:F:286:ALA:HB2	1.94	0.49
1:H:55:PRO:HG3	3:H:503:GOL:H2	1.95	0.49
1:C:462:ARG:NH1	4:C:955:HOH:O	2.31	0.48
1:B:288:ARG:NH2	1:B:336:GLU:OE2	2.46	0.48
1:B:361:ARG:HH21	1:B:420:ASN:ND2	2.08	0.48
1:C:35:LEU:HG	1:C:38:MET:HE3	1.95	0.48
1:G:354:ARG:NH2	1:G:419:GLU:OE1	2.45	0.48
1:F:80:LEU:HD11	1:F:396:THR:HG22	1.96	0.48
1:A:75:GLY:CA	1:A:400:ASN:HB2	2.32	0.48
1:D:126:TYR:O	4:D:894:HOH:O	2.20	0.48
1:G:43:PHE:O	1:G:46:GLN:HB2	2.14	0.48
1:D:443:LEU:N	1:D:444:PRO:HD3	2.29	0.48
1:F:57:THR:HA	1:F:70:LYS:HG2	1.95	0.48
1:E:242:LYS:NZ	4:E:616:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:HG23	1:D:210:PRO:HG3	1.96	0.47
1:E:43:PHE:HZ	1:E:97:GLN:OE1	1.97	0.47
1:E:75:GLY:CA	1:E:400:ASN:HB2	2.37	0.47
1:H:284:TYR:HB3	1:H:334:LEU:HG	1.96	0.47
1:G:396:THR:HG21	1:G:443:LEU:HD11	1.95	0.47
1:C:396:THR:HG21	1:C:443:LEU:HD11	1.97	0.47
1:D:107:VAL:HG21	1:D:400:ASN:OD1	2.15	0.47
1:A:261:TRP:CE2	1:A:315:MET:HA	2.50	0.47
1:C:25:ILE:HD11	1:C:103:VAL:HG22	1.95	0.47
1:C:298:TYR:OH	1:C:300:ASP:OD2	2.27	0.47
1:G:322:LYS:HG3	1:G:325:GLN:NE2	2.30	0.47
1:A:199:HIS:HE2	1:A:247:ASP:CG	2.17	0.47
1:G:210:PRO:HG2	1:G:213:GLN:HG3	1.97	0.47
1:E:371:GLU:HG2	1:E:430:TRP:CZ3	2.50	0.47
1:A:252:ILE:CD1	1:A:279:PHE:HZ	2.28	0.46
1:C:379:TRP:O	1:C:383:ARG:HB2	2.15	0.46
1:E:240:LYS:HE2	4:E:788:HOH:O	2.16	0.46
1:F:40:PRO:HB3	1:F:42:LYS:HD2	1.97	0.46
1:G:167:THR:HG23	1:G:210:PRO:HG3	1.96	0.46
1:H:214:ARG:HE	1:H:214:ARG:HA	1.79	0.46
1:A:230:LYS:NZ	1:A:234:GLU:OE2	2.45	0.46
1:C:252:ILE:HG13	1:C:265:MET:HB3	1.96	0.46
1:G:346:MET:HE2	1:G:346:MET:HA	1.98	0.46
1:B:297:TYR:OH	1:B:425:GLU:OE2	2.20	0.46
1:D:255:ASP:OD2	1:D:257:ARG:NE	2.45	0.46
1:E:388:GLN:OE1	1:E:439:ARG:NH2	2.48	0.46
1:B:199:HIS:HE2	1:B:247:ASP:CG	2.17	0.46
1:F:292:PRO:O	1:F:332:ARG:NH1	2.45	0.46
1:A:420:ASN:HB3	1:A:423:ILE:HD11	1.97	0.46
1:G:74:GLY:O	1:G:77:ASN:HB2	2.15	0.46
1:B:260:ASN:OD1	1:B:262:THR:OG1	2.34	0.46
1:F:421:SER:HA	1:F:424:ILE:HG23	1.98	0.45
1:G:115:LYS:HD3	1:G:115:LYS:HA	1.69	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.63	0.45
1:F:171:ASN:OD1	1:F:173:THR:HG23	2.16	0.45
1:E:225:LEU:O	1:E:229:LYS:HG3	2.16	0.45
1:D:284:TYR:HB3	1:D:334:LEU:HG	1.98	0.45
1:D:35:LEU:HD12	1:D:90:ILE:HG21	1.98	0.45
1:C:281:TYR:CD2	1:C:322:LYS:HE3	2.51	0.45
1:G:32:GLN:HG2	1:G:67:THR:OG1	2.17	0.45
1:B:301:TYR:OH	4:B:705:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ASP:OD1	1:E:223:ALA:N	2.49	0.45
1:G:107:VAL:HG21	1:G:400:ASN:OD1	2.16	0.45
1:C:373:ASP:HB2	1:C:444:PRO:HB2	1.99	0.44
1:A:281:TYR:CG	1:A:322:LYS:HD3	2.52	0.44
1:E:143:MET:HG3	1:E:194:GLU:HG3	1.99	0.44
1:A:202:THR:HG22	1:A:247:ASP:CB	2.41	0.44
1:A:249:LEU:HD21	1:A:252:ILE:HD13	1.99	0.44
1:B:132:ILE:HG12	1:B:431:GLY:HA2	1.99	0.44
1:H:210:PRO:HG2	1:H:213:GLN:HG3	2.00	0.44
1:F:322:LYS:NZ	4:F:631:HOH:O	2.50	0.44
1:A:248:VAL:HB	1:A:284:TYR:CZ	2.53	0.44
1:A:338:ILE:HG21	1:A:360:TYR:CE2	2.53	0.44
1:G:229:LYS:NZ	1:G:229:LYS:HB2	2.32	0.44
1:G:361:ARG:HH22	1:G:422:ASP:CG	2.21	0.44
1:B:443:LEU:O	1:B:454:LYS:NZ	2.50	0.44
1:F:42:LYS:O	1:F:43:PHE:C	2.55	0.44
1:E:303:MET:HE2	1:E:312:ILE:HD13	2.00	0.44
1:E:374:ILE:O	1:E:444:PRO:HA	2.18	0.44
1:G:344:HIS:HE1	4:G:601:HOH:O	2.01	0.44
1:C:55:PRO:HG2	1:E:182:SER:CB	2.48	0.43
1:D:373:ASP:HB2	1:D:444:PRO:HB2	1.99	0.43
1:E:386:THR:HG22	1:E:395:MET:HB2	2.00	0.43
1:A:323:TYR:CG	1:A:334:LEU:HB2	2.53	0.43
1:G:383:ARG:HD3	1:G:383:ARG:HA	1.95	0.43
1:E:23:ASN:ND2	1:E:23:ASN:C	2.70	0.43
1:E:62:ASP:OD2	1:E:62:ASP:N	2.37	0.43
1:F:117:PRO:HA	1:F:118:PRO:HD3	1.92	0.43
1:B:214:ARG:NH1	1:B:268:GLU:O	2.39	0.43
1:C:199:HIS:HE2	1:C:247:ASP:CG	2.22	0.43
1:C:225:LEU:HD23	1:C:275:ILE:HD13	2.00	0.43
1:G:346:MET:HA	1:G:346:MET:CE	2.49	0.43
1:A:204:LEU:HA	4:A:668:HOH:O	2.18	0.43
1:B:420:ASN:ND2	4:B:772:HOH:O	2.46	0.43
1:G:303:MET:HE2	1:G:312:ILE:HD13	2.00	0.43
1:E:373:ASP:HB2	1:E:444:PRO:HB2	2.01	0.43
1:G:24:GLU:HG2	1:G:104:ILE:HD11	2.01	0.43
1:G:49:SER:N	1:G:93:THR:O	2.49	0.43
1:C:323:TYR:CG	1:C:334:LEU:HB2	2.53	0.43
1:G:24:GLU:CD	1:G:102:LYS:HE2	2.33	0.42
1:G:24:GLU:HG3	1:G:102:LYS:HB3	2.01	0.42
1:B:396:THR:HG21	1:B:443:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ARG:NH2	4:E:602:HOH:O	2.38	0.42
1:G:39:VAL:HA	1:G:40:PRO:HD3	1.90	0.42
1:E:121:ASP:O	1:E:124:LYS:HG2	2.19	0.42
1:G:66:VAL:HG21	1:G:103:VAL:HG21	2.01	0.42
1:F:212:TRP:HB3	4:F:722:HOH:O	2.19	0.42
1:G:422:ASP:OD1	1:G:422:ASP:N	2.52	0.42
1:D:204:LEU:HD22	1:D:271:TRP:CD1	2.55	0.42
1:F:167:THR:HG23	1:F:210:PRO:HG3	2.02	0.42
1:F:301:TYR:HB3	1:F:341:GLN:OE1	2.19	0.42
1:B:373:ASP:HB2	1:B:444:PRO:HB2	2.02	0.42
1:C:172:GLU:OE2	4:C:1014:HOH:O	2.22	0.42
1:H:115:LYS:HD3	1:H:115:LYS:HA	1.84	0.42
1:C:400:ASN:HA	1:C:403:ILE:HD12	2.01	0.42
1:D:122:HIS:HE2	1:D:464:ARG:HG2	1.84	0.42
1:F:124:LYS:HG3	1:F:125:ASP:N	2.35	0.42
1:E:159:ASN:HB3	1:G:395:MET:SD	2.60	0.42
1:D:281:TYR:CE1	1:D:322:LYS:HG2	2.55	0.41
1:G:49:SER:HB2	1:G:93:THR:OG1	2.19	0.41
1:G:261:TRP:CG	1:G:262:THR:N	2.87	0.41
1:B:24:GLU:H	1:B:24:GLU:HG2	1.59	0.41
1:F:229:LYS:HE2	1:F:286:ALA:CB	2.50	0.41
1:A:346:MET:HE2	1:A:405:ASP:HB3	2.03	0.41
1:D:346:MET:O	1:D:409:LYS:HE3	2.19	0.41
1:H:188:VAL:O	1:H:192:ILE:HG12	2.20	0.41
1:E:23:ASN:O	1:E:101:VAL:HG23	2.21	0.41
1:E:412:GLU:HA	1:E:415:LYS:HE2	2.02	0.41
1:F:266:ARG:HA	1:F:267:PRO:HD2	1.92	0.41
1:G:120:LYS:HE2	1:G:150:HIS:O	2.20	0.41
1:G:252:ILE:HG13	1:G:265:MET:HB3	2.03	0.41
1:G:292:PRO:O	1:G:332:ARG:NH1	2.49	0.41
1:A:371:GLU:OE2	3:A:502:GOL:O1	2.37	0.41
1:E:89:ILE:HD13	1:E:102:LYS:HA	2.02	0.41
1:E:435:ARG:NH1	4:E:770:HOH:O	2.38	0.41
1:G:24:GLU:OE2	1:G:102:LYS:CE	2.68	0.41
1:G:303:MET:SD	1:G:340:MET:HG2	2.61	0.41
1:C:298:TYR:CE2	1:C:300:ASP:HB2	2.55	0.41
1:D:216:MET:CE	1:D:224:ALA:HA	2.51	0.41
1:F:252:ILE:HG13	1:F:265:MET:HG2	2.02	0.41
1:B:253:PHE:HA	1:B:254:PRO:HD3	1.85	0.41
1:E:136:ARG:NH1	1:G:394:ASP:HB2	2.36	0.41
1:A:369:VAL:CG1	1:A:372:LEU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HD3	1:C:268:GLU:OE1	2.19	0.41
1:D:396:THR:HG21	1:D:443:LEU:HD11	2.03	0.41
1:G:93:THR:HG22	1:G:98:SER:CB	2.48	0.41
1:G:216:MET:O	1:G:274:SER:HB3	2.21	0.41
1:C:346:MET:HE1	1:C:405:ASP:HB3	2.02	0.41
1:G:421:SER:O	4:G:692:HOH:O	2.22	0.40
1:C:383:ARG:HE	1:C:383:ARG:HB3	1.65	0.40
1:E:23:ASN:N	1:E:23:ASN:HD22	2.18	0.40
1:G:298:TYR:CE2	1:G:300:ASP:HB2	2.56	0.40
1:B:379:TRP:HE1	1:B:383:ARG:CZ	2.35	0.40
1:G:214:ARG:NH1	1:G:217:GLU:OE1	2.55	0.40
1:H:117:PRO:HA	1:H:118:PRO:HD3	1.95	0.40
1:D:24:GLU:H	1:D:24:GLU:HG2	1.67	0.40
1:F:35:LEU:O	1:F:37:SER:O	2.39	0.40
1:F:129:ILE:HG22	1:F:152:TYR:HD1	1.86	0.40
1:H:212:TRP:O	1:H:216:MET:HG2	2.22	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	448/456 (98%)	441 (98%)	7 (2%)	0	100	100
1	B	450/456 (99%)	438 (97%)	12 (3%)	0	100	100
1	C	450/456 (99%)	442 (98%)	8 (2%)	0	100	100
1	D	450/456 (99%)	439 (98%)	11 (2%)	0	100	100
1	E	450/456 (99%)	438 (97%)	11 (2%)	1 (0%)	47	44
1	F	450/456 (99%)	442 (98%)	8 (2%)	0	100	100
1	G	450/456 (99%)	436 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	450/456 (99%)	443 (98%)	7 (2%)	0	100	100
All	All	3598/3648 (99%)	3519 (98%)	78 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	43	PHE

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	377/381 (99%)	362 (96%)	15 (4%)	31	29
1	B	378/381 (99%)	358 (95%)	20 (5%)	22	18
1	C	378/381 (99%)	365 (97%)	13 (3%)	37	36
1	D	378/381 (99%)	367 (97%)	11 (3%)	42	43
1	E	378/381 (99%)	361 (96%)	17 (4%)	27	24
1	F	378/381 (99%)	358 (95%)	20 (5%)	22	18
1	G	378/381 (99%)	363 (96%)	15 (4%)	31	29
1	H	378/381 (99%)	362 (96%)	16 (4%)	30	27
All	All	3023/3048 (99%)	2896 (96%)	127 (4%)	30	27

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	35	LEU
1	A	37	SER
1	A	90	ILE
1	A	114	GLU
1	A	127	PHE
1	A	133	PHE

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Mol	Chain	Res	Type
1	A	142	MET
1	A	167	THR
1	A	169	ASN
1	A	218	SER
1	A	225	LEU
1	A	257	ARG
1	A	324	LYS
1	A	438	TRP
1	B	23	ASN
1	B	24	GLU
1	B	37	SER
1	B	81	LYS
1	B	127	PHE
1	B	133	PHE
1	B	142	MET
1	B	167	THR
1	B	218	SER
1	B	222	ASP
1	B	225	LEU
1	B	227	VAL
1	B	279	PHE
1	B	288	ARG
1	B	333	LEU
1	B	363	LEU
1	B	409	LYS
1	B	438	TRP
1	B	464	ARG
1	B	471	LYS
1	C	23	ASN
1	C	24	GLU
1	C	38	MET
1	C	110	LYS
1	C	127	PHE
1	C	133	PHE
1	C	257	ARG
1	C	259	ASP
1	C	260	ASN
1	C	279	PHE
1	C	383	ARG
1	C	438	TRP
1	C	464	ARG
1	D	38	MET

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Mol	Chain	Res	Type
1	D	127	PHE
1	D	133	PHE
1	D	146	ASP
1	D	160	HIS
1	D	176	GLU
1	D	257	ARG
1	D	279	PHE
1	D	391	ASP
1	D	438	TRP
1	D	464	ARG
1	E	23	ASN
1	E	24	GLU
1	E	25	ILE
1	E	43	PHE
1	E	47	GLU
1	E	60	VAL
1	E	93	THR
1	E	96	LYS
1	E	125	ASP
1	E	127	PHE
1	E	133	PHE
1	E	325	GLN
1	E	362	GLU
1	E	383	ARG
1	E	391	ASP
1	E	438	TRP
1	E	444	PRO
1	F	24	GLU
1	F	42	LYS
1	F	69	LEU
1	F	115	LYS
1	F	127	PHE
1	F	133	PHE
1	F	139	SER
1	F	173	THR
1	F	194	GLU
1	F	225	LEU
1	F	229	LYS
1	F	278	ASP
1	F	331	THR
1	F	366	LYS
1	F	380	SER

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Mol	Chain	Res	Type
1	F	383	ARG
1	F	409	LYS
1	F	438	TRP
1	F	461	VAL
1	F	474	LYS
1	G	42	LYS
1	G	127	PHE
1	G	133	PHE
1	G	169	ASN
1	G	261	TRP
1	G	268	GLU
1	G	278	ASP
1	G	346	MET
1	G	362	GLU
1	G	363	LEU
1	G	368	SER
1	G	391	ASP
1	G	438	TRP
1	G	464	ARG
1	G	465	GLU
1	H	24	GLU
1	H	42	LYS
1	H	63	LYS
1	H	91	THR
1	H	127	PHE
1	H	133	PHE
1	H	160	HIS
1	H	225	LEU
1	H	273	LYS
1	H	279	PHE
1	H	325	GLN
1	H	329	ARG
1	H	331	THR
1	H	391	ASP
1	H	438	TRP
1	H	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	420	ASN
1	C	169	ASN

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Mol	Chain	Res	Type
1	E	325	GLN
1	F	165	ASN
1	F	206	HIS
1	F	260	ASN
1	F	420	ASN
1	G	320	ASN
1	G	325	GLN
1	G	420	ASN
1	H	299	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	SO4	H	501	-	4,4,4	0.13	0	6,6,6	0.18	0
3	GOL	H	504	-	5,5,5	0.34	0	5,5,5	0.48	0
2	SO4	F	501	-	4,4,4	0.09	0	6,6,6	0.19	0
3	GOL	D	503	-	5,5,5	0.55	0	5,5,5	1.15	0
3	GOL	C	502	-	5,5,5	0.90	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	SO4	B	502	-	4,4,4	0.11	0	6,6,6	0.07	0
3	GOL	A	502	-	5,5,5	0.39	0	5,5,5	1.13	1 (20%)
3	GOL	G	502	-	5,5,5	0.31	0	5,5,5	0.79	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	H	502	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	G	501	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.29	0
3	GOL	E	502	-	5,5,5	0.36	0	5,5,5	0.30	0
2	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.07	0
3	GOL	B	503	-	5,5,5	0.42	0	5,5,5	0.43	0
2	SO4	D	501	-	4,4,4	0.13	0	6,6,6	0.27	0
3	GOL	G	503	-	5,5,5	0.33	0	5,5,5	0.25	0
3	GOL	C	503	-	5,5,5	0.27	0	5,5,5	0.44	0
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.32	0
3	GOL	C	504	-	5,5,5	0.77	0	5,5,5	1.08	0
2	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.20	0
3	GOL	H	503	-	5,5,5	0.79	0	5,5,5	1.16	0
2	SO4	B	501	-	4,4,4	0.16	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	503	-	-	0/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	H	503	-	-	1/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	E	502	-	-	0/4/4/4	-
3	GOL	H	504	-	-	3/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	G	502	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	GOL	O3-C3-C2	-2.03	100.45	110.20

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-C3
3	C	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-C3
3	C	504	GOL	O1-C1-C2-C3
3	D	503	GOL	C1-C2-C3-O3
3	G	502	GOL	O1-C1-C2-C3
3	G	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	C	504	GOL	O1-C1-C2-O2
3	A	502	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	D	503	GOL	O2-C2-C3-O3
3	C	503	GOL	O1-C1-C2-O2
3	G	502	GOL	O1-C1-C2-O2
3	G	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O1-C1-C2-O2
3	H	503	GOL	O1-C1-C2-O2
3	H	504	GOL	C1-C2-C3-O3
3	H	504	GOL	O2-C2-C3-O3
3	H	504	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GOL	1	0
3	A	502	GOL	1	0
2	E	501	SO4	1	0
2	D	501	SO4	1	0
3	C	504	GOL	2	0
3	H	503	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	450/456 (98%)	-0.35	1 (0%)	95	94	14, 28, 45, 56	0
1	B	452/456 (99%)	-0.18	2 (0%)	92	92	19, 35, 52, 74	0
1	C	452/456 (99%)	-0.62	0	100	100	10, 18, 34, 57	0
1	D	452/456 (99%)	-0.62	0	100	100	10, 20, 33, 51	0
1	E	452/456 (99%)	-0.25	6 (1%)	77	76	16, 29, 62, 96	0
1	F	452/456 (99%)	-0.14	11 (2%)	59	57	20, 35, 56, 76	0
1	G	452/456 (99%)	-0.00	8 (1%)	68	66	19, 36, 61, 82	0
1	H	452/456 (99%)	-0.31	4 (0%)	84	83	16, 29, 53, 65	0
All	All	3614/3648 (99%)	-0.31	32 (0%)	84	83	10, 28, 52, 96	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	PRO	5.7
1	E	44	ALA	5.0
1	E	43	PHE	4.0
1	F	95	GLY	3.8
1	G	45	GLY	3.6
1	E	38	MET	3.4
1	G	39	VAL	3.4
1	G	331	THR	3.1
1	B	220	ALA	3.1
1	F	264	ALA	3.0
1	F	220	ALA	3.0
1	G	43	PHE	2.9
1	F	218	SER	2.9
1	G	261	TRP	2.8
1	G	95	GLY	2.8
1	F	338	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	219	ALA	2.6
1	F	270	PRO	2.6
1	E	94	ALA	2.5
1	G	263	THR	2.5
1	B	231	TYR	2.5
1	F	173	THR	2.4
1	H	231	TYR	2.4
1	H	225	LEU	2.3
1	E	49	SER	2.3
1	F	472	ALA	2.3
1	G	74	GLY	2.2
1	H	270	PRO	2.2
1	F	222	ASP	2.2
1	A	472	ALA	2.2
1	F	146	ASP	2.1
1	H	218	SER	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	GOL	C	502	6/6	0.68	0.20	24,36,38,47	0
3	GOL	C	504	6/6	0.72	0.17	12,21,25,30	0
3	GOL	A	502	6/6	0.81	0.13	20,21,25,26	0
2	SO4	F	502	5/5	0.83	0.11	41,45,57,61	0
3	GOL	G	503	6/6	0.83	0.21	43,49,50,51	0
3	GOL	H	504	6/6	0.84	0.14	23,29,32,33	0
3	GOL	H	503	6/6	0.85	0.17	21,25,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	503	6/6	0.89	0.11	24,29,31,39	0
3	GOL	G	502	6/6	0.90	0.12	24,30,31,38	0
3	GOL	D	503	6/6	0.91	0.10	13,17,17,22	0
3	GOL	E	502	6/6	0.91	0.10	22,23,24,25	0
2	SO4	A	501	5/5	0.92	0.10	39,39,47,50	0
3	GOL	B	503	6/6	0.96	0.12	25,29,30,32	0
2	SO4	H	502	5/5	0.97	0.06	35,35,39,41	0
2	SO4	E	501	5/5	0.97	0.10	38,48,49,57	0
2	SO4	G	501	5/5	0.97	0.10	45,51,51,55	0
2	SO4	C	501	5/5	0.98	0.08	30,36,45,46	0
2	SO4	D	501	5/5	0.98	0.07	23,27,29,33	0
2	SO4	H	501	5/5	0.98	0.06	38,40,45,46	0
2	SO4	B	501	5/5	0.98	0.04	31,35,38,43	0
2	SO4	F	501	5/5	0.98	0.06	30,30,32,35	0
2	SO4	D	502	5/5	0.99	0.06	29,32,36,38	0
2	SO4	B	502	5/5	0.99	0.07	32,40,40,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.