



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 02:25 PM JST

PDB ID : 7D66
Title : Crystal structure of retroviral protease-like domain of Ddi1 from *Toxoplasma gondii*
Authors : Biswas, I.B.; Killivalavan, A.K.; Suguna, K.S.
Deposited on : 2020-09-29
Resolution : 2.13 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

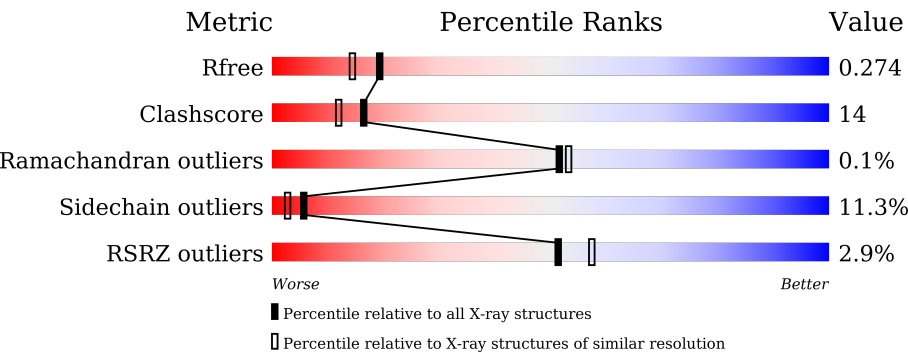
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	128	
1	B	128	
1	C	128	
1	D	128	
1	E	128	
1	F	128	

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Mol	Chain	Length	Quality of chain
1	G	128	<div><div></div><div>3%</div><div>62%</div><div>27%</div><div>5%</div><div>6%</div></div>
1	H	128	<div><div></div><div>3%</div><div>64%</div><div>24%</div><div></div><div></div><div>7%</div></div>
1	I	128	<div><div></div><div>2%</div><div>66%</div><div>27%</div><div></div><div></div><div></div></div>
1	J	128	<div><div></div><div>4%</div><div>54%</div><div>36%</div><div></div><div></div><div>6%</div></div>
1	K	128	<div><div></div><div>5%</div><div>66%</div><div>26%</div><div></div><div></div><div></div></div>
1	L	128	<div><div></div><div>2%</div><div>62%</div><div>27%</div><div>6%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23392 atoms, of which 11534 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 Ubiquitin family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	120	Total	C	H	N	O	S	32	0	0
			1877	599	948	154	169	7			
1	A	124	Total	C	H	N	O	S	31	0	0
			1901	605	955	159	175	7			
1	D	124	Total	C	H	N	O	S	36	0	0
			1897	605	959	157	169	7			
1	C	126	Total	C	H	N	O	S	37	0	0
			1920	610	969	160	174	7			
1	F	121	Total	C	H	N	O	S	30	0	0
			1886	600	951	155	173	7			
1	E	110	Total	C	H	N	O	S	28	0	0
			1706	549	862	135	153	7			
1	H	119	Total	C	H	N	O	S	27	0	0
			1897	604	962	155	169	7			
1	G	120	Total	C	H	N	O	S	32	0	0
			1860	601	936	147	169	7			
1	J	120	Total	C	H	N	O	S	32	0	0
			1878	599	953	153	166	7			
1	I	124	Total	C	H	N	O	S	31	0	0
			1931	616	977	156	175	7			
1	L	123	Total	C	H	N	O	S	29	0	0
			1945	618	983	160	177	7			
1	K	123	Total	C	H	N	O	S	34	0	0
			1885	601	951	156	171	6			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	H	O	2	0
			14	3	8	3		
2	L	1	Total	C	H	O	2	0
			14	3	8	3		

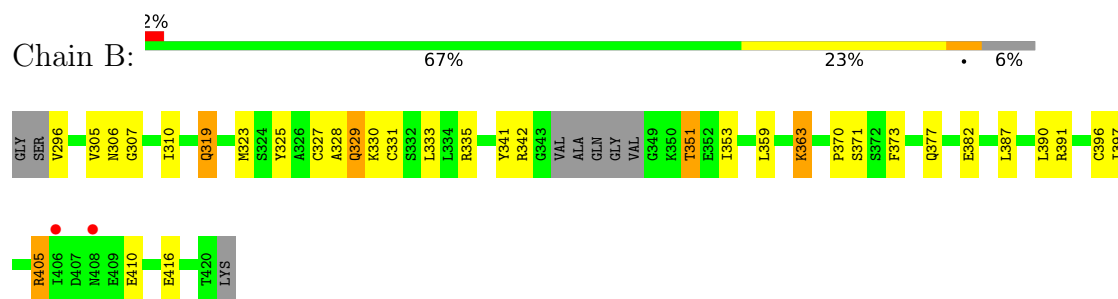
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	43	Total	O	0	0
			43	43		
3	A	53	Total	O	0	0
			53	53		
3	D	52	Total	O	0	0
			52	52		
3	C	47	Total	O	0	0
			47	47		
3	F	56	Total	O	0	0
			56	56		
3	E	41	Total	O	0	0
			41	41		
3	H	49	Total	O	0	0
			49	49		
3	G	53	Total	O	0	0
			53	53		
3	J	38	Total	O	0	0
			38	38		
3	I	48	Total	O	0	0
			48	48		
3	L	45	Total	O	0	0
			45	45		
3	K	60	Total	O	0	0
			60	60		

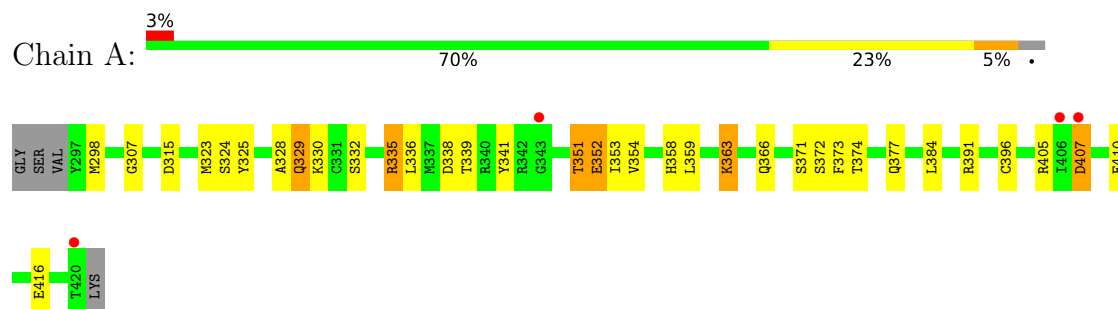
3 Residue-property plots [i](#)

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.

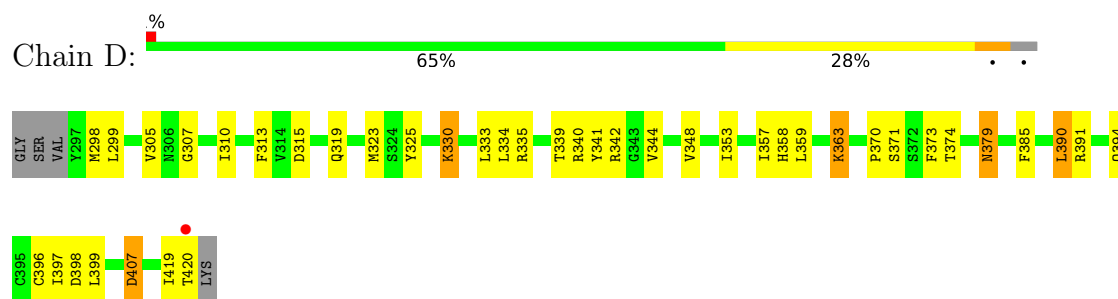
- Molecule 1: Ubiquitin family protein



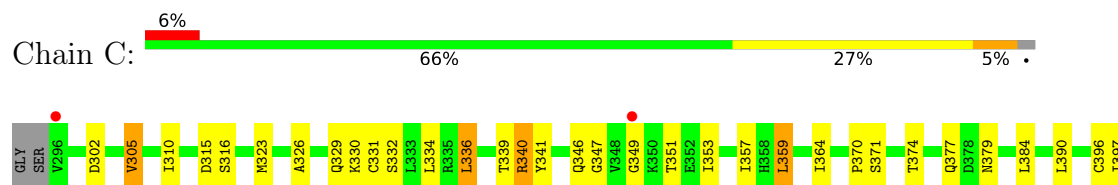
- Molecule 1: Ubiquitin family protein



- Molecule 1: Ubiquitin family protein

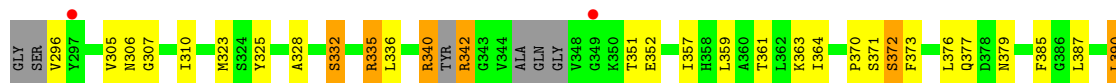


- Molecule 1: Ubiquitin family protein

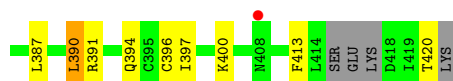
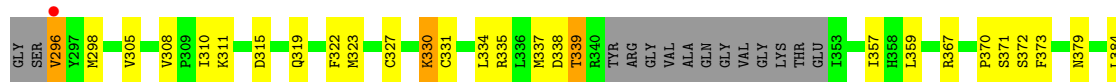




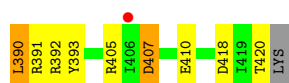
- Molecule 1: Ubiquitin family protein



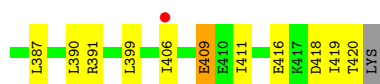
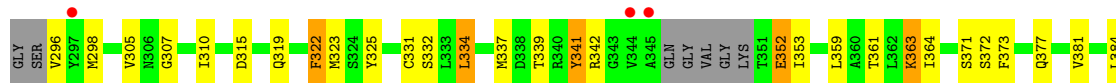
- Molecule 1: Ubiquitin family protein



- Molecule 1: Ubiquitin family protein

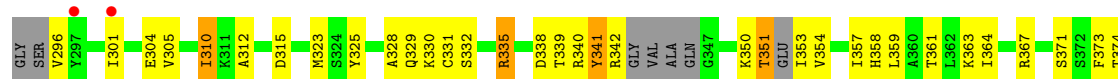


- Molecule 1: Ubiquitin family protein



- Molecule 1: Ubiquitin family protein

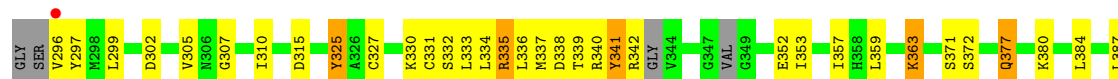




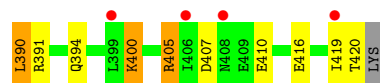
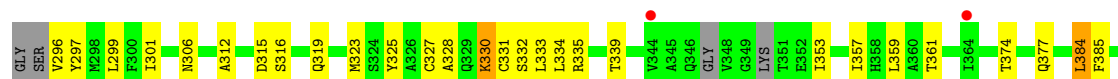
• Molecule 1: Ubiquitin family protein



• Molecule 1: Ubiquitin family protein



• Molecule 1: Ubiquitin family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 184.60Å 184.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.27 – 2.13 65.27 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.27-2.13) 99.7 (65.27-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.18 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.192 , 0.247 0.225 , 0.274	Depositor DCC
R_{free} test set	8844 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.049 for -h,-l,-k 0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23392	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 23.94 % 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 4.2204e-03. 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:
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	0.82	1/960 (0.1%)	0.96	0/1295
1	B	0.87	2/943 (0.2%)	0.96	0/1270
1	C	0.84	0/965	1.00	2/1302 (0.2%)
1	D	0.79	0/953	0.95	1/1285 (0.1%)
1	E	0.82	0/856	0.96	0/1153
1	F	0.88	2/947 (0.2%)	1.09	7/1274 (0.5%)
1	G	0.81	1/939 (0.1%)	0.97	1/1267 (0.1%)
1	H	0.86	0/948	1.06	3/1271 (0.2%)
1	I	0.86	3/969 (0.3%)	1.03	1/1306 (0.1%)
1	J	0.81	0/938	1.02	3/1262 (0.2%)
1	K	0.79	0/946	0.95	1/1276 (0.1%)
1	L	0.94	2/975 (0.2%)	1.01	0/1309
All	All	0.84	11/11339 (0.1%)	1.00	19/15270 (0.1%)

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	D	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	409	GLU	CD-OE1	9.46	1.36	1.25
1	B	416	GLU	CD-OE1	-6.23	1.18	1.25
1	L	410	GLU	CD-OE2	-5.85	1.19	1.25
1	I	309	PRO	C-O	-5.72	1.11	1.23
1	I	306	ASN	CG-OD1	5.65	1.36	1.24
1	L	302	ASP	CG-OD2	-5.32	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	409	GLU	CD-OE2	-5.30	1.19	1.25
1	B	382	GLU	CD-OE2	-5.28	1.19	1.25
1	F	372	SER	CB-OG	-5.26	1.35	1.42
1	I	304	GLU	CD-OE2	5.09	1.31	1.25
1	A	352	GLU	CD-OE1	5.05	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	342	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	F	392	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	K	297	TYR	CB-CA-C	6.73	123.86	110.40
1	H	335	ARG	CG-CD-NE	-6.61	97.92	111.80
1	F	335	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	F	335	ARG	CG-CD-NE	6.56	125.57	111.80
1	F	340	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	J	335	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	336	LEU	CB-CG-CD1	-5.87	101.03	111.00
1	F	392	ARG	CG-CD-NE	5.67	123.70	111.80
1	J	380	LYS	CB-CA-C	-5.65	99.11	110.40
1	C	407	ASP	CB-CG-OD2	5.55	123.30	118.30
1	I	306	ASN	CB-CG-ND2	-5.30	103.97	116.70
1	F	342	ARG	CG-CD-NE	5.29	122.91	111.80
1	F	420	THR	CA-C-O	5.10	130.81	120.10
1	H	420	THR	CA-C-O	5.10	130.81	120.10
1	H	335	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	315	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	J	391	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	344	VAL	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	946	955	936	36	2
1	B	929	948	929	27	5
1	C	951	969	942	34	29
1	D	938	959	934	38	0
1	E	844	862	843	35	0
1	F	935	951	934	32	29
1	G	924	936	916	23	5
1	H	935	962	950	30	2
1	I	954	977	961	31	8
1	J	925	953	933	36	8
1	K	934	951	926	37	1
1	L	962	983	969	49	0
2	A	18	24	24	3	0
2	B	24	32	32	0	0
2	E	6	8	8	0	0
2	F	24	32	32	1	0
2	H	6	8	8	0	0
2	I	6	8	8	0	0
2	J	6	8	8	0	0
2	L	6	8	8	0	0
3	A	53	0	0	0	0
3	B	43	0	0	0	0
3	C	47	0	0	0	0
3	D	52	0	0	0	0
3	E	41	0	0	1	0
3	F	56	0	0	3	0
3	G	53	0	0	1	0
3	H	49	0	0	1	0
3	I	48	0	0	0	0
3	J	38	0	0	1	0
3	K	60	0	0	0	0
3	L	45	0	0	2	1
All	All	11858	11534	11301	322	46

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 14.

All (322) 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:D:339:THR:O	1:E:420:THR:HG22	1.41	1.19
1:H:325:TYR:OH	1:K:325:TYR:CE2	2.07	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:331:CYS:HB2	1:L:333:LEU:HD12	1.41	1.01
1:B:329:GLN:HE21	1:I:334:LEU:HD12	1.29	0.96
1:C:379:ASN:HD22	1:J:341:TYR:HE2	1.14	0.95
1:A:339:THR:HB	1:H:382:GLU:OE1	1.67	0.94
1:D:339:THR:O	1:E:420:THR:CG2	2.17	0.93
1:K:353:ILE:HD12	1:K:374:THR:HG21	1.53	0.91
1:F:396:CYS:HB3	1:E:396:CYS:SG	2.12	0.90
1:B:405:ARG:HH22	1:A:405:ARG:NH2	1.72	0.88
1:E:339:THR:O	1:L:420:THR:HB	1.76	0.85
1:L:305:VAL:HG12	1:L:310:ILE:HD12	1.57	0.84
1:I:307:GLY:HA2	1:I:363:LYS:HE2	1.60	0.83
1:H:391:ARG:NH1	1:G:296:VAL:O	2.12	0.82
1:K:323:MET:HG3	1:K:327:CYS:SG	2.21	0.81
1:C:405:ARG:HG2	1:C:410:GLU:HG2	1.64	0.80
1:B:329:GLN:NE2	1:I:334:LEU:HD12	1.96	0.79
1:G:315:ASP:HB3	1:G:384:LEU:HD11	1.65	0.79
1:H:307:GLY:HA2	1:H:363:LYS:HE2	1.63	0.78
1:A:329:GLN:NE2	1:K:335:ARG:HG2	1.98	0.78
1:L:307:GLY:HA2	1:L:363:LYS:HE2	1.64	0.78
1:A:329:GLN:HE21	1:K:335:ARG:HG2	1.48	0.78
1:H:325:TYR:OH	1:K:325:TYR:HE2	1.67	0.78
1:J:305:VAL:HG12	1:J:310:ILE:HD13	1.65	0.78
1:E:323:MET:HE2	1:E:373:PHE:HE1	1.49	0.77
1:L:297:TYR:HA	1:K:391:ARG:HH12	1.47	0.77
1:K:315:ASP:HB3	1:K:384:LEU:HD11	1.68	0.76
1:I:315:ASP:HB3	1:I:384:LEU:HD11	1.68	0.76
1:L:342:ARG:HD2	1:L:353:ILE:HG13	1.68	0.75
1:D:330:LYS:HB2	1:L:334:LEU:C	2.06	0.75
1:B:307:GLY:HA2	1:B:363:LYS:HE2	1.67	0.75
1:A:405:ARG:HG2	1:A:410:GLU:HG2	1.69	0.74
1:K:405:ARG:HG3	1:K:410:GLU:HG2	1.70	0.73
1:H:329:GLN:CG	1:H:334:LEU:HD11	2.18	0.73
1:L:405:ARG:HG2	1:L:410:GLU:HG2	1.69	0.73
1:H:329:GLN:HG2	1:H:334:LEU:HD11	1.70	0.73
1:B:323:MET:HE2	1:B:373:PHE:HE1	1.53	0.73
1:K:323:MET:SD	1:K:327:CYS:SG	2.87	0.72
1:D:394:GLN:HE21	1:C:400:LYS:HA	1.53	0.72
1:C:305:VAL:HG13	1:C:310:ILE:HD12	1.71	0.71
1:L:315:ASP:HB3	1:L:384:LEU:HD21	1.72	0.70
1:F:379:ASN:O	3:F:501:HOH:O	2.10	0.70
1:H:335:ARG:HA	1:K:330:LYS:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:GLY:HA2	1:F:363:LYS:HE2	1.75	0.69
1:G:305:VAL:HG12	1:G:310:ILE:HD12	1.74	0.69
1:F:405:ARG:HG2	1:F:410:GLU:HG2	1.74	0.69
1:J:296:VAL:O	1:I:391:ARG:NH1	2.26	0.69
1:B:405:ARG:HG3	1:B:410:GLU:HG2	1.75	0.68
1:G:307:GLY:HA2	1:G:363:LYS:HE2	1.75	0.68
1:F:305:VAL:HG12	1:F:310:ILE:HD12	1.75	0.68
3:G:528:HOH:O	1:J:351:THR:HG22	1.93	0.67
1:J:338:ASP:OD2	1:J:358:HIS:HE1	1.78	0.66
1:A:307:GLY:HA2	1:A:363:LYS:HE2	1.76	0.66
1:H:335:ARG:HB3	1:K:330:LYS:HA	1.75	0.66
1:C:336:LEU:HD22	1:C:357:ILE:HG23	1.77	0.66
1:B:396:CYS:SG	1:A:396:CYS:HB3	2.36	0.65
1:L:333:LEU:HA	1:L:336:LEU:HD13	1.77	0.65
1:L:297:TYR:HA	1:K:391:ARG:NH1	2.12	0.65
1:A:315:ASP:HB3	1:A:384:LEU:HD11	1.80	0.64
1:A:354:VAL:HG22	1:A:377:GLN:HE21	1.63	0.64
1:D:298:MET:HG2	1:D:313:PHE:HE1	1.61	0.64
1:F:391:ARG:HH21	1:E:296:VAL:HG13	1.62	0.64
1:D:307:GLY:HA2	1:D:363:LYS:HE2	1.79	0.64
1:L:331:CYS:HB2	1:L:333:LEU:CD1	2.21	0.63
1:D:379:ASN:OD1	1:L:341:TYR:CE2	2.51	0.63
1:B:351:THR:HB	1:B:377:GLN:HB2	1.80	0.63
1:H:329:GLN:NE2	1:K:325:TYR:OH	2.30	0.63
1:I:323:MET:HE2	1:I:373:PHE:HE2	1.62	0.63
1:A:366:GLN:NE2	2:A:451:GOL:O2	2.31	0.63
1:B:323:MET:HE2	1:B:373:PHE:CE1	2.33	0.62
1:E:323:MET:HE2	1:E:373:PHE:CE1	2.34	0.62
1:I:340:ARG:NH2	1:I:358:HIS:HE1	1.97	0.62
1:H:322:PHE:HB3	1:H:376:LEU:HD13	1.81	0.62
1:D:333:LEU:HD23	1:D:357:ILE:HD13	1.81	0.62
1:C:379:ASN:ND2	1:J:341:TYR:CE2	2.59	0.62
1:C:379:ASN:ND2	1:J:341:TYR:HE2	1.92	0.62
1:A:323:MET:HE3	1:A:328:ALA:HB2	1.82	0.61
1:A:325:TYR:CE1	1:K:325:TYR:OH	2.48	0.61
1:E:310:ILE:HD11	1:E:331:CYS:SG	2.40	0.61
1:A:358:HIS:CD2	2:A:453:GOL:H32	2.36	0.60
1:E:296:VAL:HG21	1:E:413:PHE:HB3	1.83	0.60
1:A:307:GLY:H	1:A:363:LYS:HZ1	1.50	0.60
1:D:420:THR:HG21	1:L:338:ASP:OD1	2.01	0.60
1:F:396:CYS:HA	1:E:397:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:VAL:HG12	1:B:310:ILE:HD12	1.83	0.59
1:L:416:GLU:H	1:L:416:GLU:CD	2.05	0.59
1:H:315:ASP:HB3	1:H:384:LEU:HD21	1.83	0.59
1:K:323:MET:CG	1:K:327:CYS:SG	2.90	0.59
1:E:334:LEU:CD1	1:L:330:LYS:HB2	2.32	0.58
1:D:323:MET:HE2	1:D:373:PHE:HE2	1.67	0.58
1:I:305:VAL:HG12	1:I:310:ILE:HD12	1.85	0.58
1:F:296:VAL:HG13	1:E:391:ARG:HH12	1.68	0.58
1:J:397:ILE:O	1:I:396:CYS:HA	2.02	0.58
1:K:353:ILE:HG23	1:K:374:THR:HG23	1.83	0.58
1:D:394:GLN:NE2	1:C:400:LYS:HA	2.19	0.58
1:J:323:MET:HE2	1:J:373:PHE:HE1	1.67	0.57
1:G:323:MET:HE2	1:G:373:PHE:HE2	1.69	0.57
1:E:359:LEU:HD11	1:E:370:PRO:HB2	1.85	0.57
1:H:298:MET:HE1	1:G:319:GLN:HA	1.87	0.57
1:B:359:LEU:HD11	1:B:370:PRO:HB2	1.87	0.57
1:A:351:THR:O	1:A:352:GLU:HG2	2.04	0.56
1:L:400:LYS:HG2	1:K:394:GLN:HB3	1.87	0.56
1:A:341:TYR:N	2:A:452:GOL:O1	2.37	0.56
1:D:330:LYS:CG	1:L:335:ARG:HA	2.35	0.56
1:E:296:VAL:HG22	1:E:298:MET:O	2.04	0.56
1:E:305:VAL:HG12	1:E:310:ILE:HG13	1.87	0.56
1:A:338:ASP:OD2	1:A:358:HIS:HE1	1.89	0.56
1:C:310:ILE:HD11	1:C:331:CYS:SG	2.46	0.56
1:K:416:GLU:CD	1:K:416:GLU:H	2.08	0.56
1:K:306:ASN:ND2	1:K:361:THR:HG22	2.22	0.55
1:E:315:ASP:HB3	1:E:384:LEU:HD21	1.88	0.55
1:F:342:ARG:HB2	2:F:453:GOL:H32	1.89	0.55
1:E:310:ILE:HD13	1:E:330:LYS:NZ	2.22	0.55
1:D:339:THR:HB	1:E:311:LYS:HZ2	1.72	0.55
1:H:329:GLN:HG3	1:H:334:LEU:HD11	1.89	0.55
1:G:325:TYR:CE2	1:G:334:LEU:HD11	2.42	0.54
1:I:405:ARG:HG3	1:I:410:GLU:HG2	1.89	0.54
1:G:325:TYR:OH	1:J:325:TYR:CE1	2.59	0.54
1:L:331:CYS:CB	1:L:333:LEU:HD12	2.28	0.54
1:B:405:ARG:HH22	1:A:405:ARG:HH22	1.54	0.54
1:C:379:ASN:ND2	1:J:341:TYR:OH	2.41	0.54
1:B:323:MET:HE3	1:B:328:ALA:HB2	1.90	0.54
1:A:325:TYR:CZ	1:K:325:TYR:OH	2.60	0.54
1:G:305:VAL:CG1	1:G:310:ILE:HD12	2.38	0.53
1:L:305:VAL:CG1	1:L:310:ILE:HD12	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:306:ASN:HD22	1:K:361:THR:HG22	1.73	0.53
1:D:330:LYS:HG3	1:L:335:ARG:HA	1.89	0.53
1:J:341:TYR:HD1	1:J:342:ARG:H	1.57	0.53
1:I:337:MET:SD	1:I:357:ILE:HG12	2.49	0.53
1:A:416:GLU:CD	1:A:416:GLU:H	2.12	0.53
1:H:307:GLY:H	1:H:363:LYS:HZ1	1.57	0.53
1:G:341:TYR:HE1	1:G:352:GLU:HB3	1.73	0.52
1:A:353:ILE:HG23	1:A:374:THR:HG23	1.91	0.52
1:I:416:GLU:CD	1:I:416:GLU:H	2.13	0.52
1:F:416:GLU:CD	1:F:416:GLU:H	2.12	0.52
1:D:407:ASP:OD1	1:D:407:ASP:N	2.42	0.52
1:J:351:THR:HG23	3:J:518:HOH:O	2.09	0.51
1:E:334:LEU:HD13	1:L:330:LYS:HB2	1.92	0.51
1:J:338:ASP:OD2	1:J:358:HIS:CE1	2.60	0.51
1:F:359:LEU:HD11	1:F:370:PRO:HB2	1.93	0.51
1:J:323:MET:HE2	1:J:373:PHE:CE1	2.45	0.51
1:D:330:LYS:HB2	1:L:335:ARG:N	2.25	0.51
1:I:310:ILE:HD11	1:I:331:CYS:SG	2.51	0.51
1:C:334:LEU:HD23	1:C:334:LEU:O	2.11	0.51
1:J:416:GLU:H	1:J:416:GLU:CD	2.14	0.51
1:C:315:ASP:HB3	1:C:384:LEU:HD21	1.93	0.51
1:C:346:GLN:HG2	1:C:347:GLY:N	2.25	0.51
1:L:380:LYS:HD2	3:L:522:HOH:O	2.11	0.51
1:C:379:ASN:HB2	1:J:341:TYR:CE2	2.47	0.50
1:D:330:LYS:HB2	1:L:334:LEU:O	2.12	0.50
1:K:323:MET:HE3	1:K:328:ALA:HB2	1.93	0.50
1:D:385:PHE:CE1	1:D:390:LEU:HD13	2.47	0.50
1:F:307:GLY:H	1:F:363:LYS:HZ1	1.59	0.49
1:E:334:LEU:HB3	1:L:330:LYS:CD	2.42	0.49
1:H:385:PHE:CE1	1:H:390:LEU:HD13	2.47	0.49
1:G:310:ILE:HD11	1:G:331:CYS:SG	2.52	0.49
1:L:299:LEU:HD12	1:K:316:SER:HB2	1.94	0.49
1:B:342:ARG:HD2	1:B:353:ILE:HG12	1.94	0.49
1:F:391:ARG:NH2	1:E:296:VAL:HG13	2.26	0.49
1:D:325:TYR:HB3	1:L:325:TYR:OH	2.13	0.49
1:K:419:ILE:O	1:K:420:THR:OG1	2.29	0.49
1:E:310:ILE:HD12	1:E:327:CYS:SG	2.53	0.49
1:I:310:ILE:CD1	1:I:327:CYS:SG	3.01	0.49
1:K:385:PHE:CE1	1:K:390:LEU:HD13	2.48	0.48
1:F:305:VAL:CG1	1:F:310:ILE:HD12	2.42	0.48
1:G:364:ILE:HG22	1:G:411:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ILE:HG23	1:D:374:THR:HG23	1.95	0.48
1:C:340:ARG:HG2	1:G:420:THR:HG21	1.95	0.48
1:L:391:ARG:NH2	1:K:296:VAL:O	2.41	0.48
1:A:407:ASP:OD1	1:A:407:ASP:N	2.47	0.48
1:H:407:ASP:OD1	1:H:407:ASP:N	2.46	0.48
1:A:338:ASP:OD1	1:A:339:THR:HG22	2.13	0.48
1:I:305:VAL:CG1	1:I:310:ILE:HD12	2.44	0.48
1:L:394:GLN:O	1:K:400:LYS:HE3	2.13	0.48
1:C:420:THR:O	1:C:421:LYS:C	2.52	0.48
1:E:319:GLN:N	3:E:501:HOH:O	2.44	0.48
1:C:339:THR:HG23	1:G:420:THR:HG22	1.96	0.48
1:F:385:PHE:HE2	1:F:390:LEU:HD13	1.78	0.48
1:I:340:ARG:NH2	1:I:358:HIS:CE1	2.80	0.48
1:D:399:LEU:CD1	1:C:390:LEU:HB3	2.44	0.48
1:I:308:VAL:HG21	1:I:331:CYS:HA	1.95	0.48
1:L:339:THR:HG23	3:L:527:HOH:O	2.14	0.47
1:F:323:MET:HE3	1:F:328:ALA:HB2	1.96	0.47
1:J:395:CYS:O	1:I:399:LEU:HB2	2.14	0.47
1:B:325:TYR:HE2	1:F:377:GLN:NE2	2.12	0.47
1:F:397:ILE:O	1:E:396:CYS:HA	2.13	0.47
1:J:364:ILE:CG2	1:J:411:ILE:HG13	2.44	0.47
1:C:359:LEU:HD11	1:C:370:PRO:HB2	1.97	0.47
1:H:392:ARG:HG3	1:H:393:TYR:CD1	2.50	0.47
1:L:333:LEU:HD23	1:L:336:LEU:HD22	1.96	0.47
1:L:339:THR:HG22	1:L:339:THR:O	2.15	0.47
1:A:338:ASP:OD2	1:A:358:HIS:CE1	2.68	0.47
1:D:397:ILE:O	1:C:396:CYS:HA	2.14	0.47
1:C:353:ILE:HD12	1:C:374:THR:HG21	1.96	0.47
1:H:405:ARG:CG	1:H:410:GLU:HG2	2.45	0.47
1:H:335:ARG:H	1:H:335:ARG:HG2	1.31	0.46
1:H:405:ARG:HG2	1:H:410:GLU:HG2	1.97	0.46
1:K:296:VAL:HG12	1:K:299:LEU:HD23	1.98	0.46
1:F:323:MET:HE2	1:F:373:PHE:HE1	1.81	0.46
1:L:333:LEU:HD22	1:L:357:ILE:HD13	1.97	0.46
1:K:353:ILE:HG23	1:K:374:THR:CG2	2.45	0.46
1:D:330:LYS:HZ2	1:D:330:LYS:HG2	1.56	0.46
1:B:397:ILE:O	1:A:396:CYS:HA	2.16	0.46
1:D:339:THR:HB	1:E:311:LYS:NZ	2.28	0.46
1:E:334:LEU:HB3	1:L:330:LYS:HD3	1.97	0.46
1:K:301:ILE:CG1	1:K:312:ALA:HB3	2.45	0.46
1:D:399:LEU:HD13	1:C:390:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ASP:HA	1:C:396:CYS:SG	2.56	0.46
1:G:341:TYR:HA	1:G:353:ILE:HD11	1.98	0.46
1:J:367:ARG:HD3	1:J:407:ASP:OD2	2.16	0.46
1:I:340:ARG:CZ	1:I:358:HIS:HE1	2.29	0.46
1:L:407:ASP:OD1	1:L:407:ASP:N	2.48	0.46
1:J:304:GLU:HB2	1:J:363:LYS:HB3	1.96	0.46
1:J:364:ILE:HG22	1:J:411:ILE:HG13	1.97	0.46
1:C:305:VAL:HG21	1:C:323:MET:HE1	1.98	0.45
1:H:310:ILE:HD11	1:H:331:CYS:SG	2.56	0.45
1:H:391:ARG:CZ	1:G:296:VAL:O	2.65	0.45
1:J:396:CYS:SG	1:I:398:ASP:OD1	2.75	0.45
1:L:387:LEU:HA	1:L:390:LEU:HB2	1.98	0.45
1:D:305:VAL:HG12	1:D:310:ILE:HD12	1.97	0.45
1:H:339:THR:HG21	3:H:510:HOH:O	2.15	0.45
1:A:307:GLY:H	1:A:363:LYS:NZ	2.14	0.45
1:C:326:ALA:O	1:C:329:GLN:HG3	2.17	0.45
1:G:322:PHE:CE2	1:G:384:LEU:HD23	2.51	0.45
1:L:341:TYR:CE1	1:L:353:ILE:O	2.70	0.45
1:C:397:ILE:HD13	1:C:404:LEU:HD13	1.99	0.45
1:J:353:ILE:HG23	1:J:374:THR:HG23	1.98	0.45
1:C:353:ILE:HG23	1:C:374:THR:HG23	1.99	0.44
1:L:340:ARG:HD2	1:L:340:ARG:HA	1.59	0.44
1:I:354:VAL:HG22	1:I:377:GLN:HG3	1.98	0.44
1:F:379:ASN:HB2	3:F:501:HOH:O	2.17	0.44
1:F:387:LEU:O	1:F:391:ARG:HG2	2.17	0.44
1:L:405:ARG:NH2	1:K:405:ARG:HH12	2.15	0.44
1:H:297:TYR:O	1:H:298:MET:HE2	2.16	0.44
1:J:301:ILE:HG13	1:J:312:ALA:HB3	2.00	0.44
1:I:310:ILE:HD13	1:I:327:CYS:SG	2.57	0.44
1:K:331:CYS:O	1:K:333:LEU:HD13	2.17	0.44
1:C:359:LEU:HA	1:C:371:SER:O	2.18	0.44
1:F:406:ILE:HG23	1:F:407:ASP:OD1	2.18	0.44
1:H:307:GLY:H	1:H:363:LYS:NZ	2.15	0.44
1:G:341:TYR:CE1	1:G:352:GLU:HB3	2.52	0.44
1:B:296:VAL:O	1:A:391:ARG:NH2	2.47	0.44
1:F:400:LYS:HA	1:E:394:GLN:HE21	1.83	0.44
1:G:359:LEU:HA	1:G:371:SER:O	2.18	0.44
1:L:310:ILE:HD11	1:L:327:CYS:SG	2.58	0.44
1:J:323:MET:HE3	1:J:328:ALA:HB2	1.99	0.44
1:B:331:CYS:O	1:B:333:LEU:HD13	2.18	0.43
1:C:420:THR:HG21	1:J:339:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:LEU:CB	1:L:330:LYS:HB2	2.48	0.43
1:F:296:VAL:HG22	1:E:391:ARG:HH22	1.83	0.43
1:B:305:VAL:CG1	1:B:310:ILE:HD12	2.46	0.43
1:E:308:VAL:O	1:E:310:ILE:HG12	2.18	0.43
1:E:335:ARG:H	1:E:335:ARG:HG3	1.50	0.43
1:G:339:THR:HG21	1:J:420:THR:HG23	1.99	0.43
1:I:379:ASN:H	1:I:379:ASN:ND2	2.16	0.43
1:B:405:ARG:NH2	1:A:405:ARG:NH2	2.54	0.43
1:A:323:MET:HE2	1:A:373:PHE:CE1	2.53	0.43
1:I:323:MET:HE2	1:I:373:PHE:CE2	2.47	0.43
1:C:351:THR:HB	1:C:377:GLN:HB2	2.00	0.43
1:F:379:ASN:CA	3:F:501:HOH:O	2.66	0.43
1:H:329:GLN:HG2	1:H:334:LEU:CD1	2.45	0.43
1:I:310:ILE:HD11	1:I:327:CYS:SG	2.58	0.43
1:D:359:LEU:HA	1:D:371:SER:O	2.18	0.43
1:D:379:ASN:ND2	1:D:379:ASN:H	2.17	0.43
1:F:359:LEU:HA	1:F:371:SER:O	2.18	0.43
1:H:379:ASN:ND2	1:H:379:ASN:H	2.17	0.43
1:J:398:ASP:HA	1:I:396:CYS:SG	2.58	0.43
1:L:342:ARG:NH1	1:L:352:GLU:HA	2.34	0.42
1:D:379:ASN:OD1	1:L:341:TYR:CZ	2.72	0.42
1:L:331:CYS:CB	1:L:333:LEU:CD1	2.92	0.42
1:A:353:ILE:HG23	1:A:374:THR:CG2	2.49	0.42
1:A:359:LEU:HA	1:A:371:SER:O	2.18	0.42
1:E:357:ILE:HD12	1:E:373:PHE:CE1	2.54	0.42
1:K:306:ASN:OD1	1:K:333:LEU:HD11	2.19	0.42
1:D:323:MET:HE2	1:D:373:PHE:CE2	2.50	0.42
1:D:340:ARG:HH21	1:D:358:HIS:HE1	1.66	0.42
1:F:307:GLY:H	1:F:363:LYS:NZ	2.16	0.42
1:J:416:GLU:HA	1:J:419:ILE:HD12	2.01	0.42
1:F:394:GLN:HB3	1:E:400:LYS:HA	2.01	0.42
1:E:359:LEU:HA	1:E:371:SER:O	2.20	0.42
1:B:387:LEU:HA	1:B:390:LEU:HB2	2.02	0.42
1:A:323:MET:HE2	1:A:373:PHE:HE1	1.85	0.42
1:F:357:ILE:HD12	1:F:373:PHE:CE1	2.54	0.42
1:I:379:ASN:ND2	1:I:379:ASN:N	2.67	0.42
1:D:396:CYS:HA	1:C:397:ILE:O	2.20	0.42
1:H:359:LEU:HA	1:H:371:SER:O	2.19	0.42
1:E:387:LEU:HA	1:E:390:LEU:HB2	2.02	0.42
1:H:390:LEU:HB3	1:G:399:LEU:CD1	2.50	0.42
1:D:299:LEU:HD12	1:C:316:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:315:ASP:HB3	1:J:384:LEU:HD21	2.02	0.41
1:D:359:LEU:HD11	1:D:370:PRO:HB2	2.02	0.41
1:B:319:GLN:HB2	1:A:298:MET:HE3	2.02	0.41
1:A:325:TYR:HE1	1:K:334:LEU:HD13	1.85	0.41
1:D:325:TYR:HD2	1:L:325:TYR:CE1	2.38	0.41
1:F:352:GLU:O	1:F:376:LEU:CD2	2.68	0.41
1:D:342:ARG:HB2	1:D:353:ILE:HG12	2.02	0.41
1:B:327:CYS:O	1:B:330:LYS:HG2	2.20	0.41
1:A:351:THR:HG21	1:A:377:GLN:HB2	2.03	0.41
1:G:387:LEU:HA	1:G:390:LEU:HB2	2.03	0.41
1:F:325:TYR:OH	1:I:329:GLN:HG2	2.20	0.41
1:J:359:LEU:HA	1:J:371:SER:O	2.21	0.41
1:L:377:GLN:HE21	1:L:377:GLN:HB2	1.44	0.41
1:I:387:LEU:HA	1:I:390:LEU:HB2	2.03	0.41
1:L:336:LEU:HD12	1:L:336:LEU:N	2.36	0.41
1:C:346:GLN:HG2	1:C:347:GLY:H	1.85	0.41
1:K:333:LEU:HD23	1:K:357:ILE:HD12	2.03	0.41
1:B:310:ILE:CD1	1:B:327:CYS:SG	3.09	0.41
1:J:387:LEU:HA	1:J:390:LEU:HB2	2.03	0.41
1:L:359:LEU:HA	1:L:371:SER:O	2.20	0.40
1:K:385:PHE:HE1	1:K:390:LEU:HD13	1.85	0.40
1:B:306:ASN:HB2	1:B:333:LEU:HD11	2.04	0.40
1:B:359:LEU:HA	1:B:371:SER:O	2.20	0.40
1:F:385:PHE:CE2	1:F:390:LEU:HD13	2.56	0.40
1:D:353:ILE:HG23	1:D:374:THR:CG2	2.52	0.40
1:J:310:ILE:HD11	1:J:331:CYS:SG	2.61	0.40
1:C:418:ASP:OD1	1:C:418:ASP:N	2.55	0.40
1:G:416:GLU:CD	1:G:416:GLU:H	2.24	0.40
1:J:357:ILE:HD12	1:J:373:PHE:CE1	2.56	0.40
1:I:305:VAL:HG13	1:I:331:CYS:SG	2.62	0.40
1:B:310:ILE:HD11	1:B:331:CYS:SG	2.61	0.40
1:A:335:ARG:HD3	1:A:335:ARG:N	2.36	0.40
1:J:396:CYS:SG	1:I:398:ASP:CG	3.00	0.40

All (46) 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:336:LEU:CD1	1:F:306:ASN:O[4_454]	0.87	1.33
1:C:359:LEU:CD2	1:F:361:THR:CG2[4_454]	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:361:THR:HG1	1:I:359:LEU:HD23[4_454]	0.60	1.00
1:C:332:SER:O	1:F:332:SER:OG[4_454]	1.22	0.98
1:C:336:LEU:CG	1:F:306:ASN:O[4_454]	1.29	0.91
1:C:359:LEU:HD22	1:F:361:THR:HG22[4_454]	0.78	0.82
1:J:361:THR:OG1	1:I:359:LEU:HD23[4_454]	0.84	0.76
1:C:359:LEU:HD21	1:F:361:THR:CG2[4_454]	0.87	0.73
1:C:336:LEU:HD11	1:F:306:ASN:O[4_454]	0.88	0.72
1:B:335:ARG:HH11	1:G:332:SER:HG[3_555]	0.89	0.71
1:C:359:LEU:CD2	1:F:361:THR:HG22[4_454]	0.89	0.71
1:C:359:LEU:HD21	1:F:361:THR:HG21[4_454]	0.91	0.69
1:B:335:ARG:NH1	1:G:332:SER:OG[3_555]	1.52	0.68
1:C:359:LEU:CD2	1:F:361:THR:CB[4_454]	1.53	0.67
1:C:336:LEU:CD1	1:F:306:ASN:C[4_454]	1.54	0.66
1:J:361:THR:HG1	1:I:359:LEU:CD2[4_454]	0.95	0.65
1:C:332:SER:OG	1:F:335:ARG:HH21[4_454]	0.98	0.62
1:J:361:THR:OG1	1:I:359:LEU:CD2[4_454]	1.67	0.53
1:C:332:SER:OG	1:F:335:ARG:NH2[4_454]	1.70	0.50
1:C:359:LEU:HD23	1:F:361:THR:CB[4_454]	1.12	0.48
1:C:332:SER:HG	1:F:335:ARG:HH21[4_454]	1.14	0.46
1:C:359:LEU:HD21	1:F:361:THR:HG22[4_454]	1.18	0.42
1:C:359:LEU:HD23	1:F:361:THR:HB[4_454]	1.19	0.41
1:K:332:SER:HB3	1:K:332:SER:HB3[8_554]	1.20	0.40
1:C:359:LEU:HD22	1:F:361:THR:CG2[4_454]	1.22	0.38
1:C:332:SER:C	1:F:332:SER:OG[4_454]	1.85	0.35
1:B:335:ARG:HH12	1:G:332:SER:OG[3_555]	1.27	0.33
1:C:359:LEU:HD23	1:F:361:THR:HG1[4_454]	1.30	0.30
1:A:332:SER:HG	1:H:332:SER:O[8_554]	1.32	0.28
1:J:361:THR:HG1	1:I:359:LEU:HD21[4_454]	1.34	0.26
1:C:336:LEU:HD11	1:F:306:ASN:C[4_454]	1.35	0.25
1:C:336:LEU:HD12	1:F:306:ASN:C[4_454]	1.36	0.24
1:J:361:THR:CB	1:I:359:LEU:HD23[4_454]	1.36	0.24
1:B:335:ARG:HH11	1:G:332:SER:OG[3_555]	1.38	0.22
1:B:335:ARG:NH1	1:G:332:SER:HG[3_555]	1.39	0.21
1:C:359:LEU:HD23	1:F:361:THR:OG1[4_454]	1.40	0.20
1:C:336:LEU:HG	1:F:306:ASN:O[4_454]	1.43	0.17
1:J:332:SER:O	1:I:306:ASN:ND2[4_454]	2.06	0.14
1:J:361:THR:CB	1:I:359:LEU:CD2[4_454]	2.06	0.14
3:L:510:HOH:O	3:L:510:HOH:O[7_554]	2.06	0.14
1:C:336:LEU:HD12	1:F:306:ASN:O[4_454]	1.47	0.13
1:C:359:LEU:CD2	1:F:361:THR:OG1[4_454]	2.07	0.13
1:C:332:SER:O	1:F:332:SER:HG[4_454]	1.48	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:SER:OG	1:H:332:SER:O[8_554]	2.12	0.08
1:C:332:SER:C	1:F:332:SER:HG[4_454]	1.54	0.06
1:C:359:LEU:HD21	1:F:361:THR:CB[4_454]	1.59	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	B	116/128 (91%)	112 (97%)	4 (3%)	0	100	100
1	C	124/128 (97%)	117 (94%)	6 (5%)	1 (1%)	19	14
1	D	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	E	104/128 (81%)	100 (96%)	4 (4%)	0	100	100
1	F	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
1	G	116/128 (91%)	114 (98%)	2 (2%)	0	100	100
1	H	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
1	I	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
1	J	114/128 (89%)	113 (99%)	1 (1%)	0	100	100
1	K	117/128 (91%)	113 (97%)	4 (3%)	0	100	100
1	L	117/128 (91%)	115 (98%)	2 (2%)	0	100	100
All	All	1402/1536 (91%)	1345 (96%)	56 (4%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	349	GLY

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	101/113 (89%)	92 (91%)	9 (9%)	9	6
1	B	100/113 (88%)	93 (93%)	7 (7%)	15	11
1	C	99/113 (88%)	89 (90%)	10 (10%)	7	4
1	D	98/113 (87%)	86 (88%)	12 (12%)	5	2
1	E	92/113 (81%)	82 (89%)	10 (11%)	6	3
1	F	102/113 (90%)	90 (88%)	12 (12%)	5	2
1	G	99/113 (88%)	83 (84%)	16 (16%)	2	1
1	H	103/113 (91%)	89 (86%)	14 (14%)	3	2
1	I	103/113 (91%)	91 (88%)	12 (12%)	5	2
1	J	100/113 (88%)	87 (87%)	13 (13%)	4	2
1	K	99/113 (88%)	89 (90%)	10 (10%)	7	4
1	L	105/113 (93%)	94 (90%)	11 (10%)	7	3
All	All	1201/1356 (89%)	1065 (89%)	136 (11%)	6	3

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	319	GLN
1	B	329	GLN
1	B	341	TYR
1	B	351	THR
1	B	363	LYS
1	B	391	ARG
1	B	405	ARG
1	A	324	SER
1	A	329	GLN
1	A	330	LYS
1	A	335	ARG
1	A	336	LEU
1	A	351	THR
1	A	363	LYS

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Mol	Chain	Res	Type
1	A	372	SER
1	A	407	ASP
1	D	319	GLN
1	D	330	LYS
1	D	334	LEU
1	D	335	ARG
1	D	341	TYR
1	D	348	VAL
1	D	363	LYS
1	D	379	ASN
1	D	390	LEU
1	D	391	ARG
1	D	407	ASP
1	D	419	ILE
1	C	302	ASP
1	C	305	VAL
1	C	330	LYS
1	C	340	ARG
1	C	341	TYR
1	C	359	LEU
1	C	364	ILE
1	C	400	LYS
1	C	418	ASP
1	C	421	LYS
1	F	332	SER
1	F	336	LEU
1	F	340	ARG
1	F	351	THR
1	F	364	ILE
1	F	372	SER
1	F	390	LEU
1	F	391	ARG
1	F	407	ASP
1	F	418	ASP
1	F	419	ILE
1	F	420	THR
1	E	296	VAL
1	E	322	PHE
1	E	330	LYS
1	E	337	MET
1	E	338	ASP
1	E	339	THR

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Mol	Chain	Res	Type
1	E	367	ARG
1	E	372	SER
1	E	379	ASN
1	E	390	LEU
1	H	319	GLN
1	H	330	LYS
1	H	335	ARG
1	H	336	LEU
1	H	337	MET
1	H	339	THR
1	H	340	ARG
1	H	363	LYS
1	H	364	ILE
1	H	372	SER
1	H	379	ASN
1	H	390	LEU
1	H	407	ASP
1	H	418	ASP
1	G	298	MET
1	G	322	PHE
1	G	334	LEU
1	G	337	MET
1	G	341	TYR
1	G	352	GLU
1	G	361	THR
1	G	363	LYS
1	G	372	SER
1	G	377	GLN
1	G	381	VAL
1	G	391	ARG
1	G	406	ILE
1	G	409	GLU
1	G	418	ASP
1	G	419	ILE
1	J	310	ILE
1	J	329	GLN
1	J	330	LYS
1	J	335	ARG
1	J	340	ARG
1	J	341	TYR
1	J	350	LYS
1	J	351	THR

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Mol	Chain	Res	Type
1	J	354	VAL
1	J	377	GLN
1	J	379	ASN
1	J	400	LYS
1	J	407	ASP
1	I	301	ILE
1	I	306	ASN
1	I	324	SER
1	I	339	THR
1	I	341	TYR
1	I	352	GLU
1	I	357	ILE
1	I	363	LYS
1	I	372	SER
1	I	379	ASN
1	I	405	ARG
1	I	419	ILE
1	L	296	VAL
1	L	325	TYR
1	L	332	SER
1	L	335	ARG
1	L	337	MET
1	L	341	TYR
1	L	363	LYS
1	L	372	SER
1	L	377	GLN
1	L	391	ARG
1	L	407	ASP
1	K	319	GLN
1	K	330	LYS
1	K	339	THR
1	K	359	LEU
1	K	377	GLN
1	K	384	LEU
1	K	390	LEU
1	K	400	LYS
1	K	405	ARG
1	K	407	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	319	GLN
1	A	329	GLN
1	A	358	HIS
1	A	366	GLN
1	A	377	GLN
1	A	379	ASN
1	D	394	GLN
1	C	379	ASN
1	C	394	GLN
1	F	329	GLN
1	F	377	GLN
1	E	394	GLN
1	H	319	GLN
1	H	379	ASN
1	G	329	GLN
1	J	358	HIS
1	J	377	GLN
1	J	379	ASN
1	I	319	GLN
1	I	377	GLN
1	I	379	ASN
1	L	329	GLN
1	L	377	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	454	-	5,5,5	0.23	0	5,5,5	0.41	0
2	GOL	L	451	-	5,5,5	0.24	0	5,5,5	0.45	0
2	GOL	A	451	-	5,5,5	0.18	0	5,5,5	0.21	0
2	GOL	A	453	-	5,5,5	0.26	0	5,5,5	0.44	0
2	GOL	E	451	-	5,5,5	0.27	0	5,5,5	1.10	0
2	GOL	B	451	-	5,5,5	0.32	0	5,5,5	0.47	0
2	GOL	F	454	-	5,5,5	0.51	0	5,5,5	0.77	0
2	GOL	I	451	-	5,5,5	0.42	0	5,5,5	0.71	0
2	GOL	B	453	-	5,5,5	0.12	0	5,5,5	0.35	0
2	GOL	A	452	-	5,5,5	0.46	0	5,5,5	0.36	0
2	GOL	F	451	-	5,5,5	0.28	0	5,5,5	0.50	0
2	GOL	F	452	-	5,5,5	0.41	0	5,5,5	0.77	0
2	GOL	B	452	-	5,5,5	0.45	0	5,5,5	0.89	0
2	GOL	J	451	-	5,5,5	0.26	0	5,5,5	0.46	0
2	GOL	F	453	-	5,5,5	0.27	0	5,5,5	0.64	0
2	GOL	H	451	-	5,5,5	0.16	0	5,5,5	0.42	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
2	GOL	B	454	-	-	0/4/4/4	-
2	GOL	L	451	-	-	2/4/4/4	-
2	GOL	A	451	-	-	1/4/4/4	-
2	GOL	A	453	-	-	3/4/4/4	-
2	GOL	E	451	-	-	0/4/4/4	-
2	GOL	B	451	-	-	2/4/4/4	-
2	GOL	F	454	-	-	2/4/4/4	-
2	GOL	I	451	-	-	1/4/4/4	-
2	GOL	B	453	-	-	4/4/4/4	-
2	GOL	A	452	-	-	4/4/4/4	-
2	GOL	F	451	-	-	2/4/4/4	-
2	GOL	F	452	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	452	-	-	0/4/4/4	-
2	GOL	J	451	-	-	2/4/4/4	-
2	GOL	F	453	-	-	2/4/4/4	-
2	GOL	H	451	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	451	GOL	C1-C2-C3-O3
2	B	451	GOL	O2-C2-C3-O3
2	B	453	GOL	O1-C1-C2-O2
2	F	451	GOL	C1-C2-C3-O3
2	F	453	GOL	C1-C2-C3-O3
2	H	451	GOL	O1-C1-C2-C3
2	B	453	GOL	O1-C1-C2-C3
2	B	453	GOL	C1-C2-C3-O3
2	A	452	GOL	C1-C2-C3-O3
2	A	453	GOL	C1-C2-C3-O3
2	F	452	GOL	O1-C1-C2-C3
2	F	454	GOL	C1-C2-C3-O3
2	J	451	GOL	C1-C2-C3-O3
2	L	451	GOL	O1-C1-C2-C3
2	B	453	GOL	O2-C2-C3-O3
2	F	451	GOL	O2-C2-C3-O3
2	F	452	GOL	O1-C1-C2-O2
2	F	453	GOL	O2-C2-C3-O3
2	H	451	GOL	O1-C1-C2-O2
2	J	451	GOL	O2-C2-C3-O3
2	F	454	GOL	O2-C2-C3-O3
2	L	451	GOL	O1-C1-C2-O2
2	A	453	GOL	O1-C1-C2-C3
2	A	453	GOL	O2-C2-C3-O3
2	F	452	GOL	O2-C2-C3-O3
2	A	452	GOL	O2-C2-C3-O3
2	A	451	GOL	O1-C1-C2-C3
2	A	452	GOL	O1-C1-C2-O2
2	I	451	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	452	GOL	O1-C1-C2-C3
2	F	452	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	GOL	1	0
2	A	453	GOL	1	0
2	A	452	GOL	1	0
2	F	453	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	124/128 (96%)	0.35	4 (3%) 47 54	25, 33, 46, 53	0
1	B	120/128 (93%)	0.15	2 (1%) 70 74	22, 33, 44, 54	0
1	C	126/128 (98%)	0.24	8 (6%) 20 24	19, 34, 45, 58	0
1	D	124/128 (96%)	0.05	1 (0%) 86 88	23, 33, 44, 52	0
1	E	110/128 (85%)	0.18	2 (1%) 68 72	23, 33, 47, 55	0
1	F	121/128 (94%)	0.30	2 (1%) 70 74	24, 32, 43, 50	0
1	G	120/128 (93%)	0.18	4 (3%) 46 53	23, 34, 45, 57	0
1	H	119/128 (92%)	0.45	4 (3%) 45 51	23, 31, 44, 52	0
1	I	124/128 (96%)	0.37	2 (1%) 72 76	24, 33, 45, 53	0
1	J	120/128 (93%)	0.33	5 (4%) 36 42	21, 33, 48, 55	0
1	K	123/128 (96%)	0.19	6 (4%) 29 35	23, 35, 46, 55	0
1	L	123/128 (96%)	0.20	2 (1%) 72 76	23, 34, 44, 60	0
All	All	1454/1536 (94%)	0.25	42 (2%) 51 57	19, 33, 46, 60	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	406	ILE	5.8
1	L	296	VAL	4.4
1	C	349	GLY	4.3
1	J	406	ILE	4.1
1	B	408	ASN	4.1
1	C	409	GLU	3.6
1	I	344	VAL	3.6
1	C	406	ILE	3.5
1	I	345	ALA	3.3
1	C	408	ASN	3.2
1	D	420	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	411	ILE	3.1
1	J	419	ILE	3.1
1	A	406	ILE	3.1
1	K	408	ASN	3.0
1	G	345	ALA	2.9
1	B	406	ILE	2.8
1	A	407	ASP	2.8
1	K	364	ILE	2.7
1	E	296	VAL	2.7
1	H	406	ILE	2.7
1	K	419	ILE	2.6
1	H	331	CYS	2.6
1	A	420	THR	2.6
1	A	343	GLY	2.6
1	E	408	ASN	2.6
1	F	349	GLY	2.5
1	C	296	VAL	2.3
1	J	301	ILE	2.3
1	J	297	TYR	2.3
1	G	406	ILE	2.3
1	C	420	THR	2.3
1	C	405	ARG	2.3
1	K	399	LEU	2.3
1	H	327	CYS	2.2
1	J	408	ASN	2.2
1	F	297	TYR	2.2
1	K	344	VAL	2.2
1	G	297	TYR	2.1
1	H	328	ALA	2.0
1	K	406	ILE	2.0
1	G	344	VAL	2.0

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
2	GOL	B	452	6/6	0.57	0.27	36,46,53,54	2
2	GOL	A	453	6/6	0.79	0.17	43,47,51,52	2
2	GOL	F	451	6/6	0.80	0.24	43,49,55,60	2
2	GOL	A	452	6/6	0.83	0.14	36,46,50,52	2
2	GOL	I	451	6/6	0.83	0.17	40,55,67,69	2
2	GOL	F	454	6/6	0.85	0.17	29,41,48,49	2
2	GOL	A	451	6/6	0.86	0.11	41,43,47,48	2
2	GOL	E	451	6/6	0.86	0.15	43,50,57,62	2
2	GOL	F	453	6/6	0.86	0.19	37,43,51,67	2
2	GOL	L	451	6/6	0.86	0.17	41,44,48,49	2
2	GOL	F	452	6/6	0.88	0.18	43,47,50,50	2
2	GOL	B	451	6/6	0.89	0.14	32,49,59,59	2
2	GOL	B	453	6/6	0.89	0.23	42,45,53,54	2
2	GOL	H	451	6/6	0.90	0.18	43,44,50,50	2
2	GOL	J	451	6/6	0.92	0.13	38,43,46,49	2
2	GOL	B	454	6/6	0.97	0.16	37,43,49,53	2

6.5 Other polymers

There are no such residues in this entry.