



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:50 PM UTC

PDB ID : 1X9J / pdb_00001x9j
Title : Structure of butyrate kinase 2 reveals both open- and citrate-induced closed conformations: implications for substrate-induced fit conformational changes
Authors : Diao, J.S.; Sanders, D.A.; Hasson, M.S.
Deposited on : 2004-08-21
Resolution : 3.00 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

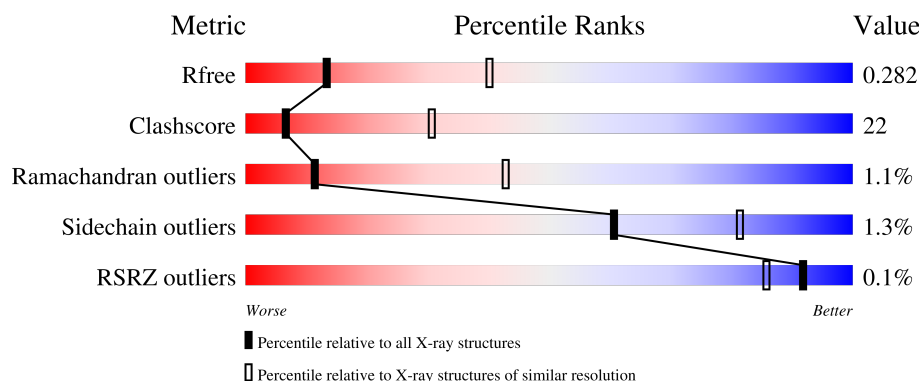
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	375	
1	B	375	
1	C	375	
1	D	375	
1	E	375	

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Mol	Chain	Length	Quality of chain
1	F	375	 58% 39% ..
1	G	375	 58% 41% ..
1	H	375	 56% 42% ..

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	A	395	-	X	-	-
2	GOL	B	394	-	X	-	-
2	GOL	C	392	-	X	-	-
2	GOL	D	393	-	X	-	-
2	GOL	F	391	-	X	-	-
5	CIT	D	381	-	X	-	-
5	CIT	D	384	-	X	-	-
5	CIT	G	382	-	X	-	-
5	CIT	G	383	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23615 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 Probable butyrate kinase 2.

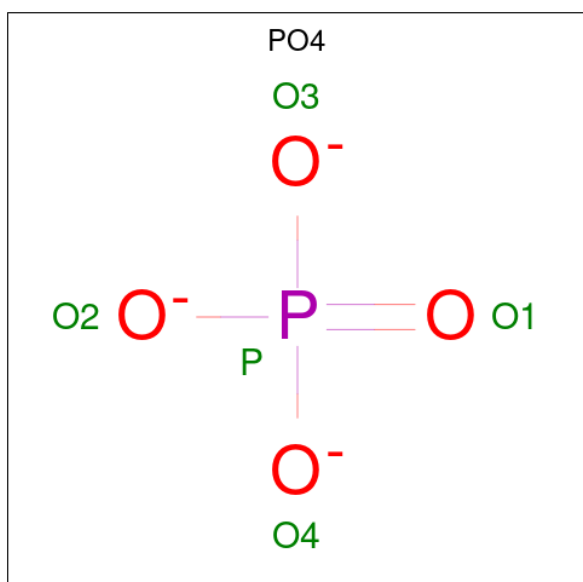
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	B	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	C	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	D	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	E	371	Total	C	N	O	S	0	0	0
			2927	1858	519	537	13			
1	F	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			
1	G	373	Total	C	N	O	S	0	0	0
			2939	1866	521	539	13			
1	H	372	Total	C	N	O	S	0	0	0
			2931	1860	520	538	13			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

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

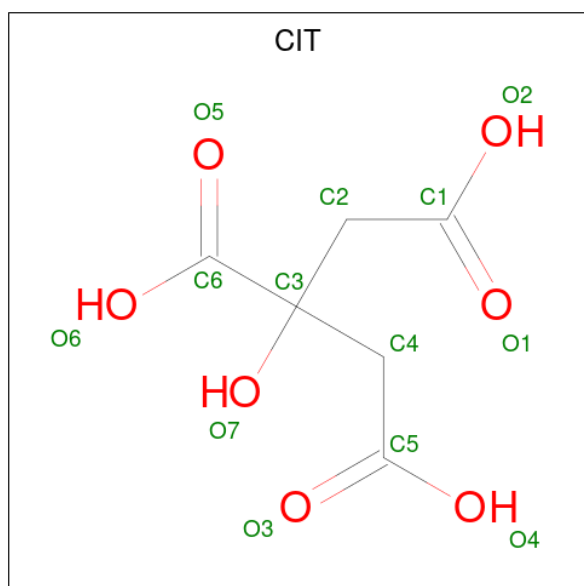


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Na 1 1	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	G	1	Total C O 13 6 7	0	0
5	G	1	Total C O 13 6 7	0	0

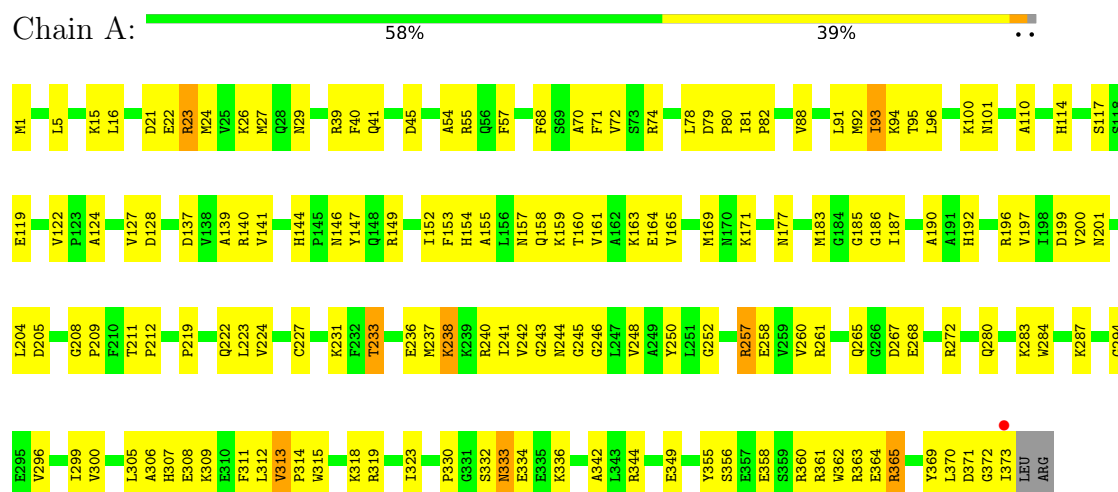
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	7	Total O 7 7	0	0
6	C	5	Total O 5 5	0	0
6	D	10	Total O 10 10	0	0
6	E	4	Total O 4 4	0	0
6	F	3	Total O 3 3	0	0
6	G	8	Total O 8 8	0	0
6	H	2	Total O 2 2	0	0

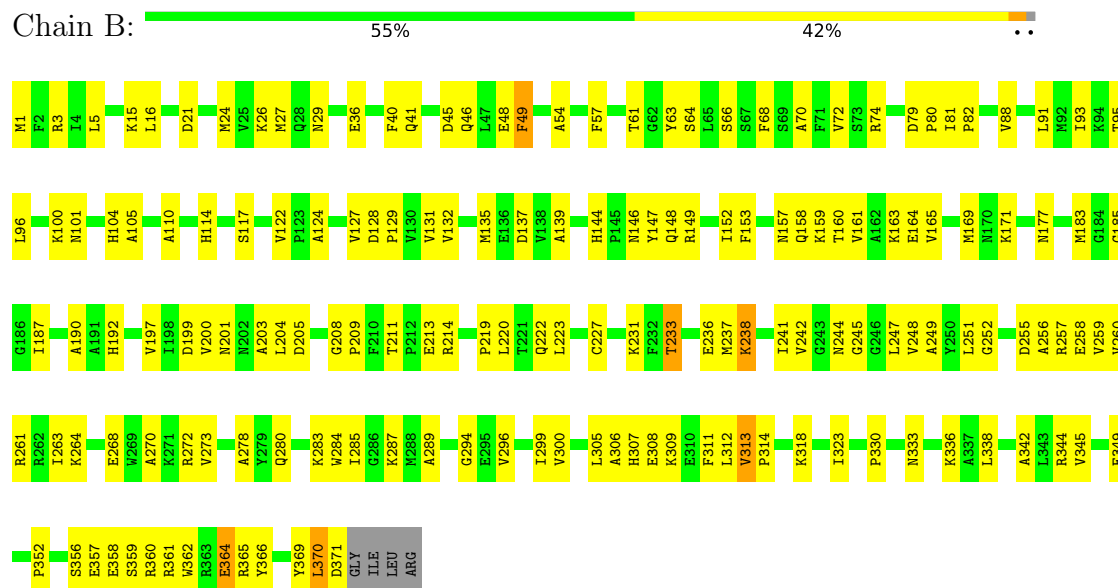
3 Residue-property plots

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: Probable butyrate kinase 2

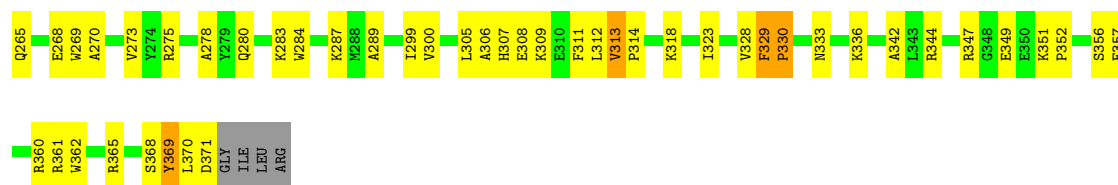


• Molecule 1: Probable butyrate kinase 2



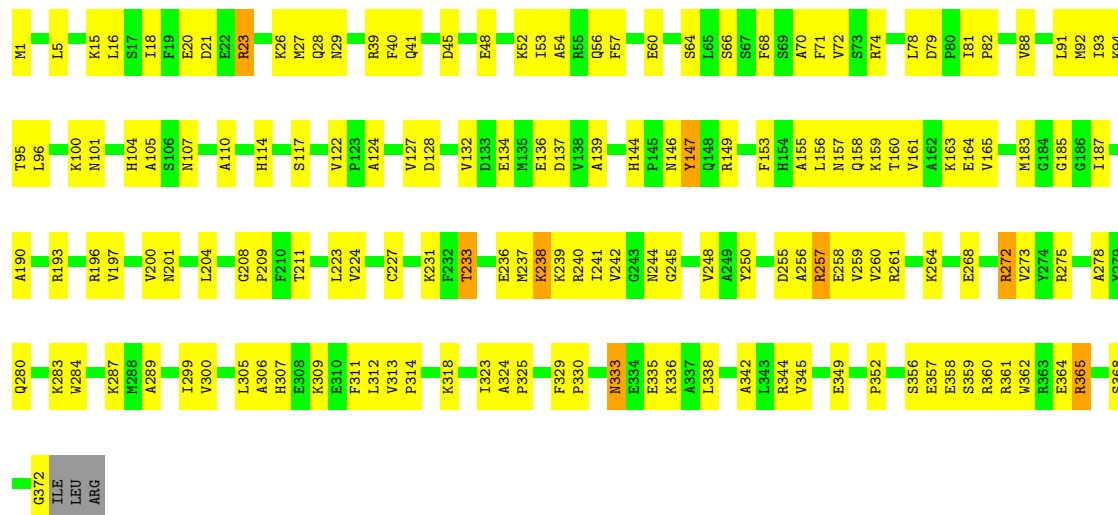
• Molecule 1: Probable butyrate kinase 2





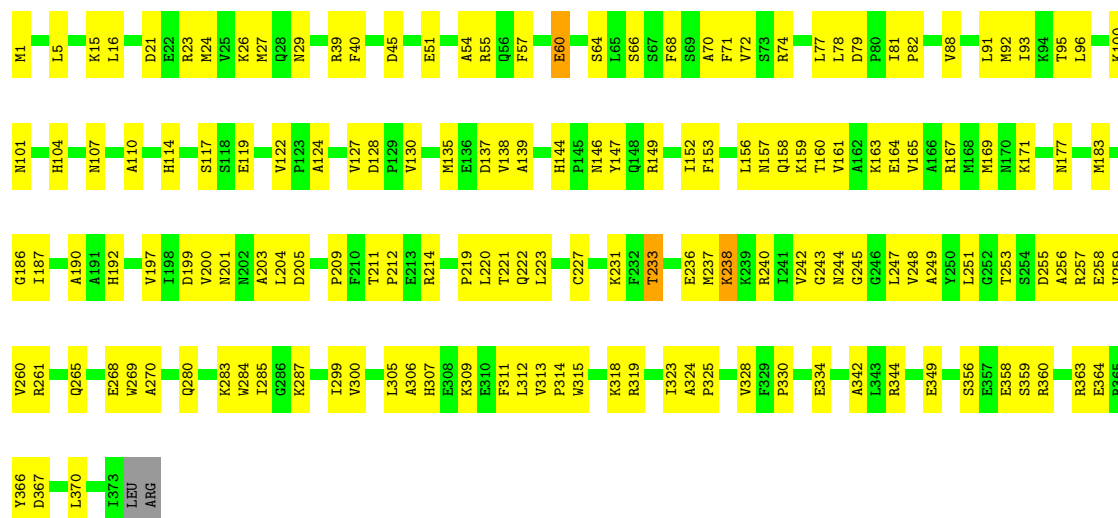
- Molecule 1: Probable butyrate kinase 2

Chain F: 58% 39% ..



- Molecule 1: Probable butyrate kinase 2

Chain G: 58% 41% ..



- Molecule 1: Probable butyrate kinase 2

Chain H: 56% 42% ..

E357	W269	G185	L96	M1
E358	A270	G186	G100	L5
S359	K271	I187	N101	N8
R360	R272			
R361	V273	A190	H104	K15
W362		A191	A105	L16
R363	A278	H192		
E364	Y279		A110	D21
R365	Q280			E22
Y366		I198	H114	E23
	K283	D199		K26
L370	W284	V200	S117	M27
D371	L285			Q28
G372	G286	L204	V122	M29
ILE	L301	G208	P123	
LEU	T302	P209	A124	R39
ARG		F210	V127	F40
	L299	T211	D128	Q41
	V300	P212	P129	K42
	L303	E213		I43
	T302	R214	V132	I44
	L305		D133	L44
	A306	L223	E134	D45
	H307		M135	K42
	E308	C227	E136	I43
	K309		D137	L44
F310	F310	K231	V138	A54
F311	F311	F322	A139	R55
L312	L312	T333	R140	Q56
V313	V313			F57
P314	P314	E236	H144	V58
	K318	M237	P145	E59
		K238	E60	E59
I323		K239	N146	T61
	F329	I241	Y147	
P330	P330	V242	R149	S64
		G243		L65
N333	N333	N244	I152	S66
E334	E334	G245	F153	S67
S335	S335	G246	H154	F68
K336	K336	L247	A155	S89
A337	A337	V248	L156	F71
L338	L338	A249	N157	V72
		Y250	Q158	S73
		L251	K159	R74
	A342		T160	
	L343		V161	L78
R344	R344	A256	K162	D79
V345	V345	R257	K163	P80
L346	L346	E258	E164	I81
R347	R347	V259	V165	
G348	G348	V260	A166	V88
			R167	
	E349	I263		L91
	P352	K264	N177	M92
		Q265		I93
	S356		M183	K94
			G194	T95

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	193.68Å 193.68Å 122.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.48 – 3.00 91.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (91.48-3.00) 97.2 (91.48-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.261 , 0.284 0.260 , 0.282	Depositor DCC
R_{free} test set	8832 reflections (8.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.278 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23615	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 41.69 % 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 2.2748e-04.*

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: NA, PO4, CIT, 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	0.37	0/2997	0.85	6/4036 (0.1%)
1	B	0.36	0/2985	0.89	9/4020 (0.2%)
1	C	0.35	0/2985	0.82	1/4020 (0.0%)
1	D	0.39	0/2997	0.89	8/4036 (0.2%)
1	E	0.38	0/2985	0.86	9/4020 (0.2%)
1	F	0.41	0/2989	0.91	9/4025 (0.2%)
1	G	0.37	0/2997	0.83	1/4036 (0.0%)
1	H	0.38	0/2989	0.91	12/4025 (0.3%)
All	All	0.38	0/23924	0.87	55/32218 (0.2%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	GLN	OE1-CD-NE2	-10.70	111.90	122.60
1	A	41	GLN	OE1-CD-NE2	-10.19	112.41	122.60
1	H	46	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	F	41	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	B	46	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	D	360	ARG	NE-CZ-NH2	9.90	128.11	119.20
1	F	272	ARG	NE-CZ-NH2	9.84	128.05	119.20
1	H	265	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	B	41	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	D	94	LYS	N-CA-C	-9.49	101.83	113.41
1	E	41	GLN	OE1-CD-NE2	-9.48	113.12	122.60
1	D	360	ARG	NE-CZ-NH1	-9.28	112.22	121.50
1	B	364	GLU	N-CA-C	-9.21	102.62	114.04
1	F	272	ARG	NE-CZ-NH1	-9.15	112.35	121.50
1	H	41	GLN	OE1-CD-NE2	-9.00	113.60	122.60
1	B	49	PHE	N-CA-C	-8.56	102.42	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	41	GLN	CG-CD-NE2	7.62	127.84	116.40
1	H	167	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	E	39	ARG	NE-CZ-NH2	7.55	126.00	119.20
1	A	41	GLN	CG-CD-NE2	7.27	127.31	116.40
1	E	39	ARG	NE-CZ-NH1	-7.15	114.35	121.50
1	D	41	GLN	CG-CD-NE2	7.09	127.03	116.40
1	H	94	LYS	N-CA-C	-7.05	103.67	111.36
1	H	167	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	B	46	GLN	CG-CD-NE2	6.99	126.88	116.40
1	E	41	GLN	CG-CD-NE2	6.88	126.72	116.40
1	H	41	GLN	CG-CD-NE2	6.79	126.58	116.40
1	D	360	ARG	CD-NE-CZ	6.75	133.84	124.40
1	F	272	ARG	CD-NE-CZ	6.70	133.78	124.40
1	H	265	GLN	CG-CD-NE2	6.67	126.41	116.40
1	H	46	GLN	CG-CD-NE2	6.65	126.37	116.40
1	B	41	GLN	CG-CD-NE2	6.28	125.82	116.40
1	G	285	ILE	N-CA-C	-6.07	104.59	110.72
1	H	93	ILE	N-CA-C	-6.03	107.62	113.53
1	F	365	ARG	N-CA-C	-5.84	105.05	111.82
1	E	94	LYS	N-CA-C	-5.71	105.06	111.28
1	D	285	ILE	N-CA-C	-5.63	105.03	110.72
1	E	329	PHE	CA-C-N	5.54	126.77	119.84
1	E	329	PHE	C-N-CA	5.54	126.77	119.84
1	A	94	LYS	N-CA-C	-5.49	104.94	111.69
1	B	285	ILE	N-CA-C	-5.48	105.19	110.72
1	B	185	GLY	N-CA-C	-5.38	106.27	112.83
1	F	185	GLY	N-CA-C	-5.35	106.30	112.83
1	F	94	LYS	N-CA-C	-5.29	105.51	111.28
1	C	185	GLY	N-CA-C	-5.26	106.41	112.83
1	A	313	VAL	CB-CA-C	-5.25	108.71	113.70
1	D	185	GLY	N-CA-C	-5.23	106.45	112.83
1	H	185	GLY	N-CA-C	-5.21	106.47	112.83
1	A	93	ILE	CA-C-O	5.18	124.18	119.20
1	F	23	ARG	N-CA-C	5.11	117.08	108.96
1	B	313	VAL	CB-CA-C	-5.10	108.85	113.70
1	A	185	GLY	N-CA-C	-5.09	106.62	112.83
1	E	185	GLY	N-CA-C	-5.08	106.63	112.83
1	H	285	ILE	N-CA-C	-5.08	105.59	110.72
1	E	313	VAL	CB-CA-C	-5.06	108.89	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2939	0	2969	122	0
1	B	2927	0	2955	139	0
1	C	2927	0	2955	139	0
1	D	2939	0	2969	141	0
1	E	2927	0	2955	147	0
1	F	2931	0	2958	132	0
1	G	2939	0	2969	135	0
1	H	2931	0	2958	142	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
2	F	6	0	4	0	0
3	B	5	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	D	1	0	0	0	0
5	D	26	0	10	3	0
5	G	26	0	10	0	0
6	A	8	0	0	1	0
6	B	7	0	0	1	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
6	E	4	0	0	0	0
6	F	3	0	0	0	0
6	G	8	0	0	0	0
6	H	2	0	0	0	0
All	All	23615	0	23728	1020	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 22.

All (1020) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:HE1	1:B:24:MET:HE1	1.42	1.01
1:A:88:VAL:HG12	1:A:93:ILE:HD11	1.43	1.00
1:A:27:MET:HG2	1:B:24:MET:HE3	1.52	0.92
1:A:257:ARG:HB3	1:A:257:ARG:HH11	1.35	0.91
1:D:88:VAL:HG12	1:D:93:ILE:HD11	1.53	0.90
1:H:344:ARG:HG3	1:H:349:GLU:HB2	1.53	0.90
1:B:88:VAL:HG12	1:B:93:ILE:HD11	1.55	0.89
1:E:344:ARG:HG3	1:E:349:GLU:HB2	1.55	0.89
1:G:88:VAL:HG12	1:G:93:ILE:HD11	1.52	0.88
1:A:344:ARG:HG3	1:A:349:GLU:HB2	1.54	0.88
1:G:344:ARG:HG3	1:G:349:GLU:HB2	1.53	0.87
1:D:344:ARG:HG3	1:D:349:GLU:HB2	1.54	0.87
1:F:272:ARG:HD2	1:G:137:ASP:OD2	1.75	0.86
1:C:333:ASN:ND2	1:C:336:LYS:HB2	1.90	0.85
1:E:261:ARG:NH1	1:E:261:ARG:HB2	1.93	0.84
1:C:196:ARG:HH22	1:C:365:ARG:HH12	1.25	0.82
1:C:309:LYS:NZ	1:D:167:ARG:HD2	1.95	0.81
1:D:72:VAL:HG21	1:D:342:ALA:HB2	1.61	0.81
1:E:261:ARG:HB2	1:E:261:ARG:HH11	1.46	0.81
1:A:72:VAL:HG21	1:A:342:ALA:HB2	1.60	0.81
1:B:72:VAL:HG21	1:B:342:ALA:HB2	1.63	0.81
1:G:167:ARG:HD2	1:H:309:LYS:NZ	1.97	0.80
1:E:306:ALA:HB3	1:E:330:PRO:HA	1.64	0.79
1:A:241:ILE:HG13	1:A:242:VAL:HG23	1.65	0.79
1:B:283:LYS:HE2	1:C:287:LYS:HE2	1.65	0.79
1:C:344:ARG:HG3	1:C:349:GLU:HB2	1.65	0.78
1:B:129:PRO:O	1:B:132:VAL:HG23	1.84	0.78
1:G:72:VAL:HG21	1:G:342:ALA:HB2	1.66	0.78
1:C:196:ARG:NH2	1:C:365:ARG:HH12	1.82	0.78
1:H:72:VAL:HG21	1:H:342:ALA:HB2	1.66	0.78
1:H:137:ASP:O	1:H:140:ARG:HG3	1.83	0.77
1:D:287:LYS:HE2	1:E:283:LYS:HE2	1.66	0.77
1:F:283:LYS:HE2	1:G:287:LYS:HE2	1.66	0.77
1:G:261:ARG:HH11	1:G:261:ARG:HB3	1.48	0.76
1:B:333:ASN:HD22	1:B:336:LYS:HB2	1.51	0.76
1:H:92:MET:HG2	1:H:92:MET:O	1.86	0.76
1:G:360:ARG:O	1:G:363:ARG:HG2	1.84	0.76
1:C:23:ARG:HD2	1:D:257:ARG:HH21	1.49	0.75
1:D:82:PRO:HD2	1:D:358:GLU:HG3	1.68	0.75
1:B:257:ARG:HH21	1:B:257:ARG:HA	1.51	0.75
1:B:241:ILE:HD11	1:C:224:VAL:HG21	1.67	0.75
1:D:77:LEU:HD21	1:D:204:LEU:CD1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:HE2	1:C:57:PHE:CE1	2.21	0.74
1:E:240:ARG:HA	1:E:244:ASN:OD1	1.88	0.74
1:G:26:LYS:HE2	1:G:57:PHE:CE1	2.22	0.74
1:G:214:ARG:HE	1:G:242:VAL:HG13	1.53	0.74
1:F:72:VAL:HG21	1:F:342:ALA:HB2	1.69	0.74
1:D:283:LYS:HE2	1:E:287:LYS:HE2	1.70	0.74
1:B:287:LYS:HE2	1:C:283:LYS:HE2	1.68	0.73
1:A:287:LYS:HE2	1:H:283:LYS:HE2	1.71	0.72
1:G:261:ARG:HB3	1:G:261:ARG:NH1	2.03	0.72
1:B:26:LYS:HE2	1:B:57:PHE:CE1	2.24	0.72
1:D:261:ARG:HG2	1:D:265:GLN:HE21	1.53	0.71
1:E:245:GLY:O	1:E:248:VAL:HG12	1.90	0.71
1:A:283:LYS:HE2	1:H:287:LYS:HE2	1.72	0.71
1:B:251:LEU:HD21	1:B:270:ALA:HA	1.71	0.71
1:B:82:PRO:HD2	1:B:358:GLU:HG3	1.72	0.71
1:C:72:VAL:HG21	1:C:342:ALA:HB2	1.73	0.70
1:E:72:VAL:HG21	1:E:342:ALA:HB2	1.73	0.70
1:E:365:ARG:O	1:E:369:TYR:HB2	1.91	0.70
1:E:26:LYS:HE2	1:E:57:PHE:CE1	2.27	0.70
1:E:91:LEU:HD23	1:E:356:SER:HA	1.74	0.70
1:C:309:LYS:HZ1	1:D:167:ARG:HD2	1.56	0.70
1:G:167:ARG:HD2	1:H:309:LYS:CE	2.21	0.70
1:H:88:VAL:HG12	1:H:93:ILE:HD11	1.73	0.70
1:E:255:ASP:OD1	1:E:257:ARG:HG3	1.92	0.69
1:E:261:ARG:HG2	1:E:265:GLN:HE21	1.57	0.69
1:F:287:LYS:HE2	1:G:283:LYS:HE2	1.74	0.69
1:D:88:VAL:CG1	1:D:93:ILE:HD11	2.22	0.69
1:D:208:GLY:HA2	1:D:284:TRP:CZ2	2.27	0.69
1:H:359:SER:O	1:H:363:ARG:HG3	1.93	0.69
1:C:333:ASN:HD22	1:C:336:LYS:HB2	1.57	0.69
1:D:256:ALA:O	1:D:260:VAL:HG23	1.94	0.68
1:B:259:VAL:O	1:B:263:ILE:HG13	1.94	0.68
1:H:360:ARG:O	1:H:364:GLU:HG3	1.94	0.68
1:D:220:LEU:HD22	1:E:223:LEU:HD22	1.75	0.67
1:E:240:ARG:HD2	1:E:244:ASN:ND2	2.08	0.67
1:A:27:MET:CG	1:B:24:MET:HE3	2.22	0.67
1:C:309:LYS:CE	1:D:167:ARG:HD2	2.23	0.67
1:H:208:GLY:HA2	1:H:284:TRP:CZ2	2.29	0.67
1:A:257:ARG:HB3	1:A:257:ARG:NH1	2.10	0.67
1:F:245:GLY:O	1:F:248:VAL:HG12	1.95	0.67
1:E:227:CYS:HA	1:E:237:MET:HE1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:CYS:HA	1:H:237:MET:HE1	1.77	0.67
1:H:250:TYR:HB3	1:H:273:VAL:HG21	1.76	0.67
1:G:248:VAL:HA	1:G:253:THR:O	1.93	0.67
1:C:227:CYS:HA	1:C:237:MET:HE1	1.76	0.66
1:D:129:PRO:O	1:D:132:VAL:HG23	1.96	0.66
1:D:227:CYS:HA	1:D:237:MET:HE1	1.76	0.66
1:A:227:CYS:HA	1:A:237:MET:HE1	1.77	0.66
1:C:240:ARG:HD2	1:C:244:ASN:HD21	1.59	0.66
1:E:144:HIS:CE1	1:E:146:ASN:HD22	2.14	0.66
1:G:77:LEU:HD21	1:G:204:LEU:CD1	2.24	0.66
1:B:227:CYS:HA	1:B:237:MET:HE1	1.76	0.66
1:E:208:GLY:HA2	1:E:284:TRP:CZ2	2.29	0.66
1:C:23:ARG:HD2	1:D:257:ARG:NH2	2.11	0.66
1:C:240:ARG:HD2	1:C:244:ASN:ND2	2.10	0.66
1:A:24:MET:HE3	1:B:27:MET:HG2	1.77	0.66
1:E:369:TYR:HB3	1:E:370:LEU:HD12	1.77	0.65
1:A:241:ILE:HG13	1:A:242:VAL:H	1.61	0.65
1:A:360:ARG:O	1:A:364:GLU:HG3	1.96	0.65
1:E:328:VAL:HG12	1:E:330:PRO:HD3	1.77	0.65
1:F:227:CYS:HA	1:F:237:MET:HE1	1.76	0.65
1:G:167:ARG:HD2	1:H:309:LYS:HE2	1.76	0.65
1:G:227:CYS:HA	1:G:237:MET:HE1	1.76	0.65
1:H:23:ARG:H	1:H:23:ARG:HD2	1.60	0.65
1:B:306:ALA:HB3	1:B:330:PRO:HA	1.78	0.65
1:E:161:VAL:O	1:E:165:VAL:HG23	1.97	0.65
1:E:214:ARG:NE	1:E:242:VAL:HG23	2.12	0.65
1:H:214:ARG:HE	1:H:242:VAL:HG23	1.61	0.65
1:H:256:ALA:O	1:H:260:VAL:HG23	1.96	0.65
1:G:256:ALA:O	1:G:260:VAL:HG23	1.96	0.65
1:D:306:ALA:HB3	1:D:330:PRO:HA	1.79	0.64
1:D:356:SER:HB3	1:D:360:ARG:NH1	2.12	0.64
1:H:55:ARG:HG2	1:H:55:ARG:HH11	1.63	0.64
1:G:167:ARG:HD2	1:H:309:LYS:HZ1	1.62	0.64
1:G:91:LEU:HD23	1:G:356:SER:HA	1.80	0.64
1:A:72:VAL:HG21	1:A:342:ALA:CB	2.26	0.64
1:E:128:ASP:HB2	1:E:156:LEU:HA	1.79	0.64
1:B:361:ARG:O	1:B:365:ARG:HG3	1.97	0.64
1:F:190:ALA:HB1	1:F:197:VAL:HG13	1.78	0.64
1:A:241:ILE:HG13	1:A:242:VAL:N	2.13	0.64
1:C:258:GLU:O	1:C:261:ARG:HB3	1.98	0.64
1:G:212:PRO:HA	1:G:247:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:MET:HA	1:E:198:ILE:HA	1.79	0.64
1:F:161:VAL:O	1:F:165:VAL:HG23	1.97	0.64
1:H:214:ARG:NE	1:H:242:VAL:HG23	2.12	0.64
1:H:135:MET:HA	1:H:198:ILE:HA	1.80	0.63
1:G:130:VAL:HG23	1:G:153:PHE:O	1.96	0.63
1:A:91:LEU:HD23	1:A:356:SER:HA	1.79	0.63
1:A:219:PRO:HG2	1:A:222:GLN:NE2	2.13	0.63
1:A:258:GLU:O	1:A:261:ARG:HB3	1.98	0.63
1:F:313:VAL:HB	1:F:314:PRO:HD3	1.81	0.63
1:H:313:VAL:HB	1:H:314:PRO:HD3	1.80	0.63
1:A:240:ARG:HH21	1:H:144:HIS:CE1	2.17	0.63
1:D:255:ASP:O	1:D:259:VAL:HG23	1.99	0.63
1:D:43:ILE:HD12	1:D:103:GLU:HB3	1.80	0.63
1:G:360:ARG:O	1:G:364:GLU:HG3	1.98	0.63
1:H:212:PRO:HA	1:H:247:LEU:HB3	1.80	0.63
1:C:309:LYS:HE2	1:D:167:ARG:HD2	1.79	0.62
1:C:144:HIS:CE1	1:C:146:ASN:HD22	2.17	0.62
1:D:313:VAL:HB	1:D:314:PRO:HD3	1.81	0.62
1:H:26:LYS:HE2	1:H:57:PHE:CE1	2.35	0.62
1:D:161:VAL:O	1:D:165:VAL:HG23	1.99	0.62
1:D:72:VAL:HG21	1:D:342:ALA:CB	2.30	0.62
1:H:95:THR:HG23	1:H:100:LYS:HD3	1.82	0.62
1:F:240:ARG:NH1	1:F:244:ASN:HD21	1.98	0.62
1:H:161:VAL:O	1:H:165:VAL:HG23	2.00	0.62
1:B:161:VAL:O	1:B:165:VAL:HG23	2.00	0.61
1:G:81:ILE:HG22	1:G:359:SER:HA	1.82	0.61
1:G:82:PRO:HD2	1:G:358:GLU:HG3	1.81	0.61
1:B:93:ILE:HD12	1:B:93:ILE:H	1.65	0.61
1:G:360:ARG:HA	1:G:363:ARG:NE	2.15	0.61
1:D:95:THR:HG23	1:D:100:LYS:HD3	1.83	0.61
1:G:161:VAL:O	1:G:165:VAL:HG23	1.99	0.61
1:A:95:THR:HG23	1:A:100:LYS:HD3	1.82	0.61
1:B:95:THR:HG23	1:B:100:LYS:HD3	1.83	0.61
1:B:81:ILE:HG22	1:B:359:SER:HA	1.82	0.61
1:E:238:LYS:HB2	1:E:238:LYS:NZ	2.15	0.61
1:C:95:THR:HG23	1:C:100:LYS:HD3	1.81	0.61
1:F:157:ASN:ND2	1:F:161:VAL:HG13	2.16	0.61
1:C:161:VAL:O	1:C:165:VAL:HG23	2.01	0.61
1:E:313:VAL:HB	1:E:314:PRO:HD3	1.83	0.61
1:E:356:SER:HB3	1:E:360:ARG:HH12	1.65	0.61
1:H:238:LYS:HB2	1:H:238:LYS:NZ	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:356:SER:HB3	1:H:360:ARG:HH12	1.66	0.61
1:A:161:VAL:O	1:A:165:VAL:HG23	2.01	0.60
1:C:238:LYS:HB2	1:C:238:LYS:NZ	2.15	0.60
1:D:238:LYS:HB2	1:D:238:LYS:NZ	2.16	0.60
1:G:313:VAL:HB	1:G:314:PRO:HD3	1.82	0.60
1:F:95:THR:HG23	1:F:100:LYS:HD3	1.82	0.60
1:G:95:THR:HG23	1:G:100:LYS:HD3	1.83	0.60
1:H:157:ASN:ND2	1:H:161:VAL:HG13	2.16	0.60
1:A:238:LYS:NZ	1:A:238:LYS:HB2	2.15	0.60
1:B:313:VAL:HB	1:B:314:PRO:HD3	1.83	0.60
1:D:81:ILE:HG22	1:D:359:SER:HA	1.82	0.60
1:C:40:PHE:HB3	1:C:45:ASP:HB2	1.82	0.60
1:E:157:ASN:ND2	1:E:161:VAL:HG13	2.17	0.60
1:B:238:LYS:HB2	1:B:238:LYS:NZ	2.17	0.60
1:E:248:VAL:HA	1:E:253:THR:O	2.02	0.60
1:E:251:LEU:HD21	1:E:270:ALA:HA	1.83	0.60
1:G:238:LYS:HB2	1:G:238:LYS:NZ	2.16	0.60
1:A:313:VAL:HB	1:A:314:PRO:HD3	1.83	0.60
1:D:93:ILE:O	1:D:93:ILE:HG22	2.00	0.60
1:D:220:LEU:HD12	1:E:241:ILE:HG23	1.83	0.60
1:B:157:ASN:ND2	1:B:161:VAL:HG13	2.17	0.60
1:D:219:PRO:HG2	1:D:222:GLN:NE2	2.16	0.60
1:E:95:THR:HG23	1:E:100:LYS:HD3	1.83	0.60
1:E:261:ARG:HH11	1:E:261:ARG:CB	2.13	0.60
1:D:134:GLU:OE2	1:D:196:ARG:HA	2.02	0.59
1:C:144:HIS:CE1	1:C:146:ASN:ND2	2.70	0.59
1:G:356:SER:HB3	1:G:360:ARG:HH12	1.68	0.59
1:B:144:HIS:CE1	1:C:240:ARG:HH21	2.21	0.59
1:H:43:ILE:C	1:H:45:ASP:H	2.10	0.59
1:B:356:SER:HB3	1:B:360:ARG:HH12	1.67	0.59
1:F:92:MET:O	1:F:92:MET:HG2	2.02	0.59
1:F:238:LYS:NZ	1:F:238:LYS:HB2	2.16	0.59
1:E:240:ARG:HA	1:E:244:ASN:CG	2.27	0.59
1:F:128:ASP:HB2	1:F:156:LEU:HA	1.84	0.59
1:B:257:ARG:HH21	1:B:257:ARG:CA	2.15	0.59
1:B:36:GLU:OE1	1:B:49:PHE:HZ	1.86	0.59
1:G:214:ARG:NE	1:G:242:VAL:HG13	2.16	0.59
1:C:313:VAL:HB	1:C:314:PRO:HD3	1.84	0.58
1:H:79:ASP:HB2	1:H:363:ARG:NH1	2.18	0.58
1:H:251:LEU:HD21	1:H:270:ALA:HA	1.85	0.58
1:H:259:VAL:O	1:H:263:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ASN:ND2	1:B:336:LYS:H	2.00	0.58
1:E:214:ARG:HE	1:E:242:VAL:HG23	1.68	0.58
1:F:333:ASN:HB3	1:F:336:LYS:HB3	1.85	0.58
1:A:26:LYS:HE2	1:A:57:PHE:CE1	2.38	0.58
1:C:91:LEU:HD23	1:C:356:SER:HA	1.86	0.58
1:B:248:VAL:HG13	1:B:249:ALA:N	2.18	0.58
1:F:356:SER:HB3	1:F:360:ARG:HH12	1.67	0.58
1:B:36:GLU:OE1	1:B:49:PHE:CZ	2.57	0.58
1:F:255:ASP:OD1	1:F:257:ARG:HB2	2.03	0.58
1:G:187:ILE:HG13	1:G:211:THR:HG22	1.86	0.57
1:C:356:SER:HB3	1:C:360:ARG:HH12	1.68	0.57
1:D:91:LEU:HD23	1:D:356:SER:HA	1.86	0.57
1:D:258:GLU:HA	1:D:261:ARG:NH1	2.19	0.57
1:A:157:ASN:ND2	1:A:161:VAL:HG13	2.18	0.57
1:E:201:ASN:HB3	1:E:284:TRP:CZ3	2.38	0.57
1:H:240:ARG:HA	1:H:244:ASN:HB2	1.85	0.57
1:B:91:LEU:HD23	1:B:356:SER:HA	1.85	0.57
1:C:60:GLU:OE2	1:D:60:GLU:HB3	2.05	0.57
1:C:157:ASN:ND2	1:C:161:VAL:HG13	2.19	0.57
1:H:302:THR:HA	1:H:329:PHE:O	2.05	0.57
1:B:70:ALA:HA	1:B:122:VAL:HG12	1.87	0.57
1:B:72:VAL:HG21	1:B:342:ALA:CB	2.34	0.57
1:C:306:ALA:HB3	1:C:330:PRO:HA	1.85	0.57
1:D:154:HIS:NE2	5:D:381:CIT:H41	2.20	0.57
1:D:239:LYS:O	1:D:244:ASN:HB3	2.05	0.57
1:F:147:TYR:CD1	1:F:147:TYR:N	2.73	0.57
1:B:40:PHE:HB3	1:B:45:ASP:HB2	1.86	0.56
1:D:157:ASN:ND2	1:D:161:VAL:HG13	2.19	0.56
1:H:245:GLY:O	1:H:248:VAL:HG12	2.05	0.56
1:D:160:THR:O	1:D:164:GLU:HG3	2.05	0.56
1:A:356:SER:HB3	1:A:360:ARG:HH12	1.70	0.56
1:B:272:ARG:HD2	1:C:369:TYR:CE1	2.40	0.56
1:C:135:MET:HA	1:C:198:ILE:HA	1.86	0.56
1:C:240:ARG:HH11	1:C:244:ASN:ND2	2.03	0.56
1:C:261:ARG:HG2	1:C:265:GLN:HE21	1.71	0.56
1:C:144:HIS:HE1	1:C:146:ASN:ND2	2.03	0.56
1:D:26:LYS:HE2	1:D:57:PHE:CE1	2.41	0.56
1:D:223:LEU:HD21	1:E:224:VAL:CG2	2.36	0.56
1:F:139:ALA:O	1:F:149:ARG:HD3	2.05	0.56
1:B:104:HIS:CD2	1:B:105:ALA:H	2.24	0.56
1:G:72:VAL:HG21	1:G:342:ALA:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:ALA:O	1:G:149:ARG:HD3	2.05	0.56
1:H:74:ARG:HG2	1:H:74:ARG:HH11	1.71	0.56
1:A:139:ALA:O	1:A:149:ARG:HD3	2.06	0.56
1:B:160:THR:O	1:B:164:GLU:HG3	2.06	0.56
1:C:74:ARG:HG2	1:C:74:ARG:HH11	1.70	0.56
1:E:240:ARG:HA	1:E:244:ASN:ND2	2.21	0.56
1:F:344:ARG:HG3	1:F:349:GLU:HB2	1.87	0.56
1:G:157:ASN:ND2	1:G:161:VAL:HG13	2.19	0.56
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.70	0.56
1:D:259:VAL:O	1:D:263:ILE:HG13	2.06	0.56
1:F:160:THR:O	1:F:164:GLU:HG3	2.06	0.56
1:G:160:THR:O	1:G:164:GLU:HG3	2.06	0.56
1:B:357:GLU:O	1:B:361:ARG:HG3	2.06	0.56
1:E:139:ALA:O	1:E:149:ARG:HD3	2.06	0.56
1:H:59:GLU:C	1:H:61:THR:H	2.13	0.56
1:F:91:LEU:HD23	1:F:356:SER:HA	1.88	0.55
1:G:190:ALA:HB1	1:G:197:VAL:HG13	1.88	0.55
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.71	0.55
1:B:148:GLN:HG3	1:B:366:TYR:OH	2.06	0.55
1:F:70:ALA:HA	1:F:122:VAL:HG12	1.88	0.55
1:A:70:ALA:HA	1:A:122:VAL:HG12	1.88	0.55
1:E:74:ARG:HG2	1:E:74:ARG:HH11	1.71	0.55
1:C:160:THR:O	1:C:164:GLU:HG3	2.06	0.55
1:E:219:PRO:HG2	1:E:222:GLN:NE2	2.22	0.55
1:G:255:ASP:HB3	1:G:258:GLU:CB	2.36	0.55
1:B:80:PRO:HB2	1:B:362:TRP:CE3	2.41	0.55
1:B:139:ALA:O	1:B:149:ARG:HD3	2.06	0.55
1:H:70:ALA:HA	1:H:122:VAL:HG12	1.89	0.55
1:H:160:THR:O	1:H:164:GLU:HG3	2.07	0.55
1:C:190:ALA:HB1	1:C:197:VAL:HG13	1.89	0.55
1:D:187:ILE:HG13	1:D:211:THR:HG22	1.89	0.55
1:F:239:LYS:O	1:F:244:ASN:HB3	2.06	0.55
1:H:139:ALA:O	1:H:149:ARG:HD3	2.07	0.55
1:A:245:GLY:O	1:A:248:VAL:HG12	2.07	0.55
1:F:114:HIS:O	1:F:117:SER:HB3	2.07	0.55
1:A:114:HIS:O	1:A:117:SER:HB3	2.07	0.54
1:B:5:LEU:HB2	1:B:68:PHE:CE2	2.42	0.54
1:D:40:PHE:HB3	1:D:45:ASP:HB2	1.88	0.54
1:F:40:PHE:HB3	1:F:45:ASP:HB2	1.90	0.54
1:C:153:PHE:CD1	1:C:158:GLN:HG3	2.43	0.54
1:D:190:ALA:HB1	1:D:197:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:LEU:HD22	1:G:220:LEU:HD22	1.89	0.54
1:F:257:ARG:HB3	1:F:257:ARG:NH1	2.23	0.54
1:D:70:ALA:HA	1:D:122:VAL:HG12	1.89	0.54
1:D:212:PRO:O	1:D:248:VAL:HG23	2.08	0.54
1:A:88:VAL:HG12	1:A:93:ILE:CD1	2.29	0.54
1:E:40:PHE:HB3	1:E:45:ASP:HB2	1.90	0.54
1:B:268:GLU:HG3	1:C:369:TYR:OH	2.07	0.54
1:D:223:LEU:HD23	1:E:223:LEU:HD23	1.89	0.54
1:D:241:ILE:HD13	1:E:220:LEU:HB3	1.90	0.54
1:E:52:LYS:O	1:E:56:GLN:HG3	2.08	0.54
1:C:258:GLU:OE1	1:C:261:ARG:HD2	2.08	0.54
1:C:328:VAL:HG12	1:C:330:PRO:HD3	1.90	0.54
1:H:240:ARG:NH1	1:H:244:ASN:HB3	2.23	0.54
1:G:261:ARG:O	1:G:265:GLN:HG3	2.08	0.54
1:H:79:ASP:CB	1:H:363:ARG:NH1	2.71	0.54
1:G:70:ALA:HA	1:G:122:VAL:HG12	1.90	0.53
1:H:91:LEU:HD23	1:H:356:SER:HA	1.90	0.53
1:C:344:ARG:CG	1:C:349:GLU:HB2	2.37	0.53
1:G:153:PHE:CD1	1:G:158:GLN:HG3	2.43	0.53
1:B:244:ASN:CG	1:B:245:GLY:N	2.66	0.53
1:B:333:ASN:HD22	1:B:336:LYS:CB	2.21	0.53
1:D:82:PRO:CD	1:D:358:GLU:HG3	2.36	0.53
1:F:257:ARG:CZ	1:F:257:ARG:HA	2.39	0.53
1:C:5:LEU:HB2	1:C:68:PHE:CE2	2.44	0.53
1:E:144:HIS:HE1	1:E:146:ASN:HD22	1.54	0.53
1:F:74:ARG:HH11	1:F:74:ARG:HG2	1.74	0.53
1:H:306:ALA:HB3	1:H:330:PRO:HA	1.89	0.53
1:A:223:LEU:HD23	1:H:223:LEU:HD23	1.91	0.53
1:F:147:TYR:HD1	1:F:147:TYR:H	1.56	0.53
1:G:245:GLY:HA2	1:G:249:ALA:HB2	1.91	0.53
1:H:43:ILE:C	1:H:45:ASP:N	2.64	0.53
1:B:248:VAL:HG13	1:B:249:ALA:H	1.73	0.53
1:C:139:ALA:O	1:C:149:ARG:HD3	2.09	0.53
1:C:241:ILE:HG13	1:C:242:VAL:HG13	1.90	0.53
1:H:42:LYS:O	1:H:45:ASP:HB2	2.08	0.53
1:D:39:ARG:HB3	1:D:40:PHE:CE1	2.44	0.53
1:F:72:VAL:HG21	1:F:342:ALA:CB	2.37	0.53
1:G:74:ARG:HG2	1:G:74:ARG:HH11	1.73	0.53
1:A:248:VAL:O	1:A:252:GLY:HA2	2.09	0.53
1:F:26:LYS:HE2	1:F:57:PHE:CE1	2.43	0.53
1:F:153:PHE:CD1	1:F:158:GLN:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ILE:HG13	1:F:211:THR:HG22	1.91	0.53
1:F:256:ALA:O	1:F:260:VAL:HG23	2.09	0.53
1:H:187:ILE:HG13	1:H:211:THR:HG22	1.90	0.53
1:A:40:PHE:HB3	1:A:45:ASP:HB2	1.90	0.53
1:A:55:ARG:HH22	1:A:119:GLU:CD	2.16	0.53
1:F:362:TRP:C	1:F:364:GLU:H	2.16	0.53
1:G:23:ARG:HG3	1:G:23:ARG:HH11	1.74	0.53
1:G:255:ASP:HB3	1:G:258:GLU:HB3	1.91	0.53
1:A:140:ARG:NH1	1:A:365:ARG:HH12	2.07	0.52
1:C:22:GLU:OE2	1:C:347:ARG:NH2	2.41	0.52
1:C:70:ALA:HA	1:C:122:VAL:HG12	1.90	0.52
1:C:114:HIS:O	1:C:117:SER:HB3	2.09	0.52
1:C:219:PRO:HG2	1:C:222:GLN:NE2	2.24	0.52
1:D:74:ARG:HH11	1:D:74:ARG:HG2	1.73	0.52
1:E:240:ARG:HD2	1:E:244:ASN:HD21	1.71	0.52
1:F:223:LEU:HD23	1:G:223:LEU:HD23	1.91	0.52
1:A:153:PHE:CD1	1:A:158:GLN:HG3	2.44	0.52
1:A:160:THR:O	1:A:164:GLU:HG3	2.09	0.52
1:E:333:ASN:C	1:E:333:ASN:HD22	2.15	0.52
1:B:114:HIS:O	1:B:117:SER:HB3	2.09	0.52
1:D:5:LEU:HB2	1:D:68:PHE:CE2	2.43	0.52
1:D:139:ALA:O	1:D:149:ARG:HD3	2.09	0.52
1:H:153:PHE:CD1	1:H:158:GLN:HG3	2.45	0.52
1:B:187:ILE:HG13	1:B:211:THR:HG22	1.91	0.52
1:B:256:ALA:O	1:B:260:VAL:HG23	2.10	0.52
1:G:153:PHE:HD1	1:G:158:GLN:HG3	1.75	0.52
1:G:255:ASP:O	1:G:259:VAL:HG23	2.09	0.52
1:B:190:ALA:HB1	1:B:197:VAL:HG13	1.91	0.52
1:E:92:MET:O	1:E:92:MET:HG2	2.08	0.52
1:C:257:ARG:NH1	1:C:308:GLU:HG2	2.25	0.52
1:E:368:SER:HA	1:E:371:ASP:HB3	1.91	0.52
1:A:209:PRO:HD3	1:A:284:TRP:CD2	2.45	0.52
1:C:257:ARG:HH12	1:C:308:GLU:HA	1.75	0.52
1:E:88:VAL:HG12	1:E:93:ILE:HD11	1.92	0.52
1:A:187:ILE:HG13	1:A:211:THR:HG22	1.91	0.52
1:B:135:MET:HE1	1:B:149:ARG:O	2.10	0.52
1:E:153:PHE:CD1	1:E:158:GLN:HG3	2.44	0.52
1:G:5:LEU:HB2	1:G:68:PHE:CE2	2.44	0.52
1:B:82:PRO:CD	1:B:358:GLU:HG3	2.40	0.52
1:F:18:ILE:HG13	1:F:57:PHE:HE2	1.75	0.52
1:F:241:ILE:HD13	1:G:220:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:PHE:CD1	1:D:158:GLN:HG3	2.45	0.51
1:G:280:GLN:O	1:G:284:TRP:HE3	1.93	0.51
1:H:114:HIS:O	1:H:117:SER:HB3	2.10	0.51
1:A:5:LEU:HB2	1:A:68:PHE:CE2	2.46	0.51
1:C:152:ILE:HG21	1:C:204:LEU:HD12	1.92	0.51
1:F:5:LEU:HB2	1:F:68:PHE:CE2	2.46	0.51
1:H:190:ALA:HB1	1:H:197:VAL:HG13	1.91	0.51
1:C:81:ILE:O	1:C:132:VAL:HA	2.10	0.51
1:C:259:VAL:O	1:C:263:ILE:HG13	2.10	0.51
1:G:40:PHE:HB3	1:G:45:ASP:HB2	1.91	0.51
1:H:251:LEU:CD2	1:H:270:ALA:HA	2.40	0.51
1:E:114:HIS:O	1:E:117:SER:HB3	2.10	0.51
1:G:261:ARG:HH11	1:G:261:ARG:CB	2.19	0.51
1:E:18:ILE:HG13	1:E:57:PHE:HE2	1.74	0.51
1:F:153:PHE:HD1	1:F:158:GLN:HG3	1.74	0.51
1:F:240:ARG:HA	1:F:244:ASN:HB3	1.92	0.51
1:H:344:ARG:CG	1:H:349:GLU:HB2	2.35	0.51
1:C:247:LEU:HD23	1:C:273:VAL:HG12	1.92	0.51
1:H:238:LYS:HB2	1:H:238:LYS:HZ3	1.75	0.51
1:E:190:ALA:HB1	1:E:197:VAL:HG13	1.93	0.51
1:E:255:ASP:O	1:E:258:GLU:HB3	2.09	0.51
1:F:134:GLU:HB3	1:F:196:ARG:HG3	1.93	0.51
1:D:104:HIS:HE2	5:D:381:CIT:H21	1.76	0.51
1:E:208:GLY:HA2	1:E:284:TRP:CE2	2.46	0.51
1:F:240:ARG:HH11	1:F:244:ASN:HD21	1.59	0.51
1:A:261:ARG:HG2	1:A:265:GLN:HE21	1.76	0.50
1:A:371:ASP:OD1	1:H:269:TRP:HB2	2.11	0.50
1:C:309:LYS:NZ	1:D:167:ARG:CD	2.71	0.50
1:D:153:PHE:HD1	1:D:158:GLN:HG3	1.76	0.50
1:G:344:ARG:CG	1:G:349:GLU:HB2	2.35	0.50
1:C:240:ARG:NH1	1:C:244:ASN:HD22	2.08	0.50
1:E:299:ILE:HD11	1:E:323:ILE:HB	1.92	0.50
1:A:153:PHE:HD1	1:A:158:GLN:HG3	1.76	0.50
1:C:153:PHE:HD1	1:C:158:GLN:HG3	1.74	0.50
1:H:153:PHE:HD1	1:H:158:GLN:HG3	1.76	0.50
1:A:190:ALA:HB1	1:A:197:VAL:HG13	1.93	0.50
1:B:80:PRO:HB2	1:B:362:TRP:CZ3	2.47	0.50
1:H:152:ILE:HG21	1:H:204:LEU:HD12	1.94	0.50
1:H:357:GLU:O	1:H:361:ARG:HD3	2.11	0.50
1:B:153:PHE:CD1	1:B:158:GLN:HG3	2.46	0.50
1:B:223:LEU:HD23	1:C:223:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:TYR:CD1	1:B:370:LEU:N	2.80	0.50
1:D:258:GLU:OE1	1:D:261:ARG:HB3	2.11	0.50
1:F:260:VAL:HG13	1:F:311:PHE:CE1	2.46	0.50
1:F:357:GLU:HG2	1:F:361:ARG:HH21	1.76	0.50
1:G:114:HIS:O	1:G:117:SER:HB3	2.11	0.50
1:G:328:VAL:O	1:G:330:PRO:HD3	2.11	0.50
1:H:140:ARG:HD3	1:H:370:LEU:HD21	1.93	0.50
1:H:370:LEU:HD12	1:H:370:LEU:N	2.26	0.50
1:H:72:VAL:HG21	1:H:342:ALA:CB	2.37	0.50
1:A:152:ILE:HG21	1:A:204:LEU:HD12	1.94	0.50
1:E:81:ILE:O	1:E:132:VAL:HA	2.10	0.50
1:D:114:HIS:O	1:D:117:SER:HB3	2.12	0.50
1:E:5:LEU:HB2	1:E:68:PHE:CE2	2.47	0.50
1:G:299:ILE:HD11	1:G:323:ILE:HB	1.94	0.50
1:H:245:GLY:HA2	1:H:249:ALA:HB2	1.93	0.50
1:E:70:ALA:HA	1:E:122:VAL:HG12	1.93	0.49
1:F:53:ILE:O	1:F:56:GLN:HB3	2.12	0.49
1:G:15:LYS:HD3	1:G:29:ASN:HD22	1.76	0.49
1:H:5:LEU:HB2	1:H:68:PHE:CE2	2.46	0.49
1:E:255:ASP:OD1	1:E:258:GLU:N	2.44	0.49
1:F:306:ALA:HB3	1:F:330:PRO:HA	1.93	0.49
1:G:245:GLY:O	1:G:248:VAL:HG12	2.12	0.49
1:C:238:LYS:O	1:C:242:VAL:HG22	2.11	0.49
1:C:251:LEU:HD21	1:C:270:ALA:HA	1.94	0.49
1:D:299:ILE:HD11	1:D:323:ILE:HB	1.94	0.49
1:E:214:ARG:HG2	1:E:242:VAL:HA	1.94	0.49
1:F:208:GLY:HA2	1:F:284:TRP:CZ2	2.48	0.49
1:F:299:ILE:HD11	1:F:323:ILE:HB	1.94	0.49
1:F:81:ILE:O	1:F:132:VAL:HA	2.12	0.49
1:F:238:LYS:HB2	1:F:238:LYS:HZ3	1.77	0.49
1:C:208:GLY:HA2	1:C:284:TRP:CZ2	2.46	0.49
1:D:152:ILE:HG21	1:D:204:LEU:HD12	1.93	0.49
1:E:153:PHE:HD1	1:E:158:GLN:HG3	1.76	0.49
1:E:240:ARG:HA	1:E:244:ASN:HD21	1.77	0.49
1:B:153:PHE:HD1	1:B:158:GLN:HG3	1.77	0.49
1:F:314:PRO:O	1:F:318:LYS:HG3	2.13	0.49
1:A:240:ARG:NH1	1:A:244:ASN:OD1	2.46	0.49
1:A:344:ARG:CG	1:A:349:GLU:HB2	2.36	0.49
1:D:245:GLY:HA2	1:D:249:ALA:HB2	1.95	0.49
1:E:187:ILE:HG13	1:E:211:THR:HG22	1.95	0.49
1:G:51:GLU:OE2	1:G:55:ARG:NH1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HD12	1:B:93:ILE:N	2.26	0.49
1:C:15:LYS:HD3	1:C:29:ASN:HD22	1.78	0.49
1:C:93:ILE:HD13	1:C:114:HIS:CD2	2.48	0.49
1:C:299:ILE:HD11	1:C:323:ILE:HB	1.94	0.49
1:E:57:PHE:O	1:E:61:THR:HG23	2.12	0.49
1:C:307:HIS:HA	1:C:309:LYS:HE3	1.95	0.49
1:E:240:ARG:HD2	1:E:244:ASN:CG	2.37	0.49
1:G:209:PRO:HB3	1:G:280:GLN:HB3	1.95	0.49
1:G:306:ALA:HB3	1:G:330:PRO:HA	1.95	0.49
1:B:204:LEU:O	1:B:242:VAL:HG22	2.13	0.49
1:A:370:LEU:C	1:A:372:GLY:H	2.21	0.48
1:D:82:PRO:HD2	1:D:358:GLU:CG	2.41	0.48
1:E:209:PRO:HB3	1:E:280:GLN:HB3	1.95	0.48
1:E:251:LEU:CD2	1:E:270:ALA:HA	2.43	0.48
1:B:220:LEU:HD22	1:C:223:LEU:HD22	1.94	0.48
1:C:196:ARG:HH22	1:C:365:ARG:NH1	2.01	0.48
1:F:241:ILE:HG23	1:G:220:LEU:HD12	1.94	0.48
1:G:152:ILE:HG21	1:G:204:LEU:HD12	1.94	0.48
1:H:333:ASN:ND2	1:H:336:LYS:HB2	2.27	0.48
1:G:23:ARG:HG3	1:G:23:ARG:NH1	2.28	0.48
1:A:15:LYS:HD3	1:A:29:ASN:HD22	1.77	0.48
1:A:92:MET:HG2	1:A:92:MET:O	2.12	0.48
1:A:154:HIS:HB3	6:A:401:HOH:O	2.13	0.48
1:B:3:ARG:NE	1:B:63:TYR:CE2	2.82	0.48
1:B:147:TYR:N	1:B:147:TYR:CD1	2.81	0.48
1:C:72:VAL:HG21	1:C:342:ALA:CB	2.42	0.48
1:C:311:PHE:C	1:C:314:PRO:HD2	2.39	0.48
1:E:152:ILE:HG21	1:E:204:LEU:HD12	1.95	0.48
1:H:59:GLU:O	1:H:61:THR:N	2.46	0.48
1:H:117:SER:HB2	1:H:124:ALA:HB2	1.96	0.48
1:E:242:VAL:O	1:E:242:VAL:HG13	2.12	0.48
1:H:299:ILE:HD11	1:H:323:ILE:HB	1.95	0.48
1:H:314:PRO:O	1:H:318:LYS:HG3	2.13	0.48
1:C:79:ASP:O	1:C:81:ILE:HG23	2.13	0.48
1:G:147:TYR:CD1	1:G:147:TYR:N	2.82	0.48
1:G:314:PRO:O	1:G:318:LYS:HG3	2.13	0.48
1:H:133:ASP:OD1	1:H:140:ARG:NH2	2.46	0.48
1:A:117:SER:HB2	1:A:124:ALA:HB2	1.96	0.48
1:C:209:PRO:HD3	1:C:284:TRP:CD2	2.49	0.48
1:C:311:PHE:O	1:C:314:PRO:HD2	2.14	0.48
1:F:360:ARG:O	1:F:364:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ARG:NH2	1:G:119:GLU:OE1	2.46	0.48
1:A:23:ARG:HH21	1:B:307:HIS:CD2	2.31	0.48
1:A:370:LEU:O	1:A:373:ILE:HG12	2.13	0.48
1:B:258:GLU:OE1	1:B:261:ARG:HD2	2.14	0.48
1:A:299:ILE:HD11	1:A:323:ILE:HB	1.95	0.48
1:C:55:ARG:HH22	1:C:119:GLU:CD	2.21	0.48
1:E:117:SER:HB2	1:E:124:ALA:HB2	1.96	0.48
1:F:238:LYS:HE3	1:G:221:THR:HG23	1.96	0.48
1:H:23:ARG:HD2	1:H:23:ARG:N	2.29	0.48
1:H:128:ASP:HB2	1:H:156:LEU:HA	1.95	0.48
1:E:72:VAL:HG21	1:E:342:ALA:CB	2.42	0.48
1:F:357:GLU:HG2	1:F:361:ARG:NH2	2.29	0.48
1:G:74:ARG:NH2	1:G:156:LEU:HB3	2.29	0.48
1:A:147:TYR:CD1	1:A:147:TYR:N	2.82	0.47
1:B:117:SER:HB2	1:B:124:ALA:HB2	1.96	0.47
1:B:152:ILE:HG21	1:B:204:LEU:HD12	1.95	0.47
1:B:209:PRO:HB3	1:B:280:GLN:HB3	1.96	0.47
1:D:40:PHE:N	1:D:40:PHE:CD1	2.81	0.47
1:G:261:ARG:HG2	1:G:265:GLN:HE21	1.78	0.47
1:A:314:PRO:O	1:A:318:LYS:HG3	2.13	0.47
1:B:1:MET:HA	1:B:21:ASP:OD2	2.13	0.47
1:B:223:LEU:HD21	1:C:224:VAL:CG2	2.44	0.47
1:B:299:ILE:HD11	1:B:323:ILE:HB	1.97	0.47
1:E:22:GLU:OE2	1:E:347:ARG:NH2	2.47	0.47
1:H:209:PRO:HB3	1:H:280:GLN:HB3	1.96	0.47
1:A:224:VAL:HG21	1:H:241:ILE:HD11	1.96	0.47
1:A:240:ARG:HD2	1:A:244:ASN:HB3	1.97	0.47
1:D:209:PRO:HB3	1:D:280:GLN:HB3	1.97	0.47
1:E:314:PRO:O	1:E:318:LYS:HG3	2.14	0.47
1:A:183:MET:HB3	1:A:305:LEU:HD12	1.95	0.47
1:A:332:SER:O	1:A:334:GLU:HG3	2.14	0.47
1:B:15:LYS:HD3	1:B:29:ASN:HD22	1.79	0.47
1:F:364:GLU:O	1:F:368:SER:N	2.47	0.47
1:B:255:ASP:O	1:B:259:VAL:HG23	2.13	0.47
1:H:242:VAL:HG13	1:H:242:VAL:O	2.15	0.47
1:B:159:LYS:O	1:B:163:LYS:HG3	2.15	0.47
1:B:244:ASN:CG	1:B:245:GLY:H	2.23	0.47
1:B:260:VAL:HG13	1:B:311:PHE:CE1	2.49	0.47
1:B:314:PRO:O	1:B:318:LYS:HG3	2.15	0.47
1:C:147:TYR:N	1:C:147:TYR:CD1	2.82	0.47
1:C:209:PRO:HB3	1:C:280:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:HE3	1:F:28:GLN:OE1	2.15	0.47
1:E:147:TYR:N	1:E:147:TYR:CD1	2.82	0.47
1:E:165:VAL:HG22	1:E:329:PHE:HE2	1.79	0.47
1:E:258:GLU:O	1:E:261:ARG:HB3	2.13	0.47
1:F:209:PRO:HB3	1:F:280:GLN:HB3	1.96	0.47
1:H:78:LEU:CD2	1:H:92:MET:HG3	2.44	0.47
1:A:209:PRO:HB3	1:A:280:GLN:HB3	1.96	0.47
1:D:135:MET:HA	1:D:198:ILE:HA	1.97	0.47
1:D:247:LEU:HD23	1:D:273:VAL:HG12	1.97	0.47
1:D:363:ARG:C	1:D:365:ARG:H	2.23	0.47
1:E:244:ASN:O	1:E:249:ALA:HB2	2.14	0.47
1:E:311:PHE:C	1:E:314:PRO:HD2	2.39	0.47
1:F:93:ILE:HD13	1:F:114:HIS:CD2	2.50	0.47
1:A:305:LEU:HB3	1:A:312:LEU:CD2	2.45	0.47
1:D:39:ARG:HB3	1:D:40:PHE:CD1	2.49	0.47
1:F:117:SER:HB2	1:F:124:ALA:HB2	1.95	0.47
1:F:204:LEU:O	1:F:242:VAL:HG22	2.15	0.47
1:C:117:SER:HB2	1:C:124:ALA:HB2	1.96	0.47
1:C:240:ARG:HH11	1:C:244:ASN:HD22	1.63	0.47
1:D:147:TYR:N	1:D:147:TYR:CD1	2.83	0.47
1:E:169:MET:O	1:E:171:LYS:HG3	2.15	0.47
1:F:15:LYS:HD3	1:F:29:ASN:HD22	1.80	0.47
1:F:144:HIS:CE1	1:G:240:ARG:HH21	2.33	0.47
1:H:147:TYR:CD1	1:H:147:TYR:N	2.82	0.47
1:A:54:ALA:O	1:A:57:PHE:HB3	2.15	0.47
1:A:307:HIS:HA	1:A:309:LYS:HE3	1.97	0.47
1:A:369:TYR:CD1	1:A:369:TYR:C	2.93	0.47
1:D:127:VAL:O	1:D:128:ASP:C	2.58	0.47
1:A:242:VAL:HG12	1:A:242:VAL:O	2.15	0.46
1:B:88:VAL:HG12	1:B:93:ILE:CD1	2.36	0.46
1:B:272:ARG:HD2	1:C:369:TYR:CD1	2.50	0.46
1:C:187:ILE:HG13	1:C:211:THR:HG22	1.97	0.46
1:C:240:ARG:NH1	1:C:244:ASN:ND2	2.63	0.46
1:D:130:VAL:O	1:D:152:ILE:HA	2.15	0.46
1:D:134:GLU:HB2	1:D:196:ARG:NH1	2.30	0.46
1:G:204:LEU:O	1:G:242:VAL:HG21	2.15	0.46
1:H:305:LEU:HB3	1:H:312:LEU:CD2	2.45	0.46
1:A:208:GLY:HA2	1:A:284:TRP:CZ2	2.49	0.46
1:G:305:LEU:HB3	1:G:312:LEU:CD2	2.46	0.46
1:H:72:VAL:HG12	1:H:338:LEU:HD22	1.96	0.46
1:A:233:THR:OG1	1:A:236:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:HB2	1:D:124:ALA:HB2	1.96	0.46
1:D:311:PHE:C	1:D:314:PRO:HD2	2.41	0.46
1:E:311:PHE:O	1:E:314:PRO:HD2	2.16	0.46
1:E:362:TRP:O	1:E:365:ARG:HB3	2.15	0.46
1:G:117:SER:HB2	1:G:124:ALA:HB2	1.97	0.46
1:H:307:HIS:HA	1:H:309:LYS:HE3	1.97	0.46
1:B:219:PRO:HG2	1:B:222:GLN:NE2	2.29	0.46
1:B:311:PHE:C	1:B:314:PRO:HD2	2.40	0.46
1:C:71:PHE:HE1	1:C:122:VAL:HB	1.81	0.46
1:F:372:GLY:HA3	1:G:269:TRP:CE3	2.50	0.46
1:A:79:ASP:O	1:A:81:ILE:HG23	2.15	0.46
1:C:208:GLY:HA2	1:C:284:TRP:CE2	2.51	0.46
1:D:188:SER:C	1:D:189:ILE:HG13	2.41	0.46
1:F:56:GLN:O	1:F:60:GLU:HG2	2.15	0.46
1:G:104:HIS:H	1:G:107:ASN:HD22	1.64	0.46
1:G:253:THR:HG21	1:G:259:VAL:HG22	1.97	0.46
1:H:15:LYS:HD3	1:H:29:ASN:HD22	1.81	0.46
1:B:369:TYR:O	1:B:370:LEU:C	2.58	0.46
1:C:128:ASP:HB2	1:C:156:LEU:HA	1.97	0.46
1:D:258:GLU:OE1	1:D:261:ARG:HD2	2.15	0.46
1:H:79:ASP:HB2	1:H:363:ARG:HH12	1.80	0.46
1:A:260:VAL:HG13	1:A:311:PHE:CE1	2.50	0.46
1:D:165:VAL:HG21	1:D:300:VAL:HG21	1.98	0.46
1:D:169:MET:O	1:D:171:LYS:HG3	2.15	0.46
1:B:233:THR:OG1	1:B:236:GLU:HB3	2.16	0.46
1:C:251:LEU:CD2	1:C:270:ALA:HA	2.46	0.46
1:C:314:PRO:O	1:C:318:LYS:HG3	2.15	0.46
1:D:208:GLY:HA2	1:D:284:TRP:CE2	2.50	0.46
1:F:305:LEU:HB3	1:F:312:LEU:CD2	2.46	0.46
1:G:200:VAL:HG22	1:G:201:ASN:N	2.31	0.46
1:C:61:THR:HG22	1:C:61:THR:O	2.16	0.46
1:D:233:THR:OG1	1:D:236:GLU:HB3	2.16	0.46
1:D:327:LEU:HB3	1:D:329:PHE:HE1	1.80	0.46
1:E:306:ALA:CB	1:E:330:PRO:HA	2.42	0.46
1:F:208:GLY:HA2	1:F:284:TRP:CE2	2.50	0.46
1:G:307:HIS:HA	1:G:309:LYS:HE3	1.98	0.46
1:A:306:ALA:HB3	1:A:330:PRO:HA	1.98	0.46
1:C:159:LYS:O	1:C:163:LYS:HG3	2.15	0.46
1:C:367:ASP:O	1:C:368:SER:C	2.59	0.46
1:D:88:VAL:HG12	1:D:93:ILE:CD1	2.34	0.46
1:E:39:ARG:O	1:E:39:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:HIS:HE1	1:E:146:ASN:ND2	2.13	0.46
1:F:200:VAL:HG22	1:F:201:ASN:N	2.31	0.46
1:F:257:ARG:HB3	1:F:257:ARG:HH11	1.81	0.46
1:B:247:LEU:HD23	1:B:273:VAL:HG12	1.99	0.45
1:E:305:LEU:HB3	1:E:312:LEU:CD2	2.46	0.45
1:A:27:MET:SD	1:A:27:MET:C	2.99	0.45
1:B:16:LEU:HD11	1:B:54:ALA:HA	1.98	0.45
1:C:333:ASN:ND2	1:C:336:LYS:CB	2.72	0.45
1:D:104:HIS:HD2	1:D:204:LEU:HD21	1.81	0.45
1:D:136:GLU:HB3	1:D:138:VAL:HG12	1.97	0.45
1:D:159:LYS:O	1:D:163:LYS:HG3	2.16	0.45
1:D:200:VAL:HG22	1:D:201:ASN:N	2.31	0.45
1:E:165:VAL:HG21	1:E:300:VAL:HG21	1.98	0.45
1:G:27:MET:SD	1:G:27:MET:C	2.99	0.45
1:G:257:ARG:NH1	1:G:257:ARG:HG2	2.31	0.45
1:B:183:MET:HB3	1:B:305:LEU:HD12	1.98	0.45
1:C:1:MET:HA	1:C:21:ASP:OD2	2.17	0.45
1:C:130:VAL:HG22	1:C:130:VAL:O	2.16	0.45
1:C:305:LEU:HB3	1:C:312:LEU:CD2	2.46	0.45
1:E:165:VAL:HG22	1:E:329:PHE:CE2	2.52	0.45
1:E:183:MET:HB3	1:E:305:LEU:HD12	1.97	0.45
1:F:48:GLU:O	1:F:52:LYS:HG3	2.16	0.45
1:B:305:LEU:HB3	1:B:312:LEU:CD2	2.47	0.45
1:D:361:ARG:O	1:D:365:ARG:HG3	2.16	0.45
1:E:233:THR:OG1	1:E:236:GLU:HB3	2.15	0.45
1:G:251:LEU:C	1:G:253:THR:H	2.25	0.45
1:B:289:ALA:HB2	1:B:323:ILE:HD13	1.99	0.45
1:C:183:MET:HB3	1:C:305:LEU:HD12	1.97	0.45
1:C:233:THR:OG1	1:C:236:GLU:HB3	2.16	0.45
1:D:70:ALA:HA	1:D:122:VAL:CG1	2.47	0.45
1:D:224:VAL:HG21	1:E:241:ILE:HD11	1.97	0.45
1:D:305:LEU:HB3	1:D:312:LEU:CD2	2.46	0.45
1:F:82:PRO:HD2	1:F:358:GLU:HG3	1.99	0.45
1:G:311:PHE:C	1:G:314:PRO:HD2	2.41	0.45
1:H:79:ASP:O	1:H:81:ILE:HG23	2.16	0.45
1:A:159:LYS:O	1:A:163:LYS:HG3	2.16	0.45
1:B:200:VAL:HG22	1:B:201:ASN:N	2.32	0.45
1:C:129:PRO:C	1:C:131:VAL:H	2.24	0.45
1:C:239:LYS:HG2	1:C:244:ASN:OD1	2.15	0.45
1:D:15:LYS:HD3	1:D:29:ASN:HD22	1.81	0.45
1:D:55:ARG:NH2	1:D:119:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ASP:O	1:F:81:ILE:HG23	2.17	0.45
1:F:289:ALA:HB2	1:F:323:ILE:HD13	1.99	0.45
1:H:157:ASN:HD21	1:H:161:VAL:HG13	1.80	0.45
1:H:233:THR:OG1	1:H:236:GLU:HB3	2.17	0.45
1:H:311:PHE:C	1:H:314:PRO:HD2	2.41	0.45
1:B:257:ARG:HB3	1:B:257:ARG:NH2	2.31	0.45
1:C:361:ARG:O	1:C:364:GLU:HB2	2.17	0.45
1:D:8:ASN:ND2	1:D:334:GLU:HB3	2.31	0.45
1:E:15:LYS:HD3	1:E:29:ASN:HD22	1.82	0.45
1:E:370:LEU:HD12	1:E:370:LEU:N	2.31	0.45
1:B:258:GLU:O	1:B:261:ARG:HB3	2.17	0.45
1:D:64:SER:C	1:D:66:SER:N	2.74	0.45
1:E:247:LEU:HD23	1:E:273:VAL:HG12	1.98	0.45
1:H:80:PRO:HB2	1:H:362:TRP:CE3	2.51	0.45
1:C:59:GLU:C	1:C:61:THR:H	2.25	0.45
1:E:159:LYS:O	1:E:163:LYS:HG3	2.17	0.45
1:D:307:HIS:HA	1:D:309:LYS:HE3	1.99	0.45
1:D:370:LEU:HD11	1:E:269:TRP:HZ3	1.81	0.45
1:F:260:VAL:O	1:F:264:LYS:HG3	2.17	0.45
1:E:357:GLU:O	1:E:361:ARG:HG2	2.17	0.44
1:F:183:MET:HB3	1:F:305:LEU:HD12	1.99	0.44
1:G:135:MET:HE2	1:G:139:ALA:HB1	1.99	0.44
1:G:144:HIS:CE1	1:G:146:ASN:HD22	2.35	0.44
1:H:88:VAL:HG23	1:H:124:ALA:O	2.17	0.44
1:H:104:HIS:ND1	1:H:105:ALA:N	2.65	0.44
1:H:183:MET:HB3	1:H:305:LEU:HD12	1.99	0.44
1:A:70:ALA:HA	1:A:122:VAL:CG1	2.47	0.44
1:B:79:ASP:O	1:B:81:ILE:HG23	2.17	0.44
1:C:48:GLU:CD	1:C:48:GLU:H	2.25	0.44
1:D:93:ILE:HD13	1:D:114:HIS:CG	2.52	0.44
1:F:233:THR:OG1	1:F:236:GLU:HB3	2.17	0.44
1:G:71:PHE:HE1	1:G:122:VAL:HB	1.83	0.44
1:G:233:THR:OG1	1:G:236:GLU:HB3	2.16	0.44
1:B:40:PHE:N	1:B:40:PHE:CD1	2.85	0.44
1:B:104:HIS:CD2	1:B:105:ALA:N	2.85	0.44
1:B:344:ARG:CG	1:B:349:GLU:HB2	2.48	0.44
1:E:200:VAL:HG22	1:E:201:ASN:N	2.32	0.44
1:F:70:ALA:HA	1:F:122:VAL:CG1	2.48	0.44
1:G:159:LYS:O	1:G:163:LYS:HG3	2.17	0.44
1:H:208:GLY:HA2	1:H:284:TRP:CE2	2.51	0.44
1:A:88:VAL:HG23	1:A:124:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:PHE:C	1:F:314:PRO:HD2	2.43	0.44
1:A:369:TYR:CD1	1:H:272:ARG:NH2	2.86	0.44
1:E:71:PHE:HE1	1:E:122:VAL:HB	1.83	0.44
1:E:255:ASP:CG	1:E:257:ARG:HG3	2.42	0.44
1:G:219:PRO:HG2	1:G:222:GLN:NE2	2.32	0.44
1:G:251:LEU:HD21	1:G:270:ALA:HA	1.99	0.44
1:G:364:GLU:O	1:G:367:ASP:N	2.49	0.44
1:A:311:PHE:C	1:A:314:PRO:HD2	2.42	0.44
1:D:344:ARG:CG	1:D:349:GLU:HB2	2.38	0.44
1:E:333:ASN:ND2	1:E:336:LYS:H	2.15	0.44
1:F:81:ILE:HG22	1:F:359:SER:HA	2.00	0.44
1:G:16:LEU:HD11	1:G:54:ALA:HA	1.98	0.44
1:A:1:MET:HA	1:A:21:ASP:OD2	2.17	0.44
1:A:361:ARG:O	1:A:365:ARG:HG3	2.18	0.44
1:B:70:ALA:HA	1:B:122:VAL:CG1	2.47	0.44
1:B:127:VAL:O	1:B:128:ASP:C	2.60	0.44
1:C:260:VAL:O	1:C:264:LYS:HG3	2.18	0.44
1:G:1:MET:HA	1:G:21:ASP:OD2	2.18	0.44
1:G:311:PHE:O	1:G:314:PRO:HD2	2.18	0.44
1:H:43:ILE:HD12	1:H:104:HIS:N	2.32	0.44
1:H:165:VAL:HG21	1:H:300:VAL:HG21	2.00	0.44
1:A:55:ARG:NH2	1:A:119:GLU:OE2	2.51	0.44
1:B:165:VAL:HG21	1:B:300:VAL:HG21	2.00	0.44
1:B:318:LYS:HB2	6:B:408:HOH:O	2.18	0.44
1:B:362:TRP:C	1:B:364:GLU:H	2.25	0.44
1:D:104:HIS:H	1:D:107:ASN:HD22	1.64	0.44
1:E:79:ASP:O	1:E:81:ILE:HG23	2.17	0.44
1:E:238:LYS:HB2	1:E:238:LYS:HZ2	1.81	0.44
1:A:272:ARG:NH2	1:H:370:LEU:HG	2.32	0.44
1:A:200:VAL:HG22	1:A:201:ASN:N	2.32	0.43
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.83	0.43
1:A:370:LEU:HB2	1:A:373:ILE:HG23	2.00	0.43
1:B:157:ASN:HD21	1:B:161:VAL:HG13	1.82	0.43
1:C:200:VAL:HG22	1:C:201:ASN:N	2.32	0.43
1:F:165:VAL:HG21	1:F:300:VAL:HG21	1.99	0.43
1:F:165:VAL:HG22	1:F:329:PHE:CZ	2.53	0.43
1:G:70:ALA:HA	1:G:122:VAL:CG1	2.48	0.43
1:B:27:MET:SD	1:B:27:MET:C	3.01	0.43
1:B:248:VAL:O	1:B:252:GLY:N	2.50	0.43
1:B:311:PHE:O	1:B:314:PRO:HD2	2.18	0.43
1:C:153:PHE:CE1	1:C:155:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ASN:HA	1:C:192:HIS:O	2.19	0.43
1:D:104:HIS:H	1:D:107:ASN:ND2	2.15	0.43
1:D:241:ILE:HD12	1:E:224:VAL:HG21	1.99	0.43
1:E:251:LEU:HD12	1:E:259:VAL:HG22	1.99	0.43
1:G:93:ILE:HD13	1:G:114:HIS:CG	2.53	0.43
1:G:366:TYR:O	1:G:370:LEU:HG	2.17	0.43
1:B:213:GLU:HA	1:B:245:GLY:O	2.18	0.43
1:C:165:VAL:HG21	1:C:300:VAL:HG21	1.99	0.43
1:D:144:HIS:CE1	1:D:146:ASN:HD22	2.36	0.43
1:F:357:GLU:O	1:F:361:ARG:HG2	2.19	0.43
1:G:169:MET:O	1:G:171:LYS:HG3	2.18	0.43
1:G:183:MET:HB3	1:G:305:LEU:HD12	2.00	0.43
1:H:289:ALA:HB2	1:H:323:ILE:HD13	2.00	0.43
1:B:64:SER:C	1:B:66:SER:N	2.77	0.43
1:B:209:PRO:HD3	1:B:284:TRP:CD2	2.53	0.43
1:G:104:HIS:H	1:G:107:ASN:ND2	2.16	0.43
1:G:127:VAL:O	1:G:128:ASP:C	2.62	0.43
1:G:165:VAL:HG21	1:G:300:VAL:HG21	2.00	0.43
1:G:167:ARG:CD	1:H:309:LYS:NZ	2.75	0.43
1:G:255:ASP:HB3	1:G:258:GLU:HB2	1.99	0.43
1:H:70:ALA:HA	1:H:122:VAL:CG1	2.48	0.43
1:A:71:PHE:HE1	1:A:122:VAL:HB	1.83	0.43
1:A:227:CYS:SG	1:H:227:CYS:SG	3.15	0.43
1:B:283:LYS:HB3	1:C:287:LYS:HG3	2.01	0.43
1:C:55:ARG:NH2	1:C:119:GLU:OE2	2.50	0.43
1:F:250:TYR:HB3	1:F:273:VAL:HG21	2.00	0.43
1:F:275:ARG:HH12	1:G:138:VAL:HB	1.83	0.43
1:G:88:VAL:HG23	1:G:124:ALA:O	2.19	0.43
1:H:366:TYR:HA	1:H:370:LEU:HD13	2.00	0.43
1:A:246:GLY:O	1:A:250:TYR:HD1	2.02	0.43
1:B:26:LYS:CD	1:B:61:THR:HG22	2.48	0.43
1:D:88:VAL:HG23	1:D:124:ALA:O	2.19	0.43
1:D:183:MET:HB3	1:D:305:LEU:HD12	1.99	0.43
1:F:157:ASN:HD21	1:F:161:VAL:HG13	1.82	0.43
1:F:268:GLU:HA	1:F:268:GLU:OE1	2.19	0.43
1:H:137:ASP:HA	1:H:140:ARG:HG3	2.01	0.43
1:H:159:LYS:O	1:H:163:LYS:HG3	2.18	0.43
1:A:165:VAL:HG21	1:A:300:VAL:HG21	2.00	0.43
1:B:88:VAL:HG23	1:B:124:ALA:O	2.18	0.43
1:E:255:ASP:OD2	1:E:257:ARG:NH1	2.51	0.43
1:F:307:HIS:HA	1:F:309:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:PRO:HA	1:G:280:GLN:OE1	2.19	0.43
1:B:268:GLU:OE1	1:B:268:GLU:HA	2.19	0.43
1:B:280:GLN:O	1:B:284:TRP:HE3	2.01	0.43
1:C:16:LEU:HD11	1:C:54:ALA:HA	2.01	0.43
1:C:23:ARG:HG3	1:C:23:ARG:HH11	1.83	0.43
1:D:16:LEU:HD11	1:D:54:ALA:HA	2.00	0.43
1:E:369:TYR:C	1:E:370:LEU:HD12	2.44	0.43
1:F:104:HIS:H	1:F:107:ASN:HD22	1.66	0.43
1:F:159:LYS:O	1:F:163:LYS:HG3	2.19	0.43
1:A:153:PHE:CE1	1:A:155:ALA:HA	2.54	0.43
1:A:311:PHE:O	1:A:314:PRO:HD2	2.19	0.43
1:B:231:LYS:C	1:B:233:THR:H	2.27	0.43
1:B:245:GLY:O	1:B:248:VAL:HG12	2.18	0.43
1:B:260:VAL:O	1:B:264:LYS:HG3	2.19	0.43
1:C:157:ASN:HD21	1:C:161:VAL:HG13	1.84	0.43
1:D:8:ASN:HD21	1:D:334:GLU:HB3	1.83	0.43
1:F:144:HIS:CE1	1:F:146:ASN:HD22	2.37	0.43
1:F:255:ASP:O	1:F:258:GLU:HB3	2.19	0.43
1:H:127:VAL:O	1:H:128:ASP:C	2.61	0.43
1:A:208:GLY:HA2	1:A:284:TRP:CE2	2.53	0.43
1:B:287:LYS:HG3	1:C:283:LYS:HB3	2.01	0.43
1:D:238:LYS:HB2	1:D:238:LYS:HZ2	1.84	0.43
1:D:311:PHE:O	1:D:314:PRO:HD2	2.18	0.43
1:E:20:GLU:O	1:E:21:ASP:HB2	2.18	0.43
1:G:315:TRP:O	1:G:319:ARG:HG3	2.19	0.43
1:H:27:MET:SD	1:H:27:MET:C	3.02	0.43
1:H:80:PRO:HB2	1:H:362:TRP:CZ3	2.54	0.43
1:H:200:VAL:HG22	1:H:201:ASN:N	2.33	0.43
1:C:24:MET:HE3	1:D:27:MET:CG	2.49	0.42
1:D:78:LEU:CD2	1:D:92:MET:HG3	2.49	0.42
1:E:351:LYS:HA	1:E:352:PRO:HD3	1.93	0.42
1:G:64:SER:C	1:G:66:SER:N	2.77	0.42
1:H:16:LEU:HD11	1:H:54:ALA:HA	2.01	0.42
1:H:64:SER:C	1:H:66:SER:N	2.77	0.42
1:A:177:ASN:HA	1:A:192:HIS:O	2.19	0.42
1:B:208:GLY:HA2	1:B:284:TRP:CE2	2.53	0.42
1:C:289:ALA:HB2	1:C:323:ILE:HD13	2.00	0.42
1:D:268:GLU:HA	1:D:268:GLU:OE1	2.19	0.42
1:E:177:ASN:HA	1:E:192:HIS:O	2.19	0.42
1:F:209:PRO:HD3	1:F:284:TRP:CD2	2.54	0.42
1:H:1:MET:HA	1:H:21:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:ASN:HD22	1:H:336:LYS:CB	2.32	0.42
1:A:80:PRO:HB2	1:A:362:TRP:CZ3	2.54	0.42
1:A:127:VAL:O	1:A:128:ASP:C	2.62	0.42
1:A:157:ASN:HD21	1:A:161:VAL:HG13	1.84	0.42
1:F:71:PHE:HE1	1:F:122:VAL:HB	1.84	0.42
1:F:100:LYS:HG3	1:F:101:ASN:N	2.34	0.42
1:F:209:PRO:HA	1:F:280:GLN:OE1	2.20	0.42
1:F:259:VAL:C	1:F:261:ARG:N	2.76	0.42
1:A:78:LEU:CD2	1:A:92:MET:HG3	2.49	0.42
1:A:100:LYS:HG3	1:A:101:ASN:N	2.35	0.42
1:B:144:HIS:CE1	1:B:146:ASN:HD22	2.37	0.42
1:C:70:ALA:HA	1:C:122:VAL:CG1	2.49	0.42
1:C:82:PRO:C	1:C:132:VAL:HG13	2.45	0.42
1:D:93:ILE:O	1:D:93:ILE:CG2	2.67	0.42
1:D:223:LEU:HD21	1:E:224:VAL:HG23	2.01	0.42
1:G:258:GLU:CD	1:G:261:ARG:NH1	2.77	0.42
1:A:22:GLU:OE1	1:A:22:GLU:N	2.49	0.42
1:A:268:GLU:HA	1:A:268:GLU:OE1	2.19	0.42
1:C:127:VAL:O	1:C:128:ASP:C	2.62	0.42
1:C:209:PRO:HA	1:C:280:GLN:OE1	2.19	0.42
1:D:74:ARG:NH1	1:D:130:VAL:HG12	2.35	0.42
1:D:100:LYS:HG3	1:D:101:ASN:N	2.35	0.42
1:E:209:PRO:HA	1:E:280:GLN:OE1	2.19	0.42
1:F:18:ILE:HG13	1:F:57:PHE:CE2	2.55	0.42
1:F:78:LEU:CD2	1:F:92:MET:HG3	2.49	0.42
1:F:88:VAL:HG12	1:F:93:ILE:HD11	2.02	0.42
1:H:345:VAL:CG1	1:H:352:PRO:HG3	2.49	0.42
1:B:369:TYR:O	1:C:269:TRP:CZ3	2.73	0.42
1:C:241:ILE:HG13	1:C:242:VAL:N	2.35	0.42
1:D:223:LEU:HD21	1:E:224:VAL:HG22	2.00	0.42
1:D:248:VAL:HG22	1:D:254:SER:HB2	2.02	0.42
1:E:28:GLN:OE1	1:F:26:LYS:HE3	2.20	0.42
1:E:64:SER:C	1:E:66:SER:N	2.78	0.42
1:E:289:ALA:HB2	1:E:323:ILE:HD13	2.02	0.42
1:F:1:MET:HA	1:F:21:ASP:OD2	2.20	0.42
1:H:92:MET:O	1:H:92:MET:CG	2.64	0.42
1:B:169:MET:O	1:B:171:LYS:HG3	2.20	0.42
1:B:307:HIS:HA	1:B:309:LYS:HE3	2.00	0.42
1:D:209:PRO:HA	1:D:280:GLN:OE1	2.20	0.42
1:D:231:LYS:C	1:D:233:THR:H	2.27	0.42
1:F:104:HIS:ND1	1:F:105:ALA:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:ARG:HG2	1:G:257:ARG:HH11	1.85	0.42
1:G:328:VAL:C	1:G:330:PRO:HD3	2.45	0.42
1:H:260:VAL:O	1:H:264:LYS:HG3	2.20	0.42
1:B:306:ALA:CB	1:B:330:PRO:HA	2.48	0.42
1:D:144:HIS:CE1	1:E:240:ARG:HH21	2.38	0.42
1:F:231:LYS:C	1:F:233:THR:H	2.27	0.42
1:G:231:LYS:C	1:G:233:THR:H	2.27	0.42
1:H:153:PHE:CE1	1:H:155:ALA:HA	2.55	0.42
1:B:345:VAL:CG1	1:B:352:PRO:HG3	2.50	0.42
1:C:64:SER:C	1:C:66:SER:N	2.77	0.42
1:D:138:VAL:HB	1:E:275:ARG:HH12	1.83	0.42
1:D:248:VAL:CG2	1:D:254:SER:HB2	2.49	0.42
1:F:153:PHE:CE1	1:F:155:ALA:HA	2.55	0.42
1:H:8:ASN:ND2	1:H:334:GLU:OE2	2.52	0.42
1:A:283:LYS:HB3	1:H:287:LYS:HG3	2.01	0.42
1:B:72:VAL:HG12	1:B:338:LEU:HD22	2.01	0.42
1:C:48:GLU:CD	1:C:48:GLU:N	2.78	0.42
1:D:1:MET:HA	1:D:21:ASP:OD2	2.20	0.42
1:E:268:GLU:OE1	1:E:268:GLU:HA	2.19	0.42
1:F:96:LEU:CD1	1:F:110:ALA:HB3	2.50	0.42
1:F:335:GLU:OE2	1:F:335:GLU:N	2.50	0.42
1:G:78:LEU:HD21	1:G:92:MET:HG3	2.01	0.42
1:H:96:LEU:CD1	1:H:110:ALA:HB3	2.50	0.42
1:B:199:ASP:OD1	1:B:200:VAL:N	2.53	0.41
1:C:231:LYS:C	1:C:233:THR:H	2.27	0.41
1:E:344:ARG:CG	1:E:349:GLU:HB2	2.36	0.41
1:H:22:GLU:OE2	1:H:347:ARG:NH2	2.51	0.41
1:H:250:TYR:HB2	1:H:273:VAL:HG11	2.02	0.41
1:D:250:TYR:O	1:D:251:LEU:HD23	2.20	0.41
1:E:16:LEU:HD11	1:E:54:ALA:HA	2.02	0.41
1:E:100:LYS:HG3	1:E:101:ASN:N	2.35	0.41
1:F:136:GLU:OE1	1:F:193:ARG:NH2	2.53	0.41
1:G:100:LYS:HG3	1:G:101:ASN:N	2.35	0.41
1:H:144:HIS:CE1	1:H:146:ASN:HD22	2.38	0.41
1:H:177:ASN:HA	1:H:192:HIS:O	2.20	0.41
1:A:238:LYS:HB2	1:A:238:LYS:HZ2	1.83	0.41
1:F:241:ILE:HD13	1:G:220:LEU:CB	2.50	0.41
1:H:209:PRO:HA	1:H:280:GLN:OE1	2.20	0.41
1:A:199:ASP:OD1	1:A:200:VAL:N	2.53	0.41
1:B:238:LYS:HB2	1:B:238:LYS:HZ3	1.86	0.41
1:D:203:ALA:O	1:D:214:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:VAL:HG23	1:E:124:ALA:O	2.20	0.41
1:E:153:PHE:CE1	1:E:155:ALA:HA	2.56	0.41
1:H:71:PHE:HE1	1:H:122:VAL:HB	1.84	0.41
1:H:361:ARG:HH11	1:H:361:ARG:HG2	1.85	0.41
1:A:82:PRO:HD2	1:A:358:GLU:HG3	2.01	0.41
1:A:96:LEU:CD1	1:A:110:ALA:HB3	2.51	0.41
1:B:82:PRO:HD2	1:B:358:GLU:CG	2.46	0.41
1:C:24:MET:HE1	1:D:24:MET:HE1	2.03	0.41
1:C:96:LEU:CD1	1:C:110:ALA:HB3	2.50	0.41
1:D:177:ASN:HA	1:D:192:HIS:O	2.21	0.41
1:E:104:HIS:H	1:E:107:ASN:HD22	1.68	0.41
1:F:136:GLU:OE1	1:F:193:ARG:NH1	2.54	0.41
1:H:209:PRO:HD3	1:H:284:TRP:CD2	2.55	0.41
1:H:278:ALA:HB2	1:H:312:LEU:HD12	2.03	0.41
1:A:231:LYS:C	1:A:233:THR:H	2.27	0.41
1:C:238:LYS:HB2	1:C:238:LYS:HZ2	1.84	0.41
1:D:153:PHE:CE1	1:D:155:ALA:HA	2.55	0.41
1:E:209:PRO:HD3	1:E:284:TRP:CD1	2.55	0.41
1:E:278:ALA:HB2	1:E:312:LEU:HD12	2.02	0.41
1:F:64:SER:C	1:F:66:SER:N	2.79	0.41
1:G:199:ASP:OD1	1:G:200:VAL:N	2.54	0.41
1:B:100:LYS:HG3	1:B:101:ASN:N	2.35	0.41
1:B:147:TYR:HD1	1:B:147:TYR:H	1.67	0.41
1:B:203:ALA:O	1:B:214:ARG:NH1	2.54	0.41
1:D:283:LYS:HB3	1:E:287:LYS:HG3	2.03	0.41
1:E:1:MET:HA	1:E:21:ASP:OD2	2.20	0.41
1:E:28:GLN:OE1	1:F:26:LYS:CE	2.69	0.41
1:F:88:VAL:HG23	1:F:124:ALA:O	2.20	0.41
1:F:257:ARG:HA	1:F:257:ARG:NE	2.36	0.41
1:G:324:ALA:HB1	1:G:325:PRO:HD2	2.03	0.41
1:H:100:LYS:HG3	1:H:101:ASN:N	2.36	0.41
1:H:311:PHE:O	1:H:314:PRO:HD2	2.21	0.41
1:H:359:SER:HB2	1:H:363:ARG:NH1	2.35	0.41
1:A:16:LEU:HD11	1:A:54:ALA:HA	2.03	0.41
1:A:169:MET:O	1:A:171:LYS:HG3	2.20	0.41
1:E:333:ASN:C	1:E:333:ASN:ND2	2.79	0.41
1:F:72:VAL:HG12	1:F:338:LEU:HD22	2.03	0.41
1:F:245:GLY:C	1:F:248:VAL:HG12	2.46	0.41
1:G:24:MET:HE3	1:H:27:MET:HG2	2.03	0.41
1:H:59:GLU:C	1:H:61:THR:N	2.79	0.41
1:H:80:PRO:O	1:H:81:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG13	1:H:250:TYR:CE2	2.56	0.41
1:A:147:TYR:HD1	1:A:147:TYR:H	1.67	0.41
1:A:186:GLY:HA2	1:A:211:THR:HG21	2.03	0.41
1:A:211:THR:HB	1:A:212:PRO:CD	2.51	0.41
1:B:177:ASN:HA	1:B:192:HIS:O	2.20	0.41
1:C:199:ASP:OD1	1:C:200:VAL:N	2.53	0.41
1:C:223:LEU:O	1:C:227:CYS:HB2	2.21	0.41
1:D:65:LEU:O	1:D:120:THR:HG21	2.21	0.41
1:D:255:ASP:OD1	1:D:257:ARG:HB2	2.21	0.41
1:E:144:HIS:CE1	1:E:146:ASN:ND2	2.84	0.41
1:E:231:LYS:C	1:E:233:THR:H	2.27	0.41
1:F:345:VAL:CG1	1:F:352:PRO:HG3	2.50	0.41
1:F:361:ARG:O	1:F:365:ARG:NE	2.53	0.41
1:G:82:PRO:CD	1:G:358:GLU:HG3	2.48	0.41
1:G:88:VAL:HG12	1:G:93:ILE:CD1	2.37	0.41
1:H:231:LYS:C	1:H:233:THR:H	2.28	0.41
1:C:59:GLU:C	1:C:61:THR:N	2.79	0.41
1:C:100:LYS:HG3	1:C:101:ASN:N	2.36	0.41
1:E:27:MET:SD	1:E:27:MET:C	3.04	0.41
1:E:80:PRO:HB2	1:E:362:TRP:CZ3	2.56	0.41
1:E:96:LEU:CD1	1:E:110:ALA:HB3	2.49	0.41
1:E:307:HIS:HA	1:E:309:LYS:HE3	2.02	0.41
1:G:96:LEU:CD1	1:G:110:ALA:HB3	2.51	0.41
1:H:137:ASP:C	1:H:140:ARG:HG3	2.45	0.41
1:H:333:ASN:HD22	1:H:336:LYS:HB2	1.86	0.41
1:A:144:HIS:CE1	1:A:146:ASN:HD22	2.38	0.40
1:A:196:ARG:HH22	1:A:365:ARG:NH2	2.19	0.40
1:C:275:ARG:HA	1:C:315:TRP:CZ3	2.56	0.40
1:E:203:ALA:O	1:E:214:ARG:NH1	2.54	0.40
1:E:256:ALA:O	1:E:260:VAL:HG23	2.21	0.40
1:F:20:GLU:O	1:F:21:ASP:HB2	2.21	0.40
1:F:278:ALA:HB2	1:F:312:LEU:HD12	2.03	0.40
1:G:211:THR:HB	1:G:212:PRO:CD	2.51	0.40
1:G:238:LYS:HB2	1:G:238:LYS:HZ3	1.85	0.40
1:A:294:GLY:O	1:A:296:VAL:N	2.53	0.40
1:B:129:PRO:C	1:B:131:VAL:H	2.29	0.40
1:C:104:HIS:ND1	1:C:105:ALA:N	2.70	0.40
1:C:334:GLU:O	1:C:335:GLU:C	2.64	0.40
1:D:77:LEU:HD21	1:D:204:LEU:HD12	2.01	0.40
1:F:224:VAL:CG2	1:G:223:LEU:HD21	2.51	0.40
1:G:203:ALA:O	1:G:214:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:GLY:C	1:G:244:ASN:HD22	2.29	0.40
1:H:268:GLU:OE1	1:H:268:GLU:HA	2.21	0.40
1:B:294:GLY:O	1:B:296:VAL:N	2.55	0.40
1:C:88:VAL:HG23	1:C:124:ALA:O	2.20	0.40
1:C:345:VAL:CG1	1:C:352:PRO:HG3	2.51	0.40
1:E:189:ILE:CD1	1:E:284:TRP:HB2	2.51	0.40
1:F:240:ARG:NH1	1:F:244:ASN:ND2	2.68	0.40
1:F:283:LYS:CE	1:G:287:LYS:HE2	2.46	0.40
1:G:186:GLY:HA2	1:G:211:THR:HG21	2.03	0.40
1:G:268:GLU:OE1	1:G:268:GLU:HA	2.21	0.40
1:H:55:ARG:HG2	1:H:55:ARG:NH1	2.32	0.40
1:A:333:ASN:OD1	1:A:336:LYS:HB2	2.22	0.40
1:B:96:LEU:CD1	1:B:110:ALA:HB3	2.52	0.40
1:B:278:ALA:HB2	1:B:312:LEU:HD12	2.03	0.40
1:D:43:ILE:C	1:D:45:ASP:N	2.79	0.40
1:D:345:VAL:CG1	1:D:352:PRO:HG3	2.52	0.40
1:E:161:VAL:HG23	1:E:162:ALA:N	2.37	0.40
1:E:369:TYR:HB3	1:E:370:LEU:CD1	2.48	0.40
1:F:16:LEU:HD11	1:F:54:ALA:HA	2.02	0.40
1:F:324:ALA:HB1	1:F:325:PRO:HD2	2.02	0.40
1:G:79:ASP:O	1:G:81:ILE:HG23	2.22	0.40
1:A:92:MET:HB2	1:A:355:TYR:CD2	2.57	0.40
1:A:315:TRP:O	1:A:319:ARG:HG3	2.21	0.40
1:B:369:TYR:O	1:B:371:ASP:N	2.55	0.40
1:D:104:HIS:NE2	5:D:381:CIT:H21	2.36	0.40
1:D:153:PHE:N	1:D:153:PHE:CD2	2.90	0.40
1:D:315:TRP:O	1:D:319:ARG:HG3	2.21	0.40
1:E:55:ARG:HH22	1:E:119:GLU:CD	2.29	0.40
1:F:27:MET:SD	1:F:27:MET:C	3.05	0.40
1:F:127:VAL:O	1:F:128:ASP:C	2.64	0.40
1:F:223:LEU:O	1:F:227:CYS:HB2	2.22	0.40
1:F:362:TRP:C	1:F:364:GLU:N	2.79	0.40
1:G:177:ASN:HA	1:G:192:HIS:O	2.21	0.40
1:H:129:PRO:O	1:H:132:VAL:HG23	2.22	0.40
1:H:333:ASN:ND2	1:H:336:LYS:CB	2.84	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	371/375 (99%)	325 (88%)	39 (10%)	7 (2%)	6	30
1	B	369/375 (98%)	326 (88%)	39 (11%)	4 (1%)	11	43
1	C	369/375 (98%)	325 (88%)	38 (10%)	6 (2%)	7	34
1	D	371/375 (99%)	327 (88%)	41 (11%)	3 (1%)	16	50
1	E	369/375 (98%)	325 (88%)	40 (11%)	4 (1%)	11	43
1	F	370/375 (99%)	325 (88%)	43 (12%)	2 (0%)	24	60
1	G	371/375 (99%)	322 (87%)	45 (12%)	4 (1%)	11	43
1	H	370/375 (99%)	326 (88%)	41 (11%)	3 (1%)	16	50
All	All	2960/3000 (99%)	2601 (88%)	326 (11%)	33 (1%)	11	43

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	LEU
1	H	60	GLU
1	A	39	ARG
1	A	243	GLY
1	C	245	GLY
1	C	368	SER
1	E	39	ARG
1	F	39	ARG
1	H	39	ARG
1	A	308	GLU
1	C	60	GLU
1	C	233	THR
1	C	267	ASP
1	D	372	GLY
1	E	233	THR
1	G	39	ARG
1	G	233	THR

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Mol	Chain	Res	Type
1	A	233	THR
1	B	205	ASP
1	B	233	THR
1	B	308	GLU
1	C	308	GLU
1	D	233	THR
1	E	308	GLU
1	F	233	THR
1	G	60	GLU
1	G	205	ASP
1	H	233	THR
1	A	205	ASP
1	A	267	ASP
1	A	333	ASN
1	D	205	ASP
1	E	330	PRO

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	313/315 (99%)	308 (98%)	5 (2%)	55	79
1	B	312/315 (99%)	309 (99%)	3 (1%)	68	84
1	C	312/315 (99%)	309 (99%)	3 (1%)	68	84
1	D	313/315 (99%)	309 (99%)	4 (1%)	61	81
1	E	312/315 (99%)	308 (99%)	4 (1%)	61	81
1	F	312/315 (99%)	306 (98%)	6 (2%)	50	76
1	G	313/315 (99%)	310 (99%)	3 (1%)	68	84
1	H	312/315 (99%)	308 (99%)	4 (1%)	61	81
All	All	2499/2520 (99%)	2467 (99%)	32 (1%)	61	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	137	ASP
1	A	238	LYS
1	A	257	ARG
1	A	365	ARG
1	B	48	GLU
1	B	137	ASP
1	B	238	LYS
1	C	39	ARG
1	C	238	LYS
1	C	369	TYR
1	D	48	GLU
1	D	136	GLU
1	D	238	LYS
1	D	361	ARG
1	E	238	LYS
1	E	257	ARG
1	E	258	GLU
1	E	369	TYR
1	F	23	ARG
1	F	137	ASP
1	F	147	TYR
1	F	238	LYS
1	F	257	ARG
1	F	333	ASN
1	G	60	GLU
1	G	238	LYS
1	G	334	GLU
1	H	23	ARG
1	H	135	MET
1	H	238	LYS
1	H	257	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	56	GLN
1	A	114	HIS
1	A	146	ASN
1	A	222	GLN
1	A	265	GLN
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	144	HIS
1	B	146	ASN
1	B	148	GLN
1	B	222	GLN
1	B	265	GLN
1	B	307	HIS
1	B	333	ASN
1	C	28	GLN
1	C	56	GLN
1	C	114	HIS
1	C	144	HIS
1	C	146	ASN
1	C	222	GLN
1	C	244	ASN
1	C	265	GLN
1	C	333	ASN
1	D	28	GLN
1	D	114	HIS
1	D	146	ASN
1	D	222	GLN
1	D	265	GLN
1	D	307	HIS
1	E	56	GLN
1	E	114	HIS
1	E	144	HIS
1	E	146	ASN
1	E	148	GLN
1	E	222	GLN
1	E	265	GLN
1	E	333	ASN
1	F	114	HIS
1	F	146	ASN
1	F	148	GLN
1	F	222	GLN
1	F	333	ASN
1	G	28	GLN
1	G	56	GLN
1	G	114	HIS
1	G	146	ASN
1	G	222	GLN
1	G	244	ASN
1	G	265	GLN

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Mol	Chain	Res	Type
1	G	333	ASN
1	H	28	GLN
1	H	56	GLN
1	H	114	HIS
1	H	144	HIS
1	H	146	ASN
1	H	148	GLN
1	H	244	ASN
1	H	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	F	403	-	4,4,4	1.46	1 (25%)	6,6,6	0.89	0
2	GOL	A	395	-	5,5,5	4.65	5 (100%)	5,5,5	5.80	4 (80%)
5	CIT	G	383	-	12,12,12	1.89	5 (41%)	17,17,17	3.05	8 (47%)
5	CIT	G	382	-	12,12,12	1.80	4 (33%)	17,17,17	3.12	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	F	391	-	5,5,5	4.62	5 (100%)	5,5,5	5.70	4 (80%)
2	GOL	C	392	-	5,5,5	4.65	5 (100%)	5,5,5	5.79	4 (80%)
3	PO4	H	404	-	4,4,4	1.51	1 (25%)	6,6,6	0.89	0
5	CIT	D	384	-	12,12,12	1.85	4 (33%)	17,17,17	3.00	8 (47%)
3	PO4	B	402	-	4,4,4	1.44	1 (25%)	6,6,6	0.90	0
3	PO4	E	401	-	4,4,4	1.42	1 (25%)	6,6,6	0.93	0
2	GOL	B	394	-	5,5,5	4.68	5 (100%)	5,5,5	5.79	4 (80%)
3	PO4	E	405	-	4,4,4	1.46	1 (25%)	6,6,6	0.90	0
5	CIT	D	381	-	12,12,12	1.83	4 (33%)	17,17,17	2.75	8 (47%)
2	GOL	D	393	-	5,5,5	4.75	5 (100%)	5,5,5	5.97	4 (80%)

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	A	395	-	-	4/4/4/4	-
5	CIT	G	383	-	-	7/16/16/16	-
5	CIT	G	382	-	-	10/16/16/16	-
2	GOL	F	391	-	-	2/4/4/4	-
2	GOL	C	392	-	-	3/4/4/4	-
5	CIT	D	384	-	-	7/16/16/16	-
2	GOL	B	394	-	-	2/4/4/4	-
5	CIT	D	381	-	-	6/16/16/16	-
2	GOL	D	393	-	-	3/4/4/4	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	393	GOL	C3-C2	-7.71	1.22	1.51
2	A	395	GOL	C3-C2	-7.51	1.23	1.51
2	C	392	GOL	C3-C2	-7.46	1.23	1.51
2	B	394	GOL	C3-C2	-7.46	1.23	1.51
2	F	391	GOL	C3-C2	-7.43	1.23	1.51
2	D	393	GOL	O1-C1	4.74	1.62	1.42
2	B	394	GOL	O1-C1	4.65	1.61	1.42
2	C	392	GOL	O1-C1	4.59	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	GOL	O1-C1	4.58	1.61	1.42
2	F	391	GOL	O1-C1	4.39	1.60	1.42
5	D	381	CIT	O7-C3	3.77	1.50	1.43
5	D	384	CIT	O7-C3	3.72	1.50	1.43
5	G	383	CIT	O7-C3	3.63	1.50	1.43
2	F	391	GOL	O3-C3	3.53	1.57	1.42
5	G	382	CIT	O7-C3	3.51	1.49	1.43
2	B	394	GOL	O3-C3	3.45	1.56	1.42
2	C	392	GOL	O3-C3	3.45	1.56	1.42
2	F	391	GOL	C1-C2	-3.42	1.38	1.51
2	D	393	GOL	O3-C3	3.30	1.56	1.42
2	D	393	GOL	O2-C2	-3.30	1.33	1.43
2	A	395	GOL	O3-C3	3.28	1.56	1.42
2	B	394	GOL	C1-C2	-3.24	1.39	1.51
2	C	392	GOL	C1-C2	-3.20	1.39	1.51
2	A	395	GOL	C1-C2	-3.20	1.39	1.51
2	A	395	GOL	O2-C2	-3.14	1.34	1.43
2	B	394	GOL	O2-C2	-3.14	1.34	1.43
2	D	393	GOL	C1-C2	-3.04	1.40	1.51
2	C	392	GOL	O2-C2	-3.01	1.34	1.43
2	F	391	GOL	O2-C2	-2.87	1.35	1.43
3	H	404	PO4	P-O1	2.64	1.56	1.50
5	D	381	CIT	O5-C6	2.59	1.30	1.22
3	E	405	PO4	P-O1	2.59	1.56	1.50
3	F	403	PO4	P-O1	2.53	1.56	1.50
3	E	401	PO4	P-O1	2.51	1.56	1.50
3	B	402	PO4	P-O1	2.48	1.56	1.50
5	G	383	CIT	C3-C6	2.46	1.56	1.53
5	D	381	CIT	O1-C1	2.32	1.29	1.22
5	G	382	CIT	C3-C6	2.26	1.55	1.53
5	G	383	CIT	O1-C1	2.25	1.29	1.22
5	D	381	CIT	C3-C6	2.24	1.55	1.53
5	G	383	CIT	O5-C6	2.21	1.29	1.22
5	D	384	CIT	O1-C1	2.21	1.29	1.22
5	D	384	CIT	C3-C6	2.17	1.55	1.53
5	D	384	CIT	O5-C6	2.15	1.28	1.22
5	G	382	CIT	O5-C6	2.15	1.28	1.22
5	G	382	CIT	O1-C1	2.12	1.29	1.22
5	G	383	CIT	O4-C5	-2.09	1.23	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	GOL	O3-C3-C2	11.36	161.50	110.38
2	C	392	GOL	O3-C3-C2	11.24	160.98	110.38
2	B	394	GOL	O3-C3-C2	11.19	160.73	110.38
2	A	395	GOL	O3-C3-C2	11.13	160.50	110.38
2	F	391	GOL	O3-C3-C2	11.04	160.08	110.38
5	G	382	CIT	O7-C3-C6	-8.48	96.94	108.96
5	G	383	CIT	O7-C3-C6	-8.42	97.02	108.96
5	D	384	CIT	O7-C3-C6	-8.16	97.39	108.96
2	D	393	GOL	O2-C2-C3	5.20	130.72	109.18
5	D	381	CIT	O7-C3-C6	-5.00	101.87	108.96
5	D	381	CIT	O6-C6-C3	4.91	122.55	113.14
2	A	395	GOL	O2-C2-C3	4.81	129.11	109.18
2	B	394	GOL	O2-C2-C3	4.73	128.77	109.18
2	F	391	GOL	O2-C2-C3	4.64	128.39	109.18
2	C	392	GOL	O2-C2-C3	4.60	128.21	109.18
5	G	382	CIT	O5-C6-C3	-4.53	113.32	122.09
5	D	384	CIT	O5-C6-C3	-4.40	113.57	122.09
5	G	383	CIT	O5-C6-C3	-4.36	113.64	122.09
5	D	381	CIT	O5-C6-C3	-4.11	114.13	122.09
5	D	384	CIT	C2-C3-C6	3.80	118.44	110.03
5	G	383	CIT	C2-C3-C6	3.77	118.38	110.03
2	A	395	GOL	O1-C1-C2	3.49	126.10	110.38
2	C	392	GOL	O1-C1-C2	3.46	125.96	110.38
2	B	394	GOL	O1-C1-C2	3.45	125.93	110.38
2	D	393	GOL	O1-C1-C2	3.45	125.89	110.38
5	G	382	CIT	C2-C3-C6	3.39	117.54	110.03
5	D	381	CIT	O2-C1-C2	3.37	125.03	114.35
5	D	381	CIT	C2-C3-C6	3.35	117.44	110.03
5	G	382	CIT	O2-C1-C2	3.34	124.93	114.35
5	D	381	CIT	C3-C2-C1	3.31	122.98	113.92
5	G	382	CIT	O4-C5-O3	-3.27	114.92	123.33
2	F	391	GOL	O1-C1-C2	3.26	125.04	110.38
5	D	384	CIT	O6-C6-O5	3.23	134.19	123.86
5	G	382	CIT	O6-C6-O5	3.21	134.12	123.86
2	D	393	GOL	C3-C2-C1	-3.19	100.10	111.80
5	G	383	CIT	O6-C6-O5	3.18	134.02	123.86
5	D	384	CIT	O2-C1-C2	3.17	124.38	114.35
5	G	383	CIT	O2-C1-C2	3.14	124.30	114.35
5	G	383	CIT	O4-C5-O3	-3.12	115.30	123.33
5	D	381	CIT	O4-C5-O3	-3.08	115.41	123.33
5	D	384	CIT	O4-C5-O3	-3.01	115.60	123.33
2	A	395	GOL	C3-C2-C1	-2.90	101.15	111.80
5	G	383	CIT	C3-C2-C1	2.88	121.79	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	391	GOL	C3-C2-C1	-2.84	101.39	111.80
2	B	394	GOL	C3-C2-C1	-2.83	101.41	111.80
5	G	382	CIT	C3-C2-C1	2.81	121.61	113.92
2	C	392	GOL	C3-C2-C1	-2.79	101.56	111.80
5	D	384	CIT	C3-C2-C1	2.69	121.28	113.92
5	G	382	CIT	C3-C4-C5	2.49	120.74	113.92
5	G	382	CIT	O1-C1-C2	-2.48	115.92	122.95
5	D	381	CIT	O1-C1-C2	-2.45	116.02	122.95
5	G	383	CIT	O1-C1-C2	-2.27	116.51	122.95
5	D	384	CIT	O1-C1-C2	-2.27	116.52	122.95

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	395	GOL	O1-C1-C2-C3
2	A	395	GOL	C1-C2-C3-O3
2	B	394	GOL	C1-C2-C3-O3
2	C	392	GOL	C1-C2-C3-O3
2	D	393	GOL	C1-C2-C3-O3
2	D	393	GOL	O2-C2-C3-O3
2	F	391	GOL	C1-C2-C3-O3
5	D	381	CIT	O7-C3-C4-C5
5	D	384	CIT	O7-C3-C4-C5
5	D	384	CIT	C2-C3-C6-O5
5	D	384	CIT	C2-C3-C6-O6
5	D	384	CIT	O7-C3-C6-O5
5	D	384	CIT	O7-C3-C6-O6
5	G	382	CIT	C1-C2-C3-O7
5	G	382	CIT	C1-C2-C3-C6
5	G	382	CIT	O7-C3-C4-C5
5	G	382	CIT	C6-C3-C4-C5
5	G	382	CIT	C2-C3-C6-O5
5	G	382	CIT	C2-C3-C6-O6
5	G	382	CIT	O7-C3-C6-O5
5	G	382	CIT	O7-C3-C6-O6
5	G	383	CIT	O7-C3-C4-C5
5	G	383	CIT	C2-C3-C6-O5
5	G	383	CIT	C2-C3-C6-O6
5	G	383	CIT	O7-C3-C6-O5
5	G	383	CIT	O7-C3-C6-O6
5	G	382	CIT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	G	382	CIT	C2-C3-C4-C5
5	G	383	CIT	C2-C3-C4-C5
2	B	394	GOL	O2-C2-C3-O3
2	C	392	GOL	O2-C2-C3-O3
5	D	381	CIT	C2-C3-C4-C5
2	F	391	GOL	O2-C2-C3-O3
5	D	381	CIT	C6-C3-C4-C5
5	D	384	CIT	C2-C3-C4-C5
5	D	384	CIT	C6-C3-C4-C5
5	G	383	CIT	C6-C3-C4-C5
2	A	395	GOL	O1-C1-C2-O2
2	A	395	GOL	O2-C2-C3-O3
2	D	393	GOL	O1-C1-C2-O2
2	C	392	GOL	O1-C1-C2-O2
5	D	381	CIT	C1-C2-C3-O7
5	D	381	CIT	O2-C1-C2-C3
5	D	381	CIT	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	381	CIT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/375 (99%)	-1.41	1 (0%) 90 79	14, 49, 111, 139	0
1	B	371/375 (98%)	-1.31	0 100 100	10, 52, 117, 136	0
1	C	371/375 (98%)	-1.38	0 100 100	15, 47, 105, 138	0
1	D	373/375 (99%)	-1.42	1 (0%) 90 79	18, 39, 109, 140	0
1	E	371/375 (98%)	-1.45	0 100 100	20, 43, 101, 135	0
1	F	372/375 (99%)	-1.36	0 100 100	23, 49, 105, 143	0
1	G	373/375 (99%)	-1.40	0 100 100	23, 46, 113, 142	0
1	H	372/375 (99%)	-1.34	0 100 100	21, 54, 117, 146	0
All	All	2976/3000 (99%)	-1.38	2 (0%) 92 86	10, 48, 111, 146	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	ILE	2.3
1	D	373	ILE	2.2

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	B	394	6/6	0.94	0.11	54,54,55,55	0
2	GOL	A	395	6/6	0.98	0.08	68,71,71,71	0
5	CIT	G	383	13/13	0.98	0.06	88,92,95,96	0
2	GOL	D	393	6/6	0.99	0.04	43,44,46,49	0
2	GOL	F	391	6/6	0.99	0.04	56,58,59,59	0
3	PO4	B	402	5/5	0.99	0.05	83,83,83,84	0
3	PO4	E	401	5/5	0.99	0.06	76,76,77,78	0
3	PO4	E	405	5/5	0.99	0.07	97,98,98,99	0
3	PO4	F	403	5/5	0.99	0.06	98,99,99,100	0
3	PO4	H	404	5/5	0.99	0.04	76,77,78,78	0
4	NA	D	380	1/1	0.99	0.03	24,24,24,24	0
5	CIT	D	381	13/13	0.99	0.06	78,80,81,81	0
5	CIT	D	384	13/13	0.99	0.07	89,91,92,92	0
5	CIT	G	382	13/13	0.99	0.06	67,68,69,70	0
2	GOL	C	392	6/6	0.99	0.07	40,43,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.