



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:59 am BST

PDB ID : 5I8I
Title : Crystal Structure of the K. lactis Urea Amidolyase
Authors : Zhao, J.; Xiang, S.
Deposited on : 2016-02-19
Resolution : 6.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

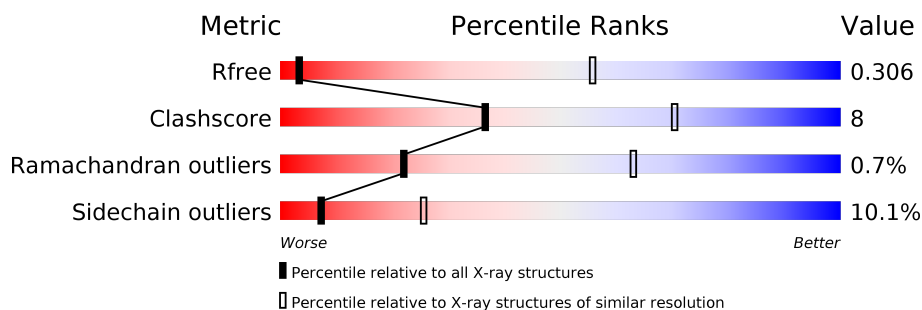
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1829	
1	B	1829	
1	C	1829	
1	D	1829	

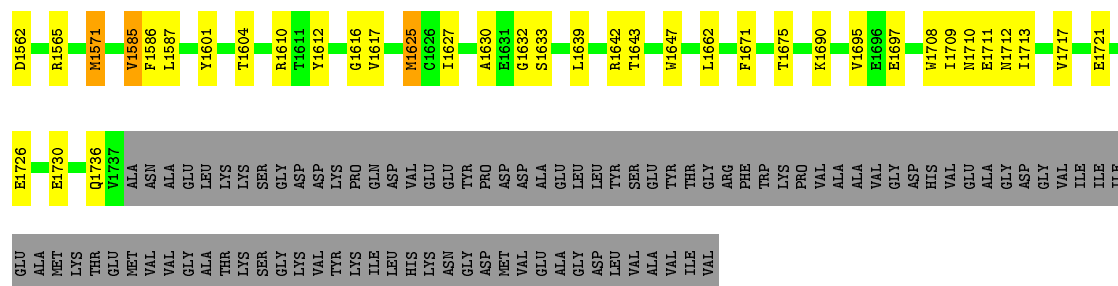
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 51722 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.

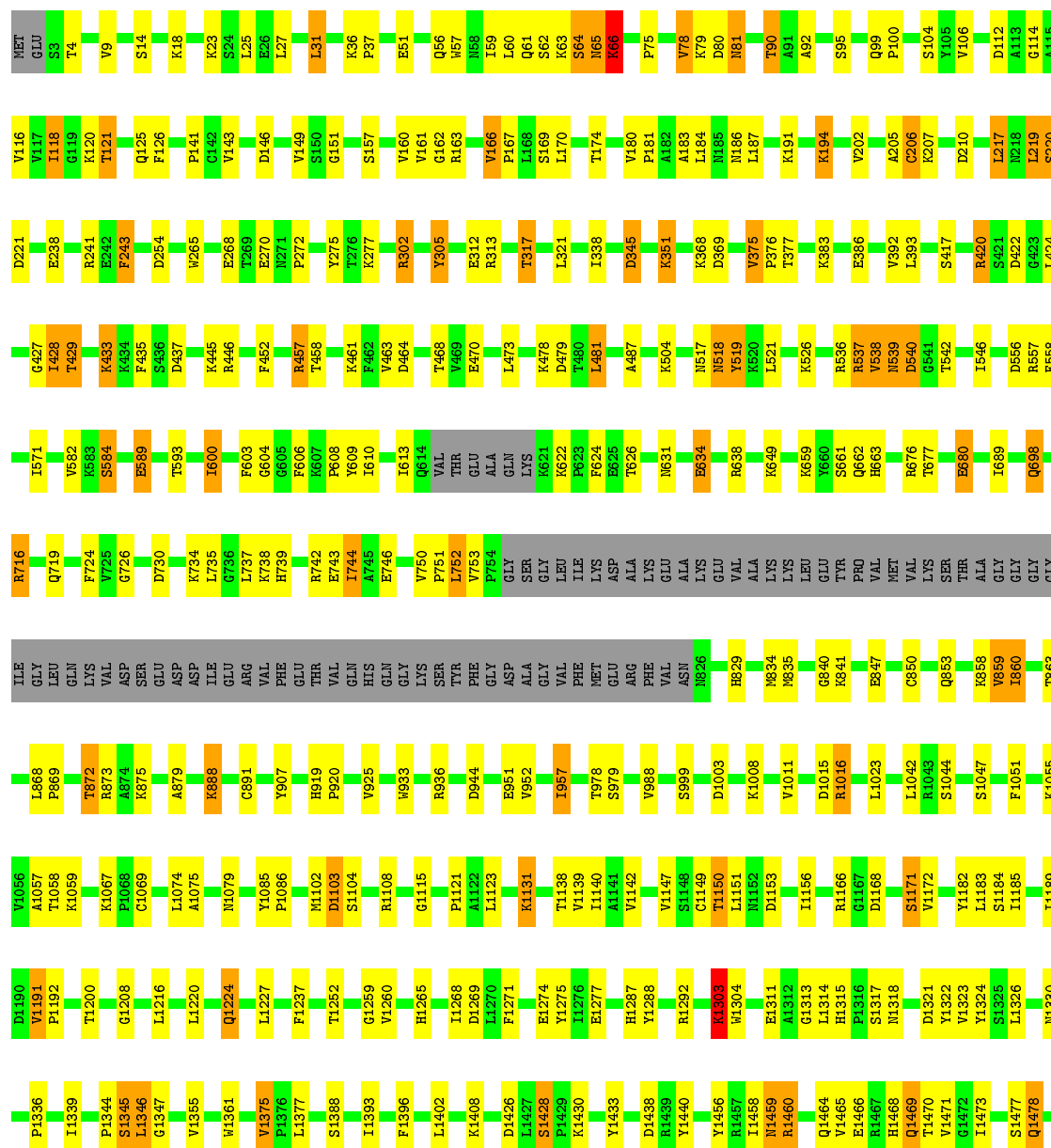
- Molecule 1 is a protein called Urea Amidolyase.

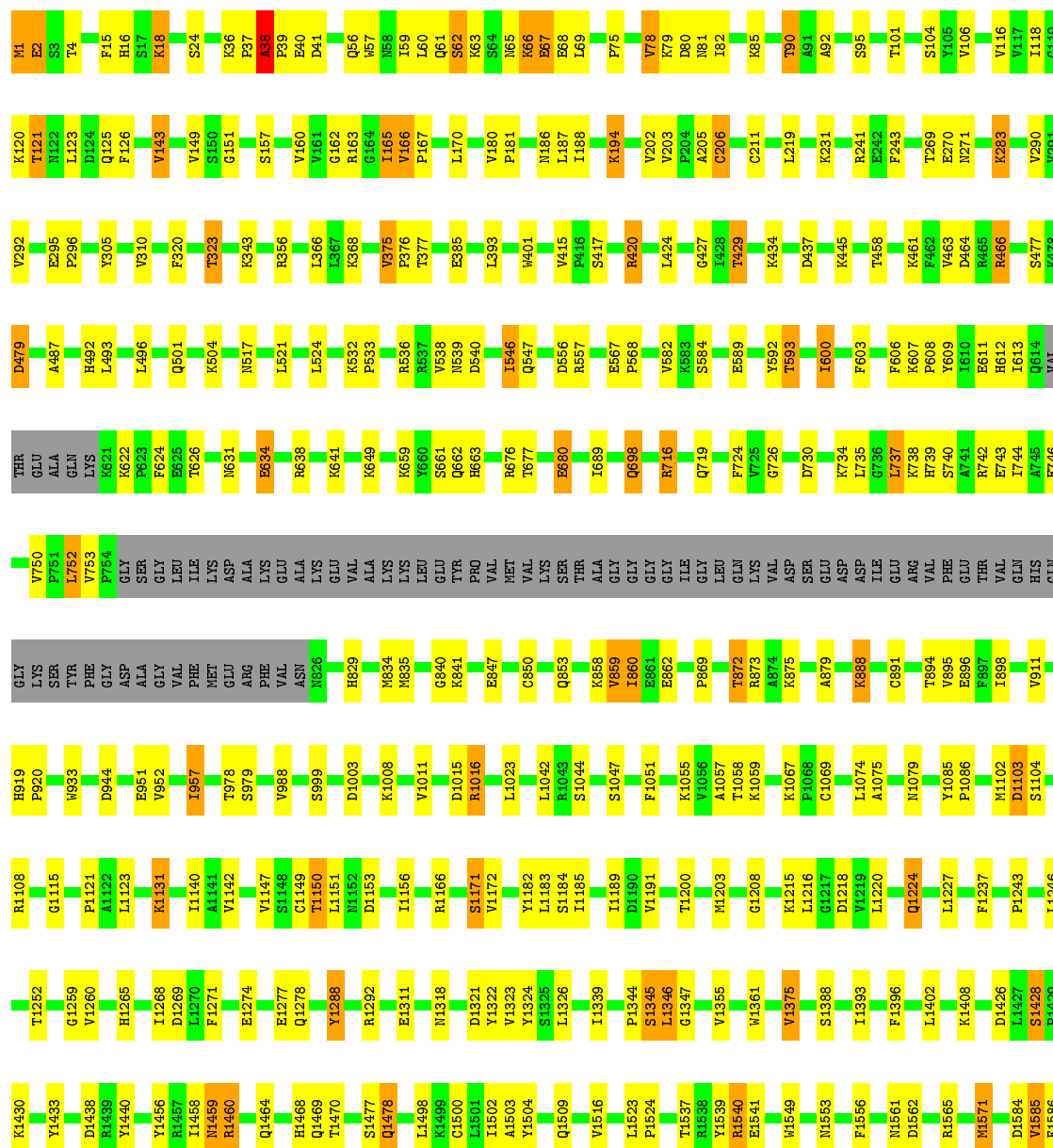
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	B	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			
1	C	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	D	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			



• Molecule 1: Urea Amidolyase

Chain B: 69% 17% 9%





L1587	LEU
Y1601	LYS
Y1606	LYS
R1610	GLY
R1611	ASP
R1612	ASP
G1616	VAL
V1617	GLU
M1625	GLU
C1626	TYR
I1627	PRO
A1630	ASP
F1631	VAL
G1632	GLU
S1633	ALA
L1639	LEU
R1642	TYR
T1643	ILE
V1647	GLY
L1662	ARG
F1671	PHE
T1675	TRP
V1695	LYS
E1696	PRO
E1697	VAL
W1708	ALA
I1709	HIS
N1710	VAL
N1711	GLU
N1712	ALA
I1713	ASP
V1717	GLY
E1721	ILE
E1726	ILE
E1730	GLU
Q1736	ALA
V1737	MET
ALA	THR
ASN	VAL
ALA	VAL
GLU	GLY

• Molecule 1: Urea Amidolyase

Chain D:  70% 17% 9%

MET	Y105	D221	K433	V652	Q719	ASP	A1075	Q1224	V1375	Y1539
GLU	V106	E238	K434	S584	D730	SER	M1079	L1227	P1376	R1540
T4	G114	R241	F435	S584	K734	ASP	P1086	F1237	L1377	T1542
W7	A115	E242	S436	E569	L735	ILE	P1086	P1243	S1388	V1549
S8	V116	F243	D437	T893	G736	GLU	D1103	P1243	K1391	F1556
V9	I118	D254	K445	T893	L737	ARG	S1104	L1246	S1392	N1561
S14	G119	W265	R446	I600	K738	VAL	R1108	T1252	I1393	D1562
S17	T121	Q125	T458	F603	H739	THR	G1115	G1259	F1396	R1565
K18	Q125	E268	K461	G604	R742	VAL	P1121	V1260	L1402	M1571
K23	V143	T269	F462	G605	I744	GLN	A1122	H1285	K1408	F1585
L25	S24	N271	V463	R606	E746	HIS	L1123	D1269	F1586	L1587
E26	V149	P272	T468	P608	A745	GLY	E951	L1270	S1428	Y1601
L27	S150	Y275	V469	P609	V750	LYS	V952	L1270	P1429	K1605
L28	G151	T276	E470	I610	P751	SER	K1131	F1271	F1433	R1610
E29	S157	K277	L473	Q614	V752	TYR	T1138	F1271	D1438	T1611
N30	V160	R302	K478	VAL	P754	PHE	V1139	E1274	R1439	Y1612
L31	V161	Y305	D479	THR	GLY	GLY	I1140	E1274	Y1456	V1617
L32	G162	R312	T480	ALA	GLY	ALA	A1141	E1274	R1457	V1618
K33	R163	E312	L481	GLN	LEU	VAL	V1142	E1277	R1458	M1625
P37	P37	R313	A487	LYS	ILE	PHE	V1147	Y1288	R1459	C1626
E51	E51	R313	K504	R621	LYS	MET	S1148	Y1288	Y1460	I1627
H55	Q56	T317	P624	P623	ALA	ARG	T1150	P1302	P1468	G1632
W57	N58	L321	S516	R624	LYS	PHE	K1151	W1304	Q1469	S1633
L59	L170	I338	N517	T626	GLU	VAL	N1152	E1311	T1470	L1639
Q61	P181	D345	N518	N631	ALA	ASN	D1153	G1313	H1468	T1643
S62	P181	K361	Y522	E634	LYS	H829	I1156	L1314	S1477	V1647
K63	L184	K368	R526	R638	LEU	M834	R1166	H1315	Q1478	D1654
K66	M185	D369	K532	K649	TYR	M835	S1171	H1315	L1498	L1662
P75	L187	V375	P533	K659	PRO	Q840	V1172	L1042	C1500	F1671
V78	K191	P376	R536	Q652	VAL	E847	Y1182	R1043	L1501	T1675
K79	R194	T377	R537	R676	MET	S850	L1183	S1044	F1051	F1691
D80	V202	P382	R538	T677	VAL	S851	S1184	S1047	D1190	V1695
N81	A205	V352	N539	D540	THR	L852	I1186	F1051	V1191	F1696
T90	C206	L393	G541	E660	ALA	Q853	G1208	K1055	F1331	E1697
A91	C207	S417	T542	I699	GLY	K858	T1200	V1056	T1339	W1708
A92	D210	R420	I546	Q698	GLY	V859	M1203	A1057	P1344	I1709
S95	C211	D422	D566	I701	ILE	R860	G1216	K1059	S1345	
Q98	L217	G427	R557	P702	GLY	E861	L1220	E862	L1346	
P100	I218	I428	P558	R716	LEU	P869		K1067	G1347	
T101	S220	T429	I571		GLN	T872		P1068	V1355	
S104					VAL	R873		C1069	W1361	

GLU
ALA
GLY
ASP
GLY
VAL
ILE
ILE
ILE
GLU
ALA
MET
LYS
THR
GLU
MET
VAL
VAL
GLY
ALA
THR
LYS
SER
GLY
LYS
VAL
TYR
LYS
ILE
LEU
HIS
LYS
ASN
GLY
ASP
MET
VAL
GLU
ALA
GLY
ASP
LEU
VAL
ALA
VAL
ILE
VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.74Å 181.94Å 549.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.50 29.98 – 6.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.98-6.50) 96.0 (29.98-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.281 , 0.306	Depositor DCC
R_{free} test set	1017 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	216.1	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 238.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	51722	wwPDB-VP
Average B, all atoms (Å ²)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.40	1/13231 (0.0%)	0.70	4/17964 (0.0%)
1	B	0.51	2/13214 (0.0%)	0.86	23/17942 (0.1%)
1	C	0.39	1/13231 (0.0%)	0.69	5/17964 (0.0%)
1	D	0.49	3/13214 (0.0%)	0.83	21/17942 (0.1%)
All	All	0.45	7/52890 (0.0%)	0.77	53/71812 (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	A	0	2
1	B	0	2
1	C	0	3
1	D	0	6
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1546	GLU	CG-CD	-7.32	1.41	1.51
1	C	1288	TYR	CD2-CE2	6.77	1.49	1.39
1	B	1546	GLU	CG-CD	-5.72	1.43	1.51
1	D	17	SER	CA-CB	5.61	1.61	1.52
1	D	1288	TYR	CD2-CE2	5.39	1.47	1.39
1	D	392	VAL	CB-CG1	5.13	1.63	1.52
1	B	392	VAL	CB-CG1	5.11	1.63	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	556	ASP	N-CA-CB	-8.99	94.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	556	ASP	N-CA-CB	-8.84	94.69	110.60
1	A	1504	TYR	CB-CG-CD1	-8.11	116.14	121.00
1	D	1504	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	D	422	ASP	N-CA-CB	-7.68	96.78	110.60
1	D	194	LYS	CD-CE-NZ	-7.39	94.70	111.70
1	D	254	ASP	CB-CA-C	-7.35	95.71	110.40
1	B	558	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	B	254	ASP	CB-CA-C	-7.26	95.88	110.40
1	B	66	LYS	CD-CE-NZ	7.15	128.15	111.70
1	D	118	ILE	CG1-CB-CG2	-6.92	96.17	111.40
1	D	558	PHE	CB-CG-CD1	-6.80	116.04	120.80
1	B	305	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	B	118	ILE	CG1-CB-CG2	-6.72	96.62	111.40
1	B	194	LYS	CD-CE-NZ	-6.68	96.34	111.70
1	B	1504	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	1303	LYS	N-CA-C	-6.47	93.52	111.00
1	D	1504	TYR	CB-CG-CD2	6.44	124.87	121.00
1	A	1504	TYR	CB-CG-CD2	6.36	124.81	121.00
1	D	305	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	457	ARG	CG-CD-NE	6.28	124.99	111.80
1	D	31	LEU	CA-CB-CG	6.10	129.32	115.30
1	B	305	TYR	CB-CG-CD1	6.04	124.62	121.00
1	D	305	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	217	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	217	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	1288	TYR	CA-CB-CG	-5.89	102.21	113.40
1	D	66	LYS	CD-CE-NZ	5.88	125.22	111.70
1	B	217	LEU	CB-CG-CD2	5.82	120.89	111.00
1	C	38	ALA	C-N-CD	5.82	140.61	128.40
1	D	531	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	C	1540	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	D	481	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	519	TYR	N-CA-C	5.71	126.42	111.00
1	B	558	PHE	CB-CG-CD2	5.71	124.80	120.80
1	B	31	LEU	CA-CB-CG	5.69	128.39	115.30
1	D	217	LEU	CB-CG-CD2	5.68	120.66	111.00
1	A	38	ALA	C-N-CD	5.66	140.29	128.40
1	D	571	ILE	CG1-CB-CG2	-5.60	99.07	111.40
1	B	571	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	D	345	ASP	CB-CA-C	-5.56	99.28	110.40
1	B	481	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	64	SER	CB-CA-C	-5.38	99.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	558	PHE	CB-CG-CD2	5.37	124.56	120.80
1	B	345	ASP	CB-CA-C	-5.36	99.68	110.40
1	B	519	TYR	N-CA-CB	-5.28	101.10	110.60
1	B	464	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	1540	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	C	546	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	C	898	ILE	N-CA-C	-5.14	97.13	111.00
1	B	446	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	188	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	D	446	ARG	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1469	GLN	Mainchain
1	A	539	ASN	Peptide
1	B	1469	GLN	Mainchain
1	B	539	ASN	Peptide
1	C	1288	TYR	Mainchain
1	C	539	ASN	Peptide
1	C	896	GLU	Mainchain
1	D	101	THR	Mainchain
1	D	1288	TYR	Mainchain
1	D	382	PRO	Mainchain
1	D	422	ASP	Mainchain
1	D	517	ASN	Mainchain
1	D	539	ASN	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	12939	0	12896	226	0
1	B	12922	0	12878	218	1
1	C	12939	0	12896	203	1
1	D	12922	0	12878	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51722	0	51548	813	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (813) 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:B:59:ILE:O	1:B:62:SER:OG	1.78	1.01
1:B:79:LYS:HA	1:B:121:THR:HG22	1.45	0.97
1:C:1509:GLN:NE2	1:D:101:THR:O	1.97	0.97
1:D:79:LYS:HA	1:D:121:THR:HG22	1.45	0.95
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.47	0.94
1:C:79:LYS:HA	1:C:121:THR:HG22	1.51	0.93
1:A:1546:GLU:HB2	1:D:1288:TYR:CD1	2.06	0.91
1:A:63:LYS:HA	1:B:1468:HIS:O	1.70	0.91
1:A:1288:TYR:OH	1:D:1541:GLU:HB3	1.72	0.89
1:A:1468:HIS:HE1	1:B:59:ILE:HG23	1.39	0.88
1:C:1459:ASN:HD21	1:C:1460:ARG:HH11	1.21	0.87
1:A:79:LYS:HA	1:A:121:THR:HG22	1.55	0.86
1:D:59:ILE:O	1:D:62:SER:OG	1.94	0.84
1:A:1459:ASN:HD21	1:A:1460:ARG:HH11	1.22	0.84
1:D:1459:ASN:HD21	1:D:1460:ARG:HH11	1.22	0.83
1:D:79:LYS:HG2	1:D:81:ASN:HB2	1.60	0.82
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.59	0.82
1:B:79:LYS:HG2	1:B:81:ASN:HB2	1.61	0.82
1:B:1459:ASN:HD21	1:B:1460:ARG:HH11	1.23	0.81
1:C:59:ILE:HG23	1:D:1468:HIS:HE1	1.43	0.80
1:C:79:LYS:HG2	1:C:81:ASN:HB2	1.64	0.80
1:A:1468:HIS:O	1:B:63:LYS:HA	1.82	0.80
1:A:58:ASN:O	1:A:62:SER:OG	2.01	0.79
1:D:859:VAL:HG23	1:D:860:ILE:HD12	1.63	0.79
1:D:186:ASN:HD21	1:D:458:THR:HG22	1.45	0.79
1:C:59:ILE:HG23	1:D:1468:HIS:CE1	2.17	0.78
1:A:859:VAL:HG23	1:A:860:ILE:HD12	1.65	0.77
1:B:1585:VAL:HG13	1:B:1586:PHE:CD1	2.21	0.76
1:D:1585:VAL:HG13	1:D:1586:PHE:CD1	2.21	0.76
1:A:64:SER:HA	1:B:1471:VAL:HG23	1.68	0.76
1:B:859:VAL:HG23	1:B:860:ILE:HD12	1.68	0.76
1:C:1585:VAL:HG13	1:C:1586:PHE:CD1	2.20	0.76
1:C:859:VAL:HG23	1:C:860:ILE:HD12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:VAL:HG13	1:A:1586:PHE:CD1	2.21	0.75
1:A:1546:GLU:HB2	1:D:1288:TYR:HD1	1.49	0.75
1:B:1016:ARG:NH2	1:B:1051:PHE:O	2.19	0.75
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.21	0.73
1:C:62:SER:O	1:D:1470:THR:HA	1.89	0.73
1:C:1016:ARG:NH2	1:C:1051:PHE:O	2.22	0.73
1:B:186:ASN:HD21	1:B:458:THR:HG22	1.54	0.72
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.71	0.72
1:C:1459:ASN:ND2	1:C:1460:ARG:HH11	1.87	0.72
1:C:493:LEU:HB2	1:C:496:LEU:HD12	1.70	0.72
1:D:1016:ARG:NH2	1:D:1051:PHE:O	2.23	0.72
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.87	0.71
1:B:275:TYR:HD1	1:B:428:ILE:HD11	1.55	0.71
1:C:1464:GLN:O	1:C:1468:HIS:HD2	1.73	0.71
1:D:1459:ASN:ND2	1:D:1460:ARG:HH11	1.88	0.71
1:A:1470:THR:HA	1:B:62:SER:O	1.91	0.71
1:A:1542:THR:O	1:D:1541:GLU:HG3	1.90	0.71
1:A:59:ILE:HG23	1:B:1468:HIS:HE1	1.56	0.71
1:B:1625:MET:HE1	1:B:1627:ILE:HG13	1.72	0.71
1:C:149:VAL:HG13	1:C:151:GLY:H	1.54	0.71
1:D:275:TYR:HD1	1:D:428:ILE:HD11	1.54	0.70
1:D:57:TRP:O	1:D:61:GLN:HG2	1.91	0.70
1:A:186:ASN:HD21	1:A:458:THR:HG22	1.57	0.70
1:A:1465:VAL:O	1:A:1469:GLN:N	2.25	0.69
1:B:1459:ASN:ND2	1:B:1460:ARG:HH11	1.90	0.69
1:C:186:ASN:HD21	1:C:458:THR:HG22	1.58	0.69
1:B:519:TYR:CE2	1:B:537:ARG:HB2	2.29	0.68
1:B:186:ASN:ND2	1:B:458:THR:HG22	2.08	0.67
1:D:1318:ASN:HD21	1:D:1605:LYS:H	1.43	0.67
1:C:1571:MET:HG2	1:C:1601:TYR:CE2	2.30	0.66
1:A:149:VAL:HG13	1:A:151:GLY:H	1.59	0.66
1:A:1287:HIS:CE1	1:A:1288:TYR:CE2	2.83	0.66
1:D:275:TYR:CD1	1:D:428:ILE:HD11	2.31	0.66
1:B:1313:GLY:HA3	1:B:1318:ASN:HD22	1.61	0.66
1:A:62:SER:O	1:B:1470:THR:HA	1.96	0.66
1:A:504:LYS:O	1:A:557:ARG:NH2	2.30	0.65
1:C:1625:MET:HE1	1:C:1627:ILE:HG13	1.77	0.65
1:B:90:THR:HG22	1:B:92:ALA:H	1.62	0.65
1:C:464:ASP:HA	1:C:466:ARG:HH21	1.62	0.65
1:D:186:ASN:ND2	1:D:458:THR:HG22	2.11	0.65
1:A:377:THR:HA	1:A:429:THR:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:TYR:CD1	1:B:428:ILE:HD11	2.32	0.65
1:C:63:LYS:HA	1:D:1468:HIS:O	1.97	0.64
1:C:377:THR:HA	1:C:429:THR:HG22	1.78	0.64
1:B:1318:ASN:HD21	1:B:1605:LYS:H	1.46	0.64
1:D:1428:SER:O	1:D:1428:SER:OG	2.13	0.64
1:C:1075:ALA:HB3	1:C:1131:LYS:HG2	1.80	0.64
1:C:504:LYS:O	1:C:557:ARG:NH2	2.30	0.64
1:A:464:ASP:HA	1:A:466:ARG:HH21	1.62	0.64
1:C:62:SER:HB3	1:D:1504:TYR:OH	1.99	0.63
1:B:626:THR:HG22	1:B:649:LYS:HB2	1.79	0.63
1:A:1468:HIS:ND1	1:B:62:SER:OG	2.31	0.63
1:D:1464:GLN:O	1:D:1468:HIS:HD2	1.81	0.63
1:D:121:THR:HG21	1:D:157:SER:OG	1.99	0.63
1:D:1625:MET:HE1	1:D:1627:ILE:HG13	1.79	0.63
1:B:1150:THR:HG23	1:B:1153:ASP:H	1.64	0.63
1:B:205:ALA:O	1:B:206:CYS:HB2	1.99	0.63
1:A:1288:TYR:OH	1:D:1541:GLU:OE2	2.10	0.63
1:B:1466:GLU:C	1:B:1469:GLN:H	2.03	0.63
1:B:220:SER:HB2	1:B:470:GLU:O	1.99	0.63
1:A:1428:SER:O	1:A:1428:SER:OG	2.17	0.62
1:D:205:ALA:O	1:D:206:CYS:HB2	1.99	0.62
1:C:1470:THR:HA	1:D:62:SER:O	1.99	0.62
1:B:121:THR:HG21	1:B:157:SER:OG	1.99	0.62
1:C:1537:THR:O	1:C:1541:GLU:HG2	2.00	0.62
1:A:163:ARG:HG3	1:A:165:ILE:HD13	1.82	0.62
1:C:1150:THR:HG23	1:C:1153:ASP:H	1.64	0.62
1:A:477:SER:OG	1:A:479:ASP:HB2	2.00	0.61
1:B:1075:ALA:HB3	1:B:1131:LYS:HG2	1.80	0.61
1:A:64:SER:N	1:B:1469:GLN:O	2.33	0.61
1:D:90:THR:HG22	1:D:92:ALA:H	1.64	0.61
1:A:1075:ALA:HB3	1:A:1131:LYS:HG2	1.82	0.61
1:C:162:GLY:HA2	1:C:187:LEU:HD21	1.83	0.61
1:D:1150:THR:HG23	1:D:1153:ASP:H	1.65	0.61
1:D:220:SER:HB2	1:D:470:GLU:O	2.00	0.61
1:A:205:ALA:O	1:A:206:CYS:HB2	2.00	0.61
1:B:1708:TRP:HE3	1:B:1709:ILE:HD12	1.63	0.61
1:C:205:ALA:O	1:C:206:CYS:HB2	2.00	0.61
1:C:101:THR:O	1:D:1509:GLN:NE2	2.33	0.61
1:D:1571:MET:HG2	1:D:1601:TYR:CE2	2.34	0.61
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.66	0.61
1:B:1339:ILE:HG23	1:B:1344:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:HIS:CE1	1:B:1288:TYR:CE2	2.89	0.61
1:A:90:THR:HG22	1:A:92:ALA:H	1.64	0.61
1:D:1075:ALA:HB3	1:D:1131:LYS:HG2	1.82	0.61
1:B:377:THR:HA	1:B:429:THR:HG22	1.83	0.61
1:B:57:TRP:O	1:B:61:GLN:HG2	2.01	0.60
1:A:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:A:59:ILE:HG23	1:B:1468:HIS:CE1	2.37	0.60
1:D:1260:VAL:HG12	1:D:1355:VAL:HA	1.84	0.60
1:D:149:VAL:HG13	1:D:151:GLY:H	1.67	0.60
1:B:149:VAL:HG13	1:B:151:GLY:H	1.66	0.60
1:D:600:ILE:HD11	1:D:609:TYR:CE1	2.36	0.60
1:C:1339:ILE:HG23	1:C:1344:PRO:HD2	1.83	0.60
1:C:90:THR:HG22	1:C:92:ALA:H	1.66	0.60
1:D:1313:GLY:HA3	1:D:1318:ASN:HD22	1.67	0.60
1:B:1465:VAL:O	1:B:1469:GLN:N	2.35	0.60
1:A:1259:GLY:HA2	1:A:1375:VAL:HG12	1.84	0.59
1:B:1500:CYS:HB3	1:B:1504:TYR:CZ	2.36	0.59
1:D:1339:ILE:HG23	1:D:1344:PRO:HD2	1.83	0.59
1:C:1468:HIS:HE1	1:D:59:ILE:HG12	1.66	0.59
1:D:60:LEU:HD11	1:D:114:GLY:HA2	1.83	0.59
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.85	0.59
1:B:375:VAL:HG12	1:B:429:THR:HG23	1.84	0.59
1:B:478:LYS:O	1:B:481:LEU:HG	2.02	0.59
1:C:1428:SER:O	1:C:1428:SER:OG	2.18	0.59
1:D:375:VAL:HG12	1:D:429:THR:HG23	1.85	0.59
1:B:143:VAL:HG13	1:B:461:LYS:HB3	1.84	0.59
1:D:1708:TRP:HE3	1:D:1709:ILE:HD12	1.67	0.59
1:C:163:ARG:HG3	1:C:165:ILE:HD13	1.84	0.59
1:D:626:THR:HG22	1:D:649:LYS:HB2	1.85	0.59
1:D:377:THR:HA	1:D:429:THR:HG22	1.84	0.59
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.68	0.59
1:B:1260:VAL:HG12	1:B:1355:VAL:HA	1.83	0.59
1:D:519:TYR:CE2	1:D:537:ARG:HB2	2.37	0.59
1:A:186:ASN:ND2	1:A:458:THR:HG22	2.16	0.59
1:B:1428:SER:OG	1:B:1428:SER:O	2.18	0.59
1:C:1708:TRP:HE3	1:C:1709:ILE:HD12	1.66	0.59
1:C:626:THR:HG22	1:C:649:LYS:HB2	1.85	0.59
1:B:1121:PRO:HG2	1:B:1189:ILE:H	1.68	0.58
1:A:1469:GLN:HB3	1:B:64:SER:OG	2.02	0.58
1:C:186:ASN:ND2	1:C:458:THR:HG22	2.18	0.58
1:C:477:SER:OG	1:C:479:ASP:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1121:PRO:HG2	1:D:1189:ILE:H	1.66	0.58
1:A:603:PHE:HB3	1:A:608:PRO:HB2	1.84	0.58
1:C:742:ARG:HH22	1:C:753:VAL:HB	1.69	0.58
1:D:1131:LYS:HB3	1:D:1171:SER:HB2	1.84	0.58
1:A:320:PHE:O	1:A:323:THR:HB	2.03	0.58
1:A:600:ILE:HD11	1:A:609:TYR:CZ	2.38	0.58
1:B:600:ILE:HD11	1:B:609:TYR:CE1	2.39	0.58
1:D:478:LYS:O	1:D:481:LEU:HG	2.03	0.58
1:A:1571:MET:HG2	1:A:1601:TYR:CE2	2.37	0.58
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.84	0.58
1:A:1260:VAL:HG12	1:A:1355:VAL:HA	1.85	0.58
1:D:317:THR:HG21	1:D:338:ILE:HG21	1.85	0.58
1:B:1131:LYS:HB3	1:B:1171:SER:HB2	1.85	0.58
1:C:56:GLN:O	1:C:59:ILE:HB	2.03	0.58
1:B:742:ARG:HH22	1:B:753:VAL:HB	1.67	0.58
1:C:1131:LYS:HB3	1:C:1171:SER:HB2	1.86	0.58
1:A:1339:ILE:HG23	1:A:1344:PRO:HD2	1.84	0.58
1:B:1259:GLY:HA2	1:B:1375:VAL:HG12	1.86	0.58
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.86	0.57
1:C:1464:GLN:O	1:C:1468:HIS:CD2	2.55	0.57
1:C:375:VAL:HG12	1:C:429:THR:HG23	1.85	0.57
1:D:853:GLN:HG2	1:D:858:LYS:HG2	1.86	0.57
1:C:600:ILE:HD11	1:C:609:TYR:CZ	2.39	0.57
1:D:1587:LEU:HB3	1:D:1647:TRP:CD2	2.39	0.57
1:A:1713:ILE:O	1:A:1717:VAL:HG23	2.05	0.57
1:C:603:PHE:HB3	1:C:608:PRO:HB2	1.86	0.57
1:D:1085:TYR:CD2	1:D:1108:ARG:HD3	2.39	0.57
1:A:1121:PRO:HG2	1:A:1189:ILE:H	1.70	0.57
1:B:603:PHE:HB3	1:B:608:PRO:HB2	1.86	0.57
1:C:1069:CYS:SG	1:C:1224:GLN:HB2	2.45	0.57
1:A:1466:GLU:C	1:A:1469:GLN:H	2.07	0.56
1:B:1587:LEU:HB3	1:B:1647:TRP:CD2	2.40	0.56
1:D:742:ARG:HH22	1:D:753:VAL:HB	1.70	0.56
1:C:1085:TYR:CD2	1:C:1108:ARG:HD3	2.40	0.56
1:D:1315:HIS:HD2	1:D:1317:SER:H	1.52	0.56
1:D:752:LEU:HD12	1:D:752:LEU:H	1.70	0.56
1:C:1121:PRO:HG2	1:C:1189:ILE:H	1.71	0.56
1:A:752:LEU:HD12	1:A:752:LEU:H	1.71	0.56
1:B:1069:CYS:SG	1:B:1224:GLN:HB2	2.46	0.56
1:B:417:SER:OG	1:B:427:GLY:HA2	2.04	0.56
1:A:1085:TYR:CD2	1:A:1108:ARG:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:O	1:A:66:LYS:NZ	2.29	0.56
1:B:504:LYS:O	1:B:557:ARG:NH2	2.39	0.56
1:C:853:GLN:HG2	1:C:858:LYS:HG2	1.86	0.56
1:C:957:ILE:HG12	1:C:1023:LEU:HD22	1.86	0.56
1:A:1458:ILE:HG21	1:A:1478:GLN:HG2	1.88	0.56
1:D:265:TRP:CD2	1:D:272:PRO:HG3	2.41	0.56
1:C:320:PHE:O	1:C:323:THR:HB	2.06	0.56
1:B:853:GLN:HG2	1:B:858:LYS:HG2	1.88	0.56
1:C:1587:LEU:HB3	1:C:1647:TRP:CD2	2.40	0.55
1:D:417:SER:OG	1:D:427:GLY:HA2	2.06	0.55
1:C:1468:HIS:CE1	1:D:59:ILE:HG23	2.40	0.55
1:A:1587:LEU:HB3	1:A:1647:TRP:CD2	2.42	0.55
1:D:1713:ILE:O	1:D:1717:VAL:HG23	2.06	0.55
1:B:61:GLN:O	1:B:66:LYS:NZ	2.32	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.88	0.55
1:D:174:THR:OG1	1:D:210:ASP:OD1	2.24	0.55
1:C:57:TRP:O	1:C:61:GLN:HG2	2.06	0.55
1:A:626:THR:HG22	1:A:649:LYS:HB2	1.88	0.55
1:B:1464:GLN:O	1:B:1468:HIS:HD2	1.88	0.55
1:A:121:THR:HG21	1:A:157:SER:OG	2.06	0.55
1:A:1500:CYS:HB3	1:A:1504:TYR:CZ	2.42	0.55
1:A:375:VAL:HG12	1:A:429:THR:HG23	1.89	0.55
1:C:1571:MET:HG2	1:C:1601:TYR:HE2	1.70	0.55
1:B:80:ASP:OD1	1:B:90:THR:HB	2.07	0.55
1:C:1713:ILE:O	1:C:1717:VAL:HG23	2.06	0.55
1:B:1085:TYR:CD2	1:B:1108:ARG:HD3	2.42	0.54
1:B:1189:ILE:HG21	1:B:1220:LEU:HD23	1.89	0.54
1:A:57:TRP:O	1:A:61:GLN:HG2	2.07	0.54
1:B:1458:ILE:HG21	1:B:1478:GLN:HG2	1.89	0.54
1:C:1260:VAL:HG12	1:C:1355:VAL:HA	1.88	0.54
1:B:957:ILE:HG12	1:B:1023:LEU:HD22	1.89	0.54
1:D:504:LYS:O	1:D:557:ARG:NH2	2.39	0.54
1:A:1561:ASN:ND2	1:A:1601:TYR:HB3	2.21	0.54
1:D:80:ASP:OD1	1:D:90:THR:HB	2.07	0.54
1:A:65:ASN:O	1:A:68:GLU:HB2	2.07	0.54
1:B:847:GLU:OE2	1:B:873:ARG:NH1	2.41	0.54
1:C:1458:ILE:HG21	1:C:1478:GLN:HG2	1.90	0.54
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.90	0.54
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.38	0.54
1:C:607:LYS:HB2	1:C:608:PRO:CD	2.38	0.54
1:A:1069:CYS:SG	1:A:1224:GLN:HB2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:HB	1:D:221:ASP:OD1	2.07	0.54
1:B:1561:ASN:ND2	1:B:1601:TYR:HB3	2.22	0.54
1:D:603:PHE:HB3	1:D:608:PRO:HB2	1.89	0.54
1:A:80:ASP:OD1	1:A:90:THR:HB	2.08	0.54
1:A:1200:THR:OG1	1:A:1208:GLY:HA3	2.09	0.53
1:A:847:GLU:OE2	1:A:873:ARG:NH1	2.42	0.53
1:A:1543:ILE:O	1:D:1542:THR:HA	2.08	0.53
1:B:487:ALA:HB3	1:B:584:SER:HB2	1.91	0.53
1:C:1710:ASN:C	1:C:1712:ASN:H	2.12	0.53
1:C:295:GLU:HB3	1:C:296:PRO:HD3	1.89	0.53
1:A:634:GLU:OE1	1:A:1008:LYS:HE2	2.09	0.53
1:D:1189:ILE:HG21	1:D:1220:LEU:HD23	1.90	0.53
1:A:624:PHE:HD1	1:A:698:GLN:HG3	1.74	0.53
1:A:62:SER:HB3	1:B:1504:TYR:CE2	2.44	0.53
1:C:592:TYR:OH	1:D:589:GLU:HG3	2.09	0.53
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.44	0.53
1:C:634:GLU:OE1	1:C:1008:LYS:HE2	2.09	0.53
1:D:957:ILE:HG12	1:D:1023:LEU:HD22	1.90	0.53
1:A:957:ILE:HG12	1:A:1023:LEU:HD22	1.90	0.53
1:B:1459:ASN:ND2	1:B:1460:ARG:HD2	2.24	0.53
1:D:1259:GLY:HA2	1:D:1375:VAL:HG12	1.91	0.53
1:C:1503:ALA:HB1	1:D:55:HIS:CD2	2.44	0.53
1:A:1149:CYS:HB2	1:A:1156:ILE:HG22	1.91	0.52
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.24	0.52
1:C:80:ASP:OD1	1:C:90:THR:HB	2.09	0.52
1:D:375:VAL:HG13	1:D:376:PRO:O	2.09	0.52
1:A:163:ARG:HG3	1:A:165:ILE:CD1	2.39	0.52
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.91	0.52
1:A:92:ALA:HB3	1:A:125:GLN:HA	1.90	0.52
1:D:56:GLN:O	1:D:59:ILE:HB	2.10	0.52
1:A:125:GLN:HG2	1:A:126:PHE:CD1	2.45	0.52
1:B:174:THR:OG1	1:B:210:ASP:OD1	2.27	0.52
1:C:600:ILE:HD11	1:C:609:TYR:CE1	2.45	0.52
1:C:375:VAL:CG1	1:C:401:TRP:HB3	2.40	0.52
1:D:1459:ASN:ND2	1:D:1460:ARG:HD2	2.24	0.52
1:D:634:GLU:OE1	1:D:1008:LYS:HE2	2.09	0.52
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.91	0.52
1:C:1459:ASN:ND2	1:C:1460:ARG:HD2	2.25	0.52
1:A:1710:ASN:C	1:A:1712:ASN:H	2.13	0.52
1:B:375:VAL:HG13	1:B:376:PRO:O	2.10	0.52
1:D:1571:MET:HG2	1:D:1601:TYR:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:HIS:HE1	1:A:1322:TYR:CZ	2.28	0.52
1:A:592:TYR:OH	1:B:589:GLU:HG3	2.10	0.52
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.91	0.52
1:B:919:HIS:ND1	1:B:920:PRO:HD3	2.25	0.52
1:C:829:HIS:CD2	1:C:850:CYS:HB2	2.45	0.52
1:C:835:MET:HG2	1:C:933:TRP:HE3	1.75	0.52
1:D:1200:THR:OG1	1:D:1208:GLY:HA3	2.09	0.52
1:D:1458:ILE:HG21	1:D:1478:GLN:HG2	1.91	0.52
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.74	0.52
1:A:1288:TYR:CZ	1:D:1541:GLU:HB3	2.45	0.52
1:A:589:GLU:O	1:A:593:THR:HB	2.09	0.51
1:A:75:PRO:O	1:A:166:VAL:HG22	2.11	0.51
1:B:60:LEU:HD11	1:B:114:GLY:HA2	1.91	0.51
1:B:9:VAL:HB	1:B:221:ASP:OD1	2.11	0.51
1:C:1189:ILE:HG21	1:C:1220:LEU:HD23	1.91	0.51
1:C:65:ASN:O	1:C:68:GLU:HB2	2.10	0.51
1:C:1259:GLY:HA2	1:C:1375:VAL:HG12	1.91	0.51
1:C:1469:GLN:HB2	1:D:63:LYS:HA	1.93	0.51
1:C:752:LEU:H	1:C:752:LEU:HD12	1.75	0.51
1:A:1288:TYR:CD1	1:A:1288:TYR:C	2.83	0.51
1:A:600:ILE:HD11	1:A:609:TYR:CE1	2.46	0.51
1:C:607:LYS:HB2	1:C:608:PRO:HD3	1.91	0.51
1:D:1498:LEU:O	1:D:1502:ILE:HG12	2.11	0.51
1:A:59:ILE:HD13	1:A:111:ARG:NH2	2.26	0.51
1:B:1315:HIS:HD2	1:B:1317:SER:H	1.58	0.51
1:B:1498:LEU:O	1:B:1502:ILE:HG12	2.11	0.51
1:C:92:ALA:HB3	1:C:125:GLN:HA	1.91	0.51
1:C:589:GLU:O	1:C:593:THR:HB	2.11	0.51
1:C:869:PRO:HD2	1:C:872:THR:CG2	2.41	0.51
1:C:847:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
1:D:487:ALA:HB3	1:D:584:SER:HB2	1.93	0.51
1:D:869:PRO:HD2	1:D:872:THR:CG2	2.41	0.51
1:B:351:LYS:O	1:B:351:LYS:HE3	2.11	0.51
1:D:1710:ASN:C	1:D:1712:ASN:H	2.13	0.51
1:A:63:LYS:O	1:A:66:LYS:NZ	2.34	0.51
1:B:1265:HIS:HE1	1:B:1322:TYR:CZ	2.28	0.51
1:D:829:HIS:CD2	1:D:850:CYS:HB2	2.47	0.50
1:C:125:GLN:HG2	1:C:126:PHE:CD1	2.47	0.50
1:C:62:SER:HB2	1:D:1468:HIS:HB3	1.93	0.50
1:D:1625:MET:HE3	1:D:1671:PHE:HZ	1.76	0.50
1:A:1470:THR:HB	1:A:1473:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1345:SER:OG	1:B:1346:LEU:N	2.44	0.50
1:B:1545:SER:C	1:B:1546:GLU:HG3	2.31	0.50
1:C:1149:CYS:HB2	1:C:1156:ILE:HG22	1.93	0.50
1:C:290:VAL:HG12	1:C:292:VAL:HG23	1.92	0.50
1:D:677:THR:OG1	1:D:680:GLU:HB2	2.12	0.50
1:A:1466:GLU:O	1:A:1469:GLN:HG3	2.12	0.50
1:D:143:VAL:HG13	1:D:461:LYS:HB3	1.94	0.50
1:A:1288:TYR:OH	1:D:1541:GLU:CB	2.54	0.50
1:B:1149:CYS:HB2	1:B:1156:ILE:HG22	1.93	0.50
1:B:610:ILE:O	1:B:610:ILE:HG22	2.12	0.50
1:C:1200:THR:OG1	1:C:1208:GLY:HA3	2.11	0.50
1:D:1140:ILE:HD11	1:D:1185:ILE:HD12	1.94	0.50
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.94	0.50
1:A:62:SER:HB2	1:B:1468:HIS:ND1	2.27	0.50
1:B:1625:MET:HE3	1:B:1671:PHE:HZ	1.77	0.50
1:D:219:LEU:HB3	1:D:473:LEU:HD21	1.94	0.50
1:A:1203:MET:HE1	1:A:1633:SER:HB3	1.94	0.49
1:B:317:THR:HG23	1:B:321:LEU:HD12	1.94	0.49
1:B:634:GLU:OE1	1:B:1008:LYS:HE2	2.13	0.49
1:A:1287:HIS:CE1	1:A:1288:TYR:CZ	3.00	0.49
1:A:194:LYS:HG2	1:A:211:CYS:SG	2.52	0.49
1:B:1625:MET:CE	1:B:1627:ILE:HG13	2.41	0.49
1:C:420:ARG:HG3	1:C:424:LEU:O	2.11	0.49
1:D:1324:TYR:CZ	1:D:1347:GLY:HA3	2.47	0.49
1:A:1498:LEU:O	1:A:1502:ILE:HG12	2.13	0.49
1:A:417:SER:OG	1:A:427:GLY:HA2	2.12	0.49
1:A:487:ALA:HB3	1:A:584:SER:HB2	1.93	0.49
1:B:1464:GLN:O	1:B:1468:HIS:CD2	2.65	0.49
1:C:1345:SER:OG	1:C:1346:LEU:N	2.45	0.49
1:A:611:GLU:C	1:A:613:ILE:H	2.15	0.49
1:C:1115:GLY:HA2	1:C:1237:PHE:HB2	1.93	0.49
1:C:163:ARG:HG3	1:C:165:ILE:CD1	2.41	0.49
1:D:835:MET:HG2	1:D:933:TRP:HE3	1.77	0.49
1:A:1203:MET:CE	1:A:1633:SER:HB3	2.42	0.49
1:C:1498:LEU:O	1:C:1502:ILE:HG12	2.13	0.49
1:D:1537:THR:O	1:D:1541:GLU:HG2	2.12	0.49
1:D:1625:MET:CE	1:D:1627:ILE:HG13	2.43	0.49
1:D:847:GLU:OE2	1:D:873:ARG:NH1	2.46	0.49
1:A:1464:GLN:O	1:A:1468:HIS:HD2	1.95	0.49
1:A:375:VAL:CG1	1:A:401:TRP:HB3	2.42	0.49
1:D:1269:ASP:OD2	1:D:1269:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1500:CYS:HB3	1:D:1504:TYR:CZ	2.48	0.49
1:A:1184:SER:C	1:A:1185:ILE:HD13	2.33	0.49
1:B:1200:THR:OG1	1:B:1208:GLY:HA3	2.13	0.49
1:A:1345:SER:OG	1:A:1346:LEU:N	2.46	0.49
1:B:162:GLY:HA2	1:B:187:LEU:HD21	1.95	0.49
1:B:452:PHE:CD1	1:B:457:ARG:HG3	2.48	0.49
1:B:677:THR:OG1	1:B:680:GLU:HB2	2.13	0.49
1:B:869:PRO:HD2	1:B:872:THR:CG2	2.43	0.49
1:D:1274:GLU:HA	1:D:1277:GLU:HG3	1.95	0.49
1:C:1468:HIS:CE1	1:D:59:ILE:HG12	2.48	0.49
1:A:1625:MET:CE	1:A:1627:ILE:HG13	2.42	0.49
1:D:1265:HIS:HE1	1:D:1322:TYR:CZ	2.31	0.49
1:D:317:THR:HG23	1:D:321:LEU:HD12	1.95	0.49
1:A:1617:VAL:HG11	1:A:1639:LEU:HD22	1.95	0.48
1:A:66:LYS:O	1:A:67:GLU:HB2	2.13	0.48
1:B:180:VAL:HB	1:B:181:PRO:HD3	1.95	0.48
1:A:75:PRO:HB2	1:A:118:ILE:CD1	2.43	0.48
1:B:1470:THR:HB	1:B:1473:ILE:HD12	1.96	0.48
1:B:1571:MET:HG2	1:B:1601:TYR:CE2	2.48	0.48
1:C:1553:ASN:OD1	1:C:1606:TYR:OH	2.24	0.48
1:C:121:THR:HG21	1:C:157:SER:OG	2.12	0.48
1:A:1537:THR:O	1:A:1541:GLU:HG2	2.14	0.48
1:A:536:ARG:HD3	1:A:538:VAL:HG23	1.95	0.48
1:B:420:ARG:HB2	1:B:422:ASP:HB2	1.95	0.48
1:D:539:ASN:O	1:D:540:ASP:O	2.31	0.48
1:A:290:VAL:HG12	1:A:292:VAL:HG23	1.95	0.48
1:B:1103:ASP:OD2	1:B:1361:TRP:HB2	2.14	0.48
1:C:1468:HIS:O	1:D:63:LYS:HA	2.13	0.48
1:C:536:ARG:HD3	1:C:538:VAL:HG23	1.94	0.48
1:D:243:PHE:CZ	1:D:435:PHE:HA	2.49	0.48
1:D:92:ALA:HB3	1:D:125:GLN:HA	1.94	0.48
1:A:1467:ARG:NH2	1:B:112:ASP:OD2	2.47	0.48
1:C:1104:SER:O	1:C:1108:ARG:HG3	2.13	0.48
1:C:16:HIS:ND1	1:C:24:SER:HB2	2.28	0.48
1:D:1069:CYS:SG	1:D:1224:GLN:HB2	2.53	0.48
1:B:99:GLN:NE2	1:B:100:PRO:HD2	2.28	0.48
1:C:1265:HIS:HE1	1:C:1322:TYR:CZ	2.31	0.48
1:D:1345:SER:OG	1:D:1346:LEU:N	2.47	0.48
1:D:7:TRP:O	1:D:167:PRO:HB3	2.14	0.48
1:A:1324:TYR:CZ	1:A:1347:GLY:HA3	2.49	0.48
1:A:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:SER:C	1:B:1185:ILE:HD13	2.34	0.48
1:C:624:PHE:HD1	1:C:698:GLN:HG3	1.79	0.48
1:D:610:ILE:HG22	1:D:610:ILE:O	2.14	0.48
1:A:1115:GLY:HA2	1:A:1237:PHE:HB2	1.94	0.48
1:D:162:GLY:HA2	1:D:187:LEU:HD21	1.96	0.48
1:A:1587:LEU:HD12	1:A:1630:ALA:HB2	1.96	0.48
1:B:219:LEU:HB3	1:B:473:LEU:HD21	1.95	0.48
1:B:539:ASN:O	1:B:540:ASP:O	2.32	0.48
1:D:1149:CYS:HB2	1:D:1156:ILE:HG22	1.96	0.48
1:D:1561:ASN:ND2	1:D:1601:TYR:HB3	2.28	0.48
1:A:1269:ASP:OD2	1:A:1269:ASP:N	2.46	0.47
1:A:634:GLU:CD	1:A:1008:LYS:HE2	2.35	0.47
1:C:1184:SER:C	1:C:1185:ILE:HD13	2.34	0.47
1:C:377:THR:HA	1:C:429:THR:CG2	2.44	0.47
1:A:1545:SER:C	1:A:1546:GLU:HG3	2.34	0.47
1:C:1324:TYR:CZ	1:C:1347:GLY:HA3	2.49	0.47
1:A:1542:THR:HB	1:D:1541:GLU:OE1	2.14	0.47
1:A:420:ARG:HG3	1:A:424:LEU:O	2.13	0.47
1:A:492:HIS:NE2	1:A:501:GLN:OE1	2.41	0.47
1:B:1585:VAL:HG13	1:B:1586:PHE:HD1	1.75	0.47
1:D:1459:ASN:HD22	1:D:1460:ARG:HD2	1.80	0.47
1:D:919:HIS:ND1	1:D:920:PRO:HD3	2.29	0.47
1:C:677:THR:OG1	1:C:680:GLU:HB2	2.14	0.47
1:C:85:LYS:HD3	1:D:1509:GLN:NE2	2.28	0.47
1:D:351:LYS:O	1:D:351:LYS:HE3	2.14	0.47
1:A:1142:VAL:HA	1:A:1182:TYR:O	2.15	0.47
1:C:1625:MET:CE	1:C:1627:ILE:HG13	2.44	0.47
1:C:1587:LEU:HD12	1:C:1630:ALA:HB2	1.96	0.47
1:C:1708:TRP:CE3	1:C:1709:ILE:HD12	2.49	0.47
1:C:492:HIS:NE2	1:C:501:GLN:OE1	2.45	0.47
1:D:1103:ASP:OD2	1:D:1361:TRP:HB2	2.14	0.47
1:D:1464:GLN:O	1:D:1468:HIS:CD2	2.64	0.47
1:A:1059:LYS:HA	1:A:1059:LYS:HD2	1.75	0.47
1:B:1708:TRP:CE3	1:B:1709:ILE:HD12	2.48	0.47
1:B:546:ILE:N	1:B:546:ILE:HD12	2.30	0.47
1:C:919:HIS:ND1	1:C:920:PRO:HD3	2.29	0.47
1:D:78:VAL:HG22	1:D:120:LYS:HE3	1.96	0.47
1:D:1115:GLY:HA2	1:D:1237:PHE:HB2	1.96	0.47
1:A:862:GLU:OE1	1:A:1016:ARG:NH1	2.47	0.47
1:B:1587:LEU:HD12	1:B:1630:ALA:HB2	1.97	0.47
1:C:634:GLU:CD	1:C:1008:LYS:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1184:SER:C	1:D:1185:ILE:HD13	2.35	0.47
1:D:99:GLN:NE2	1:D:100:PRO:HD2	2.29	0.47
1:C:1585:VAL:HG13	1:C:1586:PHE:HD1	1.75	0.47
1:B:1259:GLY:HA3	1:B:1377:LEU:HD22	1.97	0.47
1:C:1561:ASN:ND2	1:C:1601:TYR:HB3	2.30	0.47
1:C:417:SER:OG	1:C:427:GLY:HA2	2.15	0.47
1:D:546:ILE:HD12	1:D:546:ILE:N	2.29	0.47
1:D:622:LYS:HE3	1:D:622:LYS:HB2	1.67	0.47
1:A:1459:ASN:HD22	1:A:1460:ARG:HD2	1.80	0.47
1:B:1269:ASP:OD2	1:B:1269:ASP:N	2.47	0.47
1:B:302:ARG:HE	1:B:302:ARG:HB3	1.47	0.47
1:A:1140:ILE:HD11	1:A:1185:ILE:HD12	1.96	0.46
1:A:1288:TYR:CD1	1:A:1289:ASN:N	2.84	0.46
1:A:521:LEU:HB2	1:A:546:ILE:HG12	1.97	0.46
1:A:78:VAL:HG22	1:A:120:LYS:HE3	1.96	0.46
1:B:1275:TYR:HB2	1:B:1303:LYS:HG3	1.98	0.46
1:B:1713:ILE:O	1:B:1717:VAL:HG23	2.15	0.46
1:B:14:SER:O	1:B:18:LYS:HG2	2.15	0.46
1:C:1:MET:HB2	1:C:2:GLU:H	1.60	0.46
1:C:61:GLN:O	1:C:66:LYS:NZ	2.40	0.46
1:A:377:THR:HA	1:A:429:THR:CG2	2.43	0.46
1:A:38:ALA:HB1	1:A:39:PRO:HD3	1.97	0.46
1:A:829:HIS:CD2	1:A:850:CYS:HB2	2.50	0.46
1:B:1459:ASN:HD22	1:B:1460:ARG:HD2	1.80	0.46
1:B:377:THR:HA	1:B:429:THR:CG2	2.45	0.46
1:B:518:ASN:O	1:B:538:VAL:HG23	2.15	0.46
1:C:38:ALA:HB1	1:C:39:PRO:HD3	1.97	0.46
1:C:750:VAL:HG22	1:C:879:ALA:HB1	1.97	0.46
1:D:1315:HIS:CD2	1:D:1317:SER:H	2.32	0.46
1:B:92:ALA:HB3	1:B:125:GLN:HA	1.96	0.46
1:D:207:LYS:NZ	1:D:238:GLU:OE2	2.46	0.46
1:B:206:CYS:HA	1:B:312:GLU:CB	2.46	0.46
1:C:1617:VAL:HG11	1:C:1639:LEU:HD22	1.96	0.46
1:D:716:ARG:HH11	1:D:716:ARG:HG3	1.81	0.46
1:B:1537:THR:O	1:B:1541:GLU:HG2	2.16	0.46
1:B:56:GLN:O	1:B:59:ILE:HB	2.15	0.46
1:D:377:THR:HA	1:D:429:THR:CG2	2.46	0.46
1:A:1469:GLN:O	1:B:64:SER:HB3	2.16	0.46
1:B:1104:SER:O	1:B:1108:ARG:HG3	2.16	0.46
1:B:742:ARG:HD3	1:B:752:LEU:HD23	1.97	0.46
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1123:LEU:HD12	1:C:1183:LEU:HD23	1.98	0.46
1:C:1625:MET:HE3	1:C:1671:PHE:HZ	1.80	0.46
1:D:1085:TYR:CD1	1:D:1086:PRO:HA	2.51	0.46
1:D:1203:MET:HE1	1:D:1633:SER:HB3	1.98	0.46
1:D:600:ILE:HD11	1:D:609:TYR:CZ	2.51	0.46
1:A:677:THR:OG1	1:A:680:GLU:HB2	2.16	0.46
1:A:869:PRO:HD2	1:A:872:THR:CG2	2.45	0.46
1:B:1274:GLU:HA	1:B:1277:GLU:HG3	1.98	0.46
1:B:161:VAL:HG12	1:B:187:LEU:HD22	1.98	0.46
1:A:1504:TYR:OH	1:B:62:SER:HB2	2.15	0.46
1:D:1104:SER:O	1:D:1108:ARG:HG3	2.16	0.46
1:D:75:PRO:O	1:D:167:PRO:HD2	2.15	0.46
1:B:1085:TYR:CD1	1:B:1086:PRO:HA	2.52	0.45
1:B:125:GLN:HG2	1:B:126:PHE:CD1	2.52	0.45
1:B:1500:CYS:HB3	1:B:1504:TYR:OH	2.15	0.45
1:B:624:PHE:HD1	1:B:698:GLN:HG3	1.81	0.45
1:D:302:ARG:HB3	1:D:302:ARG:HE	1.48	0.45
1:D:624:PHE:HD1	1:D:698:GLN:HG3	1.81	0.45
1:A:1625:MET:HE3	1:A:1671:PHE:HZ	1.82	0.45
1:B:1268:ILE:HA	1:B:1271:PHE:O	2.16	0.45
1:D:1103:ASP:HA	1:D:1361:TRP:HA	1.98	0.45
1:A:1139:VAL:O	1:A:1140:ILE:HD12	2.17	0.45
1:A:1708:TRP:CE3	1:A:1709:ILE:HD12	2.50	0.45
1:B:1115:GLY:HA2	1:B:1237:PHE:HB2	1.99	0.45
1:B:1539:TYR:CD1	1:B:1610:ARG:HG2	2.52	0.45
1:C:611:GLU:C	1:C:613:ILE:H	2.20	0.45
1:D:180:VAL:HB	1:D:181:PRO:HD3	1.99	0.45
1:B:744:ILE:H	1:B:744:ILE:HG12	1.56	0.45
1:D:634:GLU:CD	1:D:1008:LYS:HE2	2.37	0.45
1:D:420:ARG:H	1:D:420:ARG:HG2	1.36	0.45
1:A:1085:TYR:CD1	1:A:1086:PRO:HA	2.51	0.45
1:A:56:GLN:O	1:A:59:ILE:HB	2.16	0.45
1:B:829:HIS:CD2	1:B:850:CYS:HB2	2.51	0.45
1:C:1057:ALA:C	1:C:1059:LYS:H	2.20	0.45
1:A:1057:ALA:C	1:A:1059:LYS:H	2.20	0.45
1:B:1625:MET:HE3	1:B:1671:PHE:CZ	2.51	0.45
1:C:1085:TYR:CD1	1:C:1086:PRO:HA	2.52	0.45
1:C:1142:VAL:HA	1:C:1182:TYR:O	2.17	0.45
1:A:1468:HIS:O	1:A:1469:GLN:C	2.53	0.45
1:A:1542:THR:O	1:D:1541:GLU:CG	2.60	0.45
1:A:1571:MET:HG2	1:A:1601:TYR:HE2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:O	1:A:41:ASP:HB3	2.16	0.45
1:B:1140:ILE:HD11	1:B:1185:ILE:HD12	1.98	0.45
1:B:1704:GLU:O	1:B:1707:ALA:HB3	2.17	0.45
1:A:1433:TYR:CE1	1:A:1502:ILE:HD13	2.52	0.45
1:D:1203:MET:CE	1:D:1633:SER:HB3	2.46	0.45
1:D:522:TYR:O	1:D:533:PRO:HA	2.17	0.45
1:D:546:ILE:HA	1:D:604:GLY:O	2.16	0.45
1:C:66:LYS:O	1:C:67:GLU:HB2	2.16	0.45
1:A:1274:GLU:HA	1:A:1277:GLU:HG3	1.99	0.45
1:A:75:PRO:O	1:A:167:PRO:HD2	2.17	0.45
1:B:1102:MET:HE1	1:B:1292:ARG:HA	1.99	0.45
1:B:521:LEU:HD23	1:B:600:ILE:CG2	2.47	0.45
1:C:194:LYS:HG2	1:C:211:CYS:SG	2.57	0.45
1:A:1259:GLY:HA3	1:A:1377:LEU:HD22	2.00	0.44
1:B:143:VAL:CG1	1:B:461:LYS:HB3	2.46	0.44
1:B:622:LYS:HE3	1:B:622:LYS:HB2	1.63	0.44
1:B:65:ASN:O	1:B:66:LYS:C	2.54	0.44
1:A:1103:ASP:OD2	1:A:1361:TRP:HB2	2.18	0.44
1:B:433:LYS:HG2	1:B:433:LYS:H	1.62	0.44
1:C:271:ASN:OD1	1:C:420:ARG:HD2	2.16	0.44
1:C:641:LYS:HB3	1:C:641:LYS:HE3	1.58	0.44
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.17	0.44
1:A:75:PRO:HB2	1:A:118:ILE:HD11	1.99	0.44
1:A:828:ARG:NH2	1:A:866:PRO:O	2.43	0.44
1:B:1612:TYR:CD1	1:B:1632:GLY:HA2	2.52	0.44
1:D:1539:TYR:CD1	1:D:1610:ARG:HG2	2.52	0.44
1:D:1625:MET:HE3	1:D:1671:PHE:CZ	2.51	0.44
1:D:606:PHE:CZ	1:D:610:ILE:HD11	2.52	0.44
1:A:38:ALA:HB1	1:A:39:PRO:CD	2.48	0.44
1:C:66:LYS:H	1:C:66:LYS:HG3	1.55	0.44
1:C:75:PRO:O	1:C:166:VAL:HG22	2.18	0.44
1:B:1057:ALA:C	1:B:1059:LYS:H	2.20	0.44
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.57	0.44
1:B:141:PRO:HB2	1:B:146:ASP:HA	1.99	0.44
1:C:1274:GLU:HA	1:C:1277:GLU:HG3	1.99	0.44
1:C:1612:TYR:CD1	1:C:1632:GLY:HA2	2.52	0.44
1:D:75:PRO:O	1:D:166:VAL:HG22	2.17	0.44
1:A:283:LYS:HB2	1:A:283:LYS:HE2	1.67	0.44
1:B:634:GLU:CD	1:B:1008:LYS:HE2	2.38	0.44
1:C:1103:ASP:OD2	1:C:1361:TRP:HB2	2.18	0.44
1:C:1433:TYR:CE1	1:C:1502:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:O	1:C:41:ASP:HB3	2.17	0.44
1:C:556:ASP:OD2	1:C:557:ARG:HG2	2.18	0.44
1:D:1710:ASN:O	1:D:1712:ASN:N	2.51	0.44
1:A:835:MET:HG2	1:A:933:TRP:CE3	2.53	0.44
1:B:1549:TRP:HA	1:B:1556:PHE:HB2	2.00	0.44
1:B:75:PRO:O	1:B:167:PRO:HD2	2.17	0.44
1:B:268:GLU:OE2	1:B:270:GLU:HB2	2.18	0.44
1:C:1459:ASN:HD22	1:C:1460:ARG:HD2	1.81	0.44
1:C:894:THR:HG22	1:C:895:VAL:N	2.33	0.44
1:D:1057:ALA:C	1:D:1059:LYS:H	2.22	0.44
1:A:1318:ASN:N	1:A:1318:ASN:HD22	2.16	0.44
1:A:375:VAL:HG13	1:A:401:TRP:HB3	1.99	0.44
1:A:556:ASP:OD2	1:A:557:ARG:HG2	2.18	0.44
1:C:1215:LYS:N	1:C:1218:ASP:OD2	2.41	0.44
1:C:375:VAL:HG13	1:C:401:TRP:HB3	1.98	0.44
1:C:38:ALA:HB1	1:C:39:PRO:CD	2.48	0.44
1:D:14:SER:O	1:D:18:LYS:HG2	2.17	0.44
1:B:546:ILE:HA	1:B:604:GLY:O	2.18	0.43
1:B:716:ARG:HH11	1:B:716:ARG:HG3	1.83	0.43
1:A:849:ASP:OD1	1:A:851:SER:OG	2.29	0.43
1:B:1323:VAL:HG21	1:B:1477:SER:HB3	2.00	0.43
1:A:1468:HIS:O	1:B:62:SER:O	2.35	0.43
1:B:661:SER:OG	1:B:663:HIS:ND1	2.51	0.43
1:B:78:VAL:O	1:B:120:LYS:HA	2.18	0.43
1:C:1203:MET:HE1	1:C:1633:SER:HB3	1.99	0.43
1:C:78:VAL:HG22	1:C:120:LYS:HE3	2.00	0.43
1:C:1318:ASN:HD22	1:C:1318:ASN:N	2.16	0.43
1:C:567:GLU:HG2	1:C:568:PRO:HA	1.99	0.43
1:D:29:GLU:O	1:D:33:LYS:HG3	2.18	0.43
1:D:862:GLU:OE1	1:D:1016:ARG:NH1	2.51	0.43
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.53	0.43
1:B:1103:ASP:HA	1:B:1361:TRP:HA	2.00	0.43
1:C:1140:ILE:HD11	1:C:1185:ILE:HD12	1.99	0.43
1:C:283:LYS:HE2	1:C:283:LYS:HB2	1.68	0.43
1:A:1104:SER:O	1:A:1108:ARG:HG3	2.18	0.43
1:B:1330:ASN:O	1:B:1336:PRO:HA	2.19	0.43
1:B:1324:TYR:CZ	1:B:1347:GLY:HA3	2.53	0.43
1:B:1571:MET:HG2	1:B:1601:TYR:HE2	1.83	0.43
1:B:78:VAL:HG22	1:B:120:LYS:HE3	2.00	0.43
1:C:521:LEU:HB2	1:C:546:ILE:HG12	2.00	0.43
1:D:834:MET:HG2	1:D:835:MET:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.43
1:B:1617:VAL:HG11	1:B:1639:LEU:HD22	2.01	0.43
1:D:1323:VAL:HG21	1:D:1477:SER:HB3	2.01	0.43
1:D:988:VAL:HA	1:D:1008:LYS:O	2.18	0.43
1:A:715:ASP:OD2	1:A:733:ARG:NH2	2.45	0.43
1:B:1139:VAL:O	1:B:1140:ILE:HD12	2.18	0.43
1:B:519:TYR:HB2	1:B:546:ILE:HD13	1.99	0.43
1:B:75:PRO:O	1:B:166:VAL:HG22	2.19	0.43
1:C:1268:ILE:HA	1:C:1271:PHE:O	2.18	0.43
1:C:487:ALA:HB3	1:C:584:SER:HB2	1.99	0.43
1:D:1059:LYS:HD2	1:D:1059:LYS:HA	1.77	0.43
1:D:161:VAL:HG12	1:D:187:LEU:HD22	2.00	0.43
1:A:1464:GLN:O	1:A:1468:HIS:CD2	2.71	0.43
1:C:1102:MET:HE1	1:C:1292:ARG:HA	2.01	0.43
1:C:1549:TRP:HA	1:C:1556:PHE:HB2	2.01	0.43
1:D:1549:TRP:HA	1:D:1556:PHE:HB2	2.01	0.43
1:D:521:LEU:HD11	1:D:533:PRO:HB2	2.01	0.43
1:A:716:ARG:HH11	1:A:716:ARG:HG3	1.84	0.43
1:C:1540:ARG:HD2	1:C:1540:ARG:HH11	1.66	0.43
1:C:63:LYS:O	1:C:66:LYS:NZ	2.42	0.43
1:D:1142:VAL:HA	1:D:1182:TYR:O	2.19	0.43
1:D:1617:VAL:HG11	1:D:1639:LEU:HD22	2.00	0.43
1:A:7:TRP:O	1:A:167:PRO:HB3	2.19	0.43
1:A:1690:LYS:HD3	1:A:1690:LYS:HA	1.82	0.43
1:B:1123:LEU:HD12	1:B:1183:LEU:HD23	2.01	0.43
1:B:1523:LEU:HB3	1:B:1643:THR:HG21	2.01	0.43
1:B:36:LYS:HD3	1:B:36:LYS:HA	1.72	0.43
1:C:1243:PRO:HB2	1:C:1246:LEU:HG	2.01	0.43
1:C:1203:MET:CE	1:C:1633:SER:HB3	2.49	0.43
1:C:840:GLY:N	1:C:888:LYS:HG3	2.33	0.43
1:D:1730:GLU:OE2	1:D:1730:GLU:HA	2.19	0.43
1:D:268:GLU:OE2	1:D:270:GLU:HB2	2.18	0.43
1:D:437:ASP:OD1	1:D:437:ASP:N	2.52	0.43
1:B:600:ILE:HD11	1:B:609:TYR:CZ	2.54	0.42
1:B:750:VAL:HG22	1:B:879:ALA:HB1	2.00	0.42
1:C:957:ILE:CG1	1:C:1023:LEU:HD22	2.49	0.42
1:C:75:PRO:HB2	1:C:118:ILE:CD1	2.48	0.42
1:C:1710:ASN:O	1:C:1712:ASN:N	2.52	0.42
1:A:567:GLU:HG2	1:A:568:PRO:HA	2.00	0.42
1:C:1274:GLU:O	1:C:1278:GLN:HG3	2.19	0.42
1:D:1259:GLY:HA3	1:D:1377:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:CG2	1:D:163:ARG:HG3	2.49	0.42
1:D:556:ASP:HB3	1:D:557:ARG:HG2	2.01	0.42
1:D:716:ARG:HG3	1:D:716:ARG:NH1	2.34	0.42
1:A:1323:VAL:HG21	1:A:1477:SER:HB3	2.00	0.42
1:A:661:SER:OG	1:A:663:HIS:ND1	2.52	0.42
1:A:66:LYS:O	1:A:67:GLU:CB	2.67	0.42
1:C:1585:VAL:HG13	1:C:1586:PHE:CE1	2.54	0.42
1:C:661:SER:OG	1:C:663:HIS:ND1	2.51	0.42
1:C:835:MET:HG2	1:C:933:TRP:CE3	2.54	0.42
1:D:157:SER:HB3	1:D:169:SER:OG	2.18	0.42
1:B:1102:MET:CE	1:B:1292:ARG:HA	2.50	0.42
1:A:1507:GLU:OE2	1:B:59:ILE:HG12	2.20	0.42
1:C:15:PHE:HA	1:C:18:LYS:HE2	2.01	0.42
1:A:1103:ASP:HA	1:A:1361:TRP:HA	2.01	0.42
1:B:1304:TRP:CH2	1:B:1317:SER:HB3	2.54	0.42
1:C:716:ARG:HG3	1:C:716:ARG:HH11	1.85	0.42
1:D:1123:LEU:HD12	1:D:1183:LEU:HD23	2.00	0.42
1:D:66:LYS:HG3	1:D:66:LYS:H	1.59	0.42
1:A:1616:GLY:C	1:A:1642:ARG:HG3	2.40	0.42
1:A:744:ILE:H	1:A:744:ILE:HG12	1.55	0.42
1:A:81:ASN:HB3	1:A:82:ILE:HG13	2.01	0.42
1:B:1456:TYR:CZ	1:B:1460:ARG:HD3	2.54	0.42
1:C:1346:LEU:HD13	1:C:1584:ASP:HB2	2.01	0.42
1:C:180:VAL:HB	1:C:181:PRO:HD3	2.01	0.42
1:D:1243:PRO:HB2	1:D:1246:LEU:HG	2.02	0.42
1:D:1585:VAL:HG13	1:D:1586:PHE:HD1	1.77	0.42
1:D:1708:TRP:CE3	1:D:1709:ILE:HD12	2.50	0.42
1:A:1456:TYR:CZ	1:A:1460:ARG:HD3	2.55	0.42
1:B:1184:SER:O	1:B:1185:ILE:HD13	2.20	0.42
1:B:1585:VAL:HG13	1:B:1586:PHE:CE1	2.55	0.42
1:B:420:ARG:HG2	1:B:420:ARG:H	1.31	0.42
1:B:609:TYR:CZ	1:B:613:ILE:HD11	2.55	0.42
1:D:1433:TYR:CE1	1:D:1502:ILE:HD13	2.55	0.42
1:B:936:ARG:HE	1:B:936:ARG:HB3	1.64	0.42
1:A:15:PHE:CZ	1:A:27:LEU:HD22	2.55	0.42
1:A:297:LEU:HD22	1:A:404:PHE:CD1	2.55	0.42
1:A:709:GLU:HG3	1:A:914:ARG:HD3	2.02	0.42
1:A:968:LYS:HA	1:A:968:LYS:HD2	1.87	0.42
1:B:1138:THR:OG1	1:B:1139:VAL:N	2.52	0.42
1:B:1142:VAL:HA	1:B:1182:TYR:O	2.20	0.42
1:C:1456:TYR:CZ	1:C:1460:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:LYS:HA	1:D:623:PRO:HD2	1.80	0.42
1:A:224:ILE:O	1:A:228:VAL:HG23	2.20	0.42
1:A:868:LEU:HA	1:A:869:PRO:HD3	1.89	0.42
1:B:860:ILE:HG23	1:B:957:ILE:CD1	2.50	0.42
1:C:724:PHE:CE2	1:C:726:GLY:HA3	2.55	0.42
1:D:1268:ILE:HA	1:D:1271:PHE:O	2.19	0.42
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.86	0.42
1:B:207:LYS:NZ	1:B:238:GLU:OE2	2.47	0.41
1:B:420:ARG:HG2	1:B:424:LEU:O	2.20	0.41
1:B:863:THR:HG23	1:B:925:VAL:HG11	2.01	0.41
1:C:1730:GLU:OE2	1:C:1730:GLU:HA	2.20	0.41
1:D:1184:SER:O	1:D:1185:ILE:HD13	2.19	0.41
1:D:1456:TYR:CZ	1:D:1460:ARG:HD3	2.55	0.41
1:D:265:TRP:CG	1:D:272:PRO:HG3	2.54	0.41
1:A:1191:VAL:HG22	1:A:1192:PRO:HD2	2.01	0.41
1:A:1625:MET:HE3	1:A:1671:PHE:CZ	2.55	0.41
1:B:1314:LEU:HD23	1:B:1314:LEU:HA	1.88	0.41
1:C:862:GLU:OE1	1:C:1016:ARG:NH1	2.53	0.41
1:D:1654:ASP:HB3	1:D:1691:PHE:O	2.20	0.41
1:A:1102:MET:CE	1:A:1292:ARG:HA	2.50	0.41
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.67	0.41
1:D:194:LYS:HG2	1:D:211:CYS:SG	2.60	0.41
1:D:420:ARG:C	1:D:422:ASP:N	2.73	0.41
1:A:1539:TYR:CD1	1:A:1610:ARG:HG2	2.55	0.41
1:A:1549:TRP:HA	1:A:1556:PHE:HB2	2.02	0.41
1:A:1612:TYR:CD1	1:A:1632:GLY:HA2	2.55	0.41
1:B:243:PHE:CZ	1:B:435:PHE:HA	2.55	0.41
1:B:835:MET:HG2	1:B:933:TRP:HE3	1.85	0.41
1:C:1616:GLY:C	1:C:1642:ARG:HG3	2.40	0.41
1:C:1523:LEU:HB3	1:C:1643:THR:HG21	2.03	0.41
1:C:1625:MET:HE3	1:C:1671:PHE:CZ	2.55	0.41
1:C:533:PRO:HD3	1:C:606:PHE:CZ	2.55	0.41
1:D:78:VAL:O	1:D:120:LYS:HA	2.21	0.41
1:A:1268:ILE:HA	1:A:1271:PHE:O	2.19	0.41
1:A:180:VAL:HB	1:A:181:PRO:HD3	2.03	0.41
1:A:860:ILE:HG23	1:A:957:ILE:CD1	2.51	0.41
1:B:1433:TYR:CE1	1:B:1502:ILE:HD13	2.56	0.41
1:B:183:ALA:HB2	1:B:377:THR:HG21	2.03	0.41
1:D:51:GLU:H	1:D:51:GLU:CD	2.24	0.41
1:A:79:LYS:C	1:A:81:ASN:H	2.24	0.41
1:B:1523:LEU:HB3	1:B:1643:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ILE:HG23	1:B:600:ILE:O	2.21	0.41
1:B:840:GLY:N	1:B:888:LYS:HG3	2.36	0.41
1:C:1500:CYS:HB3	1:C:1504:TYR:CZ	2.55	0.41
1:C:15:PHE:HE2	1:C:24:SER:HA	1.85	0.41
1:C:270:GLU:HB3	1:C:420:ARG:HB3	2.03	0.41
1:D:1618:VAL:HG13	1:D:1625:MET:HE2	2.02	0.41
1:D:206:CYS:HA	1:D:312:GLU:CB	2.50	0.41
1:A:1151:LEU:HB3	1:A:1156:ILE:HD13	2.02	0.41
1:A:1288:TYR:CD2	1:D:1540:ARG:NH1	2.88	0.41
1:A:14:SER:O	1:A:18:LYS:HG3	2.21	0.41
1:A:1556:PHE:CZ	1:A:1604:THR:HG22	2.55	0.41
1:B:1556:PHE:CZ	1:B:1604:THR:HG22	2.56	0.41
1:B:383:LYS:HB2	1:B:386:GLU:OE1	2.20	0.41
1:B:606:PHE:CZ	1:B:610:ILE:HD11	2.56	0.41
1:C:1103:ASP:HA	1:C:1361:TRP:HA	2.02	0.41
1:C:1459:ASN:HD21	1:C:1460:ARG:NH1	2.03	0.41
1:D:1612:TYR:CD1	1:D:1632:GLY:HA2	2.56	0.41
1:D:840:GLY:N	1:D:888:LYS:HG3	2.36	0.41
1:A:16:HIS:ND1	1:A:24:SER:HB2	2.36	0.41
1:A:635:ILE:HA	1:A:635:ILE:HD12	1.88	0.41
1:B:1466:GLU:O	1:B:1469:GLN:N	2.52	0.41
1:D:1152:ASN:O	1:D:1153:ASP:HB2	2.20	0.41
1:D:1304:TRP:CG	1:D:1316:PRO:HB2	2.56	0.41
1:A:1314:LEU:HA	1:A:1314:LEU:HD23	1.88	0.41
1:B:868:LEU:HA	1:B:869:PRO:HD3	1.90	0.41
1:C:1184:SER:O	1:C:1185:ILE:HD13	2.20	0.41
1:C:1323:VAL:HG21	1:C:1477:SER:HB3	2.02	0.41
1:C:296:PRO:HG2	1:C:366:LEU:HD22	2.03	0.41
1:C:81:ASN:HB3	1:C:82:ILE:HG13	2.02	0.41
1:D:968:LYS:HD2	1:D:968:LYS:HA	1.90	0.41
1:A:1274:GLU:O	1:A:1278:GLN:HG3	2.20	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.89	0.41
1:B:51:GLU:H	1:B:51:GLU:CD	2.24	0.41
1:C:1539:TYR:CD1	1:C:1610:ARG:HG2	2.56	0.41
1:C:143:VAL:HG13	1:C:461:LYS:HB3	2.02	0.41
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.90	0.41
1:D:516:SER:O	1:D:518:ASN:N	2.52	0.41
1:D:701:ILE:HA	1:D:702:PRO:HD3	1.92	0.41
1:D:750:VAL:HG22	1:D:879:ALA:HB1	2.02	0.41
1:D:753:VAL:HA	1:D:754:PRO:HD3	1.95	0.41
1:B:1468:HIS:O	1:B:1469:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:ASN:HD21	1:B:1601:TYR:HB3	1.86	0.41
1:B:751:PRO:O	1:B:907:TYR:HA	2.21	0.41
1:C:1269:ASP:OD2	1:C:1269:ASP:N	2.47	0.41
1:C:81:ASN:O	1:C:203:VAL:HG13	2.21	0.41
1:C:85:LYS:HD3	1:D:1509:GLN:HE22	1.85	0.41
1:C:860:ILE:HG23	1:C:957:ILE:CD1	2.50	0.41
1:D:1139:VAL:O	1:D:1140:ILE:HD12	2.20	0.41
1:D:851:SER:O	1:D:1058:THR:HA	2.21	0.41
1:A:1469:GLN:CB	1:B:64:SER:H	2.34	0.40
1:A:1:MET:HB2	1:A:2:GLU:H	1.59	0.40
1:C:1524:PRO:O	1:C:1643:THR:HG23	2.22	0.40
1:C:524:LEU:HB2	1:C:532:LYS:O	2.20	0.40
1:C:737:LEU:HB2	1:C:740:SER:OG	2.21	0.40
1:C:90:THR:HG22	1:C:92:ALA:N	2.32	0.40
1:D:1138:THR:OG1	1:D:1139:VAL:N	2.54	0.40
1:A:1194:TYR:CE2	1:A:1206:MET:HG2	2.56	0.40
1:A:78:VAL:HG23	1:A:82:ILE:HB	2.02	0.40
1:B:1151:LEU:HB3	1:B:1156:ILE:HD13	2.04	0.40
1:B:724:PHE:CE2	1:B:726:GLY:HA3	2.56	0.40
1:C:1151:LEU:HB3	1:C:1156:ILE:HD13	2.02	0.40
1:C:894:THR:O	1:C:911:VAL:HG13	2.21	0.40
1:D:1523:LEU:HB3	1:D:1643:THR:HG21	2.03	0.40
1:A:1006:LEU:HD23	1:A:1006:LEU:HA	1.96	0.40
1:A:1085:TYR:CE2	1:A:1108:ARG:HD3	2.56	0.40
1:A:1730:GLU:HA	1:A:1730:GLU:OE2	2.21	0.40
1:B:1191:VAL:HG22	1:B:1192:PRO:HD2	2.04	0.40
1:C:375:VAL:HG13	1:C:376:PRO:O	2.21	0.40
1:C:75:PRO:O	1:C:167:PRO:HD2	2.21	0.40
1:D:1085:TYR:CE2	1:D:1108:ARG:HD3	2.56	0.40
1:D:1302:PRO:HG3	1:D:1331:PHE:CE2	2.56	0.40
1:D:1391:LYS:HA	1:D:1391:LYS:HD2	1.93	0.40
1:D:1459:ASN:HD21	1:D:1460:ARG:NH1	2.04	0.40
1:A:925:VAL:HG23	1:A:926:THR:HG23	2.04	0.40
1:B:1730:GLU:HA	1:B:1730:GLU:OE2	2.20	0.40
1:C:36:LYS:HD3	1:C:40:GLU:CD	2.42	0.40
1:C:622:LYS:HE3	1:C:622:LYS:HB2	1.71	0.40
1:B:1151:LEU:HD11	1:B:1168:ASP:HB3	2.04	0.40
1:B:157:SER:HB3	1:B:169:SER:OG	2.21	0.40
1:B:519:TYR:CB	1:B:546:ILE:HD13	2.52	0.40
1:C:1059:LYS:HD2	1:C:1059:LYS:HA	1.75	0.40
1:D:1468:HIS:O	1:D:1469:GLN:C	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:ILE:HG23	1:D:957:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:TYR:OH	1:C:1541:GLU:OE2[2_455]	1.97	0.23

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	1654/1829 (90%)	1540 (93%)	101 (6%)	13 (1%)	19	60
1	B	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22	63
1	C	1654/1829 (90%)	1539 (93%)	102 (6%)	13 (1%)	19	60
1	D	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	22	63
All	All	6612/7316 (90%)	6167 (93%)	397 (6%)	48 (1%)	22	63

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	1166	ARG
1	A	1711	GLU
1	B	1166	ARG
1	C	38	ALA
1	C	1166	ARG
1	C	1711	GLU
1	D	1166	ARG
1	D	1711	GLU

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Mol	Chain	Res	Type
1	A	206	CYS
1	A	479	ASP
1	A	1438	ASP
1	B	206	CYS
1	B	479	ASP
1	B	540	ASP
1	B	1438	ASP
1	C	206	CYS
1	C	479	ASP
1	C	1438	ASP
1	D	206	CYS
1	D	479	ASP
1	D	540	ASP
1	D	1438	ASP
1	A	891	CYS
1	B	104	SER
1	B	891	CYS
1	C	891	CYS
1	D	104	SER
1	D	891	CYS
1	A	104	SER
1	A	517	ASN
1	A	612	HIS
1	C	104	SER
1	C	517	ASN
1	C	612	HIS
1	A	1003	ASP
1	A	1058	THR
1	B	65	ASN
1	B	1003	ASP
1	C	1003	ASP
1	C	1058	THR
1	D	1003	ASP
1	D	1058	THR
1	B	1058	THR
1	A	37	PRO
1	C	37	PRO
1	B	37	PRO
1	D	37	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	1413/1547 (91%)	1275 (90%)	138 (10%)	8	27
1	B	1411/1547 (91%)	1264 (90%)	147 (10%)	7	25
1	C	1413/1547 (91%)	1274 (90%)	139 (10%)	8	27
1	D	1411/1547 (91%)	1263 (90%)	148 (10%)	7	24
All	All	5648/6188 (91%)	5076 (90%)	572 (10%)	7	25

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	4	THR
1	A	18	LYS
1	A	60	LEU
1	A	62	SER
1	A	66	LYS
1	A	67	GLU
1	A	78	VAL
1	A	90	THR
1	A	95	SER
1	A	106	VAL
1	A	116	VAL
1	A	121	THR
1	A	143	VAL
1	A	149	VAL
1	A	160	VAL
1	A	165	ILE
1	A	166	VAL
1	A	170	LEU
1	A	194	LYS
1	A	202	VAL
1	A	219	LEU
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	241	ARG
1	A	243	PHE
1	A	269	THR
1	A	283	LYS
1	A	305	TYR
1	A	310	VAL
1	A	323	THR
1	A	343	LYS
1	A	356	ARG
1	A	368	LYS
1	A	375	VAL
1	A	385	GLU
1	A	393	LEU
1	A	415	VAL
1	A	420	ARG
1	A	429	THR
1	A	434	LYS
1	A	437	ASP
1	A	445	LYS
1	A	463	VAL
1	A	540	ASP
1	A	547	GLN
1	A	582	VAL
1	A	593	THR
1	A	600	ILE
1	A	631	ASN
1	A	634	GLU
1	A	638	ARG
1	A	659	LYS
1	A	662	GLN
1	A	676	ARG
1	A	680	GLU
1	A	689	ILE
1	A	698	GLN
1	A	716	ARG
1	A	719	GLN
1	A	730	ASP
1	A	734	LYS
1	A	735	LEU
1	A	737	LEU
1	A	738	LYS
1	A	739	HIS

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Mol	Chain	Res	Type
1	A	743	GLU
1	A	744	ILE
1	A	746	GLU
1	A	752	LEU
1	A	834	MET
1	A	841	LYS
1	A	859	VAL
1	A	860	ILE
1	A	872	THR
1	A	875	LYS
1	A	888	LYS
1	A	944	ASP
1	A	951	GLU
1	A	952	VAL
1	A	957	ILE
1	A	978	THR
1	A	979	SER
1	A	988	VAL
1	A	999	SER
1	A	1011	VAL
1	A	1015	ASP
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1047	SER
1	A	1055	LYS
1	A	1067	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP
1	A	1131	LYS
1	A	1147	VAL
1	A	1150	THR
1	A	1171	SER
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1321	ASP

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Mol	Chain	Res	Type
1	A	1326	LEU
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
1	A	1388	SER
1	A	1393	ILE
1	A	1396	PHE
1	A	1402	LEU
1	A	1408	LYS
1	A	1426	ASP
1	A	1428	SER
1	A	1430	LYS
1	A	1440	TYR
1	A	1459	ASN
1	A	1460	ARG
1	A	1478	GLN
1	A	1516	VAL
1	A	1562	ASP
1	A	1565	ARG
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1643	THR
1	A	1662	LEU
1	A	1675	THR
1	A	1695	VAL
1	A	1697	GLU
1	A	1721	GLU
1	A	1726	GLU
1	A	1736	GLN
1	B	4	THR
1	B	23	LYS
1	B	25	LEU
1	B	27	LEU
1	B	31	LEU
1	B	66	LYS
1	B	78	VAL
1	B	81	ASN
1	B	90	THR
1	B	95	SER
1	B	106	VAL
1	B	116	VAL

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Mol	Chain	Res	Type
1	B	118	ILE
1	B	121	THR
1	B	160	VAL
1	B	166	VAL
1	B	170	LEU
1	B	184	LEU
1	B	191	LYS
1	B	194	LYS
1	B	202	VAL
1	B	217	LEU
1	B	219	LEU
1	B	220	SER
1	B	241	ARG
1	B	243	PHE
1	B	277	LYS
1	B	302	ARG
1	B	305	TYR
1	B	313	ARG
1	B	317	THR
1	B	345	ASP
1	B	351	LYS
1	B	368	LYS
1	B	369	ASP
1	B	375	VAL
1	B	393	LEU
1	B	420	ARG
1	B	428	ILE
1	B	429	THR
1	B	433	LYS
1	B	437	ASP
1	B	445	LYS
1	B	463	VAL
1	B	468	THR
1	B	517	ASN
1	B	518	ASN
1	B	526	LYS
1	B	536	ARG
1	B	537	ARG
1	B	538	VAL
1	B	542	THR
1	B	582	VAL
1	B	584	SER

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Mol	Chain	Res	Type
1	B	589	GLU
1	B	593	THR
1	B	600	ILE
1	B	631	ASN
1	B	634	GLU
1	B	638	ARG
1	B	659	LYS
1	B	662	GLN
1	B	676	ARG
1	B	680	GLU
1	B	689	ILE
1	B	698	GLN
1	B	716	ARG
1	B	719	GLN
1	B	730	ASP
1	B	734	LYS
1	B	735	LEU
1	B	737	LEU
1	B	738	LYS
1	B	739	HIS
1	B	743	GLU
1	B	744	ILE
1	B	746	GLU
1	B	752	LEU
1	B	834	MET
1	B	841	LYS
1	B	859	VAL
1	B	860	ILE
1	B	872	THR
1	B	875	LYS
1	B	888	LYS
1	B	944	ASP
1	B	951	GLU
1	B	952	VAL
1	B	957	ILE
1	B	978	THR
1	B	979	SER
1	B	988	VAL
1	B	999	SER
1	B	1011	VAL
1	B	1015	ASP
1	B	1016	ARG

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Mol	Chain	Res	Type
1	B	1042	LEU
1	B	1044	SER
1	B	1047	SER
1	B	1055	LYS
1	B	1067	LYS
1	B	1074	LEU
1	B	1079	ASN
1	B	1103	ASP
1	B	1131	LYS
1	B	1147	VAL
1	B	1150	THR
1	B	1171	SER
1	B	1172	VAL
1	B	1191	VAL
1	B	1216	LEU
1	B	1224	GLN
1	B	1227	LEU
1	B	1252	THR
1	B	1303	LYS
1	B	1311	GLU
1	B	1321	ASP
1	B	1326	LEU
1	B	1345	SER
1	B	1346	LEU
1	B	1375	VAL
1	B	1388	SER
1	B	1393	ILE
1	B	1396	PHE
1	B	1402	LEU
1	B	1408	LYS
1	B	1426	ASP
1	B	1428	SER
1	B	1430	LYS
1	B	1440	TYR
1	B	1459	ASN
1	B	1460	ARG
1	B	1478	GLN
1	B	1516	VAL
1	B	1562	ASP
1	B	1565	ARG
1	B	1571	MET
1	B	1585	VAL

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Mol	Chain	Res	Type
1	B	1625	MET
1	B	1643	THR
1	B	1662	LEU
1	B	1675	THR
1	B	1695	VAL
1	B	1697	GLU
1	B	1721	GLU
1	B	1726	GLU
1	B	1736	GLN
1	C	1	MET
1	C	2	GLU
1	C	4	THR
1	C	18	LYS
1	C	60	LEU
1	C	62	SER
1	C	66	LYS
1	C	67	GLU
1	C	78	VAL
1	C	90	THR
1	C	95	SER
1	C	106	VAL
1	C	116	VAL
1	C	121	THR
1	C	123	LEU
1	C	143	VAL
1	C	160	VAL
1	C	165	ILE
1	C	166	VAL
1	C	170	LEU
1	C	194	LYS
1	C	202	VAL
1	C	219	LEU
1	C	231	LYS
1	C	241	ARG
1	C	243	PHE
1	C	269	THR
1	C	283	LYS
1	C	305	TYR
1	C	310	VAL
1	C	323	THR
1	C	343	LYS
1	C	356	ARG

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Mol	Chain	Res	Type
1	C	368	LYS
1	C	375	VAL
1	C	385	GLU
1	C	393	LEU
1	C	415	VAL
1	C	420	ARG
1	C	429	THR
1	C	434	LYS
1	C	437	ASP
1	C	445	LYS
1	C	463	VAL
1	C	466	ARG
1	C	540	ASP
1	C	547	GLN
1	C	582	VAL
1	C	593	THR
1	C	600	ILE
1	C	631	ASN
1	C	634	GLU
1	C	638	ARG
1	C	659	LYS
1	C	662	GLN
1	C	676	ARG
1	C	680	GLU
1	C	689	ILE
1	C	698	GLN
1	C	716	ARG
1	C	719	GLN
1	C	730	ASP
1	C	734	LYS
1	C	735	LEU
1	C	737	LEU
1	C	738	LYS
1	C	739	HIS
1	C	743	GLU
1	C	744	ILE
1	C	746	GLU
1	C	752	LEU
1	C	834	MET
1	C	841	LYS
1	C	859	VAL
1	C	860	ILE

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Mol	Chain	Res	Type
1	C	872	THR
1	C	875	LYS
1	C	888	LYS
1	C	944	ASP
1	C	951	GLU
1	C	952	VAL
1	C	957	ILE
1	C	978	THR
1	C	979	SER
1	C	988	VAL
1	C	999	SER
1	C	1011	VAL
1	C	1015	ASP
1	C	1016	ARG
1	C	1042	LEU
1	C	1044	SER
1	C	1047	SER
1	C	1055	LYS
1	C	1067	LYS
1	C	1074	LEU
1	C	1079	ASN
1	C	1103	ASP
1	C	1131	LYS
1	C	1147	VAL
1	C	1150	THR
1	C	1171	SER
1	C	1172	VAL
1	C	1191	VAL
1	C	1216	LEU
1	C	1224	GLN
1	C	1227	LEU
1	C	1252	THR
1	C	1311	GLU
1	C	1321	ASP
1	C	1326	LEU
1	C	1345	SER
1	C	1346	LEU
1	C	1375	VAL
1	C	1388	SER
1	C	1393	ILE
1	C	1396	PHE
1	C	1402	LEU

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Mol	Chain	Res	Type
1	C	1408	LYS
1	C	1426	ASP
1	C	1428	SER
1	C	1430	LYS
1	C	1440	TYR
1	C	1459	ASN
1	C	1460	ARG
1	C	1478	GLN
1	C	1516	VAL
1	C	1562	ASP
1	C	1565	ARG
1	C	1571	MET
1	C	1585	VAL
1	C	1625	MET
1	C	1643	THR
1	C	1662	LEU
1	C	1675	THR
1	C	1695	VAL
1	C	1697	GLU
1	C	1721	GLU
1	C	1726	GLU
1	C	1736	GLN
1	D	4	THR
1	D	23	LYS
1	D	25	LEU
1	D	27	LEU
1	D	31	LEU
1	D	66	LYS
1	D	78	VAL
1	D	81	ASN
1	D	90	THR
1	D	95	SER
1	D	106	VAL
1	D	116	VAL
1	D	118	ILE
1	D	121	THR
1	D	143	VAL
1	D	160	VAL
1	D	166	VAL
1	D	170	LEU
1	D	184	LEU
1	D	191	LYS

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Mol	Chain	Res	Type
1	D	194	LYS
1	D	202	VAL
1	D	217	LEU
1	D	219	LEU
1	D	220	SER
1	D	241	ARG
1	D	243	PHE
1	D	277	LYS
1	D	302	ARG
1	D	305	TYR
1	D	313	ARG
1	D	317	THR
1	D	345	ASP
1	D	351	LYS
1	D	368	LYS
1	D	369	ASP
1	D	375	VAL
1	D	393	LEU
1	D	420	ARG
1	D	428	ILE
1	D	429	THR
1	D	433	LYS
1	D	437	ASP
1	D	445	LYS
1	D	458	THR
1	D	463	VAL
1	D	468	THR
1	D	517	ASN
1	D	518	ASN
1	D	526	LYS
1	D	536	ARG
1	D	537	ARG
1	D	538	VAL
1	D	542	THR
1	D	582	VAL
1	D	584	SER
1	D	589	GLU
1	D	593	THR
1	D	600	ILE
1	D	631	ASN
1	D	634	GLU
1	D	638	ARG

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Mol	Chain	Res	Type
1	D	659	LYS
1	D	662	GLN
1	D	676	ARG
1	D	680	GLU
1	D	689	ILE
1	D	698	GLN
1	D	716	ARG
1	D	719	GLN
1	D	730	ASP
1	D	734	LYS
1	D	735	LEU
1	D	737	LEU
1	D	738	LYS
1	D	739	HIS
1	D	743	GLU
1	D	744	ILE
1	D	746	GLU
1	D	752	LEU
1	D	834	MET
1	D	841	LYS
1	D	859	VAL
1	D	860	ILE
1	D	872	THR
1	D	875	LYS
1	D	888	LYS
1	D	944	ASP
1	D	951	GLU
1	D	952	VAL
1	D	957	ILE
1	D	978	THR
1	D	979	SER
1	D	988	VAL
1	D	999	SER
1	D	1011	VAL
1	D	1015	ASP
1	D	1016	ARG
1	D	1042	LEU
1	D	1044	SER
1	D	1047	SER
1	D	1055	LYS
1	D	1067	LYS
1	D	1074	LEU

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Mol	Chain	Res	Type
1	D	1079	ASN
1	D	1103	ASP
1	D	1131	LYS
1	D	1147	VAL
1	D	1150	THR
1	D	1171	SER
1	D	1172	VAL
1	D	1191	VAL
1	D	1216	LEU
1	D	1224	GLN
1	D	1227	LEU
1	D	1252	THR
1	D	1311	GLU
1	D	1321	ASP
1	D	1326	LEU
1	D	1345	SER
1	D	1346	LEU
1	D	1375	VAL
1	D	1388	SER
1	D	1393	ILE
1	D	1396	PHE
1	D	1402	LEU
1	D	1408	LYS
1	D	1426	ASP
1	D	1428	SER
1	D	1430	LYS
1	D	1440	TYR
1	D	1459	ASN
1	D	1460	ARG
1	D	1478	GLN
1	D	1516	VAL
1	D	1562	ASP
1	D	1565	ARG
1	D	1571	MET
1	D	1585	VAL
1	D	1625	MET
1	D	1643	THR
1	D	1662	LEU
1	D	1675	THR
1	D	1695	VAL
1	D	1697	GLU
1	D	1721	GLU

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Mol	Chain	Res	Type
1	D	1726	GLU
1	D	1736	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	81	ASN
1	A	186	ASN
1	A	829	HIS
1	A	1459	ASN
1	B	99	GLN
1	B	186	ASN
1	B	539	ASN
1	B	829	HIS
1	B	1315	HIS
1	B	1318	ASN
1	B	1459	ASN
1	C	55	HIS
1	C	58	ASN
1	C	65	ASN
1	C	81	ASN
1	C	186	ASN
1	C	829	HIS
1	C	1459	ASN
1	C	1468	HIS
1	C	1509	GLN
1	D	99	GLN
1	D	186	ASN
1	D	539	ASN
1	D	829	HIS
1	D	1315	HIS
1	D	1318	ASN
1	D	1459	ASN
1	D	1468	HIS
1	D	1509	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.