



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:16 am BST

PDB ID : 4ZUZ
Title : SidC 1-871
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Deposited on : 2015-05-18
Resolution : 2.86 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

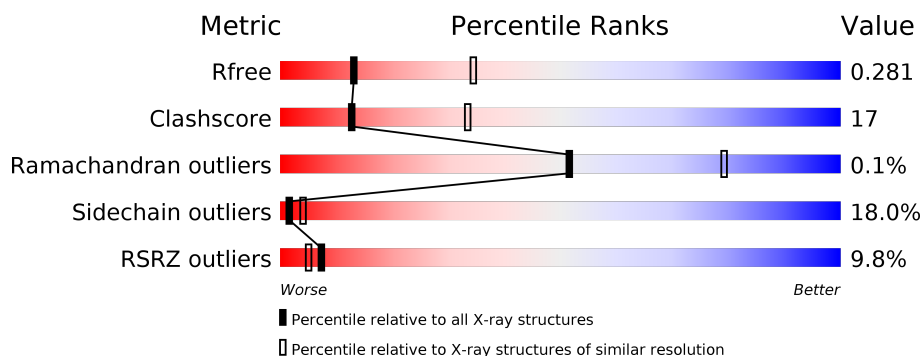
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 $\leq 5\%$. 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	917	<div> <div>9%</div> <div>62%</div> <div>24%</div> <div>7%</div> <div>7%</div> </div>
1	B	917	<div> <div>9%</div> <div>65%</div> <div>22%</div> <div>7%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14094 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 SidC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	857	Total	C	N	O	S	0	0	0
			6979	4405	1190	1374	10			
1	B	858	Total	C	N	O	S	0	0	0
			6986	4410	1191	1375	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	VAL	conflict	UNP Q6RCR4
A	326	VAL	ALA	conflict	UNP Q6RCR4
A	334	GLN	ASP	conflict	UNP Q6RCR4
A	646	ALA	LYS	conflict	UNP Q6RCR4
A	731	TYR	ALA	conflict	UNP Q6RCR4
B	325	ALA	VAL	conflict	UNP Q6RCR4
B	326	VAL	ALA	conflict	UNP Q6RCR4
B	334	GLN	ASP	conflict	UNP Q6RCR4
B	646	ALA	LYS	conflict	UNP Q6RCR4
B	731	TYR	ALA	conflict	UNP Q6RCR4

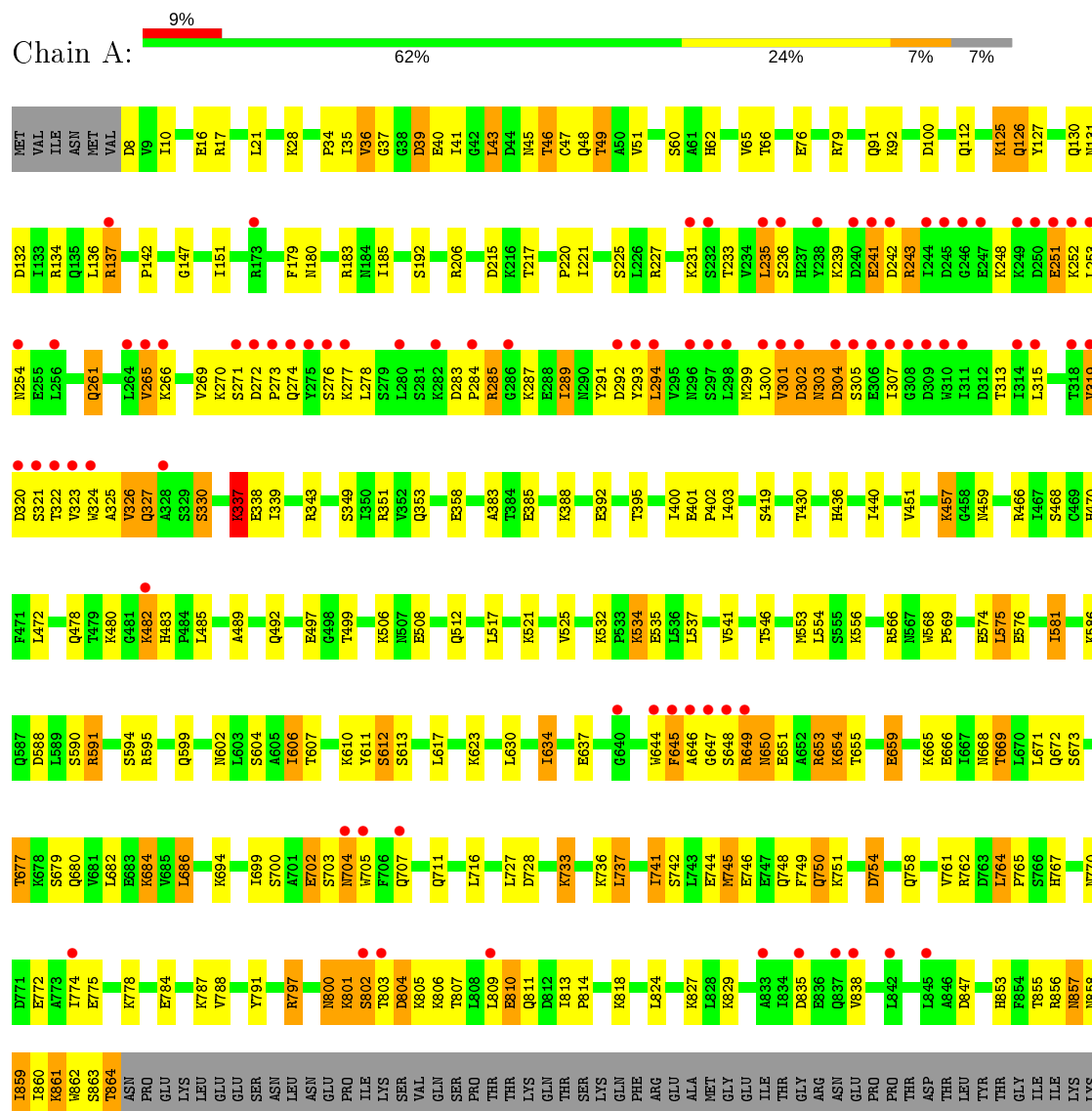
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	64	Total	O	0	0
			64	64		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: SidC



LEU	ASN	GLU	PRO	ILE	LYS	SER	VAL	GLN	SER	PRO	THR	THR	LYS	GLN	THR	SER	LYS	GLN	PHE	ARG	GLU	ALA	MET	GLY	GLU	ILE	THR	GLY	ARG	ASN	GLU	PRO	THR	ASP	THR	LEU	TYR	THR	GLY	ILE	ILE	LYS	LYS						
F776	F777	K778	E784	K787	V788	Y791	R797	N800	R801	S802	T803	D804	K805	K806	R807	L808	L809	E810	Q811	R812	I813	P814	K818	L824	K827	L828	K829	D835	K846	D847	T855	R856	I859	I860	K861	S863	T864	ASN	PRO	GLU	LYS	LEU	GLU	GLU	SER	ASN			
V681	L682	E683	K684	V685	L686	D693	K694	I699	E702	S703	N704	W705	F706	Q707	Q711	L716	F717	R718	L727	K733	K736	L737	I741	S742	N745	E746	E747	Q748	F749	Q750	K751	I752	Q753	D754	Q758	V761	R762	S763	L764	P765	S766	H767	E772	A773	I774	E775			
R595	D596	N597	I598	Q599	H600	D601	N602	L603	S604	A605	I606	T607	K610	Y611	S612	S613	L617	K623	I634	E637	G640	R641	E642	W643	W644	F645	A646	G647	S648	R649	N650	R653	K654	E659	R662	K665	E666	I667	N668	T669	L670	L671	Q672	S673	T677	K678	S679	Q680	
I460	R466	S321	T322	V323	C469	H470	F471	L472	K480	G481	K482	Q492	T499	E508	Q512	L517	K521	V525	K534	E535	L536	L537	D538	Y539	V541	T546	L554	R566	N567	W568	P569	E574	L575	E576	I581	K586	Q587	D588	L589	S590	R591	S594							
V319	D320	S321	T322	K323	A324	A325	V326	Q327	A328	A336	G337	E338	I339	D344	T348	I350	R351	V352	Q353	G374	A383	T384	E385	L386	A387	T395	I400	E401	P402	I403	I404	Y405	L415	S419	P420	L421	V301	D302	N303	D304	S305	E306	W310	T313	I314	L315			
D245	G246	E247	K248	R249	D250	E251	K252	L253	N254	E255	L256	L257	L261	L264	V265	K266	V269	K270	S271	D272	P273	Q274	Z275	K276	K277	L278	D283	P284	R285	G286	K287	E288	L289	Y291	D292	Y293	L294	K299	L300	V301	D302	N303	D304	S305	E306	W310	T313	I314	L315
Q121	K125	Q126	Y127	D128	E129	Q130	N131	D132	I133	R134	Q135	L136	R137	P142	I151	R173	S192	G204	Y205	K206	L207	L211	F212	E214	D215	K216	T217	P218	T219	P220	I221	S225	L226	R227	V230	K231	S232	T233	V234	L235	S236	H237	Y238	E241	D242	R243	I244		
MET	VAL	ILE	ASN	MET	V7	D8	V9	I10	K13	E16	R17	K28	V29	P34	I35	V36	G37	G38	D39	E40	I41	G42	L43	D44	N45	T46	C47	Q48	T49	A50	V51	S60	A61	H62	S63	G64	V65	T66	E76	R79	K86	Q91	K92	D100	Q112	Y116	I117		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.16Å 83.93Å 129.41Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	49.16 – 2.86 47.14 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.16-2.86) 99.2 (47.14-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.225 , 0.281 0.224 , 0.281	Depositor DCC
R_{free} test set	2708 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14094	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/7110	0.66	1/9595 (0.0%)
1	B	0.47	0/7117	0.65	1/9605 (0.0%)
All	All	0.49	0/14227	0.66	2/19200 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	LYS	CD-CE-NZ	-5.67	98.67	111.70
1	A	337	LYS	CD-CE-NZ	-5.50	99.05	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6979	0	6935	236	0
1	B	6986	0	6942	230	0
2	A	65	0	0	27	0
2	B	64	0	0	22	0
All	All	14094	0	13877	461	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 17.

All (461) 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:703:SER:HB3	1:B:704:ASN:CA	1.46	1.42
1:A:703:SER:HB3	1:A:704:ASN:CA	1.48	1.41
1:B:703:SER:CB	1:B:704:ASN:HA	1.41	1.41
1:A:703:SER:CB	1:A:704:ASN:HA	1.41	1.40
1:B:323:VAL:C	1:B:326:VAL:HG21	1.42	1.36
1:B:324:TRP:C	1:B:326:VAL:HB	1.46	1.36
1:A:838:VAL:HG23	1:A:862:TRP:CZ3	1.62	1.34
1:B:859:ILE:HD12	1:B:860:ILE:N	1.44	1.29
1:A:506:LYS:HA	2:A:1022:HOH:O	1.25	1.29
1:A:859:ILE:HD12	1:A:860:ILE:N	1.49	1.28
1:A:838:VAL:CG2	1:A:862:TRP:HZ3	1.46	1.28
1:B:855:THR:O	1:B:859:ILE:HG23	1.35	1.24
1:A:859:ILE:HD12	1:A:859:ILE:C	1.54	1.20
1:A:750:GLN:NE2	1:A:750:GLN:HA	1.46	1.20
1:A:320:ASP:OD2	1:A:322:THR:OG1	1.54	1.20
1:A:647:GLY:HA2	1:A:648:SER:CB	1.71	1.20
1:A:43:LEU:CD2	1:A:43:LEU:H	1.52	1.17
1:B:647:GLY:CA	1:B:648:SER:HB3	1.72	1.17
1:A:863:SER:O	1:A:864:THR:HG22	1.44	1.17
1:B:647:GLY:HA2	1:B:648:SER:CB	1.69	1.17
1:A:647:GLY:CA	1:A:648:SER:HB3	1.76	1.16
1:B:325:ALA:HA	1:B:327:GLN:H	1.01	1.15
1:B:43:LEU:HD22	1:B:43:LEU:N	1.55	1.15
1:A:457:LYS:H	1:A:457:LYS:CD	1.53	1.14
1:A:457:LYS:N	1:A:457:LYS:HD2	1.62	1.14
1:A:327:GLN:OE1	1:A:327:GLN:HA	1.42	1.12
1:B:859:ILE:HD12	1:B:859:ILE:C	1.63	1.11
1:A:43:LEU:HD23	1:A:43:LEU:N	1.65	1.10
1:A:647:GLY:CA	1:A:650:ASN:HB2	1.81	1.09
1:A:750:GLN:HE21	1:A:750:GLN:CA	1.60	1.09
1:A:330:SER:OG	1:A:401:GLU:OE2	1.70	1.08
1:B:649:ARG:HH11	1:B:649:ARG:HG3	1.17	1.08
1:B:43:LEU:H	1:B:43:LEU:HD22	1.13	1.07
1:B:860:ILE:O	1:B:863:SER:OG	1.73	1.07
1:A:647:GLY:HA3	1:A:650:ASN:H	1.19	1.06
1:B:325:ALA:H	1:B:326:VAL:HG12	1.17	1.06
1:B:324:TRP:HA	1:B:326:VAL:HG11	1.34	1.04
1:A:35:ILE:HG22	1:A:36:VAL:HG12	1.34	1.03
1:A:648:SER:O	1:A:649:ARG:HG3	1.58	1.03
1:A:647:GLY:HA3	1:A:650:ASN:HB2	1.40	1.02
1:B:778:LYS:HD2	2:B:1006:HOH:O	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:O	1:B:326:VAL:HG11	1.60	1.02
1:B:647:GLY:CA	1:B:650:ASN:HB2	1.91	1.00
1:B:324:TRP:C	1:B:326:VAL:CB	2.30	1.00
1:A:648:SER:C	1:A:649:ARG:HG3	1.79	1.00
1:B:323:VAL:C	1:B:326:VAL:CG2	2.30	0.99
1:B:325:ALA:CA	1:B:327:GLN:H	1.75	0.99
1:B:327:GLN:OE1	1:B:327:GLN:HA	1.61	0.99
1:A:863:SER:C	1:A:864:THR:HG22	1.82	0.98
1:B:647:GLY:HA3	1:B:650:ASN:H	1.22	0.98
1:A:43:LEU:H	1:A:43:LEU:HD23	0.82	0.98
1:B:460:ILE:HG23	2:B:1001:HOH:O	1.62	0.98
1:A:647:GLY:N	1:A:650:ASN:HB2	1.79	0.97
1:A:859:ILE:CD1	1:A:859:ILE:C	2.30	0.97
1:A:645:PHE:HD2	1:A:645:PHE:N	1.63	0.96
1:B:325:ALA:N	1:B:326:VAL:HB	1.81	0.96
1:A:750:GLN:HE21	1:A:750:GLN:HA	0.79	0.96
1:A:315:LEU:O	1:A:319:VAL:HG23	1.67	0.95
1:B:43:LEU:CD2	1:B:43:LEU:H	1.73	0.95
1:B:325:ALA:N	1:B:326:VAL:CB	2.30	0.95
1:A:859:ILE:CD1	1:A:860:ILE:N	2.30	0.95
1:B:323:VAL:CA	1:B:326:VAL:HG21	1.87	0.95
1:B:859:ILE:CD1	1:B:860:ILE:N	2.30	0.95
1:B:325:ALA:N	1:B:326:VAL:HG12	1.81	0.94
1:B:649:ARG:HH11	1:B:649:ARG:CG	1.78	0.94
1:A:744:GLU:OE2	2:A:1001:HOH:O	1.85	0.94
1:B:325:ALA:HA	1:B:327:GLN:N	1.82	0.94
1:B:315:LEU:O	1:B:319:VAL:HG23	1.66	0.94
1:B:325:ALA:N	1:B:326:VAL:CG1	2.30	0.94
1:A:457:LYS:H	1:A:457:LYS:HD2	0.78	0.93
1:A:861:LYS:O	1:A:864:THR:HG23	1.68	0.93
1:B:76:GLU:OE2	1:B:79:ARG:NH2	2.01	0.92
1:A:859:ILE:HD12	1:A:860:ILE:CA	1.99	0.92
1:A:838:VAL:HG23	1:A:862:TRP:HZ3	0.76	0.92
1:B:859:ILE:HD12	1:B:860:ILE:CA	2.00	0.92
1:B:647:GLY:HA3	1:B:650:ASN:HB2	1.51	0.92
1:B:649:ARG:NH1	1:B:649:ARG:HG3	1.77	0.91
1:B:324:TRP:CA	1:B:326:VAL:HG11	2.01	0.91
1:B:859:ILE:CD1	1:B:859:ILE:C	2.38	0.91
1:B:647:GLY:N	1:B:650:ASN:HB2	1.86	0.90
1:A:323:VAL:O	1:A:326:VAL:HG12	1.71	0.90
1:A:838:VAL:CG2	1:A:862:TRP:CZ3	2.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLN:HE22	1:A:758:GLN:HE22	1.20	0.89
1:B:324:TRP:N	1:B:326:VAL:HG21	1.88	0.87
1:A:645:PHE:CD2	1:A:645:PHE:N	2.37	0.87
1:A:645:PHE:HB3	1:A:646:ALA:HB2	1.57	0.86
1:B:749:PHE:HB3	2:B:1026:HOH:O	1.77	0.85
1:B:597:ASN:HB3	2:B:1004:HOH:O	1.75	0.85
1:B:648:SER:C	1:B:649:ARG:HG2	1.95	0.84
1:B:647:GLY:HA3	1:B:650:ASN:N	1.92	0.84
1:B:437:TYR:HB3	2:B:1008:HOH:O	1.76	0.84
1:B:43:LEU:CD2	1:B:43:LEU:N	2.30	0.83
1:A:647:GLY:HA2	1:A:648:SER:HB3	0.86	0.82
1:B:324:TRP:HA	1:B:326:VAL:CG1	2.08	0.82
1:B:41:ILE:HD13	1:B:440:ILE:CG2	2.09	0.82
1:B:320:ASP:O	1:B:323:VAL:HG23	1.81	0.81
1:B:323:VAL:O	1:B:326:VAL:CG1	2.30	0.80
1:A:651:GLU:O	1:A:655:THR:N	2.13	0.80
1:A:647:GLY:HA3	1:A:650:ASN:N	1.96	0.80
1:A:861:LYS:O	1:A:864:THR:CG2	2.30	0.80
1:B:327:GLN:OE1	1:B:327:GLN:CA	2.30	0.80
1:B:856:ARG:O	1:B:859:ILE:HG13	1.82	0.80
1:A:323:VAL:O	1:A:326:VAL:CG1	2.30	0.79
1:A:863:SER:C	1:A:864:THR:CG2	2.49	0.79
1:A:855:THR:O	1:A:859:ILE:HG23	1.82	0.79
1:A:863:SER:O	1:A:864:THR:CG2	2.30	0.79
1:A:648:SER:O	1:A:649:ARG:CG	2.30	0.79
1:B:702:GLU:OE2	1:B:702:GLU:CA	2.30	0.78
1:B:62:HIS:HA	2:B:1038:HOH:O	1.84	0.78
1:B:648:SER:O	1:B:649:ARG:HG2	1.83	0.78
1:B:702:GLU:OE2	1:B:702:GLU:HA	1.82	0.78
1:A:553:MET:SD	2:A:1040:HOH:O	2.42	0.78
1:A:750:GLN:NE2	1:A:750:GLN:CA	2.30	0.77
1:B:324:TRP:CA	1:B:326:VAL:CG1	2.62	0.77
1:A:728:ASP:HB2	2:A:1001:HOH:O	1.82	0.77
1:B:860:ILE:C	1:B:863:SER:HG	1.88	0.75
1:A:43:LEU:CD2	1:A:43:LEU:N	2.32	0.75
1:A:703:SER:CB	1:A:704:ASN:CA	2.30	0.74
1:B:468:SER:N	2:B:1001:HOH:O	2.18	0.74
1:B:326:VAL:HG12	1:B:327:GLN:N	2.02	0.74
1:A:647:GLY:H	1:A:650:ASN:HB2	1.51	0.73
1:A:40:GLU:OE1	1:A:436:HIS:NE2	2.12	0.73
1:A:76:GLU:OE2	1:A:79:ARG:NH2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:HB3	2:A:1002:HOH:O	1.88	0.72
1:B:647:GLY:H	1:B:650:ASN:HB2	1.54	0.72
1:A:127:TYR:CZ	2:A:1002:HOH:O	2.42	0.71
1:A:45:ASN:OD1	1:A:48:GLN:HB2	1.90	0.71
1:B:597:ASN:ND2	2:B:1002:HOH:O	2.22	0.71
1:B:648:SER:O	1:B:649:ARG:CG	2.39	0.71
1:A:127:TYR:OH	2:A:1002:HOH:O	2.09	0.71
1:B:324:TRP:O	1:B:326:VAL:HB	1.91	0.71
1:B:41:ILE:CD1	1:B:440:ILE:HG21	2.21	0.71
1:B:647:GLY:HA3	1:B:650:ASN:CB	2.20	0.71
1:A:91:GLN:HE22	1:A:604:SER:H	1.36	0.70
1:B:600:HIS:HB2	2:B:1004:HOH:O	1.91	0.70
1:A:39:ASP:O	1:A:40:GLU:HB2	1.90	0.70
1:A:750:GLN:HE22	1:A:758:GLN:NE2	1.88	0.70
1:B:704:ASN:N	1:B:705:TRP:HA	2.05	0.70
1:B:10:ILE:HB	1:B:606:ILE:HD12	1.75	0.69
1:A:10:ILE:HB	1:A:606:ILE:HD12	1.73	0.69
1:B:682:LEU:O	1:B:686:LEU:HG	1.91	0.69
1:A:611:TYR:OH	1:A:745:MET:HG2	1.93	0.69
1:A:859:ILE:HD12	1:A:860:ILE:HA	1.72	0.69
1:A:686:LEU:CD2	1:B:686:LEU:CD2	2.71	0.68
1:A:647:GLY:HA3	1:A:650:ASN:CB	2.20	0.68
1:B:91:GLN:HE22	1:B:604:SER:H	1.40	0.68
1:B:784:GLU:O	1:B:788:VAL:HG23	1.93	0.68
1:A:271:SER:HB3	1:A:327:GLN:HG2	1.76	0.68
1:A:682:LEU:O	1:A:686:LEU:HG	1.93	0.68
1:B:325:ALA:H	1:B:326:VAL:CG1	1.91	0.68
1:B:36:VAL:HG13	1:B:467:ILE:HB	1.74	0.68
1:B:611:TYR:OH	1:B:745:MET:HG2	1.93	0.68
1:B:754:ASP:C	1:B:754:ASP:OD1	2.33	0.67
1:A:754:ASP:C	1:A:754:ASP:OD1	2.33	0.67
1:B:650:ASN:O	1:B:654:LYS:HB2	1.95	0.67
1:A:647:GLY:CA	1:A:648:SER:CB	2.55	0.67
1:B:41:ILE:HD13	1:B:440:ILE:HG21	1.76	0.67
1:B:860:ILE:C	1:B:863:SER:OG	2.33	0.66
1:B:43:LEU:H	1:B:43:LEU:HD13	1.61	0.66
1:A:126:GLN:HB2	1:A:127:TYR:CD2	2.31	0.66
1:A:137:ARG:HB2	2:A:1045:HOH:O	1.96	0.65
1:A:41:ILE:HG13	1:A:451:VAL:HG22	1.78	0.65
1:A:703:SER:OG	1:A:705:TRP:HB2	1.95	0.65
1:B:323:VAL:C	1:B:326:VAL:HG11	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:GLU:O	1:A:788:VAL:HG23	1.96	0.65
1:A:650:ASN:ND2	1:A:654:LYS:NZ	2.45	0.65
1:B:43:LEU:CD1	1:B:43:LEU:H	2.07	0.65
1:B:588:ASP:OD1	1:B:591:ARG:NH2	2.30	0.65
1:B:647:GLY:HA2	1:B:648:SER:HB3	0.79	0.65
1:B:126:GLN:HB2	1:B:127:TYR:CD2	2.32	0.65
1:B:327:GLN:OE1	1:B:328:ALA:N	2.30	0.65
1:B:323:VAL:CA	1:B:326:VAL:CG2	2.73	0.64
1:B:41:ILE:CD1	1:B:440:ILE:CG2	2.76	0.64
1:A:728:ASP:CB	2:A:1001:HOH:O	2.43	0.63
1:B:702:GLU:N	1:B:702:GLU:OE2	2.30	0.63
1:A:733:LYS:NZ	2:A:1003:HOH:O	2.26	0.63
1:A:266:LYS:O	1:A:270:LYS:HG3	1.99	0.63
1:A:179:PHE:C	2:A:1019:HOH:O	2.37	0.62
1:A:859:ILE:O	1:A:859:ILE:HD12	1.99	0.62
1:B:266:LYS:O	1:B:270:LYS:HG3	2.00	0.62
1:B:859:ILE:HD12	1:B:860:ILE:HA	1.78	0.61
1:A:653:ARG:NH2	1:A:702:GLU:OE2	2.32	0.61
1:B:324:TRP:CA	1:B:326:VAL:HB	2.28	0.61
1:A:39:ASP:OD1	1:A:39:ASP:C	2.35	0.61
1:B:261:GLN:O	1:B:265:VAL:HG23	2.01	0.61
1:B:324:TRP:CA	1:B:326:VAL:CB	2.78	0.61
1:B:324:TRP:C	1:B:326:VAL:CG1	2.65	0.61
1:A:303:ASN:OD1	1:A:304:ASP:OD1	2.19	0.60
1:B:336:ALA:HA	2:B:1053:HOH:O	2.00	0.60
1:A:748:GLN:HB3	1:A:774:ILE:CD1	2.31	0.60
1:B:39:ASP:O	1:B:40:GLU:HB2	2.01	0.60
1:A:556:LYS:HD2	2:A:1058:HOH:O	2.00	0.60
1:A:686:LEU:CD2	1:B:686:LEU:HD21	2.31	0.60
1:B:8:ASP:N	1:B:8:ASP:OD2	2.31	0.60
1:A:645:PHE:H	1:A:645:PHE:HD2	1.38	0.60
1:A:36:VAL:HG23	1:A:37:GLY:N	2.16	0.60
1:A:750:GLN:NE2	1:A:758:GLN:HE22	1.98	0.59
1:B:748:GLN:HB3	1:B:774:ILE:CD1	2.33	0.59
1:A:324:TRP:O	1:A:325:ALA:HB3	2.03	0.59
1:B:41:ILE:HD13	1:B:440:ILE:HG23	1.85	0.59
1:A:269:VAL:HA	1:A:273:PRO:HA	1.85	0.58
1:B:647:GLY:CA	1:B:650:ASN:H	2.08	0.58
1:A:327:GLN:OE1	1:A:327:GLN:CA	2.30	0.58
1:B:36:VAL:CG2	1:B:37:GLY:N	2.66	0.58
1:A:261:GLN:O	1:A:265:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ALA:CA	1:B:327:GLN:N	2.55	0.58
1:B:741:ILE:HG22	1:B:742:SER:H	1.69	0.58
1:A:741:ILE:HG22	1:A:742:SER:H	1.69	0.58
1:A:750:GLN:NE2	1:A:758:GLN:NE2	2.50	0.58
1:B:269:VAL:HA	1:B:273:PRO:HA	1.85	0.58
1:A:457:LYS:N	1:A:457:LYS:CD	2.30	0.57
1:B:324:TRP:N	1:B:326:VAL:CG2	2.64	0.57
1:A:47:CYS:SG	1:A:47:CYS:O	2.61	0.57
1:A:801:LYS:HD3	1:A:802:SER:N	2.18	0.57
1:B:457:LYS:H	1:B:457:LYS:HE2	1.68	0.57
1:A:686:LEU:HD21	1:B:686:LEU:HD21	1.86	0.57
1:A:323:VAL:O	1:A:326:VAL:CB	2.53	0.57
1:A:647:GLY:H	1:A:650:ASN:CB	2.16	0.57
1:B:801:LYS:HD3	1:B:802:SER:N	2.18	0.57
1:A:147:GLY:H	1:A:478:GLN:HE22	1.53	0.57
1:B:659:GLU:HA	1:B:659:GLU:OE1	2.04	0.57
1:B:810:GLU:N	1:B:810:GLU:OE2	2.37	0.57
1:B:703:SER:C	1:B:705:TRP:HA	2.24	0.56
1:A:761:VAL:HA	1:A:764:LEU:HD22	1.87	0.56
1:B:703:SER:CB	1:B:704:ASN:CA	2.30	0.56
1:A:483:HIS:N	2:A:1002:HOH:O	2.39	0.56
1:A:650:ASN:HD22	1:A:654:LYS:HZ3	1.51	0.56
1:A:39:ASP:OD1	1:A:40:GLU:N	2.38	0.56
1:B:283:ASP:HB2	1:B:284:PRO:HD2	1.86	0.56
1:B:43:LEU:N	1:B:43:LEU:HD13	2.19	0.56
1:B:36:VAL:HG21	1:B:42:GLY:HA3	1.88	0.56
1:A:283:ASP:HB2	1:A:284:PRO:HD2	1.88	0.55
1:B:303:ASN:OD1	1:B:304:ASP:OD1	2.23	0.55
1:A:588:ASP:OD1	1:A:591:ARG:NH2	2.38	0.55
1:B:301:VAL:HG22	1:B:313:THR:HG21	1.89	0.55
1:A:650:ASN:ND2	1:A:654:LYS:HZ2	2.04	0.55
1:A:650:ASN:O	1:A:654:LYS:HB2	2.07	0.55
1:B:241:GLU:O	1:B:243:ARG:HD3	2.07	0.55
1:A:151:ILE:HG23	1:A:459:ASN:ND2	2.22	0.54
1:A:36:VAL:CG2	1:A:37:GLY:N	2.69	0.54
1:A:648:SER:C	1:A:649:ARG:CG	2.59	0.54
1:B:325:ALA:N	1:B:327:GLN:H	2.05	0.54
1:A:647:GLY:O	1:B:321:SER:OG	2.15	0.54
1:A:180:ASN:HB2	2:A:1019:HOH:O	2.07	0.54
1:B:761:VAL:HA	1:B:764:LEU:HD22	1.90	0.54
1:A:483:HIS:HB2	2:A:1002:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:HIS:HD2	1:B:472:LEU:H	1.55	0.54
1:B:855:THR:O	1:B:859:ILE:CG2	2.30	0.54
1:A:859:ILE:CD1	1:A:860:ILE:HA	2.37	0.54
1:B:401:GLU:HG2	1:B:430:THR:HG23	1.90	0.54
1:A:301:VAL:HG22	1:A:313:THR:HG21	1.90	0.53
1:A:856:ARG:O	1:A:859:ILE:HG13	2.09	0.53
1:B:151:ILE:HG23	1:B:459:ASN:ND2	2.24	0.53
1:A:859:ILE:CD1	1:A:860:ILE:CA	2.80	0.53
1:A:241:GLU:O	1:A:243:ARG:HD3	2.09	0.53
1:A:859:ILE:CG1	1:A:860:ILE:N	2.71	0.52
1:A:323:VAL:O	1:A:326:VAL:HB	2.09	0.52
1:B:40:GLU:OE1	1:B:435:LYS:HE2	2.09	0.52
1:A:650:ASN:HD22	1:A:654:LYS:NZ	2.07	0.52
1:B:677:THR:OG1	1:B:680:GLN:NE2	2.43	0.52
1:A:853:HIS:O	1:A:858:ASN:OD1	2.27	0.52
1:A:686:LEU:HD22	1:B:686:LEU:CD2	2.40	0.52
1:B:754:ASP:O	1:B:754:ASP:OD1	2.27	0.52
1:B:775:GLU:O	1:B:778:LYS:HG2	2.09	0.52
1:A:534:LYS:HG2	2:A:1006:HOH:O	2.09	0.51
1:A:704:ASN:ND2	1:A:704:ASN:N	2.57	0.51
1:A:470:HIS:HD2	1:A:472:LEU:H	1.59	0.51
1:A:810:GLU:OE2	1:A:810:GLU:N	2.42	0.51
1:B:648:SER:O	1:B:649:ARG:CB	2.58	0.51
1:A:541:VAL:HG11	1:A:581:ILE:HG13	1.92	0.51
1:B:112:GLN:C	2:B:1021:HOH:O	2.48	0.51
1:B:704:ASN:O	1:B:704:ASN:ND2	2.43	0.51
1:B:703:SER:OG	1:B:705:TRP:HB2	2.11	0.51
1:B:434:THR:HA	2:B:1008:HOH:O	2.10	0.51
1:B:47:CYS:O	1:B:47:CYS:SG	2.69	0.51
1:B:541:VAL:HG11	1:B:581:ILE:HG13	1.93	0.50
1:A:392:GLU:HG3	2:A:1044:HOH:O	2.11	0.50
1:A:401:GLU:HG2	1:A:430:THR:HG23	1.91	0.50
1:A:653:ARG:HH22	1:A:702:GLU:CD	2.15	0.50
1:B:326:VAL:CG1	1:B:327:GLN:N	2.66	0.50
1:B:666:GLU:OE2	1:B:684:LYS:HE3	2.12	0.50
1:B:283:ASP:HB3	1:B:289:ILE:HD11	1.94	0.49
1:A:17:ARG:HG3	2:A:1022:HOH:O	2.12	0.49
1:A:677:THR:OG1	1:A:680:GLN:NE2	2.45	0.49
1:A:704:ASN:N	1:A:705:TRP:HA	2.27	0.49
1:A:703:SER:HB3	1:A:705:TRP:HA	1.94	0.49
1:A:704:ASN:ND2	1:A:704:ASN:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:SER:HA	1:B:705:TRP:HD1	1.76	0.49
1:A:791:TYR:CG	1:A:813:ILE:HG12	2.48	0.49
1:B:574:GLU:HA	1:B:574:GLU:OE2	2.13	0.49
1:B:699:ILE:HG21	1:B:711:GLN:HB2	1.95	0.49
1:B:17:ARG:HD2	1:B:613:SER:O	2.12	0.49
1:B:35:ILE:O	1:B:49:THR:HG22	2.12	0.49
1:B:745:MET:CE	1:B:749:PHE:CZ	2.96	0.49
1:A:220:PRO:HG2	1:A:395:THR:HG23	1.95	0.49
1:A:35:ILE:O	1:A:49:THR:HG22	2.13	0.49
1:B:791:TYR:CG	1:B:813:ILE:HG12	2.48	0.49
1:A:28:LYS:HA	1:A:112:GLN:HE22	1.78	0.49
1:A:301:VAL:HG12	1:A:305:SER:CB	2.43	0.49
1:B:116:TYR:HD2	2:B:1021:HOH:O	1.96	0.49
1:B:301:VAL:HG12	1:B:305:SER:CB	2.42	0.48
1:B:400:ILE:HA	1:B:403:ILE:HD12	1.94	0.48
1:B:742:SER:OG	1:B:745:MET:HB2	2.13	0.48
1:A:10:ILE:HB	1:A:606:ILE:CD1	2.43	0.48
1:B:568:TRP:HZ2	1:B:594:SER:HB2	1.78	0.48
1:A:283:ASP:HB3	1:A:289:ILE:HD11	1.96	0.48
1:A:648:SER:O	1:A:649:ARG:CB	2.60	0.48
1:A:665:LYS:O	1:A:669:THR:HG22	2.13	0.48
1:B:206:ARG:HG3	1:B:383:ALA:HB1	1.96	0.48
1:B:665:LYS:O	1:B:669:THR:HG22	2.13	0.48
1:B:13:LYS:HE2	2:B:1052:HOH:O	2.14	0.48
1:A:400:ILE:HA	1:A:403:ILE:HD12	1.94	0.48
1:B:303:ASN:C	1:B:304:ASP:OD1	2.53	0.48
1:A:183:ARG:NH1	2:A:1011:HOH:O	2.47	0.47
1:A:303:ASN:C	1:A:304:ASP:OD1	2.53	0.47
1:B:810:GLU:HG3	2:B:1057:HOH:O	2.14	0.47
1:A:797:ARG:HA	1:A:797:ARG:NE	2.30	0.47
1:A:754:ASP:O	1:A:754:ASP:OD1	2.32	0.47
1:B:220:PRO:HG2	1:B:395:THR:HG23	1.97	0.47
1:A:703:SER:HA	1:A:705:TRP:HD1	1.79	0.47
1:A:206:ARG:HG3	1:A:383:ALA:HB1	1.96	0.47
1:A:770:ASN:C	1:A:770:ASN:OD1	2.53	0.47
1:A:227:ARG:HB2	1:A:324:TRP:CZ3	2.50	0.47
1:B:647:GLY:HA3	1:B:650:ASN:CA	2.44	0.47
1:A:337:LYS:HD2	1:A:337:LYS:HA	1.69	0.47
1:A:302:ASP:OD1	1:A:302:ASP:N	2.47	0.46
1:B:117:ILE:HG22	1:B:121:GLN:OE1	2.15	0.46
1:A:653:ARG:HD3	1:A:653:ARG:HA	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:ILE:HB	1:A:814:PRO:CD	2.45	0.46
1:B:736:LYS:HB3	1:B:737:LEU:HD23	1.97	0.46
1:B:813:ILE:HB	1:B:814:PRO:CD	2.46	0.46
1:A:647:GLY:N	1:A:650:ASN:CB	2.64	0.46
1:B:647:GLY:CA	1:B:648:SER:CB	2.52	0.46
1:A:736:LYS:HB3	1:A:737:LEU:HD23	1.98	0.46
1:A:745:MET:CE	1:A:749:PHE:CZ	2.99	0.46
1:A:765:PRO:HB2	1:A:767:HIS:CE1	2.51	0.46
1:B:859:ILE:CD1	1:B:860:ILE:CA	2.86	0.46
1:A:125:LYS:HE3	1:A:125:LYS:HB3	1.71	0.46
1:A:126:GLN:HB2	1:A:127:TYR:CE2	2.51	0.46
1:A:91:GLN:NE2	2:A:1009:HOH:O	2.44	0.46
1:B:324:TRP:CD1	1:B:324:TRP:N	2.82	0.46
1:B:746:GLU:OE1	1:B:762:ARG:NH2	2.49	0.46
1:A:800:ASN:O	1:A:804:ASP:HB2	2.16	0.45
1:B:859:ILE:CG1	1:B:860:ILE:N	2.78	0.45
1:A:506:LYS:CB	2:A:1022:HOH:O	2.56	0.45
1:A:703:SER:CB	1:A:705:TRP:HA	2.45	0.45
1:A:746:GLU:OE1	1:A:762:ARG:NH2	2.49	0.45
1:A:775:GLU:O	1:A:778:LYS:HG2	2.16	0.45
1:A:818:LYS:HB2	1:A:847:ASP:HB3	1.96	0.45
1:A:39:ASP:OD1	1:A:40:GLU:HG3	2.16	0.45
1:A:508:GLU:HG3	1:A:512:GLN:OE1	2.16	0.45
1:A:349:SER:OG	1:A:353:GLN:NE2	2.49	0.45
1:B:285:ARG:HA	1:B:285:ARG:HD3	1.68	0.45
1:B:29:VAL:HB	2:B:1021:HOH:O	2.17	0.45
1:B:856:ARG:O	1:B:860:ILE:HG13	2.16	0.45
1:A:17:ARG:CB	2:A:1022:HOH:O	2.64	0.45
1:B:40:GLU:OE1	1:B:435:LYS:CE	2.65	0.45
1:A:343:ARG:NH2	1:A:705:TRP:CH2	2.85	0.45
1:A:41:ILE:HD13	1:A:440:ILE:HG21	1.99	0.45
1:B:204:GLY:N	2:B:1010:HOH:O	2.47	0.45
1:B:231:LYS:O	1:B:235:LEU:HB2	2.18	0.45
1:B:323:VAL:C	1:B:326:VAL:CG1	2.82	0.44
1:B:34:PRO:HB3	1:B:466:ARG:HD3	1.98	0.44
1:A:358:GLU:OE2	1:A:436:HIS:ND1	2.50	0.44
1:B:125:LYS:HE3	1:B:125:LYS:HB3	1.72	0.44
1:A:478:GLN:NE2	1:A:478:GLN:HA	2.32	0.44
1:B:302:ASP:OD1	1:B:302:ASP:N	2.51	0.44
1:B:349:SER:OG	1:B:353:GLN:NE2	2.51	0.44
1:A:653:ARG:NH2	1:A:702:GLU:CD	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:SER:OG	1:A:863:SER:O	2.32	0.44
1:B:65:VAL:HG12	1:B:66:THR:N	2.31	0.44
1:A:401:GLU:HB2	1:A:402:PRO:HD3	2.00	0.44
1:B:10:ILE:HB	1:B:606:ILE:CD1	2.47	0.44
1:B:818:LYS:HB2	1:B:847:ASP:HB3	2.00	0.44
1:A:41:ILE:HD13	1:A:440:ILE:CG2	2.48	0.44
1:A:653:ARG:NH2	1:A:702:GLU:OE1	2.51	0.44
1:B:291:TYR:OH	1:B:303:ASN:HB2	2.18	0.44
1:B:508:GLU:HG3	1:B:512:GLN:OE1	2.18	0.44
1:B:797:ARG:NE	1:B:797:ARG:HA	2.33	0.43
1:A:127:TYR:CE1	2:A:1002:HOH:O	2.67	0.43
1:A:34:PRO:HB3	1:A:466:ARG:HD3	2.00	0.43
1:B:28:LYS:HA	1:B:112:GLN:HE22	1.83	0.43
1:B:800:ASN:O	1:B:804:ASP:HB2	2.18	0.43
1:B:802:SER:HA	1:B:803:THR:HA	1.73	0.43
1:A:666:GLU:OE2	1:A:684:LYS:HE3	2.18	0.43
1:A:16:GLU:H	1:A:612:SER:HB2	1.83	0.43
1:A:802:SER:HA	1:A:803:THR:HA	1.74	0.43
1:B:36:VAL:HG22	1:B:37:GLY:N	2.34	0.43
1:B:568:TRP:N	1:B:569:PRO:HD2	2.34	0.43
1:B:324:TRP:N	1:B:326:VAL:CB	2.82	0.43
1:B:136:LEU:HA	1:B:142:PRO:HB3	2.01	0.43
1:B:403:ILE:HG22	2:B:1028:HOH:O	2.18	0.43
1:B:610:LYS:N	1:B:610:LYS:HD2	2.34	0.43
1:B:765:PRO:HB2	1:B:767:HIS:CE1	2.53	0.43
1:A:610:LYS:N	1:A:610:LYS:HD2	2.33	0.43
1:A:17:ARG:HB2	2:A:1022:HOH:O	2.19	0.42
1:A:243:ARG:HG3	1:A:304:ASP:HB3	2.01	0.42
1:A:532:LYS:C	2:A:1006:HOH:O	2.58	0.42
1:A:136:LEU:HA	1:A:142:PRO:HB3	2.01	0.42
1:A:315:LEU:C	1:A:319:VAL:HG23	2.35	0.42
1:A:568:TRP:N	1:A:569:PRO:HD2	2.35	0.42
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.89	0.42
1:A:294:LEU:N	1:A:294:LEU:HD23	2.34	0.42
1:A:575:LEU:CD2	1:A:586:LYS:HG3	2.49	0.42
1:A:568:TRP:HZ2	1:A:594:SER:HB2	1.85	0.42
1:A:838:VAL:HG23	1:A:862:TRP:CH2	2.40	0.42
1:B:294:LEU:N	1:B:294:LEU:HD23	2.34	0.42
1:A:291:TYR:OH	1:A:303:ASN:HB2	2.19	0.42
1:B:387:ALA:HB3	2:B:1023:HOH:O	2.19	0.42
1:B:647:GLY:CA	1:B:650:ASN:CB	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLN:CA	1:A:478:GLN:HE21	2.32	0.42
1:A:185:ILE:HA	2:A:1012:HOH:O	2.19	0.42
1:A:221:ILE:HD11	1:A:339:ILE:HG13	2.01	0.42
1:A:231:LYS:O	1:A:235:LEU:HB2	2.19	0.42
1:A:485:LEU:HD12	1:A:489:ALA:HA	2.01	0.42
1:A:478:GLN:HE21	1:A:478:GLN:HA	1.85	0.42
1:A:330:SER:OG	1:A:401:GLU:CD	2.52	0.42
1:B:129:GLU:OE2	1:B:129:GLU:HA	2.20	0.42
1:B:221:ILE:HD11	1:B:339:ILE:HG13	2.01	0.42
1:A:659:GLU:OE1	1:A:659:GLU:HA	2.19	0.41
1:A:772:GLU:HG2	1:A:801:LYS:HG3	2.02	0.41
1:B:45:ASN:OD1	1:B:45:ASN:N	2.52	0.41
1:A:130:GLN:CA	1:A:130:GLN:OE1	2.68	0.41
1:B:401:GLU:HB2	1:B:402:PRO:HD3	2.01	0.41
1:B:575:LEU:HD22	1:B:586:LYS:HG3	2.01	0.41
1:B:745:MET:HE1	2:B:1041:HOH:O	2.19	0.41
1:B:772:GLU:HG2	1:B:801:LYS:HG3	2.02	0.41
1:A:742:SER:OG	1:A:745:MET:HB2	2.19	0.41
1:A:388:LYS:HG2	2:A:1044:HOH:O	2.21	0.41
1:A:575:LEU:HD22	1:A:586:LYS:HG3	2.01	0.41
1:B:320:ASP:C	1:B:323:VAL:HG23	2.39	0.41
1:A:248:LYS:HD3	1:A:251:GLU:OE2	2.21	0.41
1:A:857:ASN:O	1:A:861:LYS:HG3	2.20	0.41
1:B:860:ILE:CA	1:B:863:SER:OG	2.68	0.41
1:A:630:LEU:O	1:A:634:ILE:HG23	2.19	0.41
1:B:301:VAL:HG12	1:B:305:SER:HB2	2.02	0.41
1:B:659:GLU:OE2	1:B:662:ARG:NH1	2.54	0.41
1:A:45:ASN:O	1:A:46:THR:C	2.59	0.41
1:A:45:ASN:N	1:A:45:ASN:OD1	2.53	0.41
1:A:65:VAL:HG12	1:A:66:THR:N	2.34	0.41
1:A:285:ARG:HD3	1:A:285:ARG:HA	1.69	0.41
1:A:784:GLU:CD	1:A:806:LYS:HZ1	2.24	0.41
1:B:649:ARG:NH1	1:B:649:ARG:CG	2.47	0.41
1:B:130:GLN:CA	1:B:130:GLN:OE1	2.68	0.41
1:B:324:TRP:N	1:B:326:VAL:HG11	2.36	0.41
1:B:539:TYR:CE1	2:B:1016:HOH:O	2.70	0.41
1:B:810:GLU:OE2	1:B:810:GLU:CA	2.69	0.41
1:A:17:ARG:HD2	1:A:613:SER:O	2.21	0.41
1:B:575:LEU:CD2	1:B:586:LYS:HG3	2.51	0.41
1:B:784:GLU:CD	1:B:806:LYS:HZ1	2.24	0.41
1:A:239:LYS:O	1:A:307:ILE:CD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HG3	1:B:304:ASP:HB3	2.03	0.40
1:A:130:GLN:OE1	1:A:130:GLN:HA	2.21	0.40
1:B:753:GLN:HG2	1:B:754:ASP:N	2.37	0.40
1:B:219:THR:O	1:B:338:GLU:HB2	2.22	0.40
1:B:653:ARG:HA	1:B:653:ARG:HD3	1.88	0.40
1:B:693:ASP:OD1	1:B:718:ARG:NE	2.54	0.40
1:A:699:ILE:HG21	1:A:711:GLN:HB2	2.03	0.40
1:B:16:GLU:H	1:B:612:SER:HB2	1.85	0.40
1:B:64:GLY:C	2:B:1017:HOH:O	2.59	0.40
1:B:859:ILE:CD1	1:B:860:ILE:HA	2.49	0.40

There are no symmetry-related clashes.

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	855/917 (93%)	829 (97%)	25 (3%)	1 (0%)	51	79
1	B	856/917 (93%)	823 (96%)	33 (4%)	0	100	100
All	All	1711/1834 (93%)	1652 (97%)	58 (3%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU

5.3.2 Protein sidechains [i](#)

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	784/841 (93%)	642 (82%)	142 (18%)	1	4
1	B	785/841 (93%)	645 (82%)	140 (18%)	2	4
All	All	1569/1682 (93%)	1287 (82%)	282 (18%)	1	4

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	21	LEU
1	A	36	VAL
1	A	39	ASP
1	A	43	LEU
1	A	46	THR
1	A	49	THR
1	A	51	VAL
1	A	60	SER
1	A	62	HIS
1	A	92	LYS
1	A	100	ASP
1	A	125	LYS
1	A	126	GLN
1	A	131	ASN
1	A	132	ASP
1	A	134	ARG
1	A	137	ARG
1	A	192	SER
1	A	215	ASP
1	A	217	THR
1	A	225	SER
1	A	233	THR
1	A	235	LEU
1	A	236	SER
1	A	241	GLU
1	A	242	ASP
1	A	243	ARG
1	A	251	GLU
1	A	252	LYS
1	A	253	LEU
1	A	254	ASN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	265	VAL
1	A	272	ASP
1	A	274	GLN
1	A	276	SER
1	A	277	LYS
1	A	278	LEU
1	A	285	ARG
1	A	287	LYS
1	A	289	ILE
1	A	292	ASP
1	A	293	TYR
1	A	294	LEU
1	A	299	MET
1	A	300	LEU
1	A	301	VAL
1	A	302	ASP
1	A	303	ASN
1	A	304	ASP
1	A	319	VAL
1	A	321	SER
1	A	326	VAL
1	A	327	GLN
1	A	330	SER
1	A	337	LYS
1	A	338	GLU
1	A	351	ARG
1	A	385	GLU
1	A	419	SER
1	A	457	LYS
1	A	468	SER
1	A	480	LYS
1	A	482	LYS
1	A	492	GLN
1	A	499	THR
1	A	517	LEU
1	A	521	LYS
1	A	525	VAL
1	A	534	LYS
1	A	535	GLU
1	A	537	LEU
1	A	546	THR
1	A	554	LEU

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Mol	Chain	Res	Type
1	A	566	ARG
1	A	574	GLU
1	A	575	LEU
1	A	576	GLU
1	A	581	ILE
1	A	590	SER
1	A	591	ARG
1	A	595	ARG
1	A	599	GLN
1	A	602	ASN
1	A	606	ILE
1	A	607	THR
1	A	612	SER
1	A	617	LEU
1	A	623	LYS
1	A	634	ILE
1	A	637	GLU
1	A	644	TRP
1	A	645	PHE
1	A	649	ARG
1	A	650	ASN
1	A	653	ARG
1	A	654	LYS
1	A	659	GLU
1	A	668	ASN
1	A	669	THR
1	A	671	LEU
1	A	672	GLN
1	A	673	SER
1	A	677	THR
1	A	679	SER
1	A	684	LYS
1	A	686	LEU
1	A	694	LYS
1	A	700	SER
1	A	702	GLU
1	A	704	ASN
1	A	707	GLN
1	A	716	LEU
1	A	727	LEU
1	A	733	LYS
1	A	737	LEU

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Mol	Chain	Res	Type
1	A	741	ILE
1	A	745	MET
1	A	750	GLN
1	A	751	LYS
1	A	754	ASP
1	A	764	LEU
1	A	787	LYS
1	A	797	ARG
1	A	800	ASN
1	A	801	LYS
1	A	802	SER
1	A	804	ASP
1	A	805	LYS
1	A	807	THR
1	A	809	LEU
1	A	810	GLU
1	A	811	GLN
1	A	824	LEU
1	A	827	LYS
1	A	829	LYS
1	A	835	ASP
1	A	857	ASN
1	A	859	ILE
1	A	861	LYS
1	A	864	THR
1	B	8	ASP
1	B	36	VAL
1	B	39	ASP
1	B	41	ILE
1	B	43	LEU
1	B	46	THR
1	B	49	THR
1	B	51	VAL
1	B	60	SER
1	B	62	HIS
1	B	86	LYS
1	B	92	LYS
1	B	100	ASP
1	B	125	LYS
1	B	126	GLN
1	B	131	ASN
1	B	132	ASP

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Mol	Chain	Res	Type
1	B	134	ARG
1	B	137	ARG
1	B	192	SER
1	B	215	ASP
1	B	217	THR
1	B	225	SER
1	B	233	THR
1	B	235	LEU
1	B	236	SER
1	B	242	ASP
1	B	243	ARG
1	B	251	GLU
1	B	252	LYS
1	B	253	LEU
1	B	254	ASN
1	B	261	GLN
1	B	265	VAL
1	B	272	ASP
1	B	274	GLN
1	B	276	SER
1	B	277	LYS
1	B	278	LEU
1	B	285	ARG
1	B	287	LYS
1	B	289	ILE
1	B	292	ASP
1	B	293	TYR
1	B	294	LEU
1	B	299	MET
1	B	300	LEU
1	B	301	VAL
1	B	302	ASP
1	B	303	ASN
1	B	304	ASP
1	B	319	VAL
1	B	321	SER
1	B	323	VAL
1	B	324	TRP
1	B	327	GLN
1	B	337	LYS
1	B	338	GLU
1	B	351	ARG

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Mol	Chain	Res	Type
1	B	385	GLU
1	B	419	SER
1	B	457	LYS
1	B	468	SER
1	B	480	LYS
1	B	482	LYS
1	B	492	GLN
1	B	499	THR
1	B	517	LEU
1	B	521	LYS
1	B	525	VAL
1	B	534	LYS
1	B	535	GLU
1	B	537	LEU
1	B	546	THR
1	B	554	LEU
1	B	566	ARG
1	B	574	GLU
1	B	575	LEU
1	B	576	GLU
1	B	581	ILE
1	B	590	SER
1	B	591	ARG
1	B	595	ARG
1	B	599	GLN
1	B	602	ASN
1	B	606	ILE
1	B	607	THR
1	B	612	SER
1	B	617	LEU
1	B	623	LYS
1	B	634	ILE
1	B	637	GLU
1	B	644	TRP
1	B	649	ARG
1	B	653	ARG
1	B	654	LYS
1	B	659	GLU
1	B	668	ASN
1	B	669	THR
1	B	671	LEU
1	B	672	GLN

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Mol	Chain	Res	Type
1	B	673	SER
1	B	677	THR
1	B	679	SER
1	B	684	LYS
1	B	686	LEU
1	B	694	LYS
1	B	699	ILE
1	B	702	GLU
1	B	703	SER
1	B	707	GLN
1	B	716	LEU
1	B	727	LEU
1	B	733	LYS
1	B	737	LEU
1	B	741	ILE
1	B	745	MET
1	B	750	GLN
1	B	751	LYS
1	B	754	ASP
1	B	764	LEU
1	B	787	LYS
1	B	797	ARG
1	B	800	ASN
1	B	801	LYS
1	B	802	SER
1	B	804	ASP
1	B	805	LYS
1	B	807	THR
1	B	809	LEU
1	B	810	GLU
1	B	811	GLN
1	B	824	LEU
1	B	827	LYS
1	B	829	LYS
1	B	835	ASP
1	B	859	ILE
1	B	861	LYS
1	B	863	SER
1	B	864	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	89	ASN
1	A	91	GLN
1	A	112	GLN
1	A	126	GLN
1	A	143	GLN
1	A	222	ASN
1	A	366	ASN
1	A	382	HIS
1	A	411	ASN
1	A	425	GLN
1	A	445	HIS
1	A	470	HIS
1	A	478	GLN
1	A	483	HIS
1	A	507	ASN
1	A	550	ASN
1	A	572	GLN
1	A	602	ASN
1	A	650	ASN
1	A	661	GLN
1	A	680	GLN
1	A	704	ASN
1	A	707	GLN
1	A	750	GLN
1	A	769	HIS
1	A	800	ASN
1	A	857	ASN
1	A	858	ASN
1	B	89	ASN
1	B	91	GLN
1	B	112	GLN
1	B	126	GLN
1	B	131	ASN
1	B	143	GLN
1	B	222	ASN
1	B	366	ASN
1	B	382	HIS
1	B	411	ASN
1	B	425	GLN
1	B	445	HIS
1	B	470	HIS
1	B	483	HIS

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Mol	Chain	Res	Type
1	B	507	ASN
1	B	519	GLN
1	B	550	ASN
1	B	572	GLN
1	B	602	ASN
1	B	661	GLN
1	B	680	GLN
1	B	769	HIS
1	B	858	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 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

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	857/917 (93%)	0.35	83 (9%) 7 5	31, 65, 134, 199	8 (0%)
1	B	858/917 (93%)	0.44	85 (9%) 7 5	36, 76, 140, 181	8 (0%)
All	All	1715/1834 (93%)	0.40	168 (9%) 7 5	31, 71, 139, 199	16 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	707	GLN	9.4
1	A	244	ILE	8.1
1	A	294	LEU	7.0
1	A	236	SER	6.9
1	A	301	VAL	6.8
1	A	273	PRO	6.7
1	B	304	ASP	6.7
1	A	310	TRP	6.5
1	B	249	LYS	6.4
1	B	247	GLU	6.4
1	B	302	ASP	6.0
1	B	704	ASN	6.0
1	A	247	GLU	5.9
1	B	705	TRP	5.6
1	A	324	TRP	5.5
1	B	253	LEU	5.5
1	B	238	TYR	5.5
1	B	246	GLY	5.5
1	A	300	LEU	5.4
1	A	250	ASP	5.4
1	B	245	ASP	5.3
1	A	838	VAL	5.2
1	B	862	TRP	5.0
1	B	649	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	321	SER	4.9
1	A	238	TYR	4.7
1	B	645	PHE	4.7
1	B	313	THR	4.7
1	A	307	ILE	4.6
1	B	250	ASP	4.6
1	B	303	ASN	4.5
1	B	300	LEU	4.5
1	B	706	PHE	4.4
1	B	257	ILE	4.4
1	A	315	LEU	4.3
1	A	318	THR	4.3
1	B	273	PRO	4.3
1	A	275	TYR	4.2
1	A	264	LEU	4.2
1	A	232	SER	4.2
1	A	297	SER	4.1
1	B	846	ALA	4.1
1	A	314	ILE	4.0
1	A	644	TRP	4.0
1	B	211	LEU	3.9
1	A	647	GLY	3.9
1	A	304	ASP	3.9
1	B	647	GLY	3.9
1	B	264	LEU	3.8
1	B	137	ARG	3.8
1	A	254	ASN	3.7
1	B	310	TRP	3.7
1	A	272	ASP	3.7
1	A	311	ILE	3.7
1	B	251	GLU	3.6
1	A	646	ALA	3.6
1	A	276	SER	3.6
1	A	305	SER	3.6
1	A	320	ASP	3.5
1	A	298	LEU	3.5
1	B	226	LEU	3.5
1	B	242	ASP	3.4
1	B	244	ILE	3.4
1	B	305	SER	3.4
1	B	648	SER	3.3
1	A	308	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	256	LEU	3.3
1	B	241	GLU	3.2
1	A	265	VAL	3.2
1	B	809	LEU	3.2
1	A	274	GLN	3.2
1	A	645	PHE	3.2
1	A	322	THR	3.2
1	B	265	VAL	3.2
1	A	241	GLU	3.1
1	A	271	SER	3.1
1	B	173	ARG	3.1
1	B	405	TYR	3.1
1	A	482	LYS	3.1
1	B	640	GLY	3.1
1	B	254	ASN	3.0
1	B	294	LEU	3.0
1	A	306	GLU	3.0
1	B	752	ILE	3.0
1	B	646	ALA	2.9
1	A	833	ALA	2.9
1	B	415	LEU	2.9
1	A	649	ARG	2.9
1	B	643	TRP	2.9
1	A	240	ASP	2.9
1	A	251	GLU	2.9
1	B	301	VAL	2.9
1	B	237	HIS	2.8
1	A	293	TYR	2.8
1	A	235	LEU	2.8
1	B	320	ASP	2.8
1	A	231	LYS	2.8
1	B	650	ASN	2.8
1	B	235	LEU	2.8
1	B	322	THR	2.8
1	A	246	GLY	2.7
1	A	280	LEU	2.7
1	B	230	VAL	2.7
1	A	328	ALA	2.7
1	B	277	LYS	2.7
1	A	292	ASP	2.7
1	A	809	LEU	2.7
1	A	707	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	248	LYS	2.6
1	A	803	THR	2.6
1	B	260	LEU	2.6
1	A	249	LYS	2.6
1	B	207	LEU	2.6
1	A	705	TRP	2.6
1	A	837	GLN	2.6
1	B	348	ILE	2.6
1	A	242	ASP	2.6
1	B	306	GLU	2.6
1	A	253	LEU	2.6
1	B	598	LEU	2.5
1	B	227	ARG	2.5
1	A	277	LYS	2.5
1	A	319	VAL	2.5
1	A	296	ASN	2.5
1	B	596	ASP	2.5
1	B	641	ARG	2.5
1	B	252	LYS	2.5
1	A	774	ILE	2.5
1	A	835	ASP	2.4
1	B	644	TRP	2.4
1	B	777	PHE	2.4
1	A	640	GLY	2.4
1	B	386	ILE	2.4
1	A	802	SER	2.4
1	A	137	ARG	2.4
1	A	321	SER	2.4
1	A	252	LYS	2.4
1	B	234	VAL	2.4
1	A	245	ASP	2.4
1	B	274	GLN	2.4
1	A	302	ASP	2.3
1	A	323	VAL	2.3
1	A	309	ASP	2.3
1	B	324	TRP	2.3
1	A	256	LEU	2.3
1	B	276	SER	2.3
1	B	344	ASP	2.2
1	B	835	ASP	2.2
1	A	266	LYS	2.2
1	A	704	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	LYS	2.2
1	B	597	ASN	2.2
1	B	599	GLN	2.2
1	B	482	LYS	2.2
1	B	213	PRO	2.2
1	B	421	LEU	2.1
1	B	703	SER	2.1
1	B	758	GLN	2.1
1	A	286	GLY	2.1
1	B	374	GLY	2.1
1	A	842	LEU	2.1
1	A	284	PRO	2.0
1	A	173	ARG	2.0
1	B	285	ARG	2.0
1	B	293	TYR	2.0
1	A	845	LEU	2.0
1	B	314	ILE	2.0
1	A	648	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.