



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:21 PM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

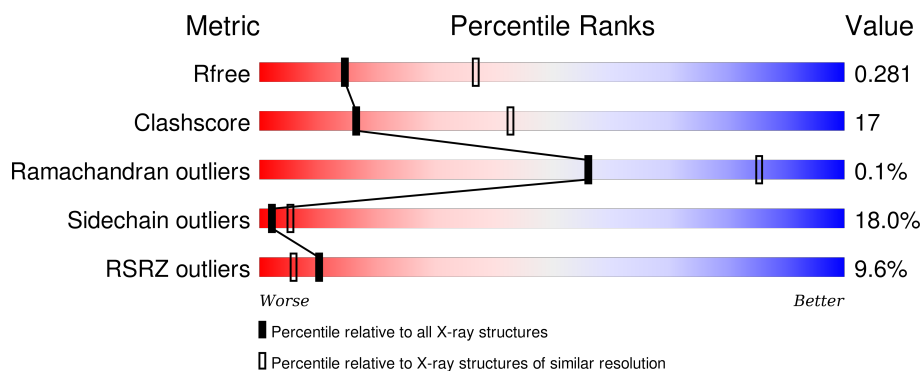
1 Overall quality at a glance

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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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. 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

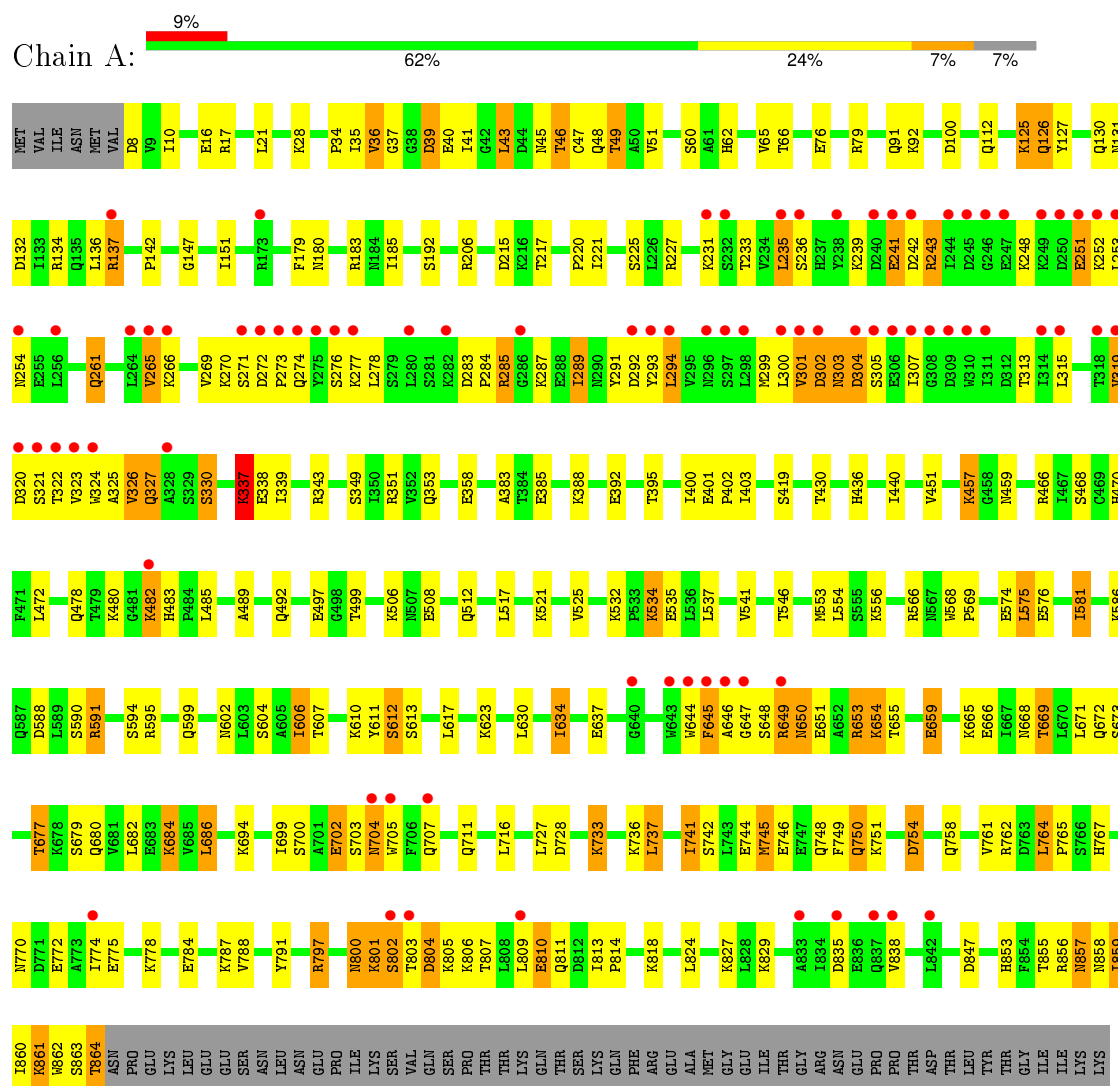
- Molecule 2 is water.

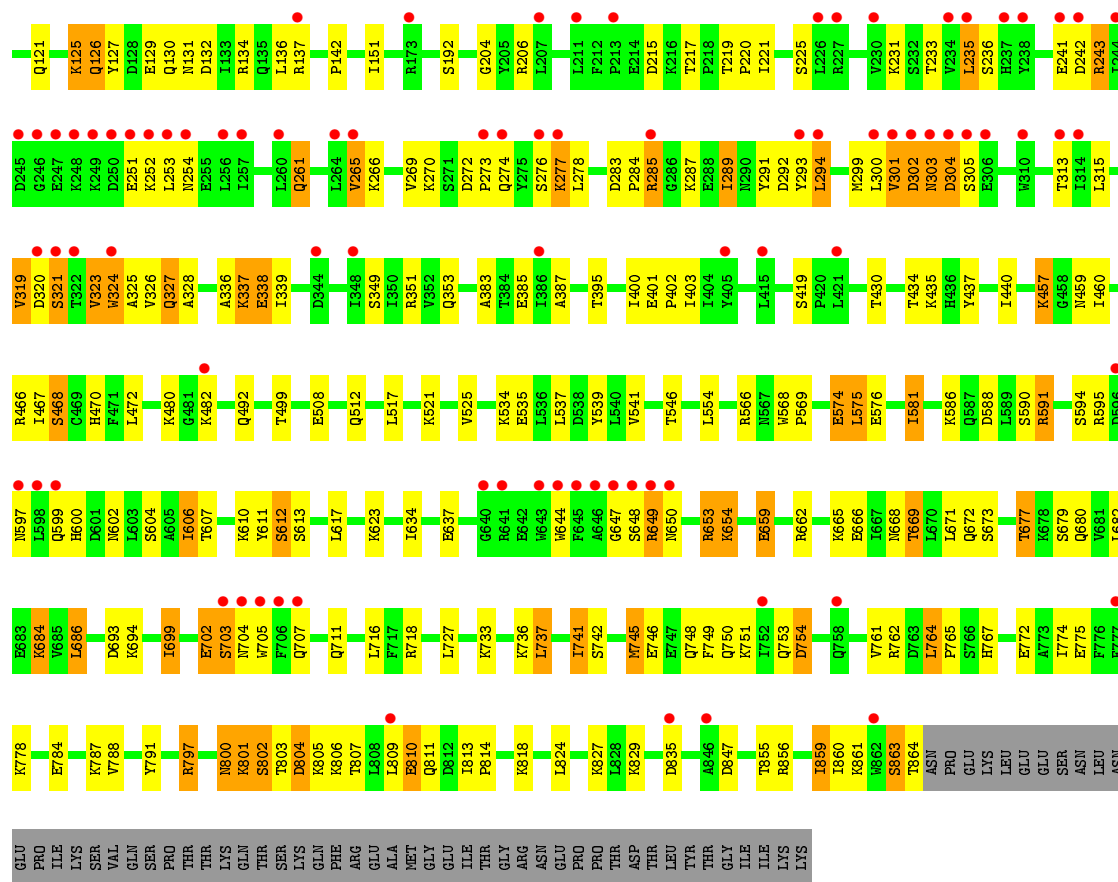
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	64	Total	O	0	0
			64	64		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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





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	Depositor
R, R_{free}	0.225 , 0.281 0.224 , 0.281	Depositor DCC
R_{free} test set	2708 reflections (5.35%)	DCC
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 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53343 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:B:703:SER:CB	1:B:704:ASN:HA	1.41	1.41
1:A:703:SER:HB3	1:A:704:ASN:CA	1.48	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:B:647:GLY:CA	1:B:648:SER:HB3	1.72	1.17
1:A:43:LEU:H	1:A:43:LEU:CD2	1.52	1.17
1:B:647:GLY:HA2	1:B:648:SER:CB	1.69	1.17
1:A:863:SER:O	1:A:864:THR:HG22	1.44	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:CD	1:A:457:LYS:H	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:B:325:ALA:H	1:B:326:VAL:HG12	1.17	1.06
1:A:647:GLY:HA3	1:A:650:ASN:H	1.19	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:859:ILE:CD1	1:A:859:ILE:C	2.30	0.97
1:A:647:GLY:N	1:A:650:ASN:HB2	1.79	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:B:325:ALA:HA	1:B:327:GLN:N	1.82	0.94
1:A:744:GLU:OE2	2:A:1001:HOH:O	1.85	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:HD2	1:A:457:LYS:H	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:CA	1:B:702:GLU:OE2	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:HA	1:B:702:GLU:OE2	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:B:647:GLY:H	1:B:650:ASN:HB2	1.54	0.72
1:A:482:LYS:HB3	2:A:1002:HOH:O	1.88	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:648:SER:O	1:B:649:ARG:CG	2.39	0.71
1:B:597:ASN:ND2	2:B:1002:HOH:O	2.22	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:A:127:TYR:OH	2:A:1002:HOH:O	2.09	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:859:ILE:HD12	1:A:860:ILE:HA	1.72	0.69
1:A:611:TYR:OH	1:A:745:MET:HG2	1.93	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:611:TYR:OH	1:B:745:MET:HG2	1.93	0.68
1:B:36:VAL:HG13	1:B:467:ILE:HB	1.74	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:703:SER:OG	1:A:705:TRP:HB2	1.95	0.65
1:A:41:ILE:HG13	1:A:451:VAL:HG22	1.78	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:647:GLY:HA2	1:B:648:SER:HB3	0.79	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:327:GLN:OE1	1:B:328:ALA:N	2.30	0.65
1:B:126:GLN:HB2	1:B:127:TYR:CD2	2.32	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:859:ILE:O	1:A:859:ILE:HD12	1.99	0.62
1:A:179:PHE:C	2:A:1019:HOH:O	2.37	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:OD2	1:B:8:ASP:N	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:B:41:ILE:HD13	1:B:440:ILE:HG23	1.85	0.59
1:A:324:TRP:O	1:A:325:ALA:HB3	2.03	0.59
1:B:647:GLY:CA	1:B:650:ASN:H	2.08	0.58
1:A:269:VAL:HA	1:A:273:PRO:HA	1.85	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:B:325:ALA:CA	1:B:327:GLN:N	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ILE:HG22	1:B:742:SER:H	1.69	0.58
1:A:261:GLN:O	1:A:265:VAL:HG23	2.04	0.58
1:A:750:GLN:NE2	1:A:758:GLN:NE2	2.50	0.58
1:A:741:ILE:HG22	1:A:742:SER:H	1.69	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:686:LEU:HD21	1:B:686:LEU:HD21	1.86	0.57
1:A:47:CYS:SG	1:A:47:CYS:O	2.61	0.57
1:B:457:LYS:H	1:B:457:LYS:HE2	1.68	0.57
1:A:801:LYS:HD3	1:A:802:SER:N	2.18	0.57
1:A:647:GLY:H	1:A:650:ASN:CB	2.16	0.57
1:A:323:VAL:O	1:A:326:VAL:CB	2.53	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:810:GLU:N	1:B:810:GLU:OE2	2.37	0.57
1:B:659:GLU:OE1	1:B:659:GLU:HA	2.04	0.57
1:B:703:SER:C	1:B:705:TRP:HA	2.24	0.56
1:B:703:SER:CB	1:B:704:ASN:CA	2.30	0.56
1:A:761:VAL:HA	1:A:764:LEU:HD22	1.87	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:648:SER:C	1:A:649:ARG:CG	2.59	0.54
1:A:36:VAL:CG2	1:A:37:GLY:N	2.69	0.54
1:A:151:ILE:HG23	1:A:459:ASN:ND2	2.22	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:B:775:GLU:O	1:B:778:LYS:HG2	2.09	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:A:853:HIS:O	1:A:858:ASN:OD1	2.27	0.52
1:A:704:ASN:ND2	1:A:704:ASN:N	2.57	0.51
1:A:534:LYS:HG2	2:A:1006:HOH:O	2.09	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:704:ASN:O	1:B:704:ASN:ND2	2.43	0.51
1:B:112:GLN:C	2:B:1021:HOH:O	2.48	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:703:SER:HB3	1:A:705:TRP:HA	1.94	0.49
1:A:704:ASN:N	1:A:705:TRP:HA	2.27	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:B:703:SER:HA	1:B:705:TRP:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASN:ND2	1:A:704:ASN:H	2.10	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:35:ILE:O	1:B:49:THR:HG22	2.12	0.49
1:B:17:ARG:HD2	1:B:613:SER:O	2.12	0.49
1:B:745:MET:CE	1:B:749:PHE:CZ	2.96	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:220:PRO:HG2	1:A:395:THR:HG23	1.95	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:A:28:LYS:HA	1:A:112:GLN:HE22	1.78	0.49
1:B:742:SER:OG	1:B:745:MET:HB2	2.13	0.48
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: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:B:303:ASN:C	1:B:304:ASP:OD1	2.53	0.48
1:A:400:ILE:HA	1:A:403:ILE:HD12	1.94	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:A:703:SER:HA	1:A:705:TRP:HD1	1.79	0.47
1:B:220:PRO:HG2	1:B:395:THR:HG23	1.97	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:B:647:GLY:HA3	1:B:650:ASN:CA	2.44	0.47
1:A:227:ARG:HB2	1:A:324:TRP:CZ3	2.50	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:B:859:ILE:CD1	1:B:860:ILE:CA	2.86	0.46
1:A:745:MET:CE	1:A:749:PHE:CZ	2.99	0.46
1:A:736:LYS:HB3	1:A:737:LEU:HD23	1.98	0.46
1:A:765:PRO:HB2	1:A:767:HIS:CE1	2.51	0.46
1:A:126:GLN:HB2	1:A:127:TYR:CE2	2.51	0.46
1:A:125:LYS:HE3	1:A:125:LYS:HB3	1.71	0.46
1:B:324:TRP:CD1	1:B:324:TRP:N	2.82	0.46
1:A:91:GLN:NE2	2:A:1009:HOH:O	2.44	0.46
1:B:746:GLU:OE1	1:B:762:ARG:NH2	2.49	0.46
1:B:859:ILE:CG1	1:B:860:ILE:N	2.78	0.45
1:A:800:ASN:O	1:A:804:ASP:HB2	2.16	0.45
1:A:703:SER:CB	1:A:705:TRP:HA	2.45	0.45
1:A:506:LYS:CB	2:A:1022:HOH:O	2.56	0.45
1:A:775:GLU:O	1:A:778:LYS:HG2	2.16	0.45
1:A:746:GLU:OE1	1:A:762:ARG:NH2	2.49	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:29:VAL:HB	2:B:1021:HOH:O	2.17	0.45
1:B:285:ARG:HA	1:B:285:ARG:HD3	1.68	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: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:A:34:PRO:HB3	1:A:466:ARG:HD3	2.00	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:B:36:VAL:HG22	1:B:37:GLY:N	2.34	0.43
1:A:802:SER:HA	1:A:803:THR:HA	1.74	0.43
1:B:568:TRP:N	1:B:569:PRO:HD2	2.34	0.43
1:A:16:GLU:H	1:A:612:SER:HB2	1.83	0.43
1:B:324:TRP:N	1:B:326:VAL:CB	2.82	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:B:136:LEU:HA	1:B:142:PRO:HB3	2.01	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: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:136:LEU:HA	1:A:142:PRO:HB3	2.01	0.42
1:A:838:VAL:HG23	1:A:862:TRP:CH2	2.40	0.42
1:A:568:TRP:HZ2	1:A:594:SER:HB2	1.85	0.42
1:A:575:LEU:CD2	1:A:586:LYS:HG3	2.49	0.42
1:A:294:LEU:N	1:A:294:LEU:HD23	2.34	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:647:GLY:CA	1:B:650:ASN:CB	2.78	0.42
1:B:387:ALA:HB3	2:B:1023:HOH:O	2.19	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:485:LEU:HD12	1:A:489:ALA:HA	2.01	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:185:ILE:HA	2:A:1012:HOH:O	2.19	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:772:GLU:HG2	1:A:801:LYS:HG3	2.02	0.41
1:A:659:GLU:OE1	1:A:659:GLU:HA	2.19	0.41
1:B:45:ASN:OD1	1:B:45:ASN:N	2.52	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:B:401:GLU:HB2	1:B:402:PRO:HD3	2.01	0.41
1:A:130:GLN:CA	1:A:130:GLN:OE1	2.68	0.41
1:B:575:LEU:HD22	1:B:586:LYS:HG3	2.01	0.41
1:A:742:SER:OG	1:A:745:MET:HB2	2.19	0.41
1:B:320:ASP:C	1:B:323:VAL:HG23	2.39	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:860:ILE:CA	1:B:863:SER:OG	2.68	0.41
1:A:857:ASN:O	1:A:861:LYS:HG3	2.20	0.41
1:A:248:LYS:HD3	1:A:251:GLU:OE2	2.21	0.41
1:B:659:GLU:OE2	1:B:662:ARG:NH1	2.54	0.41
1:B:301:VAL:HG12	1:B:305:SER:HB2	2.02	0.41
1:A:630:LEU:O	1:A:634:ILE:HG23	2.19	0.41
1:A:45:ASN:N	1:A:45:ASN:OD1	2.53	0.41
1:A:45:ASN:O	1:A:46:THR:C	2.59	0.41
1:A:65:VAL:HG12	1:A:66:THR:N	2.34	0.41
1:B:649:ARG:NH1	1:B:649:ARG:CG	2.47	0.41
1:A:784:GLU:CD	1:A:806:LYS:HZ1	2.24	0.41
1:A:285:ARG:HD3	1:A:285:ARG:HA	1.69	0.41
1:B:324:TRP:N	1:B:326:VAL:HG11	2.36	0.41
1:B:810:GLU:OE2	1:B:810:GLU:CA	2.69	0.41
1:B:130:GLN:CA	1:B:130:GLN:OE1	2.68	0.41
1:B:539:TYR:CE1	2:B:1016:HOH:O	2.70	0.41
1:A:17:ARG:HD2	1:A:613:SER:O	2.21	0.41
1:B:784:GLU:CD	1:B:806:LYS:HZ1	2.24	0.41
1:B:575:LEU:CD2	1:B:586:LYS:HG3	2.51	0.41
1:B:243:ARG:HG3	1:B:304:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:O	1:A:307:ILE:CD1	2.69	0.40
1:B:753:GLN:HG2	1:B:754:ASP:N	2.37	0.40
1:A:130:GLN:OE1	1:A:130:GLN:HA	2.21	0.40
1:B:693:ASP:OD1	1:B:718:ARG:NE	2.54	0.40
1:B:653:ARG:HA	1:B:653:ARG:HD3	1.88	0.40
1:B:219:THR:O	1:B:338:GLU:HB2	2.22	0.40
1:B:859:ILE:CD1	1:B:860:ILE:HA	2.49	0.40
1:B:64:GLY:C	2:B:1017:HOH:O	2.59	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

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%)	56	85
1	B	856/917 (93%)	823 (96%)	33 (4%)	0	100	100
All	All	1711/1834 (93%)	1652 (97%)	58 (3%)	1 (0%)	56	85

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%)	2	5
1	B	785/841 (93%)	645 (82%)	140 (18%)	2	5
All	All	1569/1682 (93%)	1287 (82%)	282 (18%)	2	5

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	81 (9%) 10 6	31, 65, 134, 199	8 (0%)
1	B	858/917 (93%)	0.44	84 (9%) 10 5	36, 76, 140, 181	8 (0%)
All	All	1715/1834 (93%)	0.40	165 (9%) 10 6	31, 71, 139, 199	16 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	707	GLN	9.5
1	A	244	ILE	8.0
1	A	301	VAL	7.1
1	A	294	LEU	7.0
1	A	273	PRO	6.8
1	A	236	SER	6.7
1	B	304	ASP	6.6
1	A	310	TRP	6.5
1	B	249	LYS	6.5
1	B	247	GLU	6.2
1	B	704	ASN	6.2
1	B	302	ASP	5.9
1	A	247	GLU	5.8
1	B	705	TRP	5.7
1	B	253	LEU	5.5
1	A	324	TRP	5.5
1	B	246	GLY	5.5
1	B	245	ASP	5.4
1	B	238	TYR	5.4
1	A	300	LEU	5.3
1	A	838	VAL	5.2
1	A	250	ASP	5.1
1	B	862	TRP	5.0
1	B	321	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	303	ASN	4.8
1	A	238	TYR	4.8
1	B	649	ARG	4.7
1	B	645	PHE	4.7
1	B	250	ASP	4.6
1	A	307	ILE	4.6
1	B	313	THR	4.6
1	B	257	ILE	4.5
1	B	300	LEU	4.5
1	B	706	PHE	4.4
1	B	273	PRO	4.3
1	A	318	THR	4.3
1	A	315	LEU	4.2
1	A	264	LEU	4.2
1	A	297	SER	4.2
1	A	275	TYR	4.2
1	A	232	SER	4.1
1	A	647	GLY	4.1
1	A	314	ILE	4.0
1	B	846	ALA	4.0
1	A	644	TRP	3.9
1	B	211	LEU	3.9
1	B	264	LEU	3.9
1	B	647	GLY	3.8
1	A	272	ASP	3.8
1	A	276	SER	3.8
1	B	137	ARG	3.8
1	A	304	ASP	3.7
1	A	311	ILE	3.7
1	A	646	ALA	3.7
1	B	310	TRP	3.7
1	B	226	LEU	3.6
1	A	308	GLY	3.6
1	A	254	ASN	3.6
1	A	305	SER	3.5
1	B	305	SER	3.5
1	B	251	GLU	3.5
1	A	298	LEU	3.4
1	B	244	ILE	3.4
1	B	242	ASP	3.4
1	A	320	ASP	3.4
1	B	241	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	3.3
1	A	322	THR	3.2
1	B	265	VAL	3.2
1	A	645	PHE	3.2
1	A	271	SER	3.2
1	A	274	GLN	3.2
1	A	241	GLU	3.2
1	B	256	LEU	3.2
1	B	809	LEU	3.1
1	A	482	LYS	3.1
1	B	173	ARG	3.1
1	B	405	TYR	3.1
1	B	648	SER	3.1
1	B	752	ILE	3.0
1	B	643	TRP	3.0
1	B	294	LEU	3.0
1	A	306	GLU	3.0
1	B	254	ASN	2.9
1	A	649	ARG	2.9
1	B	322	THR	2.9
1	B	301	VAL	2.9
1	B	640	GLY	2.9
1	A	240	ASP	2.8
1	A	833	ALA	2.8
1	A	293	TYR	2.8
1	B	235	LEU	2.8
1	B	415	LEU	2.8
1	B	277	LYS	2.8
1	A	251	GLU	2.7
1	A	328	ALA	2.7
1	B	320	ASP	2.7
1	B	237	HIS	2.7
1	A	231	LYS	2.7
1	A	242	ASP	2.7
1	A	280	LEU	2.7
1	B	646	ALA	2.7
1	A	292	ASP	2.7
1	B	248	LYS	2.7
1	A	707	GLN	2.7
1	B	650	ASN	2.6
1	A	705	TRP	2.6
1	B	348	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	809	LEU	2.6
1	A	837	GLN	2.6
1	B	596	ASP	2.6
1	A	235	LEU	2.6
1	B	207	LEU	2.6
1	B	260	LEU	2.6
1	A	246	GLY	2.6
1	B	230	VAL	2.6
1	A	319	VAL	2.6
1	A	296	ASN	2.6
1	A	803	THR	2.6
1	A	253	LEU	2.6
1	B	306	GLU	2.6
1	A	277	LYS	2.6
1	B	598	LEU	2.5
1	B	777	PHE	2.5
1	B	276	SER	2.5
1	A	640	GLY	2.5
1	A	774	ILE	2.5
1	B	386	ILE	2.5
1	A	802	SER	2.4
1	B	641	ARG	2.4
1	B	252	LYS	2.4
1	A	249	LYS	2.4
1	A	835	ASP	2.4
1	B	644	TRP	2.4
1	A	137	ARG	2.4
1	B	227	ARG	2.4
1	A	323	VAL	2.3
1	B	274	GLN	2.3
1	B	234	VAL	2.3
1	B	599	GLN	2.3
1	A	309	ASP	2.3
1	A	282	LYS	2.3
1	A	245	ASP	2.3
1	A	302	ASP	2.3
1	A	252	LYS	2.3
1	B	324	TRP	2.3
1	B	835	ASP	2.2
1	A	256	LEU	2.2
1	B	344	ASP	2.2
1	B	597	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	2.2
1	A	266	LYS	2.2
1	B	482	LYS	2.2
1	A	321	SER	2.2
1	A	704	ASN	2.1
1	B	703	SER	2.1
1	A	842	LEU	2.1
1	A	286	GLY	2.1
1	B	213	PRO	2.1
1	B	285	ARG	2.1
1	B	758	GLN	2.1
1	B	314	ILE	2.1
1	B	293	TYR	2.0
1	A	173	ARG	2.0
1	A	643	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.