



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 AM GMT

PDB ID : 2FSF
Title : Escherichia coli SecA, the preprotein translocase dimeric ATPase
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.
Deposited on : 2006-01-23
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

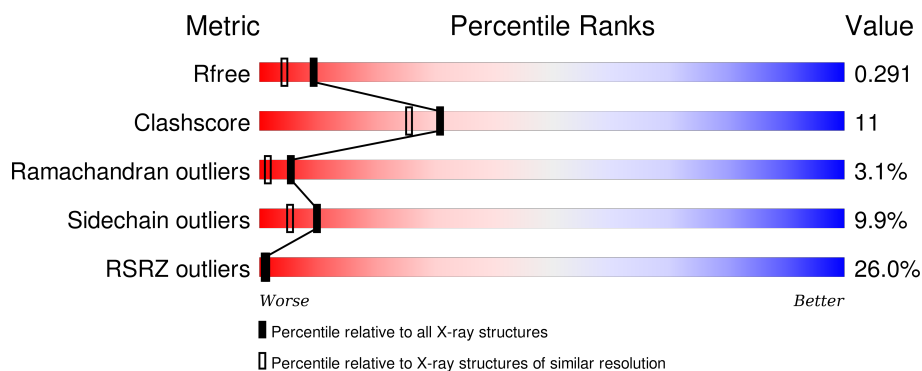
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	853	<div> <div>15%</div> <div>61%</div> <div>15%</div> <div>• •</div> <div>20%</div> </div>
1	B	853	<div> <div>28%</div> <div>55%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11637 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 Preprotein translocase secA subunit.

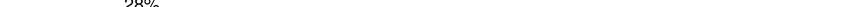
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5462	3426	966	1044	26			
1	B	723	Total	C	N	O	S	0	0	0
			5741	3600	1009	1104	28			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	257	Total	O	0	0
			257	257		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:**
-
- The sequence logo displays the following amino acids (from top to bottom): VAL, PHE, GLY, SER, R13, N14, D15, R16, T17, L18, R19, E20, M21, V24, A30, K31, E32, P33, K37, I38, S39, D40, E41, E42, E55, K56, E61, P65, A69, V70, W71, R72, R82, L88, C98, I99, A100, E101, M102, R103, T113, L114, P115, A116, Y117, H127, V128, F130.
- Conservation percentages are indicated by the color scale: 15% (red), 61% (green), 15% (yellow), and 20% (grey).

- Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.03Å 90.17Å 163.05Å 90.00° 100.48° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.98-2.00) 97.1 (19.98-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.261 0.257 , 0.291	Depositor DCC
R_{free} test set	7014 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.3	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 140049 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11637	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 ⓘ

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	1.34	35/5552 (0.6%)	1.10	19/7491 (0.3%)
1	B	1.49	61/5833 (1.0%)	1.20	36/7870 (0.5%)
All	All	1.42	96/11385 (0.8%)	1.15	55/15361 (0.4%)

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	4
1	B	0	9
All	All	0	13

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	CYS	CB-SG	-13.49	1.59	1.82
1	A	698	GLU	CD-OE2	13.10	1.40	1.25
1	A	698	GLU	CD-OE1	10.85	1.37	1.25
1	A	560	GLU	CG-CD	9.58	1.66	1.51
1	A	697	LEU	C-N	9.56	1.56	1.34
1	B	284	GLU	CD-OE2	9.48	1.36	1.25
1	A	695	GLN	C-O	8.68	1.39	1.23
1	A	698	GLU	C-O	8.58	1.39	1.23
1	B	393	THR	N-CA	8.55	1.63	1.46
1	B	103	ARG	CG-CD	8.49	1.73	1.51
1	B	395	ASP	N-CA	8.31	1.62	1.46
1	B	652	ALA	CA-CB	8.26	1.69	1.52
1	B	385	GLU	CG-CD	8.09	1.64	1.51
1	B	98	CYS	CB-SG	-8.04	1.68	1.82
1	B	393	THR	C-O	7.89	1.38	1.23
1	B	210	GLU	CG-CD	7.84	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	VAL	CB-CG1	-7.25	1.37	1.52
1	B	61	GLU	CD-OE1	7.23	1.33	1.25
1	A	752	GLU	CG-CD	7.22	1.62	1.51
1	B	802	GLU	CD-OE1	7.20	1.33	1.25
1	B	66	GLU	CD-OE2	7.10	1.33	1.25
1	B	41	GLU	CG-CD	7.06	1.62	1.51
1	B	168	GLU	CB-CG	-7.04	1.38	1.52
1	A	197	GLU	CG-CD	6.81	1.62	1.51
1	A	460	GLU	CG-CD	6.64	1.61	1.51
1	B	512	ASP	CB-CG	6.63	1.65	1.51
1	B	625	LYS	CD-CE	6.50	1.67	1.51
1	B	97	ARG	CG-CD	6.49	1.68	1.51
1	B	385	GLU	CD-OE1	6.40	1.32	1.25
1	B	806	GLU	CG-CD	6.37	1.61	1.51
1	B	801	GLN	N-CA	6.35	1.59	1.46
1	A	136	ALA	CA-CB	6.35	1.65	1.52
1	A	660	TYR	CE1-CZ	6.33	1.46	1.38
1	B	197	GLU	CD-OE2	6.25	1.32	1.25
1	A	745	GLU	CG-CD	6.22	1.61	1.51
1	B	66	GLU	CG-CD	6.20	1.61	1.51
1	B	428	TYR	CE1-CZ	-6.12	1.30	1.38
1	A	163	ALA	CA-CB	-6.10	1.39	1.52
1	B	381	PHE	CE1-CZ	6.10	1.49	1.37
1	A	61	GLU	CD-OE1	6.10	1.32	1.25
1	B	23	LYS	CE-NZ	6.09	1.64	1.49
1	B	589	SER	CB-OG	-6.07	1.34	1.42
1	A	141	GLU	CD-OE1	6.06	1.32	1.25
1	A	406	LYS	CD-CE	6.05	1.66	1.51
1	B	96	GLU	CD-OE1	6.04	1.32	1.25
1	B	394	ALA	CA-CB	6.01	1.65	1.52
1	B	182	TYR	CD1-CE1	6.00	1.48	1.39
1	B	61	GLU	CD-OE2	5.95	1.32	1.25
1	B	393	THR	CA-CB	5.90	1.68	1.53
1	B	708	GLU	CB-CG	5.87	1.63	1.52
1	B	821	GLU	CG-CD	-5.82	1.43	1.51
1	B	385	GLU	CD-OE2	5.80	1.32	1.25
1	B	66	GLU	CB-CG	-5.78	1.41	1.52
1	B	822	VAL	CB-CG2	5.77	1.65	1.52
1	A	197	GLU	CD-OE1	5.77	1.31	1.25
1	A	698	GLU	C-N	5.74	1.47	1.34
1	A	460	GLU	CB-CG	5.74	1.63	1.52
1	A	61	GLU	CB-CG	5.68	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	752	GLU	CD-OE1	5.65	1.31	1.25
1	B	452	VAL	CB-CG2	-5.55	1.41	1.52
1	A	673	SER	CB-OG	-5.54	1.35	1.42
1	A	466	SER	C-O	5.51	1.33	1.23
1	A	394	ALA	CA-CB	5.51	1.64	1.52
1	B	173	ASP	CB-CG	5.50	1.63	1.51
1	B	560	GLU	CG-CD	5.49	1.60	1.51
1	B	380	TYR	CE2-CZ	-5.47	1.31	1.38
1	A	56	LYS	CD-CE	5.46	1.64	1.51
1	B	196	GLU	CD-OE1	-5.45	1.19	1.25
1	A	665	GLU	CG-CD	5.36	1.59	1.51
1	B	126	VAL	CB-CG2	5.36	1.64	1.52
1	A	396	THR	N-CA	5.33	1.57	1.46
1	A	776	LYS	CD-CE	5.33	1.64	1.51
1	B	625	LYS	CE-NZ	5.32	1.62	1.49
1	B	411	VAL	CB-CG1	5.30	1.64	1.52
1	B	124	LYS	CD-CE	5.29	1.64	1.51
1	B	647	GLU	CD-OE2	5.27	1.31	1.25
1	B	197	GLU	CG-CD	5.22	1.59	1.51
1	B	182	TYR	CD2-CE2	5.22	1.47	1.39
1	A	560	GLU	CD-OE1	5.20	1.31	1.25
1	B	106	GLU	CG-CD	5.19	1.59	1.51
1	B	141	GLU	CG-CD	5.18	1.59	1.51
1	B	127	HIS	C-O	-5.16	1.13	1.23
1	B	176	TYR	CB-CG	5.16	1.59	1.51
1	B	395	ASP	CA-C	5.15	1.66	1.52
1	B	388	ALA	CA-CB	5.14	1.63	1.52
1	B	386	LYS	CD-CE	5.14	1.64	1.51
1	B	196	GLU	CB-CG	-5.12	1.42	1.52
1	B	503	ALA	CA-CB	-5.08	1.41	1.52
1	B	626	ALA	CA-CB	-5.06	1.41	1.52
1	A	197	GLU	CD-OE2	5.05	1.31	1.25
1	A	406	LYS	CE-NZ	5.04	1.61	1.49
1	B	406	LYS	CD-CE	5.04	1.63	1.51
1	B	68	PHE	CD1-CE1	5.03	1.49	1.39
1	A	201	ARG	CB-CG	-5.03	1.39	1.52
1	B	56	LYS	CE-NZ	5.03	1.61	1.49
1	A	101	GLU	CG-CD	5.01	1.59	1.51

All (55) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	B	425	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	B	425	ASP	CB-CG-OD1	9.05	126.45	118.30
1	A	72	ARG	NE-CZ-NH2	8.68	124.64	120.30
1	B	561	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	782	MET	CG-SD-CE	7.75	112.59	100.20
1	B	408	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	A	72	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	A	574	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	800	LYS	N-CA-C	-7.32	91.25	111.00
1	B	167	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	209	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	657	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	A	574	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	B	801	GLN	N-CA-CB	7.04	123.27	110.60
1	A	420	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	85	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	625	LYS	CD-CE-NZ	6.55	126.76	111.70
1	B	779	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	429	MET	CG-SD-CE	-6.51	89.78	100.20
1	B	185	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	561	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	40	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	566	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	209	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	544	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	441	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	82	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	82	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	832	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	B	374	SER	CA-CB-OG	-5.75	95.69	111.20
1	B	663	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	34	GLU	CB-CA-C	-5.70	99.01	110.40
1	B	568	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	205	TYR	CD1-CE1-CZ	-5.64	114.72	119.80
1	B	420	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	198	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	418	MET	CG-SD-CE	5.61	109.17	100.20
1	B	103	ARG	CG-CD-NE	5.59	123.54	111.80
1	B	16	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	589	SER	CB-CA-C	-5.49	99.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	ARG	CG-CD-NE	-5.49	100.27	111.80
1	B	385	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	B	540	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	408	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	698	GLU	O-C-N	5.38	131.31	122.70
1	A	139	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	697	LEU	C-N-CA	-5.32	108.41	121.70
1	B	608	ARG	N-CA-CB	5.29	120.13	110.60
1	A	198	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	800	LYS	C-N-CA	-5.26	108.55	121.70
1	B	40	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	286	LEU	CA-CB-CG	5.16	127.18	115.30
1	B	800	LYS	O-C-N	-5.16	114.44	122.70
1	A	689	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Peptide
1	A	393	THR	Peptide
1	A	395	ASP	Peptide
1	A	697	LEU	Mainchain
1	B	229	ALA	Peptide
1	B	300	SER	Peptide
1	B	365	ILE	Peptide
1	B	393	THR	Peptide
1	B	394	ALA	Peptide
1	B	597	ILE	Peptide
1	B	607	MET	Peptide
1	B	610	LEU	Peptide
1	B	793	GLY	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	5462	0	5460	90	0
1	B	5741	0	5731	155	1
2	A	177	0	0	12	0
2	B	257	0	0	30	0
All	All	11637	0	11191	245	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 11.

All (245) 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:96:GLU:HG3	2:B:1033:HOH:O	1.46	1.13
1:A:799:PRO:HA	2:A:1026:HOH:O	1.50	1.08
1:B:800:LYS:O	1:B:801:GLN:HB2	1.61	1.01
1:B:103:ARG:HH11	1:B:103:ARG:HG3	1.26	0.97
1:A:799:PRO:C	1:A:800:LYS:O	1.95	0.93
1:A:394:ALA:HA	2:A:980:HOH:O	1.68	0.92
1:A:15:ASP:HA	1:A:18:LEU:HB2	1.53	0.91
1:B:457:ILE:O	1:B:505:ASN:ND2	2.10	0.85
1:A:732:GLU:OE2	1:A:736:ARG:NH1	2.11	0.84
1:A:736:ARG:CZ	2:A:1005:HOH:O	2.25	0.84
1:A:799:PRO:CA	2:A:1026:HOH:O	2.18	0.82
1:A:731:HIS:HB3	2:A:1016:HOH:O	1.80	0.81
1:A:736:ARG:NE	2:A:1005:HOH:O	2.14	0.80
1:B:693:PRO:O	1:B:696:SER:HB2	1.80	0.80
1:A:598:PHE:O	1:A:600:SER:N	2.15	0.80
1:B:103:ARG:HD2	1:B:104:THR:N	1.99	0.78
1:A:535:GLU:HA	1:A:535:GLU:OE1	1.82	0.78
1:B:230:GLU:OE2	1:B:369:ASN:HA	1.85	0.77
1:B:395:ASP:CB	2:B:964:HOH:O	2.32	0.76
1:B:395:ASP:CA	2:B:964:HOH:O	2.34	0.76
1:A:731:HIS:NE2	1:A:733:GLU:HB3	2.01	0.75
1:B:800:LYS:O	1:B:801:GLN:CB	2.23	0.75
1:B:33:PRO:O	1:B:37:LYS:HD3	1.86	0.74
1:A:103:ARG:NH1	1:A:573:GLY:O	2.21	0.74
1:B:103:ARG:HH11	1:B:103:ARG:CG	2.01	0.74
1:B:598:PHE:O	1:B:600:SER:N	2.21	0.73
1:B:788:GLY:O	1:B:792:ARG:N	2.21	0.72
1:B:16:ARG:NE	1:B:19:ARG:HH21	1.88	0.71
1:B:395:ASP:HB2	2:B:964:HOH:O	1.88	0.71
1:B:395:ASP:HA	2:B:964:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ARG:HG3	2:B:1078:HOH:O	1.92	0.70
1:B:392:GLY:O	1:B:394:ALA:CA	2.40	0.70
1:B:228:PRO:O	1:B:230:GLU:N	2.23	0.69
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.90	0.68
1:A:657:ARG:HD3	2:A:1006:HOH:O	1.92	0.68
1:B:103:ARG:HD3	2:B:888:HOH:O	1.93	0.68
1:A:101:GLU:OE2	1:A:393:THR:HA	1.93	0.68
1:B:103:ARG:NH1	1:B:103:ARG:HG3	2.05	0.67
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.75	0.67
1:A:530:THR:H	1:A:533:GLN:HE21	1.44	0.65
1:B:805:ARG:NE	2:B:1115:HOH:O	2.17	0.65
1:B:481:ALA:O	1:B:484:HIS:NE2	2.29	0.65
1:A:800:LYS:N	2:A:1026:HOH:O	2.30	0.65
1:B:520:GLN:HE21	1:B:520:GLN:H	1.44	0.65
1:B:718:LEU:O	1:B:720:ILE:N	2.30	0.65
1:B:14:ASN:ND2	2:B:1083:HOH:O	2.28	0.64
1:B:14:ASN:HB3	2:B:1083:HOH:O	1.97	0.63
1:A:742:GLN:N	1:A:742:GLN:HE21	1.97	0.62
1:B:227:GLY:HA3	1:B:372:LEU:HD11	1.80	0.62
1:B:703:ILE:HA	1:B:706:LEU:HB3	1.82	0.62
1:B:282:ILE:HD12	1:B:286:LEU:CD1	2.30	0.62
1:B:179:ASN:CG	2:B:1017:HOH:O	2.37	0.61
1:B:718:LEU:O	1:B:720:ILE:HG13	1.99	0.61
1:B:459:ILE:O	1:B:463:GLU:HG3	2.00	0.61
1:B:104:THR:OG1	1:B:509:ARG:NE	2.33	0.61
1:B:529:PRO:HA	1:B:533:GLN:NE2	2.16	0.61
1:B:609:LYS:HB3	2:B:1050:HOH:O	1.99	0.60
1:A:594:LEU:C	1:A:596:ARG:H	2.05	0.60
1:B:385:GLU:OE2	2:B:1026:HOH:O	2.16	0.60
1:B:597:ILE:HD12	1:B:634:VAL:HG21	1.84	0.59
1:B:563:GLU:HG3	1:B:597:ILE:HD13	1.84	0.59
1:A:429:MET:HB2	1:A:433:GLU:OE2	2.03	0.59
1:B:503:ALA:HB1	1:B:506:MET:HG3	1.84	0.59
1:B:504:THR:O	1:B:505:ASN:C	2.41	0.58
1:B:789:ILE:O	1:B:789:ILE:HG22	2.03	0.58
1:B:293:ASP:OD2	1:B:293:ASP:N	2.36	0.58
1:B:618:ILE:HG22	1:B:619:GLU:N	2.19	0.58
1:A:731:HIS:NE2	1:A:733:GLU:CB	2.66	0.58
1:A:614:PRO:HA	2:A:1024:HOH:O	2.04	0.58
1:B:496:TYR:CD2	1:B:497:PRO:HD2	2.40	0.57
1:A:736:ARG:NH2	2:A:1005:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLY:O	1:B:394:ALA:N	2.37	0.57
1:A:530:THR:H	1:A:533:GLN:NE2	2.02	0.57
1:B:103:ARG:HD2	1:B:104:THR:H	1.70	0.56
1:A:395:ASP:CG	1:A:396:THR:N	2.58	0.56
1:A:732:GLU:OE2	1:A:736:ARG:CZ	2.52	0.56
1:A:753:VAL:HG21	1:A:833:MET:HE2	1.87	0.56
1:B:179:ASN:OD1	2:B:1017:HOH:O	2.17	0.56
1:B:378:GLN:O	1:B:382:ARG:HG3	2.04	0.56
1:B:594:LEU:C	1:B:596:ARG:H	2.08	0.56
1:B:223:LEU:HD21	1:B:377:PHE:CZ	2.41	0.56
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.36	0.56
1:B:771:LEU:HD23	1:B:771:LEU:C	2.26	0.56
1:A:534:ILE:HG22	1:A:534:ILE:O	2.06	0.56
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.54	0.55
1:B:608:ARG:CG	2:B:1078:HOH:O	2.53	0.55
1:B:429:MET:HB3	1:B:433:GLU:OE2	2.06	0.55
1:B:282:ILE:HD11	1:B:298:LEU:HB3	1.88	0.55
1:B:290:GLY:HA2	1:B:293:ASP:HB3	1.89	0.55
1:B:703:ILE:O	1:B:705:GLY:N	2.40	0.54
1:A:738:ARG:O	1:A:742:GLN:NE2	2.40	0.54
1:B:619:GLU:N	2:B:1103:HOH:O	2.20	0.54
1:B:603:VAL:HG12	1:B:603:VAL:O	2.07	0.54
1:A:789:ILE:HG23	1:A:789:ILE:O	2.08	0.53
1:A:435:ILE:HG21	1:A:468:GLU:HG3	1.89	0.53
1:B:395:ASP:C	2:B:921:HOH:O	2.46	0.53
1:B:488:ALA:O	2:B:1101:HOH:O	2.19	0.53
1:B:301:PRO:O	1:B:302:ALA:CB	2.56	0.53
1:B:526:LEU:HD22	1:B:533:GLN:HE22	1.74	0.53
1:A:618:ILE:O	1:A:619:GLU:HB2	2.08	0.53
1:B:703:ILE:HG22	1:B:707:GLN:HG2	1.92	0.52
1:A:530:THR:HG1	1:A:533:GLN:H	1.56	0.52
1:A:440:GLU:O	1:A:444:GLU:CG	2.58	0.52
1:A:798:ASP:OD1	1:A:799:PRO:O	2.28	0.52
1:A:429:MET:HG2	1:A:612:MET:SD	2.49	0.52
1:B:607:MET:HB3	1:B:612:MET:CE	2.40	0.52
1:B:288:LYS:HG3	1:B:289:GLU:HG2	1.90	0.52
1:B:531:ALA:O	1:B:535:GLU:OE1	2.28	0.52
1:B:647:GLU:OE2	1:B:800:LYS:CE	2.59	0.51
1:B:706:LEU:C	1:B:706:LEU:HD12	2.30	0.51
1:A:730:LEU:O	1:A:731:HIS:ND1	2.42	0.51
1:A:519:TRP:HA	1:A:522:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:GLU:OE2	1:B:800:LYS:HE2	2.11	0.51
1:A:696:SER:HB2	1:A:700:MET:HG3	1.92	0.51
1:B:679:ILE:O	1:B:683:VAL:HG23	2.11	0.51
1:B:282:ILE:O	1:B:286:LEU:HB2	2.11	0.50
1:B:691:TYR:HB3	1:B:702:ASP:O	2.12	0.50
1:B:506:MET:HG2	2:B:983:HOH:O	2.12	0.50
1:A:457:ILE:HG23	1:A:560:GLU:HB2	1.93	0.50
1:B:282:ILE:HD12	1:B:286:LEU:HD13	1.93	0.50
1:A:594:LEU:O	1:A:597:ILE:HG12	2.11	0.50
1:B:589:SER:HB2	1:B:592:ASP:OD2	2.11	0.50
1:B:18:LEU:HD23	1:B:21:MET:HE3	1.94	0.50
1:A:395:ASP:O	1:A:397:GLU:OE2	2.29	0.50
1:B:16:ARG:NE	1:B:19:ARG:NH2	2.57	0.50
1:B:507:ALA:N	2:B:983:HOH:O	2.30	0.50
1:B:56:LYS:NZ	2:B:1089:HOH:O	2.45	0.50
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.41	0.50
1:B:395:ASP:HB2	2:B:892:HOH:O	2.11	0.49
1:B:520:GLN:NE2	1:B:520:GLN:H	2.09	0.49
1:A:799:PRO:C	2:A:1026:HOH:O	2.46	0.49
1:A:799:PRO:O	1:A:800:LYS:O	2.30	0.49
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.94	0.49
1:A:39:SER:OG	1:A:42:GLU:HG3	2.12	0.49
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.12	0.48
1:A:144:ARG:CG	1:A:148:GLU:OE1	2.61	0.48
1:A:394:ALA:O	1:A:396:THR:N	2.45	0.48
1:B:532:GLU:HA	1:B:535:GLU:HB2	1.95	0.48
1:A:144:ARG:HG2	1:A:148:GLU:OE1	2.13	0.48
1:A:590:MET:SD	1:A:607:MET:HB2	2.53	0.48
1:B:16:ARG:HE	1:B:19:ARG:NH2	2.12	0.48
1:B:679:ILE:CG1	1:B:823:ILE:HD11	2.44	0.48
1:B:395:ASP:HA	2:B:1077:HOH:O	2.14	0.48
1:A:800:LYS:HB3	1:A:800:LYS:NZ	2.28	0.47
1:A:402:SER:O	1:A:406:LYS:HD3	2.14	0.47
1:A:99:ILE:HB	1:A:409:THR:HB	1.96	0.47
1:B:519:TRP:HB3	1:B:541:TRP:CG	2.49	0.47
1:B:301:PRO:O	1:B:302:ALA:HB2	2.13	0.47
1:A:435:ILE:O	1:A:439:ILE:HG12	2.13	0.47
1:B:228:PRO:O	1:B:230:GLU:OE2	2.31	0.47
1:B:529:PRO:HA	1:B:533:GLN:HE21	1.79	0.47
1:A:440:GLU:O	1:A:444:GLU:HG3	2.14	0.47
1:A:742:GLN:O	1:A:746:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:HG22	1:B:21:MET:CE	2.45	0.47
1:B:430:THR:OG1	2:B:1099:HOH:O	2.18	0.47
1:B:12:SER:HB2	1:B:15:ASP:OD1	2.15	0.47
1:B:801:GLN:HA	1:B:801:GLN:OE1	2.15	0.47
1:B:651:VAL:CG2	1:B:804:LYS:HG2	2.45	0.47
1:B:282:ILE:HD12	1:B:286:LEU:HD12	1.97	0.46
1:B:805:ARG:CD	2:B:1115:HOH:O	2.61	0.46
1:B:308:HIS:CE1	1:B:784:TYR:CE1	3.04	0.46
1:B:712:ASN:C	1:B:828:LYS:HZ1	2.17	0.46
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.97	0.46
1:B:292:MET:O	1:B:294:GLU:N	2.48	0.46
1:A:519:TRP:O	1:A:522:GLU:HB2	2.15	0.46
1:A:17:THR:O	1:A:21:MET:HG3	2.16	0.46
1:B:637:ARG:NH1	2:B:1032:HOH:O	2.49	0.46
1:B:392:GLY:O	1:B:394:ALA:HB3	2.16	0.45
1:A:561:ARG:HB2	1:A:594:LEU:HD13	1.97	0.45
1:B:607:MET:HB3	1:B:612:MET:HE1	1.98	0.45
1:B:592:ASP:O	1:B:595:MET:N	2.45	0.45
1:B:734:THR:HA	1:B:737:GLU:OE2	2.16	0.45
1:B:506:MET:SD	1:B:574:ARG:NE	2.90	0.45
1:B:593:ALA:O	1:B:596:ARG:HB3	2.17	0.45
1:A:32:GLU:OE2	1:A:82:ARG:HD2	2.17	0.45
1:B:520:GLN:HA	1:B:523:VAL:HG13	1.99	0.45
1:A:593:ALA:O	1:A:596:ARG:HB2	2.17	0.45
1:B:17:THR:O	1:B:21:MET:HE2	2.17	0.45
1:B:224:ILE:HG23	1:B:371:THR:HG23	1.98	0.45
1:B:648:TYR:CZ	1:B:800:LYS:HB2	2.51	0.44
1:B:550:GLU:HG3	1:B:550:GLU:O	2.17	0.44
1:B:99:ILE:HD12	1:B:211:VAL:HG21	2.00	0.44
1:A:715:ASP:HB2	1:A:828:LYS:HG2	1.99	0.44
1:B:798:ASP:HA	1:B:799:PRO:HD2	1.75	0.44
1:A:503:ALA:CB	1:A:506:MET:HG2	2.47	0.44
1:A:503:ALA:HB1	1:A:506:MET:HG2	1.99	0.44
1:A:370:GLN:OE1	1:A:776:LYS:HD3	2.17	0.44
1:B:223:LEU:HD11	1:B:377:PHE:CE1	2.53	0.44
1:B:99:ILE:HB	1:B:409:THR:HB	1.99	0.44
1:B:230:GLU:OE2	1:B:368:GLU:O	2.34	0.44
1:A:594:LEU:HD21	1:A:597:ILE:HD11	2.00	0.44
1:B:644:GLN:HE22	1:B:800:LYS:NZ	2.15	0.43
1:A:613:LYS:HA	1:A:614:PRO:HD2	1.88	0.43
1:A:228:PRO:HB3	1:A:367:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:ILE:O	1:B:789:ILE:CG2	2.65	0.43
1:B:563:GLU:HG2	1:B:634:VAL:HG11	2.00	0.43
1:B:747:TYR:OH	1:B:763:GLU:OE2	2.32	0.43
1:B:228:PRO:HB3	1:B:367:ASN:OD1	2.18	0.43
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.51	0.43
1:A:648:TYR:OH	1:A:800:LYS:N	2.51	0.43
1:B:679:ILE:HG13	1:B:823:ILE:HD11	2.01	0.43
1:B:14:ASN:HD21	1:B:411:VAL:H	1.67	0.43
1:A:701:TRP:N	1:A:701:TRP:CD1	2.85	0.43
1:B:395:ASP:C	1:B:397:GLU:H	2.21	0.42
1:B:703:ILE:O	1:B:706:LEU:N	2.49	0.42
1:B:514:VAL:O	2:B:957:HOH:O	2.21	0.42
1:B:283:GLU:O	1:B:287:VAL:HG12	2.19	0.42
1:A:440:GLU:O	1:A:444:GLU:HG2	2.19	0.42
1:B:13:ARG:HD2	1:B:13:ARG:HA	1.84	0.42
1:A:620:HIS:HA	1:A:621:PRO:HD2	1.81	0.42
1:B:103:ARG:CD	1:B:104:THR:H	2.32	0.42
1:B:496:TYR:CG	1:B:497:PRO:HD2	2.54	0.42
1:A:773:SER:O	1:A:776:LYS:HG2	2.19	0.42
1:B:782:MET:CE	1:B:810:MET:HE2	2.49	0.42
1:B:16:ARG:HD3	1:B:16:ARG:HA	1.90	0.42
1:B:618:ILE:CA	2:B:1103:HOH:O	2.67	0.42
1:A:666:LEU:HD22	1:A:672:VAL:HG21	2.00	0.42
1:B:605:GLY:O	1:B:608:ARG:HG2	2.19	0.42
1:B:285:LEU:HD23	1:B:310:VAL:HG21	2.02	0.42
1:A:526:LEU:HD13	1:A:529:PRO:HA	2.01	0.42
1:B:723:TRP:HB2	1:B:724:LEU:HD23	2.02	0.42
1:B:223:LEU:O	1:B:374:SER:HA	2.20	0.41
1:B:103:ARG:NH2	1:B:575:SER:O	2.53	0.41
1:A:594:LEU:C	1:A:596:ARG:N	2.71	0.41
1:B:198:ARG:HH21	1:B:664:ASN:HD22	1.67	0.41
1:A:365:ILE:HG22	1:A:366:GLN:O	2.20	0.41
1:B:392:GLY:O	1:B:394:ALA:CB	2.69	0.41
1:A:412:VAL:HA	1:A:413:PRO:HD2	1.81	0.41
1:A:693:PRO:HA	1:A:694:PRO:HD3	1.92	0.41
1:A:727:GLU:HA	1:A:728:PRO:HD2	1.91	0.41
1:A:532:GLU:OE1	1:A:535:GLU:HB2	2.20	0.41
1:B:742:GLN:O	1:B:745:GLU:HG2	2.21	0.41
1:A:762:PHE:O	1:A:766:VAL:HG23	2.21	0.41
1:A:24:VAL:HG13	1:A:65:PRO:HG3	2.02	0.41
1:B:782:MET:CE	1:B:810:MET:CE	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LEU:HD12	1:A:529:PRO:HB3	2.03	0.41
1:A:460:GLU:H	1:A:460:GLU:CD	2.24	0.41
1:B:396:THR:N	2:B:892:HOH:O	2.54	0.41
1:A:394:ALA:CA	2:A:980:HOH:O	2.44	0.40
1:A:528:ASN:O	1:A:529:PRO:C	2.59	0.40
1:B:557:ILE:HG23	1:B:587:TYR:CD2	2.57	0.40
1:B:510:GLY:HA3	1:B:574:ARG:HH12	1.87	0.40
1:B:696:SER:HB3	1:B:700:MET:HB2	2.03	0.40
1:B:441:ASP:HA	2:B:984:HOH:O	2.20	0.40
1:B:215:LEU:O	1:B:219:ALA:HB2	2.22	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:600:SER:OG	1:B:830:GLN:O[1_655]	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	682/853 (80%)	635 (93%)	31 (4%)	16 (2%)	8	3
1	B	717/853 (84%)	650 (91%)	39 (5%)	28 (4%)	4	1
All	All	1399/1706 (82%)	1285 (92%)	70 (5%)	44 (3%)	5	1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	ALA
1	A	396	THR
1	A	507	ALA

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Mol	Chain	Res	Type
1	A	599	ALA
1	A	614	PRO
1	A	730	LEU
1	B	229	ALA
1	B	293	ASP
1	B	302	ALA
1	B	394	ALA
1	B	395	ASP
1	B	599	ALA
1	B	612	MET
1	B	614	PRO
1	B	719	PRO
1	B	729	GLU
1	B	801	GLN
1	A	395	ASP
1	A	510	GLY
1	A	795	ALA
1	B	288	LYS
1	B	292	MET
1	B	393	THR
1	B	396	THR
1	B	510	GLY
1	B	597	ILE
1	B	619	GLU
1	B	704	PRO
1	A	603	VAL
1	A	619	GLU
1	B	289	GLU
1	B	368	GLU
1	B	796	GLN
1	B	797	LYS
1	A	800	LYS
1	A	801	GLN
1	A	791	LEU
1	B	298	LEU
1	B	367	ASN
1	B	593	ALA
1	A	613	LYS
1	A	789	ILE
1	B	534	ILE
1	B	789	ILE

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	582/728 (80%)	532 (91%)	50 (9%)	13 7
1	B	613/728 (84%)	545 (89%)	68 (11%)	8 4
All	All	1195/1456 (82%)	1077 (90%)	118 (10%)	10 5

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	ASN
1	A	15	ASP
1	A	16	ARG
1	A	19	ARG
1	A	37	LYS
1	A	41	GLU
1	A	55	GLU
1	A	72	ARG
1	A	201	ARG
1	A	226	SER
1	A	365	ILE
1	A	366	GLN
1	A	369	ASN
1	A	393	THR
1	A	395	ASP
1	A	406	LYS
1	A	409	THR
1	A	444	GLU
1	A	457	ILE
1	A	506	MET
1	A	509	ARG
1	A	523	VAL
1	A	527	GLU
1	A	535	GLU
1	A	591	GLU
1	A	602	ARG

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Mol	Chain	Res	Type
1	A	613	LYS
1	A	614	PRO
1	A	618	ILE
1	A	632	ARG
1	A	635	GLU
1	A	636	SER
1	A	642	ARG
1	A	669	VAL
1	A	672	VAL
1	A	699	GLU
1	A	708	GLU
1	A	711	LYS
1	A	725	ASP
1	A	730	LEU
1	A	731	HIS
1	A	734	THR
1	A	735	LEU
1	A	742	GLN
1	A	754	VAL
1	A	791	LEU
1	A	797	LYS
1	A	800	LYS
1	A	816	GLU
1	B	12	SER
1	B	14	ASN
1	B	16	ARG
1	B	37	LYS
1	B	38	LEU
1	B	103	ARG
1	B	226	SER
1	B	230	GLU
1	B	231	ASP
1	B	282	ILE
1	B	283	GLU
1	B	284	GLU
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	291	ILE
1	B	293	ASP
1	B	299	TYR
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	307	MET
1	B	367	ASN
1	B	368	GLU
1	B	393	THR
1	B	409	THR
1	B	431	GLU
1	B	457	ILE
1	B	506	MET
1	B	512	ASP
1	B	520	GLN
1	B	523	VAL
1	B	526	LEU
1	B	527	GLU
1	B	532	GLU
1	B	535	GLU
1	B	589	SER
1	B	594	LEU
1	B	595	MET
1	B	596	ARG
1	B	602	ARG
1	B	604	SER
1	B	609	LYS
1	B	612	MET
1	B	625	LYS
1	B	637	ARG
1	B	657	ARG
1	B	670	SER
1	B	672	VAL
1	B	679	ILE
1	B	680	ARG
1	B	696	SER
1	B	703	ILE
1	B	706	LEU
1	B	707	GLN
1	B	718	LEU
1	B	722	GLU
1	B	725	ASP
1	B	726	LYS
1	B	727	GLU
1	B	729	GLU
1	B	779	LEU
1	B	783	ASP

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Mol	Chain	Res	Type
1	B	791	LEU
1	B	792	ARG
1	B	796	GLN
1	B	800	LYS
1	B	821	GLU
1	B	831	VAL
1	B	832	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	533	GLN
1	A	638	ASN
1	A	662	GLN
1	A	742	GLN
1	A	748	GLN
1	B	14	ASN
1	B	520	GLN
1	B	528	ASN
1	B	533	GLN
1	B	545	HIS
1	B	629	ASN
1	B	638	ASN
1	B	644	GLN
1	B	664	ASN
1	B	707	GLN
1	B	742	GLN
1	B	761	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	686/853 (80%)	1.07	130 (18%)	2 2	40, 53, 84, 102	0
1	B	723/853 (84%)	1.68	237 (32%)	0 1	38, 54, 87, 102	0
All	All	1409/1706 (82%)	1.39	367 (26%)	1 1	38, 53, 86, 102	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	LEU	12.9
1	B	728	PRO	11.4
1	B	789	ILE	10.2
1	B	365	ILE	9.9
1	B	615	GLY	9.5
1	A	365	ILE	9.5
1	B	791	LEU	9.4
1	B	614	PRO	9.2
1	B	796	GLN	9.1
1	B	700	MET	9.0
1	A	794	TYR	9.0
1	B	291	ILE	9.0
1	A	614	PRO	8.7
1	B	794	TYR	8.5
1	A	834	PRO	8.4
1	B	696	SER	8.3
1	A	597	ILE	8.3
1	B	792	ARG	8.3
1	A	728	PRO	8.3
1	B	695	GLN	8.3
1	B	723	TRP	8.2
1	B	280	VAL	8.2
1	B	731	HIS	8.1
1	A	792	ARG	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	507	ALA	7.7
1	B	697	LEU	7.6
1	A	367	ASN	7.6
1	A	616	GLU	7.5
1	B	299	TYR	7.4
1	A	603	VAL	7.4
1	B	694	PRO	7.3
1	B	287	VAL	7.2
1	B	793	GLY	7.1
1	A	796	GLN	7.1
1	A	394	ALA	7.0
1	A	615	GLY	7.0
1	B	699	GLU	7.0
1	A	790	HIS	7.0
1	B	366	GLN	6.9
1	B	290	GLY	6.9
1	B	603	VAL	6.9
1	B	721	ALA	6.8
1	B	795	ALA	6.8
1	B	294	GLU	6.7
1	B	704	PRO	6.7
1	B	367	ASN	6.6
1	B	790	HIS	6.5
1	A	789	ILE	6.4
1	A	14	ASN	6.4
1	B	618	ILE	6.3
1	B	295	GLY	6.3
1	B	730	LEU	6.0
1	B	508	GLY	6.0
1	B	709	ARG	5.9
1	B	283	GLU	5.9
1	A	16	ARG	5.9
1	A	368	GLU	5.9
1	B	232	SER	5.9
1	B	229	ALA	5.9
1	B	729	GLU	5.9
1	B	12	SER	5.7
1	B	313	ALA	5.7
1	B	703	ILE	5.6
1	B	602	ARG	5.5
1	B	284	GLU	5.5
1	A	833	MET	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	705	GLY	5.4
1	B	734	THR	5.4
1	B	230	GLU	5.4
1	B	368	GLU	5.3
1	B	282	ILE	5.3
1	A	366	GLN	5.3
1	B	231	ASP	5.3
1	B	285	LEU	5.2
1	A	723	TRP	5.2
1	B	598	PHE	5.2
1	A	731	HIS	5.2
1	B	293	ASP	5.2
1	B	228	PRO	5.1
1	B	725	ASP	5.1
1	B	617	ALA	5.1
1	B	532	GLU	5.1
1	B	832	ARG	5.1
1	B	126	VAL	5.0
1	B	691	TYR	5.0
1	B	312	ALA	5.0
1	A	596	ARG	5.0
1	B	597	ILE	4.9
1	A	13	ARG	4.8
1	A	617	ALA	4.8
1	A	604	SER	4.8
1	A	724	LEU	4.8
1	B	281	LEU	4.8
1	B	174	ILE	4.7
1	B	718	LEU	4.7
1	A	15	ASP	4.7
1	B	702	ASP	4.7
1	B	727	GLU	4.7
1	B	726	LYS	4.7
1	B	292	MET	4.7
1	A	602	ARG	4.7
1	B	616	GLU	4.7
1	A	717	ASP	4.6
1	B	289	GLU	4.6
1	B	393	THR	4.5
1	B	797	LYS	4.5
1	B	610	LEU	4.5
1	A	725	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	507	ALA	4.4
1	A	784	TYR	4.4
1	B	831	VAL	4.4
1	B	722	GLU	4.3
1	B	296	GLU	4.3
1	A	727	GLU	4.2
1	A	613	LYS	4.2
1	B	596	ARG	4.2
1	A	700	MET	4.2
1	B	114	LEU	4.2
1	B	607	MET	4.1
1	A	793	GLY	4.1
1	B	720	ILE	4.1
1	B	724	LEU	4.1
1	A	612	MET	4.1
1	B	738	ARG	4.0
1	B	71	VAL	4.0
1	B	735	LEU	4.0
1	B	674	GLU	4.0
1	B	733	GLU	4.0
1	B	509	ARG	3.9
1	B	156	ILE	3.9
1	B	301	PRO	3.9
1	B	182	TYR	3.9
1	B	175	THR	3.9
1	B	717	ASP	3.9
1	B	117	TYR	3.8
1	A	730	LEU	3.8
1	B	128	VAL	3.8
1	B	528	ASN	3.8
1	A	557	ILE	3.8
1	A	509	ARG	3.8
1	A	527	GLU	3.8
1	A	704	PRO	3.8
1	B	482	LYS	3.8
1	B	170	TYR	3.7
1	A	600	SER	3.7
1	A	795	ALA	3.7
1	B	67	ALA	3.7
1	A	228	PRO	3.7
1	B	613	LYS	3.7
1	A	618	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	394	ALA	3.7
1	A	797	LYS	3.6
1	B	116	ALA	3.6
1	A	718	LEU	3.6
1	A	369	ASN	3.6
1	A	831	VAL	3.6
1	B	206	ALA	3.6
1	B	121	LEU	3.5
1	B	708	GLU	3.5
1	A	594	LEU	3.5
1	A	832	ARG	3.5
1	B	594	LEU	3.5
1	A	70	VAL	3.5
1	B	150	LEU	3.5
1	B	99	ILE	3.5
1	A	726	LYS	3.5
1	A	182	TYR	3.5
1	B	611	GLY	3.5
1	B	129	VAL	3.4
1	A	601	ASP	3.4
1	A	508	GLY	3.4
1	A	788	GLY	3.4
1	B	510	GLY	3.4
1	B	100	ALA	3.4
1	A	176	TYR	3.4
1	B	68	PHE	3.4
1	A	722	GLU	3.4
1	B	380	TYR	3.4
1	A	745	GLU	3.4
1	B	74	ALA	3.4
1	B	118	LEU	3.4
1	B	502	ILE	3.3
1	B	606	MET	3.3
1	B	690	ALA	3.3
1	B	176	TYR	3.3
1	B	719	PRO	3.3
1	A	177	GLY	3.3
1	B	70	VAL	3.3
1	B	211	VAL	3.3
1	B	600	SER	3.3
1	B	608	ARG	3.2
1	B	706	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	601	ASP	3.2
1	B	136	ALA	3.2
1	A	208	VAL	3.2
1	B	177	GLY	3.2
1	B	483	PHE	3.2
1	B	207	LEU	3.2
1	B	94	LEU	3.2
1	B	186	TYR	3.2
1	B	158	LEU	3.2
1	A	395	ASP	3.1
1	B	113	THR	3.1
1	B	208	VAL	3.1
1	B	89	LEU	3.1
1	B	407	LEU	3.1
1	B	740	LEU	3.1
1	A	729	GLU	3.1
1	B	554	LEU	3.1
1	A	393	THR	3.1
1	A	502	ILE	3.1
1	A	71	VAL	3.1
1	A	215	LEU	3.1
1	B	93	VAL	3.0
1	A	129	VAL	3.0
1	B	712	ASN	3.0
1	B	404	ILE	3.0
1	A	716	LEU	3.0
1	B	389	GLY	3.0
1	B	749	ARG	3.0
1	B	127	HIS	3.0
1	B	412	VAL	3.0
1	B	693	PRO	3.0
1	B	88	LEU	2.9
1	B	830	GLN	2.9
1	B	595	MET	2.9
1	B	388	ALA	2.9
1	B	205	TYR	2.9
1	A	510	GLY	2.9
1	A	454	VAL	2.9
1	B	556	ILE	2.9
1	B	453	LEU	2.9
1	B	86	VAL	2.9
1	A	405	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	THR	2.9
1	A	37	LYS	2.9
1	B	609	LYS	2.9
1	B	147	PHE	2.8
1	B	103	ARG	2.8
1	B	111	THR	2.8
1	B	381	PHE	2.8
1	B	670	SER	2.8
1	B	90	GLY	2.8
1	A	556	ILE	2.8
1	B	120	ALA	2.8
1	A	608	ARG	2.8
1	A	114	LEU	2.8
1	A	174	ILE	2.8
1	B	215	LEU	2.8
1	B	115	PRO	2.8
1	A	523	VAL	2.8
1	A	691	TYR	2.7
1	A	128	VAL	2.7
1	A	170	TYR	2.7
1	B	530	THR	2.7
1	A	754	VAL	2.7
1	A	381	PHE	2.7
1	A	127	HIS	2.7
1	A	715	ASP	2.7
1	B	605	GLY	2.7
1	B	737	GLU	2.7
1	B	429	MET	2.7
1	A	554	LEU	2.6
1	A	720	ILE	2.6
1	B	745	GLU	2.6
1	B	125	GLY	2.6
1	B	742	GLN	2.6
1	A	709	ARG	2.6
1	B	286	LEU	2.6
1	A	799	PRO	2.6
1	A	737	GLU	2.6
1	B	203	LEU	2.6
1	A	429	MET	2.6
1	B	701	TRP	2.6
1	B	410	VAL	2.6
1	B	612	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	609	LYS	2.6
1	A	598	PHE	2.6
1	B	384	TYR	2.5
1	B	523	VAL	2.5
1	B	310	VAL	2.5
1	B	501	THR	2.5
1	B	288	LYS	2.5
1	B	689	ASP	2.5
1	A	511	THR	2.5
1	B	405	TYR	2.5
1	B	178	THR	2.5
1	B	632	ARG	2.5
1	A	150	LEU	2.5
1	B	154	VAL	2.5
1	B	214	ILE	2.5
1	A	453	LEU	2.4
1	A	705	GLY	2.4
1	B	472	ALA	2.4
1	B	686	ALA	2.4
1	B	519	TRP	2.4
1	B	91	GLY	2.4
1	B	604	SER	2.4
1	B	308	HIS	2.4
1	A	528	ASN	2.4
1	B	69	ALA	2.3
1	A	721	ALA	2.3
1	A	742	GLN	2.3
1	B	652	ALA	2.3
1	B	391	THR	2.3
1	B	651	VAL	2.3
1	B	829	VAL	2.3
1	A	708	GLU	2.3
1	B	752	GLU	2.3
1	B	557	ILE	2.3
1	A	30	ALA	2.3
1	B	395	ASP	2.3
1	B	707	GLN	2.3
1	B	375	ILE	2.2
1	A	206	ALA	2.2
1	A	610	LEU	2.2
1	A	697	LEU	2.2
1	B	401	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	749	ARG	2.2
1	B	369	ASN	2.2
1	A	733	GLU	2.2
1	B	741	ALA	2.2
1	B	63	LEU	2.2
1	B	146	LEU	2.2
1	B	387	LEU	2.2
1	B	452	VAL	2.2
1	B	753	VAL	2.2
1	B	505	ASN	2.2
1	A	113	THR	2.2
1	B	297	SER	2.2
1	B	637	ARG	2.2
1	A	69	ALA	2.2
1	B	681	GLU	2.2
1	B	377	PHE	2.2
1	B	586	PHE	2.2
1	A	116	ALA	2.2
1	B	119	ASN	2.2
1	A	702	ASP	2.1
1	B	28	ILE	2.1
1	A	17	THR	2.1
1	A	117	TYR	2.1
1	A	211	VAL	2.1
1	A	712	ASN	2.1
1	A	532	GLU	2.1
1	B	65	PRO	2.1
1	B	711	LYS	2.1
1	B	526	LEU	2.1
1	B	621	PRO	2.1
1	A	136	ALA	2.1
1	B	303	ASN	2.1
1	B	732	GLU	2.1
1	A	798	ASP	2.1
1	A	595	MET	2.1
1	B	460	GLU	2.0
1	A	156	ILE	2.0
1	B	534	ILE	2.0
1	B	692	ILE	2.0
1	B	739	ILE	2.0
1	A	88	LEU	2.0
1	B	110	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	392	GLY	2.0
1	A	606	MET	2.0
1	A	56	LYS	2.0
1	B	98	CYS	2.0
1	A	216	ILE	2.0
1	B	682	ASP	2.0
1	A	482	LYS	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.