



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 1OZB / pdb_00001ozb
Title : Crystal Structure of SecB complexed with SecA C-terminus
Authors : Zhou, J.; Xu, Z.
Deposited on : 2003-04-08
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

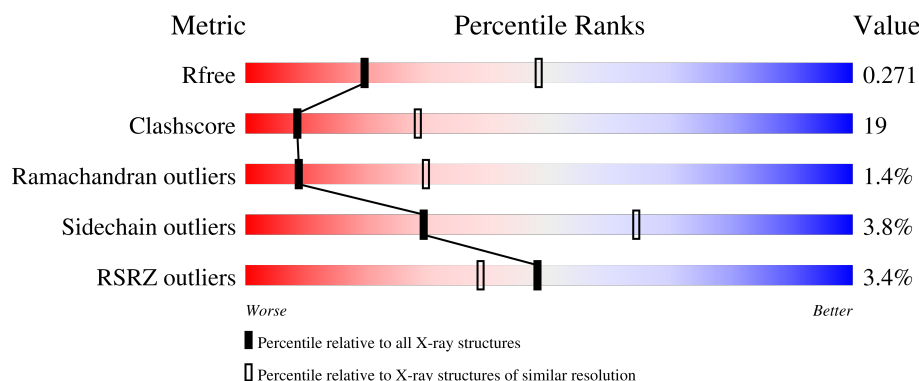
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	169	4% 53% 32% • 15%
1	B	169	2% 52% 27% • 19%
1	C	169	3% 51% 27% • 20%
1	D	169	2% 43% 34% • 20%
1	E	169	4% 46% 34% • 17%

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Mol	Chain	Length	Quality of chain
1	F	169	2% 43% 38% 7% 12%
1	G	169	% 49% 36% • 13%
1	H	169	4% 49% 31% • 20%
2	I	27	7% 52% 33% • 11%
2	J	27	7% 33% 52% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9144 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 Protein-export protein secB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1120	716	180	218	6			
1	B	137	Total	C	N	O	S	0	0	0
			1079	693	171	209	6			
1	C	136	Total	C	N	O	S	0	0	0
			1072	688	170	208	6			
1	D	135	Total	C	N	O	S	0	0	0
			1067	685	169	207	6			
1	E	140	Total	C	N	O	S	0	0	0
			1092	700	174	212	6			
1	F	148	Total	C	N	O	S	0	0	0
			1145	730	187	222	6			
1	G	147	Total	C	N	O	S	0	0	0
			1147	732	183	226	6			
1	H	136	Total	C	N	O	S	0	0	0
			1072	688	170	208	6			

- Molecule 2 is a protein called Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	24	Total	C	N	O	S	0	0	0
			174	105	38	28	3			
2	J	24	Total	C	N	O	S	0	0	0
			174	105	38	28	3			

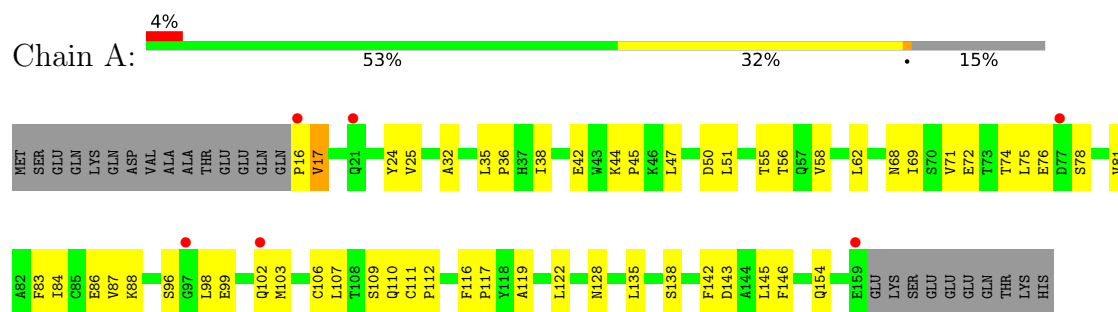
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		

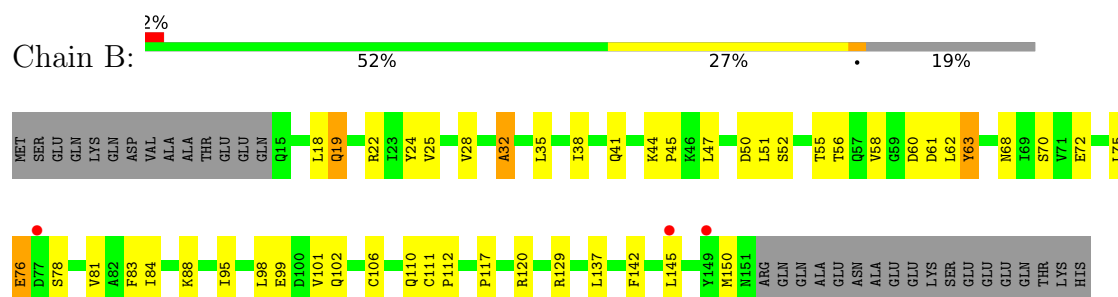
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

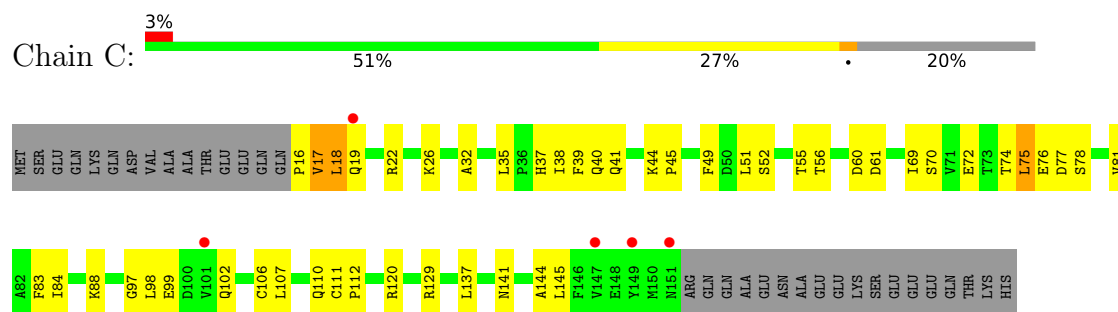
- Molecule 1: Protein-export protein secB



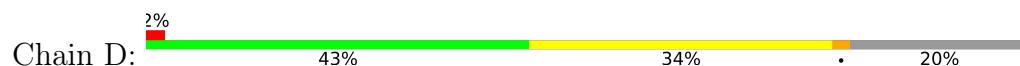
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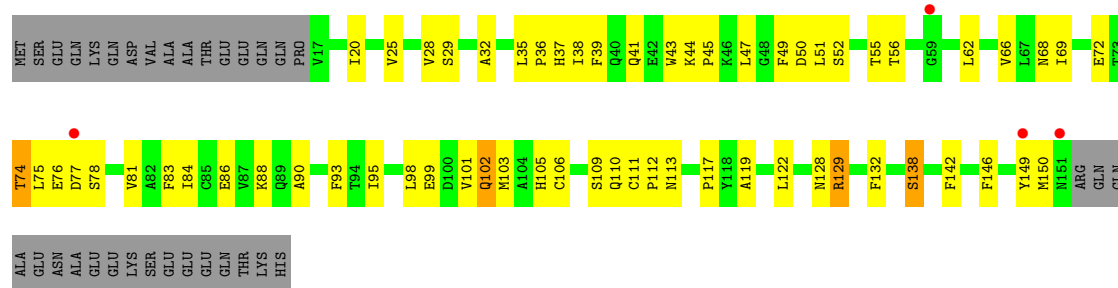


- Molecule 1: Protein-export protein secB

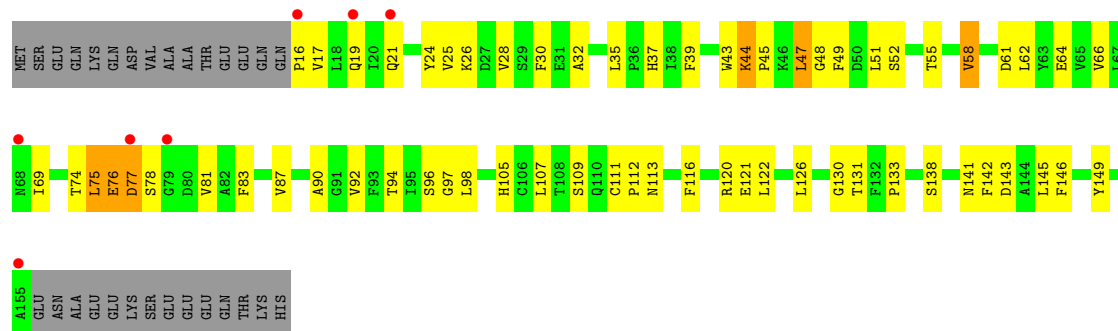


- Molecule 1: Protein-export protein secB

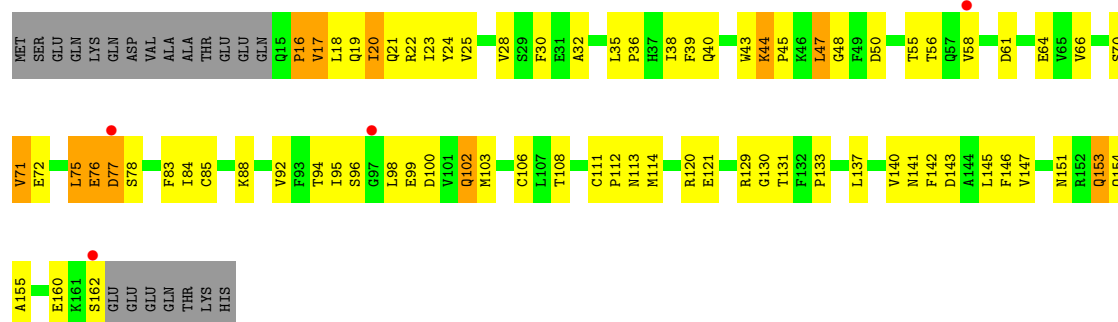
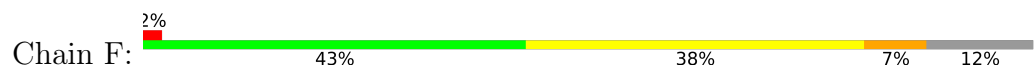




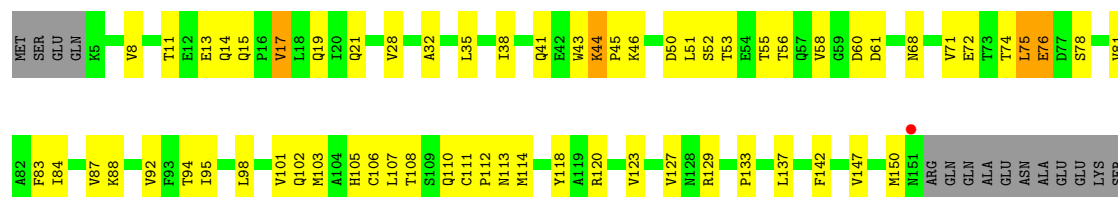
• Molecule 1: Protein-export protein secB



• Molecule 1: Protein-export protein secB

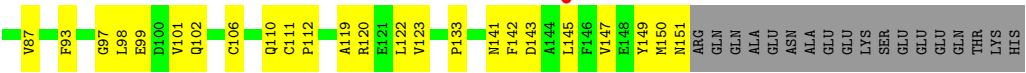
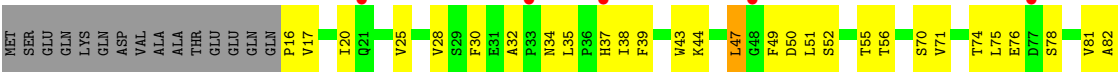


• Molecule 1: Protein-export protein secB

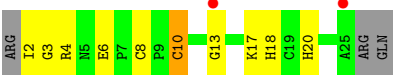


GLU
GLU
GLN
GLN
THR
LYS
HIS

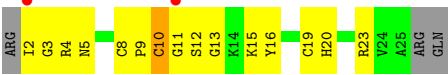
• Molecule 1: Protein-export protein secB



• Molecule 2: Preprotein translocase secA subunit



• Molecule 2: Preprotein translocase secA subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.50Å 114.50Å 286.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.16 – 2.80 38.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.16-2.80) 97.0 (38.16-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.273 0.226 , 0.271	Depositor DCC
R_{free} test set	3771 reflections (7.96%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9144	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 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.52	0/1143	1.00	6/1559 (0.4%)
1	B	0.49	0/1103	1.05	5/1505 (0.3%)
1	C	0.48	0/1095	1.03	9/1493 (0.6%)
1	D	0.49	0/1090	1.03	10/1486 (0.7%)
1	E	0.49	0/1115	1.07	9/1521 (0.6%)
1	F	0.51	0/1168	1.03	9/1593 (0.6%)
1	G	0.45	0/1171	1.01	7/1598 (0.4%)
1	H	0.44	0/1095	1.00	10/1493 (0.7%)
2	I	0.47	0/178	1.07	1/236 (0.4%)
2	J	0.53	0/178	1.13	2/236 (0.8%)
All	All	0.49	0/9336	1.03	68/12720 (0.5%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ALA	CA-C-N	10.13	129.78	119.24
1	B	32	ALA	C-N-CA	10.13	129.78	119.24
1	E	32	ALA	CA-C-N	9.13	128.73	119.24
1	E	32	ALA	C-N-CA	9.13	128.73	119.24
1	E	76	GLU	N-CA-C	8.79	120.47	111.07
1	B	76	GLU	N-CA-C	8.71	120.39	111.07
1	G	32	ALA	CA-C-N	8.56	128.14	119.24
1	G	32	ALA	C-N-CA	8.56	128.14	119.24
1	C	32	ALA	CA-C-N	8.23	127.80	119.24
1	C	32	ALA	C-N-CA	8.23	127.80	119.24
1	H	76	GLU	N-CA-C	8.01	119.64	111.07
1	A	76	GLU	N-CA-C	7.96	120.04	111.36
1	D	76	GLU	N-CA-C	7.93	119.92	111.28
1	G	76	GLU	N-CA-C	7.85	120.53	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	76	GLU	N-CA-C	7.78	119.76	111.28
1	H	17	VAL	N-CA-C	7.75	118.89	108.27
1	E	44	LYS	CA-C-N	7.75	127.51	119.76
1	E	44	LYS	C-N-CA	7.75	127.51	119.76
2	J	13	GLY	N-CA-C	-7.57	104.94	113.79
1	C	76	GLU	N-CA-C	7.56	119.16	111.07
1	A	17	VAL	N-CA-C	7.46	119.06	108.17
1	F	44	LYS	CA-C-N	6.97	126.73	119.76
1	F	44	LYS	C-N-CA	6.97	126.73	119.76
1	C	44	LYS	CA-C-N	6.92	126.68	119.76
1	C	44	LYS	C-N-CA	6.92	126.68	119.76
2	I	13	GLY	N-CA-C	-6.90	106.24	115.21
1	D	32	ALA	CA-C-N	6.69	126.47	119.05
1	D	32	ALA	C-N-CA	6.69	126.47	119.05
1	F	16	PRO	N-CA-CB	6.48	110.05	103.25
1	H	32	ALA	CA-C-N	6.48	125.98	119.24
1	H	32	ALA	C-N-CA	6.48	125.98	119.24
1	A	16	PRO	N-CA-CB	6.47	110.12	103.00
1	G	17	VAL	N-CA-C	6.39	117.06	108.11
1	E	16	PRO	N-CA-CB	6.36	110.00	103.00
1	F	32	ALA	CA-C-N	6.33	125.82	119.24
1	F	32	ALA	C-N-CA	6.33	125.82	119.24
1	D	132	PHE	CA-C-N	-6.16	113.42	119.76
1	D	132	PHE	C-N-CA	-6.16	113.42	119.76
1	A	47	LEU	N-CA-C	6.11	118.67	108.96
1	G	44	LYS	CA-C-N	6.05	125.81	119.76
1	G	44	LYS	C-N-CA	6.05	125.81	119.76
1	G	45	PRO	N-CA-C	6.01	120.63	111.19
1	C	45	PRO	N-CA-C	6.00	120.61	111.19
1	D	37	HIS	N-CA-C	5.85	117.66	111.28
1	D	45	PRO	N-CA-C	5.82	120.33	111.19
1	A	154	GLN	N-CA-C	-5.82	106.03	113.01
1	F	45	PRO	N-CA-C	5.79	120.28	111.19
1	H	47	LEU	N-CA-C	5.70	118.02	108.96
1	B	47	LEU	N-CA-C	5.69	118.00	108.96
1	H	44	LYS	CA-C-N	5.68	125.44	119.76
1	H	44	LYS	C-N-CA	5.68	125.44	119.76
2	J	3	GLY	N-CA-C	5.64	120.50	111.64
1	F	47	LEU	N-CA-C	5.62	118.80	109.46
1	H	37	HIS	N-CA-C	5.61	117.40	111.28
1	H	34	ASN	N-CA-C	5.60	119.23	111.55
1	H	16	PRO	N-CA-CB	5.60	109.16	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	HIS	N-CA-C	5.59	118.14	111.71
1	E	45	PRO	N-CA-C	5.56	119.92	111.19
1	B	45	PRO	N-CA-C	5.54	119.88	111.19
1	C	16	PRO	N-CA-CB	5.47	109.02	103.00
1	C	17	VAL	N-CA-C	5.43	117.60	108.81
1	D	47	LEU	N-CA-C	5.42	117.58	108.96
1	F	17	VAL	N-CA-C	5.39	116.50	108.46
1	C	37	HIS	N-CA-C	5.26	117.75	111.71
1	D	44	LYS	CA-C-N	5.19	124.95	119.76
1	D	44	LYS	C-N-CA	5.19	124.95	119.76
1	A	45	PRO	N-CA-C	5.10	119.20	111.19
1	E	47	LEU	N-CA-C	5.07	117.88	109.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1120	0	1077	37	0
1	B	1079	0	1050	38	0
1	C	1072	0	1043	35	0
1	D	1067	0	1041	53	0
1	E	1092	0	1054	45	0
1	F	1145	0	1093	58	0
1	G	1147	0	1101	50	0
1	H	1072	0	1043	36	0
2	I	174	0	159	7	0
2	J	174	0	159	13	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	9144	0	8820	341	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 19.

All (341) 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:G:28:VAL:HG12	1:H:30:PHE:HB3	1.55	0.88
1:F:114:MET:HG2	1:H:120:ARG:HH12	1.41	0.86
1:F:25:VAL:HG11	1:F:28:VAL:HG23	1.57	0.85
1:D:98:LEU:HB2	1:D:103:MET:HE2	1.60	0.84
1:F:95:ILE:HG22	1:F:103:MET:HE1	1.58	0.84
1:D:98:LEU:HD22	1:D:102:GLN:HB2	1.62	0.82
1:D:129:ARG:HA	1:D:129:ARG:HH11	1.46	0.81
1:F:20:ILE:HD11	1:F:23:ILE:HG13	1.63	0.80
2:J:9:PRO:O	2:J:10:CYS:HB3	1.81	0.79
1:F:19:GLN:HG2	1:F:94:THR:HB	1.63	0.79
1:A:72:GLU:HG3	1:A:84:ILE:HG12	1.64	0.78
1:E:25:VAL:HG11	1:E:28:VAL:HG23	1.66	0.78
1:E:51:LEU:HD23	1:E:52:SER:N	1.99	0.78
1:D:99:GLU:HB2	1:D:102:GLN:NE2	2.00	0.77
1:F:66:VAL:HG11	1:F:88:LYS:HZ2	1.47	0.77
1:F:72:GLU:HG3	1:F:84:ILE:HG12	1.67	0.76
1:F:66:VAL:HG11	1:F:88:LYS:NZ	2.00	0.76
1:C:141:ASN:HD22	1:C:144:ALA:HB2	1.51	0.74
1:H:50:ASP:HB2	1:H:70:SER:HB3	1.70	0.74
1:F:25:VAL:HG11	1:F:28:VAL:CG2	2.18	0.73
1:E:122:LEU:HD13	1:F:129:ARG:HD3	1.71	0.71
1:E:30:PHE:HB2	1:E:126:LEU:HD13	1.71	0.71
1:D:35:LEU:HD23	1:D:38:ILE:HG22	1.72	0.70
1:H:25:VAL:HG11	1:H:28:VAL:HG23	1.72	0.70
1:F:114:MET:HG2	1:H:120:ARG:NH1	2.05	0.70
1:C:72:GLU:HG3	1:C:84:ILE:HG12	1.73	0.69
1:D:99:GLU:HB2	1:D:102:GLN:HE21	1.54	0.69
1:A:86:GLU:OE2	2:I:4:ARG:HG2	1.93	0.68
1:C:120:ARG:HD2	1:C:137:LEU:O	1.93	0.68
1:H:38:ILE:HD13	1:H:82:ALA:HA	1.76	0.68
1:G:98:LEU:HB2	1:G:103:MET:CE	2.24	0.68
1:A:38:ILE:HD11	1:A:75:LEU:HD23	1.75	0.68
1:D:25:VAL:HG11	1:D:28:VAL:HG23	1.75	0.68
1:D:101:VAL:HG13	1:D:150:MET:HE1	1.76	0.67
1:F:50:ASP:HB2	1:F:70:SER:HB2	1.77	0.67
1:A:24:TYR:CD1	1:B:35:LEU:HD23	2.29	0.67
1:C:35:LEU:HD23	1:C:38:ILE:HG22	1.75	0.66
1:G:113:ASN:HD22	1:G:142:PHE:HD1	1.43	0.66
1:B:38:ILE:HD11	1:B:75:LEU:HD22	1.78	0.66
1:F:43:TRP:CZ3	1:F:75:LEU:HD11	2.31	0.66
1:A:98:LEU:HB2	1:A:103:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:HD2	1:B:137:LEU:O	1.96	0.66
1:F:47:LEU:HD11	1:F:71:VAL:HG22	1.78	0.65
1:E:35:LEU:HD22	1:E:39:PHE:CZ	2.31	0.65
1:D:84:ILE:HD11	2:J:23:ARG:HG3	1.79	0.65
1:D:102:GLN:CD	1:D:102:GLN:H	2.04	0.65
1:D:74:THR:HG22	1:D:81:VAL:HA	1.78	0.65
1:E:51:LEU:HD23	1:E:51:LEU:C	2.22	0.64
1:C:98:LEU:HB3	1:C:102:GLN:HB3	1.79	0.64
1:D:102:GLN:NE2	1:D:102:GLN:H	1.96	0.64
1:F:98:LEU:HD12	1:F:103:MET:HE2	1.81	0.63
1:C:141:ASN:ND2	1:C:144:ALA:HB2	2.13	0.63
1:B:19:GLN:NE2	1:D:138:SER:HB3	2.14	0.62
1:F:19:GLN:CG	1:F:94:THR:HB	2.29	0.62
1:D:51:LEU:HD23	1:D:52:SER:N	2.14	0.62
1:G:21:GLN:HB2	1:G:92:VAL:HG12	1.82	0.62
1:E:111:CYS:HB2	1:E:112:PRO:HD3	1.80	0.61
1:H:111:CYS:HB2	1:H:112:PRO:HD3	1.82	0.61
1:A:87:VAL:HG11	1:A:122:LEU:HD23	1.82	0.61
1:B:72:GLU:HG3	1:B:84:ILE:HD13	1.82	0.61
1:C:17:VAL:HG12	1:C:19:GLN:HE21	1.66	0.61
1:C:40:GLN:HE21	1:F:40:GLN:NE2	1.98	0.61
1:E:146:PHE:O	1:E:149:TYR:HB3	2.00	0.61
1:C:49:PHE:HE1	1:C:69:ILE:HG23	1.65	0.61
1:E:97:GLY:C	1:E:98:LEU:HD12	2.26	0.61
1:A:98:LEU:HD22	1:A:102:GLN:HB3	1.83	0.60
1:H:119:ALA:O	1:H:123:VAL:HG23	2.01	0.60
1:B:51:LEU:HD23	1:B:52:SER:N	2.16	0.60
1:H:101:VAL:HG22	1:H:150:MET:HE1	1.82	0.60
1:D:51:LEU:HD23	1:D:51:LEU:C	2.26	0.59
1:E:120:ARG:HH12	1:G:114:MET:HG2	1.68	0.59
1:G:28:VAL:CG1	1:H:30:PHE:HB3	2.29	0.59
1:E:58:VAL:HG12	1:E:62:LEU:HB3	1.84	0.59
1:F:43:TRP:NE1	1:F:133:PRO:HG3	2.18	0.59
1:E:77:ASP:OD2	1:E:77:ASP:N	2.31	0.58
1:H:74:THR:HG22	1:H:81:VAL:HA	1.85	0.58
1:D:25:VAL:CG1	1:D:28:VAL:HG23	2.33	0.58
1:H:47:LEU:HD11	1:H:71:VAL:HG13	1.84	0.58
1:B:120:ARG:HG3	1:B:137:LEU:HB2	1.85	0.58
1:G:120:ARG:HD2	1:G:137:LEU:O	2.02	0.58
1:H:35:LEU:HD22	1:H:39:PHE:CE1	2.39	0.58
1:F:25:VAL:CG1	1:F:28:VAL:HG23	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:VAL:CG1	1:H:28:VAL:HG23	2.34	0.58
1:F:95:ILE:CG2	1:F:103:MET:HE1	2.33	0.57
1:C:40:GLN:HE21	1:F:40:GLN:HE21	1.52	0.57
1:G:103:MET:HE2	1:G:103:MET:HA	1.86	0.57
1:A:58:VAL:O	1:A:58:VAL:CG1	2.53	0.57
1:F:20:ILE:CD1	1:F:23:ILE:HG13	2.35	0.57
1:F:71:VAL:HG12	1:F:85:CYS:HB3	1.85	0.57
1:G:95:ILE:HG22	1:G:103:MET:HE1	1.86	0.57
1:H:142:PHE:CD2	1:H:145:LEU:HD12	2.39	0.57
1:C:97:GLY:O	1:C:98:LEU:HD23	2.05	0.56
1:F:44:LYS:O	1:F:76:GLU:HG2	2.04	0.56
1:G:72:GLU:HG3	1:G:84:ILE:HG12	1.87	0.56
1:A:68:ASN:OD1	1:A:88:LYS:HE3	2.04	0.56
1:D:68:ASN:OD1	1:D:88:LYS:HG3	2.04	0.56
1:E:25:VAL:CG1	1:E:28:VAL:HG23	2.34	0.56
1:G:43:TRP:NE1	1:G:133:PRO:HG3	2.20	0.56
1:A:51:LEU:CD2	1:A:145:LEU:HD11	2.35	0.56
1:A:74:THR:HG22	1:A:81:VAL:HA	1.88	0.56
1:E:44:LYS:O	1:E:76:GLU:HG2	2.06	0.56
1:A:51:LEU:C	1:A:51:LEU:HD23	2.31	0.56
1:B:68:ASN:OD1	1:B:88:LYS:HG3	2.06	0.55
1:D:25:VAL:HG11	1:D:28:VAL:CG2	2.36	0.55
1:G:106:CYS:HA	1:G:110:GLN:HB2	1.89	0.55
1:B:117:PRO:HG3	1:D:117:PRO:HB2	1.87	0.55
1:A:32:ALA:HB1	1:A:35:LEU:HD13	1.88	0.55
1:B:25:VAL:HG11	1:B:28:VAL:CG2	2.36	0.55
1:D:106:CYS:HA	1:D:110:GLN:HB2	1.88	0.55
1:B:58:VAL:HG22	1:B:58:VAL:O	2.07	0.55
1:C:38:ILE:HD12	1:C:41:GLN:NE2	2.21	0.55
1:B:101:VAL:HG13	1:B:150:MET:CE	2.36	0.55
1:E:49:PHE:HE1	1:E:69:ILE:HG23	1.71	0.55
1:H:142:PHE:HD2	1:H:145:LEU:HD12	1.72	0.55
1:A:58:VAL:O	1:A:58:VAL:HG12	2.07	0.54
1:E:25:VAL:HG11	1:E:28:VAL:CG2	2.36	0.54
1:H:35:LEU:HD22	1:H:39:PHE:CZ	2.42	0.54
1:H:101:VAL:HG13	1:H:150:MET:HE2	1.90	0.54
1:G:98:LEU:HB3	1:G:102:GLN:HB2	1.89	0.54
1:A:111:CYS:HB2	1:A:112:PRO:HD3	1.90	0.54
1:C:17:VAL:CG1	1:C:19:GLN:HE21	2.20	0.54
1:H:51:LEU:C	1:H:51:LEU:HD23	2.33	0.54
1:B:106:CYS:HA	1:B:110:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:CYS:HB2	1:D:112:PRO:HD3	1.91	0.53
1:G:105:HIS:CE1	1:G:110:GLN:HE21	2.25	0.53
1:D:69:ILE:HD12	1:D:119:ALA:HB1	1.91	0.53
1:F:44:LYS:HD2	1:F:77:ASP:OD2	2.09	0.53
1:F:141:ASN:OD1	1:F:143:ASP:HB2	2.08	0.53
1:G:83:PHE:CD1	1:G:83:PHE:C	2.87	0.53
1:A:87:VAL:CG1	1:A:122:LEU:HD23	2.39	0.52
1:E:87:VAL:CG1	1:E:122:LEU:HD23	2.38	0.52
1:G:44:LYS:O	1:G:76:GLU:HG2	2.09	0.52
1:D:35:LEU:HD23	1:D:38:ILE:CG2	2.38	0.52
1:B:63:TYR:N	1:B:63:TYR:CD1	2.78	0.52
1:G:74:THR:HG22	1:G:81:VAL:HA	1.91	0.52
1:E:55:THR:HG21	1:E:107:LEU:HD13	1.91	0.52
1:G:51:LEU:C	1:G:51:LEU:HD23	2.35	0.52
1:E:39:PHE:CE1	1:F:22:ARG:NE	2.77	0.52
1:G:38:ILE:HD11	1:G:75:LEU:HD22	1.91	0.52
1:G:51:LEU:HD23	1:G:52:SER:N	2.25	0.52
1:H:43:TRP:NE1	1:H:133:PRO:HG3	2.25	0.52
1:B:51:LEU:HD23	1:B:51:LEU:C	2.35	0.51
1:H:143:ASP:O	1:H:147:VAL:HG23	2.10	0.51
1:H:25:VAL:HG11	1:H:28:VAL:CG2	2.40	0.51
2:J:5:ASN:HA	2:J:15:LYS:HD3	1.91	0.51
1:G:38:ILE:HD12	1:G:41:GLN:NE2	2.25	0.51
1:H:98:LEU:HB3	1:H:102:GLN:HB3	1.92	0.51
1:D:86:GLU:OE1	2:J:4:ARG:HG2	2.10	0.51
1:G:28:VAL:HG23	1:G:87:VAL:HG22	1.93	0.51
1:G:60:ASP:O	1:G:61:ASP:HB2	2.09	0.51
1:B:19:GLN:HE22	1:D:138:SER:HB3	1.75	0.51
1:D:113:ASN:HD22	1:D:142:PHE:HD1	1.57	0.51
1:A:128:ASN:HD21	1:D:128:ASN:HB3	1.75	0.51
1:F:35:LEU:HD23	1:F:38:ILE:HG22	1.92	0.50
1:F:130:GLY:O	1:F:131:THR:OG1	2.29	0.50
1:E:43:TRP:NE1	1:E:133:PRO:HG3	2.26	0.50
1:E:44:LYS:HB3	1:E:76:GLU:CG	2.41	0.50
1:B:22:ARG:HD2	1:B:24:TYR:CD2	2.46	0.50
1:F:147:VAL:HG12	1:F:151:ASN:ND2	2.26	0.50
1:D:102:GLN:CD	1:D:102:GLN:N	2.68	0.50
1:C:18:LEU:C	1:C:18:LEU:HD12	2.36	0.50
1:C:51:LEU:HD23	1:C:51:LEU:C	2.37	0.50
1:G:55:THR:HG21	1:G:107:LEU:HD13	1.92	0.50
1:D:20:ILE:HG23	1:D:20:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD22	1:D:39:PHE:CE1	2.47	0.50
1:G:58:VAL:HG22	1:G:58:VAL:O	2.11	0.50
1:F:142:PHE:HD2	1:F:145:LEU:CD1	2.25	0.49
1:G:120:ARG:HG3	1:G:137:LEU:HB2	1.93	0.49
1:D:55:THR:HG22	1:D:56:THR:N	2.28	0.49
1:E:109:SER:HA	1:E:142:PHE:HB2	1.95	0.49
1:C:51:LEU:HD23	1:C:52:SER:N	2.28	0.49
1:E:109:SER:O	1:E:113:ASN:HB2	2.12	0.49
1:A:116:PHE:N	1:A:117:PRO:HD2	2.28	0.49
1:F:21:GLN:HB2	1:F:92:VAL:HG12	1.93	0.49
1:H:55:THR:HG22	1:H:56:THR:N	2.27	0.49
1:B:101:VAL:HG13	1:B:150:MET:HE1	1.95	0.49
1:G:17:VAL:O	1:G:95:ILE:HA	2.13	0.49
1:A:51:LEU:HD21	1:A:145:LEU:HD11	1.94	0.49
1:D:66:VAL:HG13	1:D:90:ALA:HB2	1.95	0.49
1:G:35:LEU:HD23	1:G:38:ILE:HG22	1.94	0.49
1:A:32:ALA:HB1	1:A:35:LEU:CD1	2.43	0.48
1:E:47:LEU:HD12	1:E:48:GLY:N	2.27	0.48
1:B:81:VAL:HG11	1:B:84:ILE:HD11	1.95	0.48
1:C:35:LEU:HD22	1:C:39:PHE:CZ	2.48	0.48
1:A:128:ASN:HD21	1:D:128:ASN:CG	2.22	0.48
1:G:98:LEU:HD12	1:G:103:MET:CE	2.44	0.48
1:F:120:ARG:HD2	1:F:137:LEU:O	2.14	0.48
1:A:38:ILE:HD11	1:A:75:LEU:CD2	2.43	0.48
1:A:55:THR:HG22	1:A:56:THR:N	2.29	0.48
1:A:69:ILE:HD12	1:A:119:ALA:HB1	1.96	0.48
1:B:32:ALA:HB1	1:B:35:LEU:CD1	2.43	0.48
1:C:141:ASN:O	1:C:145:LEU:HD13	2.13	0.48
1:E:26:LYS:HE2	1:E:64:GLU:OE1	2.13	0.48
1:C:26:LYS:HB2	1:C:88:LYS:CD	2.44	0.48
2:I:2:ILE:HG23	2:I:2:ILE:O	2.13	0.48
1:A:55:THR:HG21	1:A:107:LEU:HD13	1.95	0.47
1:B:60:ASP:O	1:B:61:ASP:HB2	2.13	0.47
1:C:38:ILE:HD11	1:C:75:LEU:HD22	1.95	0.47
1:F:24:TYR:OH	1:F:64:GLU:HG3	2.13	0.47
1:H:51:LEU:HD23	1:H:52:SER:N	2.28	0.47
1:F:18:LEU:HD22	1:F:106:CYS:SG	2.54	0.47
1:H:87:VAL:CG1	1:H:122:LEU:HD23	2.45	0.47
1:B:111:CYS:HB2	1:B:112:PRO:HD3	1.97	0.47
2:J:9:PRO:O	2:J:10:CYS:CB	2.55	0.47
1:C:106:CYS:HA	1:C:110:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HD13	1:D:93:PHE:CE2	2.49	0.47
1:E:24:TYR:CD1	1:F:35:LEU:HD13	2.50	0.47
1:G:98:LEU:HB2	1:G:103:MET:HE2	1.95	0.47
1:H:28:VAL:HG22	1:H:122:LEU:HD21	1.96	0.47
1:D:105:HIS:HA	1:D:146:PHE:CD1	2.50	0.47
2:J:2:ILE:HG13	2:J:16:TYR:CD2	2.50	0.47
1:E:28:VAL:HG22	1:E:122:LEU:HD21	1.98	0.46
2:J:8:CYS:SG	2:J:19:CYS:HB3	2.55	0.46
1:C:17:VAL:HG12	1:C:18:LEU:N	2.30	0.46
1:C:55:THR:HG21	1:C:107:LEU:HD22	1.96	0.46
1:E:121:GLU:HG3	1:G:118:TYR:HA	1.97	0.46
1:C:35:LEU:HD22	1:C:39:PHE:CE1	2.50	0.46
1:F:108:THR:OG1	1:F:146:PHE:HA	2.15	0.46
1:D:86:GLU:CD	2:J:4:ARG:HG2	2.41	0.46
1:E:43:TRP:NE1	1:E:133:PRO:CG	2.79	0.46
1:E:145:LEU:O	1:E:146:PHE:C	2.57	0.46
1:F:17:VAL:HG22	1:F:96:SER:OG	2.15	0.46
1:D:146:PHE:O	1:D:149:TYR:HB3	2.16	0.46
1:H:97:GLY:O	1:H:98:LEU:HD23	2.16	0.46
1:F:111:CYS:HA	1:F:114:MET:HE3	1.98	0.46
1:D:55:THR:CG2	1:D:56:THR:N	2.77	0.46
1:A:109:SER:HA	1:A:142:PHE:HB3	1.97	0.46
1:D:38:ILE:HD12	1:D:41:GLN:NE2	2.31	0.46
1:D:129:ARG:HH11	1:D:129:ARG:CA	2.24	0.46
1:F:35:LEU:HD22	1:F:39:PHE:CE1	2.50	0.46
1:C:26:LYS:HB2	1:C:88:LYS:HD2	1.98	0.45
1:G:68:ASN:OD1	1:G:88:LYS:HG3	2.16	0.45
1:A:83:PHE:CD1	1:A:83:PHE:C	2.94	0.45
1:G:46:LYS:HD3	1:G:46:LYS:HA	1.84	0.45
1:H:49:PHE:HD1	1:H:71:VAL:HG22	1.81	0.45
1:F:83:PHE:CD1	1:F:83:PHE:C	2.94	0.45
1:H:145:LEU:O	1:H:149:TYR:HB2	2.16	0.45
1:A:35:LEU:HD12	1:A:35:LEU:N	2.31	0.45
1:B:50:ASP:HB2	1:B:70:SER:HB3	1.98	0.45
1:G:35:LEU:HD23	1:G:38:ILE:CG2	2.46	0.45
1:H:20:ILE:HD13	1:H:93:PHE:CE2	2.52	0.45
1:B:38:ILE:CD1	1:B:75:LEU:HD22	2.46	0.45
1:B:142:PHE:HD2	1:B:145:LEU:HD12	1.81	0.45
1:B:72:GLU:HG3	1:B:84:ILE:CD1	2.47	0.45
1:C:111:CYS:HB2	1:C:112:PRO:HD3	1.99	0.45
1:G:19:GLN:HA	1:G:19:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:PHE:CD1	1:E:83:PHE:C	2.95	0.44
2:I:8:CYS:O	2:I:10:CYS:N	2.49	0.44
1:C:55:THR:HG22	1:C:56:THR:N	2.33	0.44
1:H:141:ASN:OD1	1:H:143:ASP:HB2	2.17	0.44
1:A:17:VAL:CG2	1:A:96:SER:OG	2.65	0.44
1:H:151:ASN:HD22	1:H:151:ASN:N	2.16	0.44
1:B:98:LEU:HB3	1:B:102:GLN:HB2	1.99	0.44
1:D:29:SER:HB2	2:J:5:ASN:ND2	2.33	0.44
1:D:109:SER:O	1:D:113:ASN:HB2	2.16	0.44
1:E:28:VAL:HB	1:F:30:PHE:HB3	2.00	0.44
1:G:44:LYS:HB3	1:G:76:GLU:OE2	2.18	0.44
1:H:35:LEU:HD23	1:H:38:ILE:HG22	2.00	0.44
1:A:106:CYS:HA	1:A:110:GLN:HB2	1.99	0.44
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.85	0.44
2:I:17:LYS:HE3	2:I:18:HIS:CE1	2.53	0.44
1:C:129:ARG:HD3	1:D:122:LEU:HD13	1.99	0.44
1:F:61:ASP:O	1:F:94:THR:HA	2.18	0.44
1:C:60:ASP:O	1:C:61:ASP:HB2	2.17	0.43
1:C:74:THR:HG22	1:C:81:VAL:HA	1.99	0.43
1:A:42:GLU:OE1	1:A:44:LYS:HE3	2.18	0.43
1:D:49:PHE:HE1	1:D:69:ILE:HG23	1.83	0.43
1:F:160:GLU:C	1:F:162:SER:N	2.76	0.43
1:B:101:VAL:HG13	1:B:150:MET:HE2	1.99	0.43
1:D:35:LEU:HD22	1:D:39:PHE:CZ	2.53	0.43
2:J:19:CYS:HB3	2:J:20:HIS:H	1.67	0.43
1:C:40:GLN:CG	1:F:40:GLN:HB2	2.48	0.43
1:D:43:TRP:CE3	1:D:75:LEU:HD11	2.53	0.43
1:G:108:THR:HG22	1:G:108:THR:O	2.18	0.43
1:G:111:CYS:HA	1:G:114:MET:HE3	1.99	0.43
1:E:74:THR:HG22	1:E:81:VAL:HA	2.00	0.43
1:G:111:CYS:HB2	1:G:112:PRO:HD3	2.00	0.43
2:I:3:GLY:N	2:I:6:GLU:HG3	2.34	0.43
1:A:122:LEU:HD13	1:B:129:ARG:HD3	2.01	0.43
1:E:105:HIS:NE2	1:E:143:ASP:OD1	2.44	0.43
1:H:106:CYS:HA	1:H:110:GLN:HB2	2.00	0.43
1:B:83:PHE:CD1	1:B:83:PHE:C	2.97	0.43
1:C:22:ARG:HD3	1:D:39:PHE:CE1	2.53	0.43
1:F:160:GLU:C	1:F:162:SER:H	2.26	0.43
1:D:72:GLU:CD	2:J:23:ARG:HH12	2.26	0.43
1:G:55:THR:CG2	1:G:56:THR:N	2.81	0.43
2:J:10:CYS:O	2:J:12:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:VAL:HB	1:F:142:PHE:CE1	2.53	0.42
1:G:55:THR:HG22	1:G:56:THR:N	2.34	0.42
1:G:53:THR:HG21	1:G:112:PRO:HB3	2.02	0.42
1:G:61:ASP:O	1:G:94:THR:HA	2.18	0.42
1:F:18:LEU:HD13	1:F:95:ILE:HG12	2.01	0.42
1:A:71:VAL:HG11	1:A:135:LEU:HD21	2.01	0.42
1:A:142:PHE:O	1:A:143:ASP:C	2.61	0.42
1:B:41:GLN:HB2	1:B:75:LEU:HD23	2.01	0.42
1:C:83:PHE:C	1:C:83:PHE:CD1	2.98	0.42
2:I:4:ARG:O	2:I:17:LYS:HG2	2.19	0.42
1:A:143:ASP:O	1:A:146:PHE:HB3	2.20	0.42
1:E:51:LEU:HD23	1:E:52:SER:CA	2.49	0.42
1:G:101:VAL:HG13	1:G:150:MET:HE2	2.00	0.42
1:C:120:ARG:HG3	1:C:137:LEU:HB2	2.02	0.42
1:D:38:ILE:HD11	1:D:75:LEU:HD22	2.01	0.42
1:G:123:VAL:O	1:G:127:VAL:HG23	2.20	0.42
1:E:21:GLN:HB3	1:E:92:VAL:HG12	2.02	0.42
1:E:61:ASP:O	1:E:94:THR:HA	2.20	0.42
1:E:138:SER:HB3	1:G:19:GLN:HE22	1.85	0.42
1:F:113:ASN:HD22	1:F:142:PHE:HD1	1.66	0.42
1:D:83:PHE:CD1	1:D:83:PHE:C	2.97	0.42
1:F:102:GLN:HE21	1:F:102:GLN:HB3	1.51	0.42
1:B:44:LYS:HB2	1:B:76:GLU:HG2	2.01	0.41
1:E:87:VAL:HG11	1:E:122:LEU:HD23	2.01	0.41
1:F:55:THR:CG2	1:F:56:THR:N	2.82	0.41
1:F:121:GLU:C	1:F:121:GLU:CD	2.88	0.41
1:F:142:PHE:CD2	1:F:145:LEU:CD1	3.03	0.41
1:G:129:ARG:HD3	1:H:122:LEU:HD13	2.02	0.41
1:B:25:VAL:HG11	1:B:28:VAL:HG22	2.01	0.41
1:B:55:THR:HG22	1:B:56:THR:N	2.35	0.41
1:B:142:PHE:CD2	1:B:145:LEU:HD12	2.55	0.41
1:E:66:VAL:HG22	1:E:90:ALA:HB2	2.02	0.41
1:E:69:ILE:HD11	1:E:116:PHE:CE1	2.55	0.41
1:E:130:GLY:O	1:E:131:THR:OG1	2.37	0.41
1:F:153:GLN:C	1:F:155:ALA:H	2.28	0.41
1:E:17:VAL:HB	1:E:96:SER:OG	2.20	0.41
1:E:141:ASN:OD1	1:E:143:ASP:HB2	2.21	0.41
2:I:8:CYS:SG	2:I:20:HIS:HB2	2.61	0.41
1:G:98:LEU:HB2	1:G:103:MET:HE3	1.98	0.41
1:B:32:ALA:HB1	1:B:35:LEU:HD13	2.02	0.41
1:D:77:ASP:OD2	1:D:77:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ILE:HG22	1:D:103:MET:HE1	2.03	0.41
1:A:128:ASN:HD21	1:D:128:ASN:CB	2.33	0.41
1:F:47:LEU:HD12	1:F:48:GLY:N	2.36	0.41
1:F:111:CYS:HB2	1:F:112:PRO:HD3	2.01	0.41
1:E:75:LEU:N	1:E:75:LEU:CD1	2.84	0.41
1:C:145:LEU:HD12	1:C:145:LEU:N	2.37	0.40
1:F:99:GLU:O	1:F:100:ASP:C	2.65	0.40
2:J:8:CYS:HA	2:J:9:PRO:HD3	1.88	0.40
1:B:18:LEU:HD13	1:B:95:ILE:HG12	2.02	0.40
1:F:147:VAL:CG1	1:F:151:ASN:HD21	2.34	0.40
1:G:14:GLN:O	1:G:15:GLN:C	2.63	0.40
1:G:111:CYS:HA	1:G:114:MET:CE	2.52	0.40
1:A:75:LEU:HD22	1:A:75:LEU:N	2.36	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	142/169 (84%)	133 (94%)	8 (6%)	1 (1%)	18	47
1	B	135/169 (80%)	128 (95%)	6 (4%)	1 (1%)	18	47
1	C	134/169 (79%)	126 (94%)	6 (4%)	2 (2%)	8	28
1	D	133/169 (79%)	125 (94%)	7 (5%)	1 (1%)	16	44
1	E	138/169 (82%)	128 (93%)	9 (6%)	1 (1%)	18	47
1	F	146/169 (86%)	137 (94%)	5 (3%)	4 (3%)	4	15
1	G	145/169 (86%)	135 (93%)	8 (6%)	2 (1%)	9	30
1	H	134/169 (79%)	127 (95%)	6 (4%)	1 (1%)	18	47
2	I	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	2	7
2	J	22/27 (82%)	16 (73%)	4 (18%)	2 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1151/1406 (82%)	1072 (93%)	63 (6%)	16 (1%)	9	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	16	PRO
2	J	10	CYS
1	F	154	GLN
2	J	11	GLY
1	A	78	SER
1	B	78	SER
1	C	77	ASP
1	C	78	SER
1	D	78	SER
1	F	78	SER
1	G	78	SER
1	H	78	SER
2	I	10	CYS
1	E	78	SER
1	F	77	ASP
1	G	8	VAL

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	124/152 (82%)	118 (95%)	6 (5%)	23	56
1	B	123/152 (81%)	120 (98%)	3 (2%)	43	77
1	C	122/152 (80%)	118 (97%)	4 (3%)	33	69
1	D	122/152 (80%)	115 (94%)	7 (6%)	18	49
1	E	122/152 (80%)	118 (97%)	4 (3%)	33	69
1	F	125/152 (82%)	118 (94%)	7 (6%)	19	50
1	G	128/152 (84%)	122 (95%)	6 (5%)	23	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	122/152 (80%)	120 (98%)	2 (2%)	55	83
2	I	16/22 (73%)	16 (100%)	0	100	100
2	J	16/22 (73%)	16 (100%)	0	100	100
All	All	1020/1260 (81%)	981 (96%)	39 (4%)	29	64

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	36	PRO
1	A	50	ASP
1	A	62	LEU
1	A	99	GLU
1	A	138	SER
1	B	19	GLN
1	B	63	TYR
1	B	99	GLU
1	C	18	LEU
1	C	70	SER
1	C	75	LEU
1	C	99	GLU
1	D	36	PRO
1	D	50	ASP
1	D	62	LEU
1	D	74	THR
1	D	102	GLN
1	D	129	ARG
1	D	138	SER
1	E	19	GLN
1	E	58	VAL
1	E	75	LEU
1	E	77	ASP
1	F	20	ILE
1	F	36	PRO
1	F	58	VAL
1	F	71	VAL
1	F	75	LEU
1	F	102	GLN
1	F	153	GLN
1	G	11	THR
1	G	13	GLU

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Mol	Chain	Res	Type
1	G	50	ASP
1	G	71	VAL
1	G	75	LEU
1	G	147	VAL
1	H	75	LEU
1	H	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	128	ASN
1	A	136	ASN
1	A	151	ASN
1	B	19	GLN
1	B	21	GLN
1	B	102	GLN
1	B	128	ASN
1	B	136	ASN
1	C	19	GLN
1	C	110	GLN
1	C	128	ASN
1	C	136	ASN
1	C	141	ASN
1	D	21	GLN
1	D	40	GLN
1	D	102	GLN
1	D	113	ASN
1	E	89	GLN
1	E	151	ASN
1	F	19	GLN
1	F	21	GLN
1	F	40	GLN
1	F	89	GLN
1	F	102	GLN
1	F	113	ASN
1	F	128	ASN
1	F	136	ASN
1	F	151	ASN
1	G	19	GLN
1	G	21	GLN
1	G	34	ASN

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Mol	Chain	Res	Type
1	G	57	GLN
1	G	110	GLN
1	G	113	ASN
1	G	128	ASN
1	G	136	ASN
1	H	19	GLN
1	H	21	GLN
1	H	57	GLN
1	H	89	GLN
1	H	113	ASN
1	H	128	ASN
1	H	151	ASN
2	J	18	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	144/169 (85%)	0.11	6 (4%)	40	32	18, 44, 92, 128	0
1	B	137/169 (81%)	0.04	3 (2%)	62	52	19, 46, 107, 139	0
1	C	136/169 (80%)	0.08	5 (3%)	45	36	22, 47, 103, 151	0
1	D	135/169 (79%)	0.17	4 (2%)	52	42	20, 50, 97, 140	0
1	E	140/169 (82%)	0.39	7 (5%)	34	26	28, 56, 95, 115	0
1	F	148/169 (87%)	0.10	4 (2%)	56	46	29, 51, 83, 119	0
1	G	147/169 (86%)	0.18	1 (0%)	84	77	32, 59, 88, 123	0
1	H	136/169 (80%)	0.43	6 (4%)	39	31	36, 65, 112, 164	0
2	I	24/27 (88%)	0.37	2 (8%)	17	12	36, 57, 83, 88	0
2	J	24/27 (88%)	0.75	2 (8%)	17	12	36, 63, 92, 97	0
All	All	1171/1406 (83%)	0.20	40 (3%)	48	39	18, 53, 99, 164	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	ASP	6.8
1	A	159	GLU	4.5
1	D	151	ASN	4.3
1	G	151	ASN	4.2
1	C	19	GLN	4.0
1	D	77	ASP	4.0
1	F	162	SER	3.8
2	I	25	ALA	3.6
1	B	77	ASP	3.5
1	E	19	GLN	3.4
1	H	77	ASP	3.4
1	F	77	ASP	3.2
1	E	155	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	GLY	3.1
1	F	58	VAL	3.0
1	B	149	TYR	3.0
1	E	21	GLN	3.0
1	H	21	GLN	3.0
2	J	2	ILE	3.0
1	A	16	PRO	3.0
1	E	79	GLY	2.8
1	A	102	GLN	2.7
1	C	149	TYR	2.7
1	H	37	HIS	2.7
1	H	33	PRO	2.6
2	J	11	GLY	2.6
1	E	16	PRO	2.5
1	C	147	VAL	2.5
1	F	97	GLY	2.5
1	B	145	LEU	2.4
1	H	145	LEU	2.4
1	H	48	GLY	2.3
1	E	68	ASN	2.3
1	A	21	GLN	2.2
1	D	59	GLY	2.1
1	D	149	TYR	2.1
2	I	13	GLY	2.1
1	E	77	ASP	2.0
1	C	151	ASN	2.0
1	C	101	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	J	51	1/1	0.99	0.07	54,54,54,54	0
3	ZN	I	50	1/1	1.00	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.