



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:48 pm BST

PDB ID : 3R8B
Title : Crystal structure of Staphylococcal Enterotoxin B in complex with an affinity matured mouse TCR VBeta8.2 protein, G5-8
Authors : Bonsor, D.A.; Sundberg, E.J.
Deposited on : 2011-03-23
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

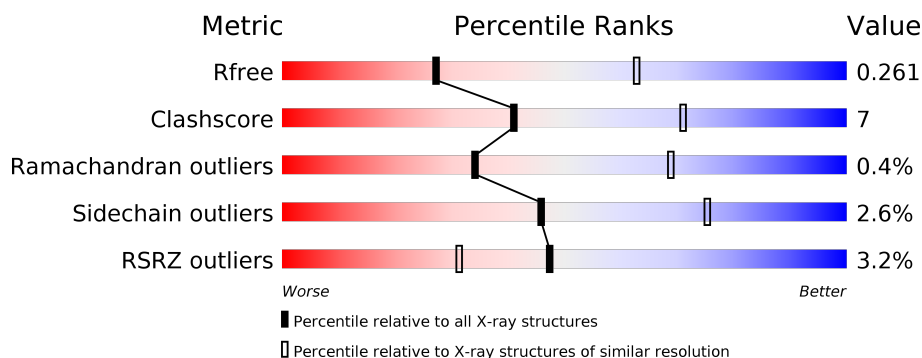
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	C	239	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	E	239	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
1	G	239	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	I	239	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	K	239	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	239	<div><div><div></div><div></div><div></div></div><div>%</div><div>85%</div><div>8%</div><div>•</div><div>6%</div></div>
1	O	239	<div><div><div></div><div></div><div></div></div><div>13%</div><div>83%</div><div>10%</div><div>•</div><div>6%</div></div>
2	B	125	<div><div><div></div><div></div><div></div></div><div>%</div><div>72%</div><div>18%</div><div>•</div><div>9%</div></div>
2	D	125	<div><div><div></div><div></div><div></div></div><div>75%</div><div>15%</div><div>•</div><div>9%</div></div>
2	F	125	<div><div><div></div><div></div><div></div></div><div>%</div><div>72%</div><div>18%</div><div>•</div><div>10%</div></div>
2	H	125	<div><div><div></div><div></div><div></div></div><div>74%</div><div>15%</div><div>•</div><div>10%</div></div>
2	J	125	<div><div><div></div><div></div><div></div></div><div>2%</div><div>68%</div><div>20%</div><div>•</div><div>10%</div></div>
2	L	125	<div><div><div></div><div></div><div></div></div><div>70%</div><div>20%</div><div>•</div><div>9%</div></div>
2	N	125	<div><div><div></div><div></div><div></div></div><div>2%</div><div>70%</div><div>18%</div><div>•</div><div>10%</div></div>
2	P	125	<div><div><div></div><div></div><div></div></div><div>5%</div><div>71%</div><div>17%</div><div>•</div><div>11%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21911 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 Enterotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1862	1193	299	360	10			
1	C	224	Total	C	N	O	S	0	0	0
			1863	1193	300	360	10			
1	E	224	Total	C	N	O	S	0	0	0
			1855	1188	299	358	10			
1	G	223	Total	C	N	O	S	0	0	0
			1852	1187	297	358	10			
1	I	226	Total	C	N	O	S	0	0	0
			1881	1205	303	363	10			
1	K	224	Total	C	N	O	S	0	0	0
			1866	1196	300	360	10			
1	M	225	Total	C	N	O	S	0	0	0
			1864	1194	300	360	10			
1	O	225	Total	C	N	O	S	0	0	0
			1868	1196	300	362	10			

- Molecule 2 is a protein called G5-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	114	Total	C	N	O	S	0	0	0
			864	546	147	167	4			
2	D	114	Total	C	N	O	S	0	0	0
			877	552	153	168	4			
2	F	113	Total	C	N	O	S	0	0	0
			870	547	152	167	4			
2	H	113	Total	C	N	O	S	0	0	0
			867	547	149	167	4			
2	J	112	Total	C	N	O	S	0	0	0
			883	557	154	168	4			
2	L	114	Total	C	N	O	S	0	0	0
			870	549	150	167	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	112	Total 868	C 547	N 151	O 166	S 4	0	0	0
2	P	111	Total 858	C 542	N 147	O 165	S 4	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Cl 1	0	0
3	J	2	Total 2	Cl 2	0	0
3	D	2	Total 2	Cl 2	0	0
3	B	2	Total 2	Cl 2	0	0
3	I	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	N	1	Total 1	Cl 1	0	0
3	O	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0
3	M	1	Total 1	Cl 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	2	Total	Zn	0	0
			2	2		
5	G	1	Total	Zn	0	0
			1	1		
5	J	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	K	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	H	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		
5	I	2	Total	Zn	0	0
			2	2		
5	C	1	Total	Zn	0	0
			1	1		
5	N	2	Total	Zn	0	0
			2	2		

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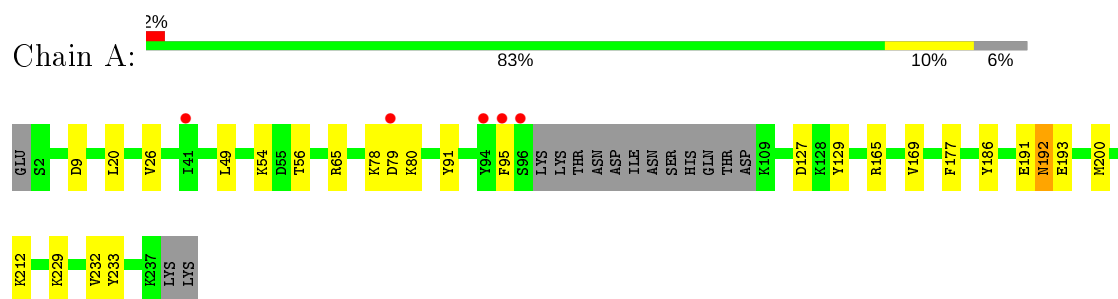
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	1	Total 1	Zn 1	0	0
5	L	2	Total 2	Zn 2	0	0
5	F	2	Total 2	Zn 2	0	0
5	M	1	Total 1	Zn 1	0	0

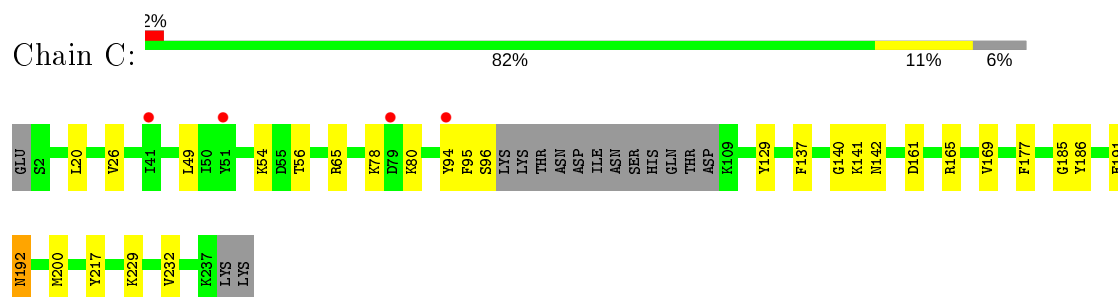
3 Residue-property plots [i](#)

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

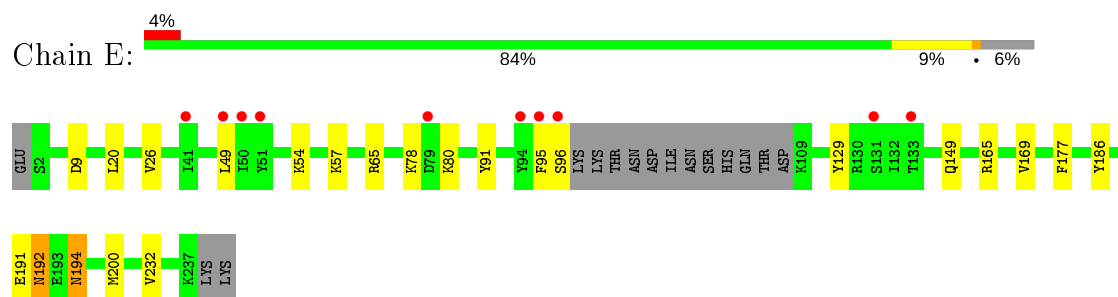
- Molecule 1: Enterotoxin type B



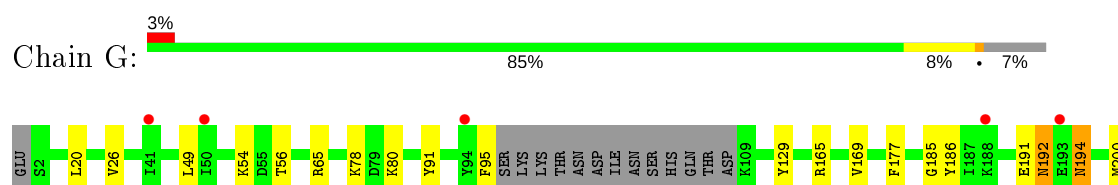
- Molecule 1: Enterotoxin type B

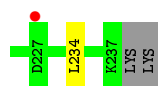


- Molecule 1: Enterotoxin type B

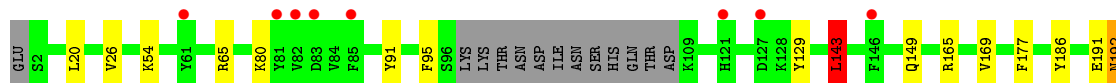
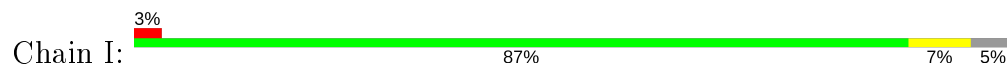


- Molecule 1: Enterotoxin type B

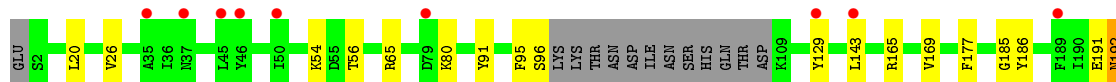
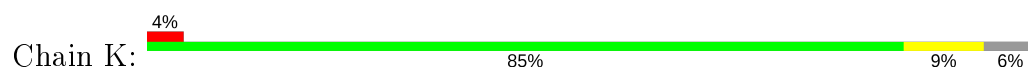




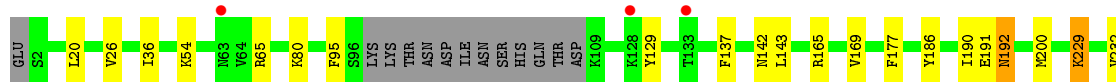
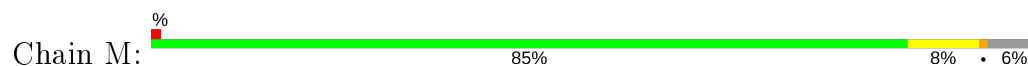
- Molecule 1: Enterotoxin type B



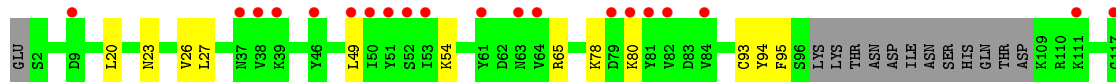
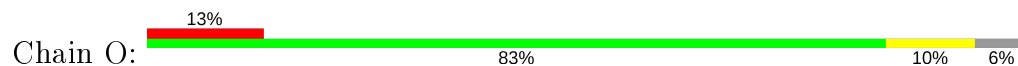
- Molecule 1: Enterotoxin type B



- Molecule 1: Enterotoxin type B



- Molecule 1: Enterotoxin type B



- Molecule 2: G5-8





- Molecule 2: G5-8



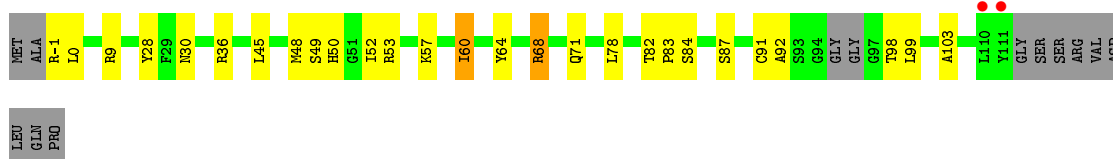
- Molecule 2: G5-8



- Molecule 2: G5-8



- Molecule 2: G5-8



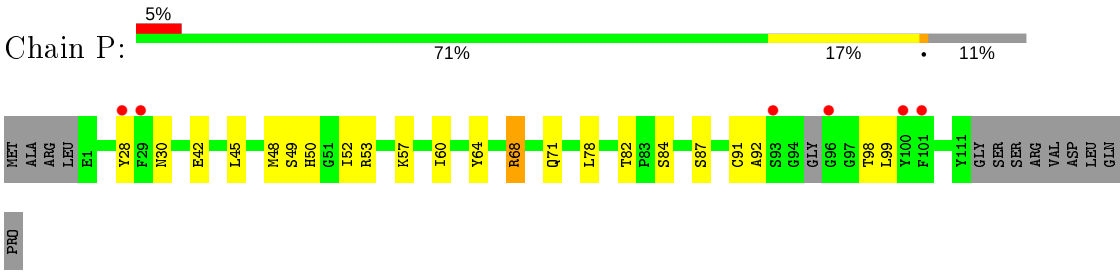
- Molecule 2: G5-8



- Molecule 2: G5-8



- Molecule 2: G5-8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.95Å 160.37Å 186.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 2.95 46.57 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (46.57-2.95) 92.5 (46.57-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.246 , 0.265 0.242 , 0.261	Depositor DCC
R_{free} test set	3259 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21911	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% 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, SO4, CL

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	0.68	0/1905	0.65	0/2566
1	C	0.65	0/1906	0.64	0/2566
1	E	0.68	0/1898	0.64	0/2557
1	G	0.67	0/1895	0.64	0/2554
1	I	0.70	1/1924 (0.1%)	0.66	1/2588 (0.0%)
1	K	0.67	0/1909	0.65	0/2570
1	M	0.68	0/1906	0.65	0/2565
1	O	0.68	0/1910	0.64	0/2570
2	B	0.69	0/883	0.71	0/1197
2	D	0.67	0/896	0.72	0/1212
2	F	0.65	0/888	0.72	0/1200
2	H	0.67	0/885	0.71	0/1197
2	J	0.68	0/901	0.74	0/1217
2	L	0.70	0/889	0.70	0/1204
2	N	0.68	0/887	0.72	0/1200
2	P	0.66	0/876	0.69	0/1185
All	All	0.67	1/22358 (0.0%)	0.67	1/30148 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	193	GLU	CB-CG	5.50	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	143	LEU	CA-CB-CG	5.67	128.34	115.30

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	1862	0	1784	27	0
1	C	1863	0	1786	23	0
1	E	1855	0	1771	20	0
1	G	1852	0	1768	20	0
1	I	1881	0	1810	15	0
1	K	1866	0	1795	23	0
1	M	1864	0	1781	22	0
1	O	1868	0	1785	16	0
2	B	864	0	823	32	0
2	D	877	0	848	24	0
2	F	870	0	835	28	0
2	H	867	0	833	26	0
2	J	883	0	864	24	0
2	L	870	0	834	31	0
2	N	868	0	843	24	0
2	P	858	0	828	21	0
3	A	1	0	0	0	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
3	D	2	0	0	1	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	1	0
4	A	5	0	0	1	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	1	0	0	0	0
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	N	2	0	0	0	0
5	O	1	0	0	0	0
5	P	2	0	0	0	0
All	All	21911	0	20988	304	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 7.

All (304) 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)
2:B:7:SER:CB	1:K:56:THR:HB	1.35	1.52
1:A:56:THR:HB	2:L:7:SER:CB	1.35	1.51
1:A:56:THR:CB	2:L:7:SER:CB	2.13	1.27
2:B:7:SER:CB	1:K:56:THR:CB	2.22	1.17
1:E:191:GLU:O	1:E:192:ASN:HB2	1.52	1.08
3:B:124:CL:CL	3:D:124:CL:CL	2.65	0.89
2:D:7:SER:HB2	1:G:56:THR:HB	1.60	0.81
2:D:29:PHE:CD1	2:D:95:GLY:HA3	2.15	0.81
2:J:82:THR:HG22	2:J:84:SER:H	1.45	0.80
2:D:82:THR:HG22	2:D:84:SER:H	1.47	0.80
1:A:129:TYR:CG	2:L:14:VAL:HG22	2.18	0.78
2:B:82:THR:HG22	2:B:84:SER:H	1.47	0.78
1:I:20:LEU:HD11	2:J:57:LYS:HG3	1.65	0.78
1:G:20:LEU:HD11	2:H:57:LYS:HG3	1.67	0.77
2:P:82:THR:HG22	2:P:84:SER:H	1.48	0.77
2:B:30:ASN:O	2:B:68:ARG:NH1	2.19	0.75
2:N:82:THR:HG22	2:N:84:SER:H	1.52	0.75
2:L:82:THR:HG22	2:L:84:SER:H	1.52	0.74
1:O:20:LEU:HD11	2:P:57:LYS:HG3	1.70	0.74
1:C:20:LEU:HD11	2:D:57:LYS:HG3	1.70	0.73
2:D:30:ASN:O	2:D:68:ARG:NH1	2.23	0.72
1:M:20:LEU:HD11	2:N:57:LYS:HG3	1.72	0.72
1:A:56:THR:OG1	2:L:7:SER:CB	2.38	0.71
2:H:28:TYR:CZ	2:H:71:GLN:HG3	2.26	0.71
1:A:129:TYR:CD1	2:L:14:VAL:HG22	2.26	0.71
2:H:82:THR:HG22	2:H:84:SER:H	1.54	0.70
1:E:20:LEU:HD11	2:F:57:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:GLU:O	1:G:192:ASN:HB2	1.91	0.70
2:F:12:VAL:H	1:M:36:ILE:CD1	2.03	0.70
1:A:191:GLU:O	1:A:192:ASN:HB2	1.92	0.70
1:K:191:GLU:O	1:K:192:ASN:HB2	1.91	0.70
2:F:82:THR:HG22	2:F:84:SER:H	1.54	0.69
1:M:191:GLU:O	1:M:192:ASN:HB2	1.91	0.69
2:F:28:TYR:CZ	2:F:71:GLN:HG3	2.28	0.69
2:L:30:ASN:O	2:L:68:ARG:NH1	2.27	0.68
2:D:29:PHE:CE1	2:D:95:GLY:HA3	2.29	0.68
2:H:60:ILE:O	2:H:60:ILE:HG23	1.93	0.68
1:C:191:GLU:O	1:C:192:ASN:HB2	1.93	0.67
2:L:28:TYR:CZ	2:L:71:GLN:HG3	2.29	0.67
2:J:98:THR:HG22	2:J:99:LEU:N	2.11	0.66
2:F:98:THR:HG22	2:F:99:LEU:N	2.11	0.66
2:N:28:TYR:CZ	2:N:71:GLN:HG3	2.31	0.66
2:D:28:TYR:CZ	2:D:71:GLN:HG3	2.31	0.66
2:P:98:THR:HG22	2:P:99:LEU:N	2.10	0.66
1:I:191:GLU:O	1:I:192:ASN:HB2	1.95	0.66
1:O:186:TYR:N	1:O:200:MET:HE2	2.12	0.65
1:E:149:GLN:OE1	2:N:10:ASN:O	2.14	0.65
2:B:28:TYR:CZ	2:B:71:GLN:HG3	2.31	0.65
2:H:98:THR:HG22	2:H:99:LEU:N	2.12	0.65
1:A:20:LEU:HD11	2:B:57:LYS:HG3	1.80	0.64
1:A:129:TYR:CD2	2:L:14:VAL:HG22	2.31	0.64
2:D:98:THR:HG22	2:D:99:LEU:N	2.12	0.64
2:J:28:TYR:CZ	2:J:71:GLN:HG3	2.32	0.64
1:O:191:GLU:O	1:O:192:ASN:HB2	1.98	0.63
2:P:30:ASN:O	2:P:68:ARG:NH1	2.30	0.63
2:P:60:ILE:O	2:P:60:ILE:HG23	1.98	0.63
2:H:30:ASN:O	2:H:68:ARG:NH1	2.31	0.63
2:J:30:ASN:O	2:J:68:ARG:NH1	2.31	0.63
1:M:165:ARG:O	1:M:169:VAL:HG23	1.99	0.63
2:B:98:THR:HG22	2:B:99:LEU:N	2.14	0.63
1:C:165:ARG:O	1:C:169:VAL:HG23	1.98	0.63
1:M:186:TYR:N	1:M:200:MET:HE2	2.15	0.62
2:P:28:TYR:CZ	2:P:71:GLN:HG3	2.34	0.62
1:A:165:ARG:O	1:A:169:VAL:HG23	2.00	0.62
1:K:20:LEU:HD11	2:L:57:LYS:HG3	1.80	0.62
1:E:57:LYS:HE2	2:N:24:LYS:HD3	1.80	0.62
2:L:98:THR:HG22	2:L:99:LEU:N	2.15	0.61
2:P:48:MET:HE1	2:P:50:HIS:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:GLU:O	1:E:192:ASN:CB	2.33	0.61
1:K:165:ARG:O	1:K:169:VAL:HG23	2.01	0.61
1:I:20:LEU:HD11	2:J:57:LYS:CG	2.29	0.61
1:C:140:GLY:O	1:I:129:TYR:CD2	2.54	0.60
1:I:143:LEU:HD12	1:I:143:LEU:O	2.01	0.60
2:J:36:ARG:HE	2:J:60:ILE:HD11	1.66	0.60
1:O:23:ASN:ND2	3:O:242:CL:CL	2.72	0.60
1:G:185:GLY:C	1:G:200:MET:HE2	2.23	0.60
2:N:95:GLY:O	2:N:97:GLY:N	2.35	0.60
2:N:98:THR:HG22	2:N:99:LEU:N	2.17	0.59
2:D:68:ARG:NH2	2:D:71:GLN:O	2.36	0.59
2:F:30:ASN:O	2:F:68:ARG:NH1	2.35	0.59
1:I:165:ARG:O	1:I:169:VAL:HG23	2.03	0.58
2:B:14:VAL:HG22	1:K:129:TYR:CG	2.38	0.58
2:J:82:THR:HG22	2:J:84:SER:N	2.16	0.58
2:N:30:ASN:O	2:N:68:ARG:NH1	2.36	0.58
2:B:82:THR:HG22	2:B:84:SER:N	2.17	0.57
2:B:14:VAL:HG22	1:K:129:TYR:CD1	2.39	0.57
1:G:194:ASN:N	1:G:194:ASN:OD1	2.29	0.57
2:H:28:TYR:CE2	2:H:71:GLN:HG3	2.40	0.57
2:F:28:TYR:CE2	2:F:71:GLN:HG3	2.40	0.57
1:I:91:TYR:CE1	2:J:50:HIS:HB3	2.39	0.57
1:E:129:TYR:HB2	2:N:10:ASN:ND2	2.20	0.57
2:P:82:THR:HG22	2:P:84:SER:N	2.19	0.56
1:A:129:TYR:HB2	2:L:14:VAL:HG13	1.85	0.56
2:F:12:VAL:N	1:M:36:ILE:CD1	2.69	0.56
2:F:68:ARG:NH2	2:F:71:GLN:O	2.38	0.56
2:N:28:TYR:CE2	2:N:71:GLN:HG3	2.39	0.56
2:N:68:ARG:NH2	2:N:71:GLN:O	2.38	0.56
1:C:56:THR:HB	2:H:7:SER:HB2	1.88	0.55
1:E:20:LEU:HD11	2:F:57:LYS:CG	2.35	0.55
2:L:28:TYR:CE2	2:L:71:GLN:HG3	2.40	0.55
2:B:14:VAL:HG22	1:K:129:TYR:CD2	2.41	0.55
2:L:68:ARG:NH2	2:L:71:GLN:O	2.39	0.55
1:G:20:LEU:HD11	2:H:57:LYS:CG	2.35	0.55
1:E:165:ARG:O	1:E:169:VAL:HG23	2.06	0.55
1:K:20:LEU:HD11	2:L:57:LYS:CG	2.36	0.55
2:N:48:MET:HE1	2:N:50:HIS:NE2	2.22	0.55
1:C:141:LYS:HB3	1:I:149:GLN:OE1	2.06	0.54
2:D:82:THR:HG22	2:D:84:SER:N	2.18	0.54
2:H:68:ARG:NH2	2:H:71:GLN:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:98:THR:HG22	2:J:99:LEU:H	1.71	0.54
2:B:48:MET:HE1	2:B:50:HIS:NE2	2.23	0.54
1:A:20:LEU:HD11	2:B:57:LYS:CG	2.38	0.54
2:D:64:TYR:CD1	2:D:78:LEU:CD2	2.91	0.54
1:M:20:LEU:HD23	1:M:177:PHE:CZ	2.43	0.54
2:D:28:TYR:CE2	2:D:71:GLN:HG3	2.43	0.53
2:B:28:TYR:CE2	2:B:71:GLN:HG3	2.44	0.53
1:I:20:LEU:CD1	2:J:57:LYS:HG3	2.38	0.53
2:F:12:VAL:H	1:M:36:ILE:HD12	1.74	0.53
2:P:68:ARG:NH2	2:P:71:GLN:O	2.42	0.53
2:B:68:ARG:NH2	2:B:71:GLN:O	2.43	0.52
1:C:186:TYR:N	1:C:200:MET:HE2	2.24	0.52
1:K:65:ARG:HD2	1:K:95:PHE:HB3	1.91	0.52
2:F:64:TYR:CD1	2:F:78:LEU:CD2	2.92	0.52
2:H:64:TYR:CD1	2:H:78:LEU:CD2	2.93	0.52
1:M:20:LEU:HD11	2:N:57:LYS:CG	2.39	0.51
2:J:28:TYR:CE2	2:J:71:GLN:HG3	2.45	0.51
1:M:190:ILE:CG2	1:M:229:LYS:NZ	2.74	0.51
1:I:65:ARG:HD2	1:I:95:PHE:HB3	1.92	0.51
2:P:98:THR:HG22	2:P:99:LEU:H	1.76	0.51
1:E:186:TYR:N	1:E:200:MET:HE2	2.26	0.51
2:D:98:THR:HG22	2:D:99:LEU:H	1.73	0.51
2:D:14:VAL:HG22	1:G:129:TYR:CE1	2.44	0.51
1:A:127:ASP:OD2	4:A:241:SO4:O4	2.29	0.51
1:C:20:LEU:HD11	2:D:57:LYS:CG	2.38	0.51
1:A:20:LEU:HD23	1:A:177:PHE:CZ	2.46	0.51
1:A:65:ARG:HD2	1:A:95:PHE:HB3	1.93	0.51
2:J:48:MET:HE1	2:J:50:HIS:NE2	2.25	0.50
1:E:20:LEU:HD23	1:E:177:PHE:CZ	2.46	0.50
1:E:57:LYS:HE2	2:N:24:LYS:CD	2.41	0.50
2:P:28:TYR:CE2	2:P:71:GLN:HG3	2.46	0.50
1:M:65:ARG:HD2	1:M:95:PHE:HB3	1.93	0.50
2:F:48:MET:HE1	2:F:50:HIS:NE2	2.27	0.50
2:P:48:MET:HG2	2:P:49:SER:N	2.26	0.50
2:F:98:THR:CG2	2:F:99:LEU:N	2.75	0.50
1:M:190:ILE:CG2	1:M:229:LYS:HZ3	2.25	0.50
2:F:14:VAL:HG22	1:M:129:TYR:CZ	2.46	0.50
1:C:65:ARG:HD2	1:C:95:PHE:HB3	1.93	0.50
2:L:98:THR:HG22	2:L:99:LEU:H	1.76	0.50
2:N:98:THR:HG22	2:N:99:LEU:H	1.77	0.49
1:O:20:LEU:HD23	1:O:177:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:98:THR:CG2	2:P:99:LEU:N	2.74	0.49
1:C:129:TYR:CZ	2:H:14:VAL:HG22	2.47	0.49
1:G:65:ARG:HD2	1:G:95:PHE:HB3	1.94	0.49
2:J:68:ARG:NH2	2:J:71:GLN:O	2.44	0.49
1:G:20:LEU:CD1	2:H:57:LYS:HG3	2.41	0.49
2:H:98:THR:HG22	2:H:99:LEU:H	1.77	0.49
2:B:14:VAL:HG22	1:K:129:TYR:CE1	2.48	0.49
2:L:29:PHE:CE1	2:L:95:GLY:HA3	2.48	0.49
2:H:48:MET:HE1	2:H:50:HIS:NE2	2.28	0.49
2:L:64:TYR:CD1	2:L:78:LEU:CD2	2.96	0.49
2:J:64:TYR:CD1	2:J:78:LEU:CD2	2.96	0.49
1:G:165:ARG:O	1:G:169:VAL:HG23	2.12	0.49
1:C:161:ASP:OD2	1:C:217:TYR:OH	2.26	0.48
1:A:186:TYR:N	1:A:200:MET:HE2	2.28	0.48
2:F:98:THR:HG22	2:F:99:LEU:H	1.77	0.48
2:H:98:THR:CG2	2:H:99:LEU:N	2.77	0.48
1:K:177:PHE:CD2	2:L:65:LYS:HG2	2.49	0.48
2:J:98:THR:HG22	2:J:99:LEU:O	2.14	0.48
1:K:186:TYR:N	1:K:200:MET:HE2	2.28	0.48
2:B:60:ILE:HG23	2:B:60:ILE:O	2.13	0.48
2:B:64:TYR:CD1	2:B:78:LEU:CD2	2.97	0.48
1:C:20:LEU:CD1	2:D:57:LYS:HG3	2.42	0.48
1:M:20:LEU:HD23	1:M:177:PHE:CE2	2.48	0.48
2:B:98:THR:CG2	2:B:99:LEU:N	2.77	0.48
1:C:20:LEU:HD23	1:C:177:PHE:CZ	2.49	0.48
1:I:20:LEU:HD23	1:I:177:PHE:CE2	2.48	0.48
2:F:82:THR:HG22	2:F:84:SER:N	2.25	0.48
2:L:48:MET:HE1	2:L:50:HIS:NE2	2.28	0.48
2:N:64:TYR:CD1	2:N:78:LEU:CD2	2.96	0.48
1:E:65:ARG:HD2	1:E:95:PHE:HB3	1.96	0.47
2:L:82:THR:HG22	2:L:84:SER:N	2.24	0.47
1:I:20:LEU:HD23	1:I:177:PHE:CZ	2.48	0.47
1:C:129:TYR:CE1	2:H:14:VAL:HG22	2.49	0.47
1:K:91:TYR:CE1	2:L:50:HIS:HB3	2.48	0.47
1:A:129:TYR:CE1	2:L:14:VAL:HG22	2.49	0.47
1:O:237:LYS:O	1:O:239:LYS:CB	2.62	0.47
1:C:129:TYR:CE2	2:H:14:VAL:HG22	2.50	0.47
2:D:98:THR:CG2	2:D:99:LEU:N	2.77	0.47
2:F:48:MET:HG2	2:F:49:SER:N	2.30	0.47
1:K:20:LEU:HD23	1:K:177:PHE:CZ	2.50	0.47
1:E:20:LEU:HD23	1:E:177:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:45:LEU:O	2:J:60:ILE:HG22	2.15	0.46
2:J:98:THR:CG2	2:J:99:LEU:N	2.76	0.46
2:D:14:VAL:HG22	1:G:129:TYR:CD1	2.50	0.46
1:G:91:TYR:CE1	2:H:50:HIS:HB3	2.51	0.46
2:N:82:THR:HG22	2:N:84:SER:N	2.24	0.46
1:O:65:ARG:HD2	1:O:95:PHE:HB3	1.95	0.46
2:D:48:MET:HE1	2:D:50:HIS:NE2	2.31	0.46
2:P:64:TYR:CD1	2:P:78:LEU:CD2	2.98	0.46
2:H:82:THR:HG22	2:H:84:SER:N	2.26	0.46
2:J:82:THR:HG23	2:J:83:PRO:HD2	1.98	0.46
2:F:42:GLU:HB3	2:P:45:LEU:HD22	1.97	0.46
1:C:49:LEU:HD21	1:C:78:LYS:HB2	1.98	0.46
1:E:200:MET:HE1	1:E:232:VAL:HG13	1.98	0.46
2:J:48:MET:HG2	2:J:49:SER:N	2.31	0.46
2:F:12:VAL:HG23	1:M:36:ILE:HD13	1.98	0.46
2:L:98:THR:CG2	2:L:99:LEU:N	2.78	0.46
2:N:48:MET:HG2	2:N:49:SER:N	2.31	0.46
1:O:165:ARG:O	1:O:169:VAL:HG23	2.15	0.46
2:P:98:THR:HG22	2:P:99:LEU:O	2.15	0.46
2:B:52:ILE:HG22	2:B:53:ARG:HG3	1.98	0.45
1:E:91:TYR:CE1	2:F:50:HIS:HB3	2.50	0.45
1:A:200:MET:HE1	1:A:232:VAL:HG13	1.99	0.45
2:D:48:MET:CE	2:D:56:GLU:CD	2.85	0.45
1:A:20:LEU:CD1	2:B:57:LYS:HG3	2.44	0.45
1:E:194:ASN:ND2	1:E:194:ASN:H	2.14	0.45
1:G:186:TYR:N	1:G:200:MET:HE2	2.31	0.45
2:H:60:ILE:O	2:H:60:ILE:CG2	2.65	0.45
2:N:60:ILE:O	2:N:60:ILE:HG23	2.17	0.45
2:H:48:MET:HG2	2:H:49:SER:N	2.32	0.45
1:E:49:LEU:HD21	1:E:78:LYS:HB2	1.99	0.45
1:G:20:LEU:HD23	1:G:177:PHE:CZ	2.52	0.45
2:B:98:THR:HG22	2:B:99:LEU:H	1.79	0.44
1:M:190:ILE:HG21	1:M:229:LYS:NZ	2.33	0.44
2:B:14:VAL:HG22	1:K:129:TYR:CE2	2.52	0.44
1:K:185:GLY:HA3	1:K:200:MET:HE3	1.98	0.44
1:M:200:MET:HE1	1:M:232:VAL:HG13	1.99	0.44
1:G:20:LEU:HD23	1:G:177:PHE:CE2	2.52	0.44
2:J:98:THR:CG2	2:J:99:LEU:H	2.31	0.44
1:M:20:LEU:CD1	2:N:57:LYS:HG3	2.44	0.44
1:K:20:LEU:HD23	1:K:177:PHE:CE2	2.53	0.44
1:E:20:LEU:CD1	2:F:57:LYS:HG3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:98:THR:CG2	2:N:99:LEU:N	2.81	0.44
2:F:98:THR:HG22	2:F:99:LEU:O	2.18	0.44
1:A:186:TYR:CE1	1:A:233:TYR:HB2	2.53	0.43
1:A:212:LYS:NZ	1:O:212:LYS:HB2	2.32	0.43
2:F:52:ILE:HG22	2:F:53:ARG:HG3	2.00	0.43
1:C:94:TYR:HE2	1:E:9:ASP:HB3	1.84	0.43
1:O:20:LEU:HD23	1:O:177:PHE:CE2	2.54	0.43
1:A:20:LEU:HD23	1:A:177:PHE:CE2	2.54	0.43
2:B:48:MET:HG2	2:B:49:SER:N	2.34	0.43
1:C:129:TYR:CD1	2:H:14:VAL:HG22	2.53	0.43
2:P:91:CYS:SG	2:P:92:ALA:N	2.92	0.43
1:I:186:TYR:N	1:I:200:MET:HE2	2.33	0.43
2:B:8:PRO:HA	1:K:56:THR:HG21	2.01	0.43
2:L:98:THR:CG2	2:L:99:LEU:H	2.32	0.43
2:P:98:THR:CG2	2:P:99:LEU:H	2.31	0.43
2:D:50:HIS:CD2	2:D:56:GLU:OE2	2.71	0.43
1:A:49:LEU:HD21	1:A:78:LYS:HB2	2.01	0.43
2:L:60:ILE:HG23	2:L:60:ILE:O	2.18	0.43
1:A:129:TYR:CE2	2:L:14:VAL:HG22	2.54	0.42
1:O:186:TYR:CA	1:O:200:MET:HE2	2.49	0.42
2:F:98:THR:CG2	2:F:99:LEU:H	2.32	0.42
1:A:91:TYR:CE1	2:B:50:HIS:HB3	2.54	0.42
2:H:50:HIS:CD2	2:H:56:GLU:OE2	2.73	0.42
2:B:7:SER:CB	1:K:56:THR:OG1	2.65	0.42
1:I:20:LEU:HD12	1:I:20:LEU:N	2.35	0.42
2:J:52:ILE:HG22	2:J:53:ARG:HG3	2.01	0.42
2:B:14:VAL:HG22	1:K:129:TYR:CZ	2.54	0.42
1:O:200:MET:HE1	1:O:232:VAL:HG13	2.01	0.42
1:C:185:GLY:HA3	1:C:200:MET:HE3	2.00	0.42
1:G:49:LEU:HD21	1:G:78:LYS:HB2	2.02	0.42
1:M:190:ILE:HG21	1:M:229:LYS:HZ3	1.83	0.42
2:N:52:ILE:HG22	2:N:53:ARG:HG3	2.00	0.42
2:P:60:ILE:CG2	2:P:60:ILE:O	2.66	0.42
1:I:143:LEU:C	1:I:143:LEU:HD12	2.40	0.42
2:L:24:LYS:HA	2:L:72:GLU:O	2.20	0.42
2:D:98:THR:CG2	2:D:99:LEU:H	2.32	0.42
1:M:186:TYR:CA	1:M:200:MET:HE2	2.50	0.42
1:O:186:TYR:CE1	1:O:233:TYR:HB2	2.54	0.42
1:C:20:LEU:HD23	1:C:177:PHE:CE2	2.55	0.41
1:C:200:MET:HE1	1:C:232:VAL:HG13	2.01	0.41
2:F:24:LYS:HA	2:F:72:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:50:HIS:CD2	2:N:56:GLU:OE2	2.72	0.41
1:A:186:TYR:C	1:A:200:MET:HE2	2.41	0.41
2:D:48:MET:HG2	2:D:49:SER:N	2.35	0.41
2:L:52:ILE:HG22	2:L:53:ARG:HG3	2.02	0.41
1:A:78:LYS:O	1:A:79:ASP:HB2	2.19	0.41
2:D:14:VAL:HG22	1:G:129:TYR:CZ	2.56	0.41
1:C:129:TYR:CD2	2:H:14:VAL:HG22	2.55	0.41
1:M:137:PHE:CE2	1:M:142:ASN:HB2	2.55	0.41
2:P:52:ILE:HG22	2:P:53:ARG:HG3	2.02	0.41
1:G:20:LEU:HD12	1:G:20:LEU:N	2.35	0.41
1:K:186:TYR:CE1	1:K:233:TYR:HB2	2.55	0.41
2:L:50:HIS:CD2	2:L:56:GLU:OE2	2.73	0.41
1:O:49:LEU:HD21	1:O:78:LYS:HB2	2.03	0.41
1:A:9:ASP:HB3	1:O:94:TYR:HE2	1.85	0.41
2:F:12:VAL:N	1:M:36:ILE:HD13	2.35	0.41
2:J:9:ARG:NE	2:J:103:ALA:HB3	2.35	0.41
2:B:98:THR:CG2	2:B:99:LEU:H	2.33	0.41
1:G:200:MET:HE3	1:G:234:LEU:CD2	2.51	0.41
2:J:91:CYS:SG	2:J:92:ALA:N	2.93	0.41
2:B:50:HIS:CD2	2:B:56:GLU:OE2	2.74	0.41
1:E:186:TYR:C	1:E:200:MET:HE2	2.41	0.40
1:G:191:GLU:O	1:G:192:ASN:CB	2.64	0.40
2:L:48:MET:HG2	2:L:49:SER:N	2.35	0.40
2:B:24:LYS:HA	2:B:72:GLU:O	2.21	0.40
2:B:98:THR:HG22	2:B:99:LEU:O	2.21	0.40
2:F:45:LEU:HD22	2:P:42:GLU:HB3	2.03	0.40
1:K:191:GLU:O	1:K:192:ASN:CB	2.65	0.40
1:O:27:LEU:HD11	1:O:210:GLN:HG2	2.03	0.40
1:C:137:PHE:CE2	1:C:142:ASN:HB2	2.56	0.40
2:H:91:CYS:SG	2:H:92:ALA:N	2.95	0.40
2:N:95:GLY:O	2:N:96:GLY:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	220/239 (92%)	210 (96%)	9 (4%)	1 (0%)	29	64
1	C	220/239 (92%)	209 (95%)	10 (4%)	1 (0%)	29	64
1	E	220/239 (92%)	208 (94%)	11 (5%)	1 (0%)	29	64
1	G	219/239 (92%)	208 (95%)	10 (5%)	1 (0%)	29	64
1	I	222/239 (93%)	211 (95%)	10 (4%)	1 (0%)	29	64
1	K	220/239 (92%)	209 (95%)	10 (4%)	1 (0%)	29	64
1	M	220/239 (92%)	208 (94%)	11 (5%)	1 (0%)	29	64
1	O	220/239 (92%)	208 (94%)	11 (5%)	1 (0%)	29	64
2	B	112/125 (90%)	102 (91%)	10 (9%)	0	100	100
2	D	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
2	F	109/125 (87%)	105 (96%)	4 (4%)	0	100	100
2	H	109/125 (87%)	103 (94%)	6 (6%)	0	100	100
2	J	108/125 (86%)	102 (94%)	5 (5%)	1 (1%)	17	51
2	L	112/125 (90%)	101 (90%)	11 (10%)	0	100	100
2	N	110/125 (88%)	102 (93%)	7 (6%)	1 (1%)	17	51
2	P	107/125 (86%)	101 (94%)	6 (6%)	0	100	100
All	All	2640/2912 (91%)	2493 (94%)	137 (5%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	192	ASN
2	N	96	GLY
1	A	192	ASN
1	G	192	ASN
2	J	0	LEU
1	K	192	ASN
1	M	192	ASN
1	O	192	ASN
1	I	192	ASN
1	C	192	ASN

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	207/225 (92%)	202 (98%)	5 (2%)	49	77
1	C	207/225 (92%)	202 (98%)	5 (2%)	49	77
1	E	205/225 (91%)	200 (98%)	5 (2%)	49	77
1	G	205/225 (91%)	201 (98%)	4 (2%)	55	80
1	I	209/225 (93%)	205 (98%)	4 (2%)	57	81
1	K	208/225 (92%)	201 (97%)	7 (3%)	37	69
1	M	206/225 (92%)	200 (97%)	6 (3%)	42	73
1	O	207/225 (92%)	202 (98%)	5 (2%)	49	77
2	B	90/105 (86%)	88 (98%)	2 (2%)	52	79
2	D	93/105 (89%)	91 (98%)	2 (2%)	52	79
2	F	92/105 (88%)	90 (98%)	2 (2%)	52	79
2	H	92/105 (88%)	89 (97%)	3 (3%)	38	70
2	J	96/105 (91%)	92 (96%)	4 (4%)	30	63
2	L	91/105 (87%)	89 (98%)	2 (2%)	52	79
2	N	93/105 (89%)	89 (96%)	4 (4%)	29	62
2	P	92/105 (88%)	90 (98%)	2 (2%)	52	79
All	All	2393/2640 (91%)	2331 (97%)	62 (3%)	46	75

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	54	LYS
1	A	80	LYS
1	A	193	GLU
1	A	229	LYS
2	B	68	ARG
2	B	87	SER
1	C	26	VAL

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Mol	Chain	Res	Type
1	C	54	LYS
1	C	80	LYS
1	C	96	SER
1	C	229	LYS
2	D	68	ARG
2	D	87	SER
1	E	26	VAL
1	E	54	LYS
1	E	80	LYS
1	E	96	SER
1	E	194	ASN
2	F	68	ARG
2	F	87	SER
1	G	26	VAL
1	G	54	LYS
1	G	80	LYS
1	G	194	ASN
2	H	60	ILE
2	H	68	ARG
2	H	87	SER
1	I	26	VAL
1	I	54	LYS
1	I	80	LYS
1	I	143	LEU
2	J	-1	ARG
2	J	60	ILE
2	J	68	ARG
2	J	87	SER
1	K	26	VAL
1	K	54	LYS
1	K	80	LYS
1	K	96	SER
1	K	143	LEU
1	K	193	GLU
1	K	229	LYS
2	L	68	ARG
2	L	87	SER
1	M	26	VAL
1	M	54	LYS
1	M	80	LYS
1	M	143	LEU
1	M	229	LYS

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Mol	Chain	Res	Type
1	M	239	LYS
2	N	7	SER
2	N	60	ILE
2	N	68	ARG
2	N	87	SER
1	O	26	VAL
1	O	54	LYS
1	O	80	LYS
1	O	93	CYS
1	O	229	LYS
2	P	68	ARG
2	P	87	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	71	GLN
1	E	194	ASN
2	H	71	GLN
1	I	194	ASN
2	J	71	GLN
1	K	125	GLN
1	M	149	GLN
1	M	194	ASN
2	N	10	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 38 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	241	-	4,4,4	0.12	0	6,6,6	0.39	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	241	SO4	1	0

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	224/239 (93%)	0.27	5 (2%) 62 45	33, 45, 57, 62	0
1	C	224/239 (93%)	0.26	4 (1%) 68 51	33, 45, 56, 62	0
1	E	224/239 (93%)	0.35	10 (4%) 33 21	33, 45, 57, 60	0
1	G	223/239 (93%)	0.47	6 (2%) 54 38	32, 45, 56, 63	0
1	I	226/239 (94%)	0.48	8 (3%) 44 29	33, 45, 56, 62	0
1	K	224/239 (93%)	0.36	9 (4%) 38 25	33, 45, 57, 63	0
1	M	225/239 (94%)	0.38	3 (1%) 77 61	33, 45, 57, 62	0
1	O	225/239 (94%)	0.79	30 (13%) 3 2	33, 45, 57, 62	0
2	B	114/125 (91%)	0.09	1 (0%) 84 71	32, 40, 49, 53	0
2	D	114/125 (91%)	0.03	0 100 100	32, 40, 49, 54	0
2	F	113/125 (90%)	0.11	1 (0%) 84 71	32, 40, 49, 55	0
2	H	113/125 (90%)	-0.08	0 100 100	32, 40, 49, 53	0
2	J	112/125 (89%)	0.27	2 (1%) 68 51	32, 40, 49, 62	0
2	L	114/125 (91%)	0.11	0 100 100	32, 40, 49, 53	0
2	N	112/125 (89%)	0.08	2 (1%) 68 51	32, 41, 48, 53	0
2	P	111/125 (88%)	0.34	6 (5%) 25 16	32, 40, 49, 53	0
All	All	2698/2912 (92%)	0.32	87 (3%) 47 31	32, 43, 56, 63	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	94	TYR	3.8
1	O	142	ASN	3.8
1	O	64	VAL	3.7
1	G	41	ILE	3.7
1	O	51	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	79	ASP	3.5
1	C	94	TYR	3.5
1	O	50	ILE	3.5
1	O	119	THR	3.4
1	O	143	LEU	3.4
1	G	94	TYR	3.4
1	O	111	LYS	3.3
2	P	93	SER	3.3
1	O	38	VAL	3.3
1	O	118	VAL	3.3
1	E	49	LEU	3.3
1	O	49	LEU	3.3
1	A	95	PHE	3.2
1	O	52	SER	3.1
1	O	122	ASN	3.1
1	K	143	LEU	3.1
2	F	98	THR	3.0
1	O	80	LYS	2.9
1	O	133	THR	2.9
1	O	81	TYR	2.9
1	G	50	ILE	2.9
1	A	94	TYR	2.9
1	A	96	SER	2.8
1	K	189	PHE	2.8
1	I	82	VAL	2.8
1	O	46	TYR	2.8
2	P	29	PHE	2.7
1	O	117	GLY	2.7
1	O	120	GLU	2.7
1	E	96	SER	2.6
1	E	51	TYR	2.5
1	I	85	PHE	2.5
1	O	39	LYS	2.5
1	O	63	ASN	2.5
1	K	79	ASP	2.5
1	G	193	GLU	2.5
2	P	28	TYR	2.5
1	I	127	ASP	2.4
2	B	96	GLY	2.4
1	G	188	LYS	2.4
1	O	154	LYS	2.4
1	I	61	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	50	ILE	2.3
2	P	96	GLY	2.3
1	O	155	VAL	2.3
1	C	51	TYR	2.3
2	J	110	LEU	2.3
1	M	63	ASN	2.3
1	M	128	LYS	2.3
1	A	79	ASP	2.3
1	O	9	ASP	2.3
1	K	37	ASN	2.3
1	E	133	THR	2.2
2	J	111	TYR	2.2
1	I	83	ASP	2.2
1	K	50	ILE	2.2
1	O	84	VAL	2.2
1	A	41	ILE	2.2
1	O	53	ILE	2.2
2	P	101	PHE	2.2
1	O	82	VAL	2.2
1	I	146	PHE	2.2
1	I	121	HIS	2.2
2	N	111	TYR	2.2
1	E	95	PHE	2.1
1	C	41	ILE	2.1
1	E	131	SER	2.1
1	E	41	ILE	2.1
1	I	81	TYR	2.1
1	K	129	TYR	2.1
1	K	45	LEU	2.1
2	N	98	THR	2.1
1	K	46	TYR	2.1
1	O	79	ASP	2.1
2	P	100	TYR	2.1
1	O	61	TYR	2.0
1	E	79	ASP	2.0
1	O	37	ASN	2.0
1	K	35	ALA	2.0
1	M	133	THR	2.0
1	G	227	ASP	2.0
1	O	141	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](#)

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(\AA^2)	Q<0.9
5	ZN	I	240	1/1	0.51	0.21	95,95,95,95	0
5	ZN	K	240	1/1	0.76	0.11	77,77,77,77	0
4	SO4	A	241	5/5	0.88	0.15	74,75,76,76	0
3	CL	O	242	1/1	0.88	0.20	52,52,52,52	0
5	ZN	O	241	1/1	0.90	0.06	76,76,76,76	0
3	CL	M	242	1/1	0.91	0.17	49,49,49,49	0
5	ZN	G	240	1/1	0.91	0.04	71,71,71,71	0
3	CL	B	123	1/1	0.92	0.21	21,21,21,21	0
5	ZN	M	241	1/1	0.92	0.07	78,78,78,78	0
5	ZN	I	241	1/1	0.92	0.08	100,100,100,100	0
5	ZN	J	122	1/1	0.94	0.08	58,58,58,58	0
3	CL	J	123	1/1	0.95	0.24	16,16,16,16	0
3	CL	D	124	1/1	0.95	0.26	33,33,33,33	0
5	ZN	P	121	1/1	0.95	0.13	63,63,63,63	0
5	ZN	L	122	1/1	0.95	0.07	69,69,69,69	0
3	CL	C	241	1/1	0.96	0.14	44,44,44,44	0
3	CL	I	242	1/1	0.96	0.11	29,29,29,29	0
5	ZN	C	240	1/1	0.96	0.04	71,71,71,71	0
3	CL	B	124	1/1	0.97	0.14	37,37,37,37	0
3	CL	A	240	1/1	0.97	0.19	41,41,41,41	0
3	CL	L	123	1/1	0.97	0.24	31,31,31,31	0
5	ZN	N	121	1/1	0.97	0.07	64,64,64,64	0
5	ZN	E	240	1/1	0.97	0.06	65,65,65,65	0
3	CL	J	124	1/1	0.98	0.19	27,27,27,27	0
5	ZN	P	122	1/1	0.98	0.09	30,30,30,30	0
5	ZN	D	121	1/1	0.98	0.05	56,56,56,56	0
5	ZN	F	121	1/1	0.98	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	H	122	1/1	0.98	0.13	64,64,64,64	0
3	CL	D	123	1/1	0.98	0.37	24,24,24,24	0
5	ZN	J	121	1/1	0.99	0.11	29,29,29,29	0
5	ZN	H	121	1/1	0.99	0.13	34,34,34,34	0
5	ZN	B	121	1/1	0.99	0.07	60,60,60,60	0
5	ZN	F	122	1/1	0.99	0.12	36,36,36,36	0
5	ZN	D	122	1/1	0.99	0.12	33,33,33,33	0
3	CL	G	241	1/1	0.99	0.07	34,34,34,34	0
3	CL	N	123	1/1	0.99	0.20	52,52,52,52	0
5	ZN	N	122	1/1	0.99	0.08	30,30,30,30	0
5	ZN	L	121	1/1	0.99	0.08	35,35,35,35	0
5	ZN	B	122	1/1	0.99	0.12	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.