



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 04:38 PM UTC

PDB ID : 8VS8 / pdb_00008vs8
Title : Crystal structure of ADI-19425 Fab in complex with anti-idiotypic 1D3 Fab
Authors : Kher, G.; Homad, L.J.; McGuire, A.T.; Pancera, M.
Deposited on : 2024-01-23
Resolution : 2.67 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

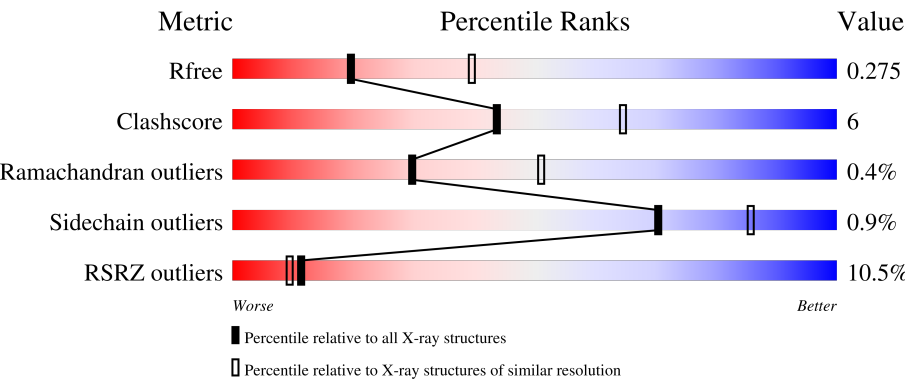
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	227	10% 75% 14% 11%
1	E	227	2% 77% 13% 9%
1	I	227	2% 44% 9% 47%
1	M	227	5% 83% 9% 7%
1	Q	227	3% 48% 7% 45%

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Mol	Chain	Length	Quality of chain
1	U	227	
1	Y	227	
1	c	227	
2	B	218	
2	F	218	
2	J	218	
2	N	218	
2	R	218	
2	V	218	
2	Z	218	
2	d	218	
3	C	214	
3	G	214	
3	K	214	
3	O	214	
3	S	214	
3	W	214	
3	a	214	
3	e	214	
4	D	226	
4	H	226	
4	L	226	
4	P	226	
4	T	226	
4	X	226	

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Mol	Chain	Length	Quality of chain
4	b	226	9% 89% 8%
4	f	226	14% 81% 14% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 45030 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 ADI-19425 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1512	958	253	293	8			
1	E	206	Total	C	N	O	S	0	0	0
			1547	979	259	301	8			
1	I	121	Total	C	N	O	S	0	0	0
			920	578	156	180	6			
1	M	210	Total	C	N	O	S	0	0	0
			1576	996	264	308	8			
1	Q	125	Total	C	N	O	S	0	0	0
			940	588	159	187	6			
1	U	178	Total	C	N	O	S	0	0	0
			1347	850	227	262	8			
1	Y	121	Total	C	N	O	S	0	0	0
			920	578	156	180	6			
1	c	98	Total	C	N	O	S	0	0	0
			748	474	126	143	5			

- Molecule 2 is a protein called ADI-19425 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	1	0	0
			1568	983	261	320	4			
2	F	214	Total	C	N	O	S	1	0	0
			1587	996	263	324	4			
2	J	110	Total	C	N	O	S	0	0	0
			802	502	133	165	2			
2	N	214	Total	C	N	O	S	1	0	0
			1581	993	260	324	4			
2	R	110	Total	C	N	O	S	0	0	0
			806	504	134	166	2			
2	V	201	Total	C	N	O	S	0	0	0
			1484	933	245	302	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	108	Total	C	N	O	S	0	0	0
			792	496	131	163	2			
2	d	81	Total	C	N	O	S	0	0	0
			602	379	97	124	2			

- Molecule 3 is a protein called 1D3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1649	1027	279	338	5			
3	G	214	Total	C	N	O	S	0	0	0
			1649	1027	280	337	5			
3	K	212	Total	C	N	O	S	0	0	0
			1641	1024	279	334	4			
3	O	214	Total	C	N	O	S	0	0	0
			1657	1032	281	339	5			
3	S	214	Total	C	N	O	S	0	0	0
			1647	1026	277	339	5			
3	W	200	Total	C	N	O	S	0	0	0
			1549	967	261	317	4			
3	a	214	Total	C	N	O	S	0	0	0
			1645	1023	278	339	5			
3	e	214	Total	C	N	O	S	0	0	0
			1635	1018	275	337	5			

- Molecule 4 is a protein called 1D3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	9	0	0
			1660	1053	274	327	6			
4	H	220	Total	C	N	O	S	0	0	0
			1648	1047	270	325	6			
4	L	218	Total	C	N	O	S	2	0	0
			1632	1036	271	319	6			
4	P	217	Total	C	N	O	S	3	0	0
			1637	1041	270	320	6			
4	T	214	Total	C	N	O	S	2	0	0
			1616	1029	266	315	6			
4	X	216	Total	C	N	O	S	0	0	0
			1622	1031	266	319	6			
4	b	218	Total	C	N	O	S	5	0	0
			1639	1041	270	322	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	f	215	Total	C	N	O	S	5	0	0
			1594	1014	260	314	6			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	7	Total	O	0	0
			7	7		
5	C	5	Total	O	0	0
			5	5		
5	D	13	Total	O	0	0
			13	13		
5	E	6	Total	O	0	0
			6	6		
5	F	6	Total	O	0	0
			6	6		
5	G	10	Total	O	0	0
			10	10		
5	H	6	Total	O	0	0
			6	6		
5	I	5	Total	O	0	0
			5	5		
5	J	1	Total	O	0	0
			1	1		
5	K	3	Total	O	0	0
			3	3		
5	L	6	Total	O	0	0
			6	6		
5	M	14	Total	O	0	0
			14	14		
5	N	5	Total	O	0	0
			5	5		
5	O	13	Total	O	0	0
			13	13		
5	P	2	Total	O	0	0
			2	2		
5	Q	6	Total	O	0	0
			6	6		
5	S	5	Total	O	0	0
			5	5		

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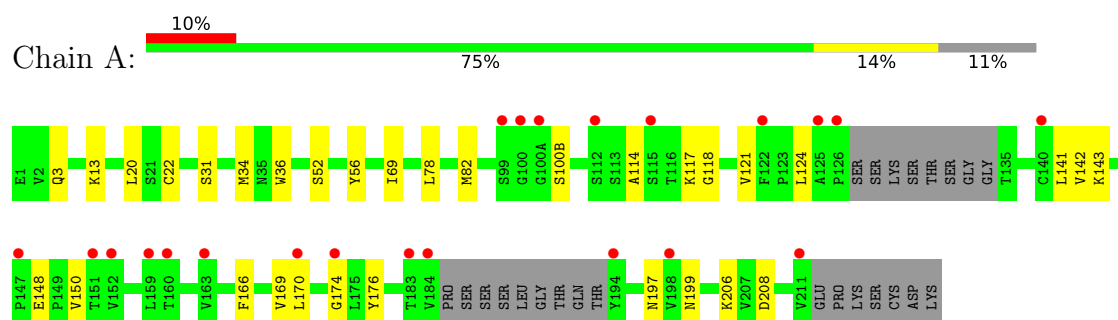
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	8	Total 8	O 8	0	0
5	U	5	Total 5	O 5	0	0
5	V	4	Total 4	O 4	0	0
5	W	7	Total 7	O 7	0	0
5	X	6	Total 6	O 6	0	0
5	Y	3	Total 3	O 3	0	0
5	Z	1	Total 1	O 1	0	0
5	a	7	Total 7	O 7	0	0
5	b	10	Total 10	O 10	0	0
5	c	2	Total 2	O 2	0	0
5	e	2	Total 2	O 2	0	0
5	f	1	Total 1	O 1	0	0

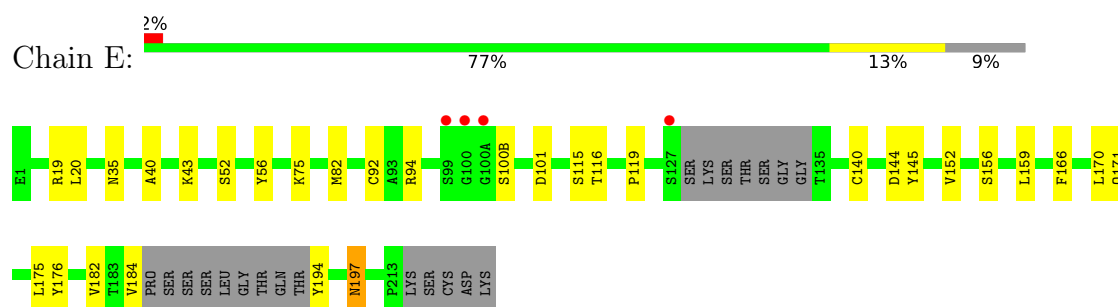
3 Residue-property plots [i](#)

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.

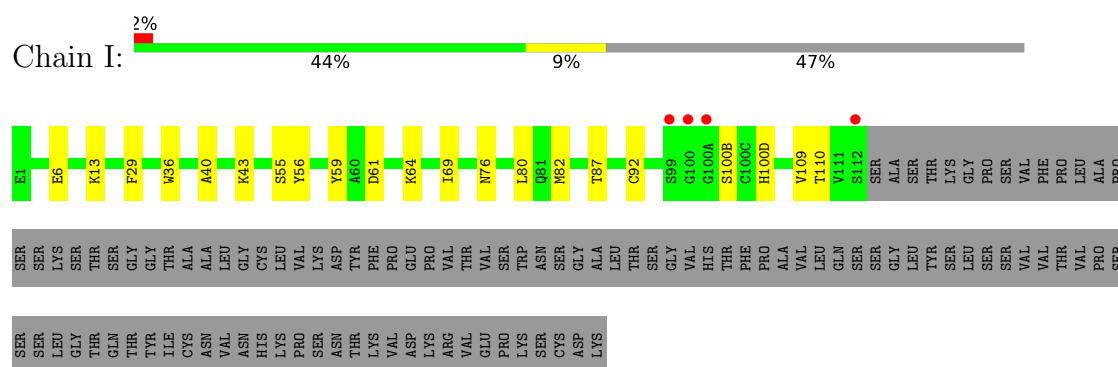
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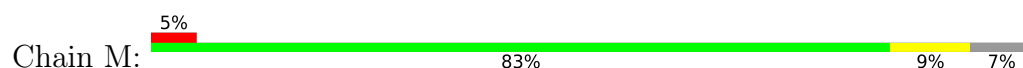
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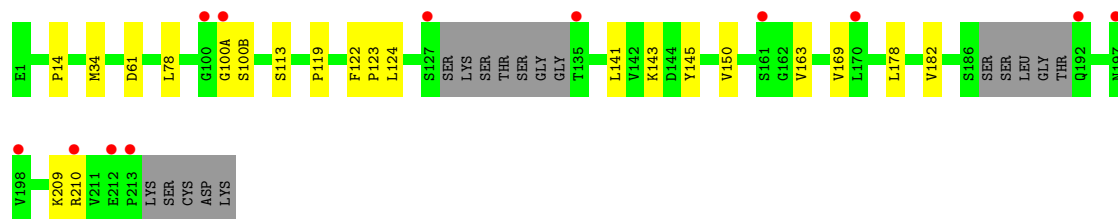


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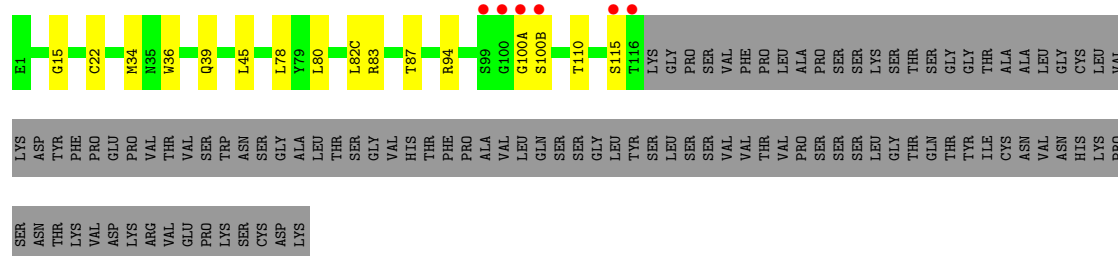


- Molecule 1: ADI-19425 Heavy Chain

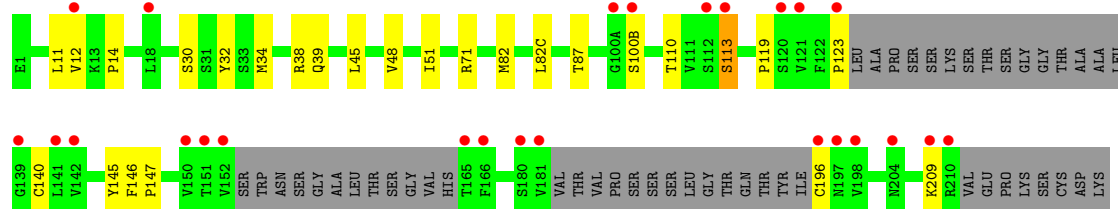




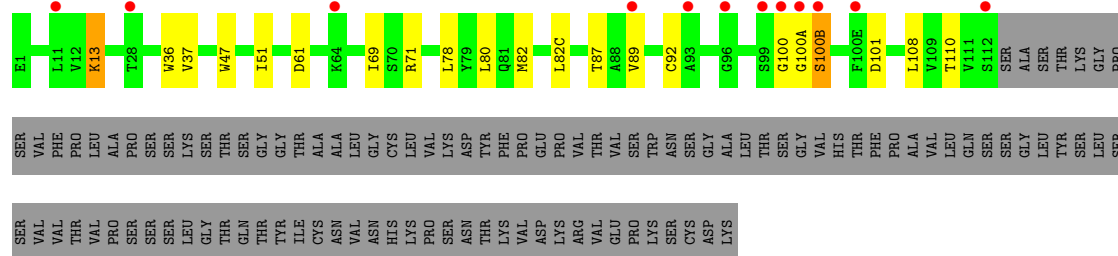
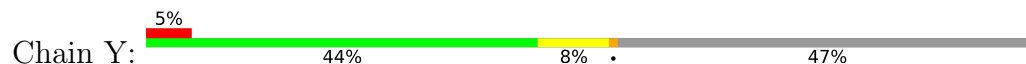
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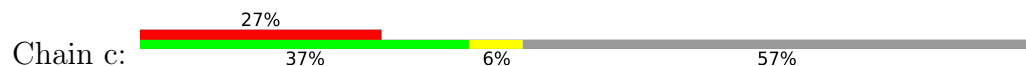
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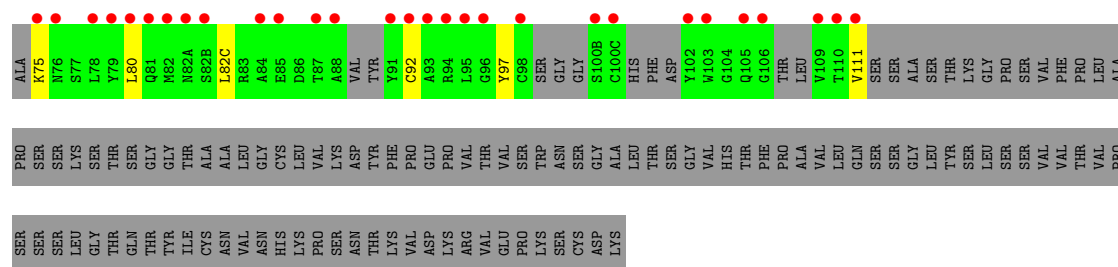


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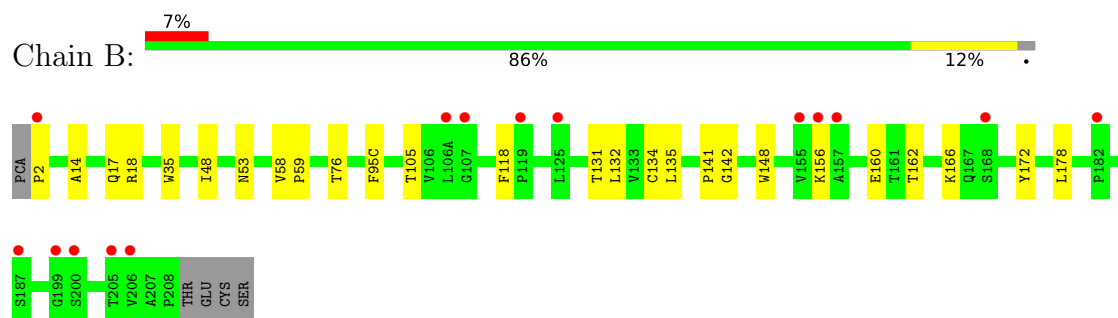


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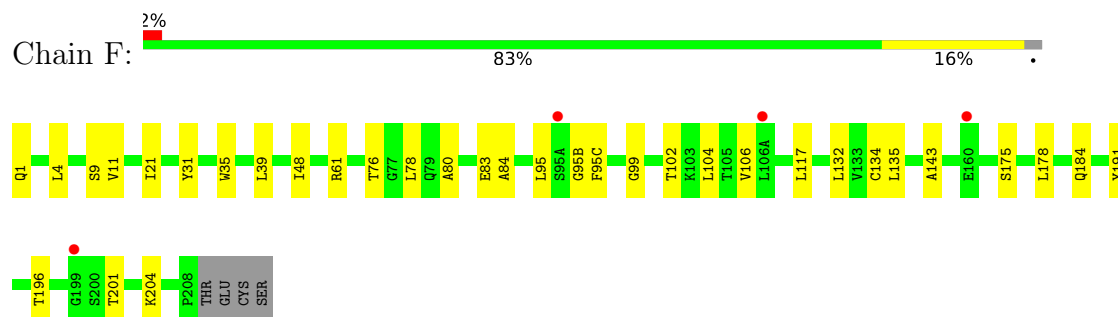




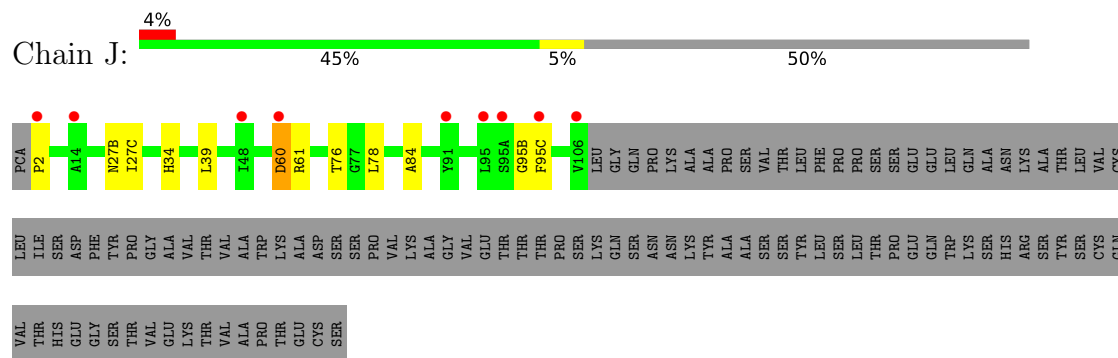
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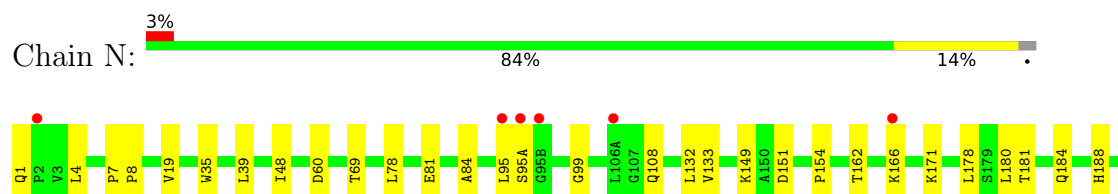
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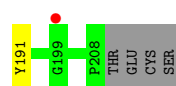


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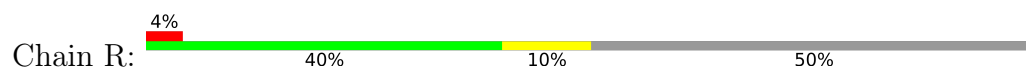


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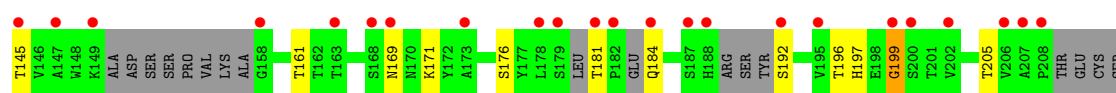
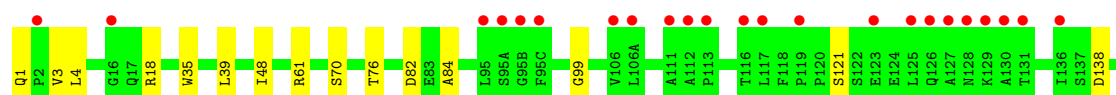
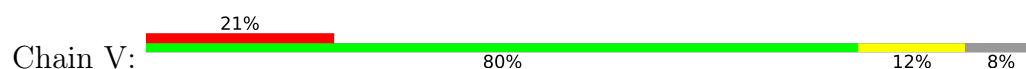




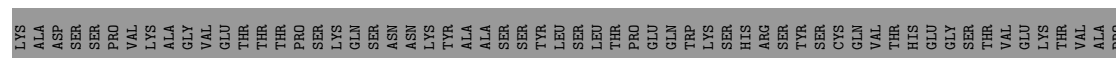
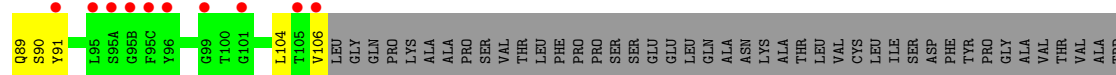
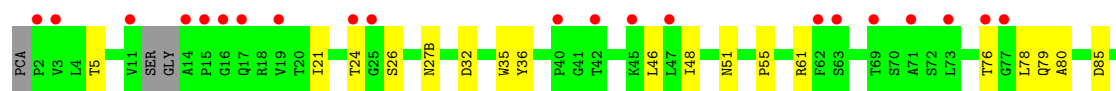
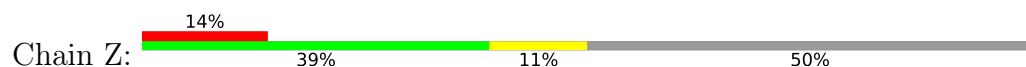
• Molecule 2: ADI-19425 Light Chain



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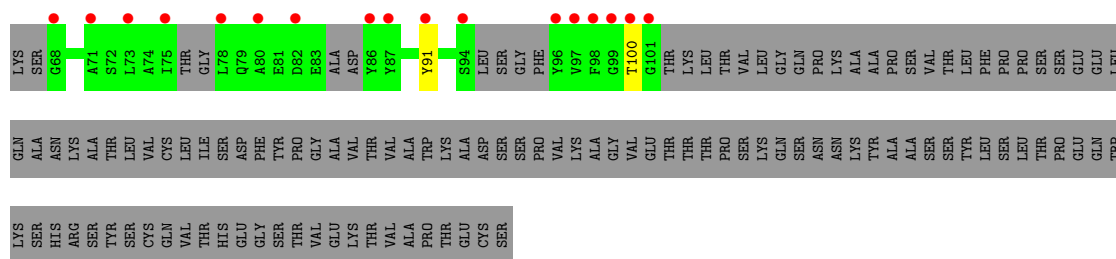


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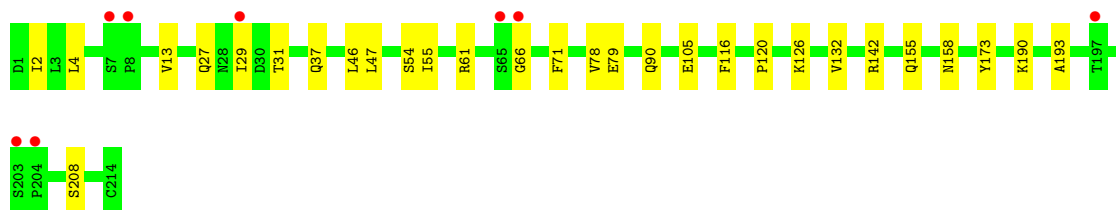
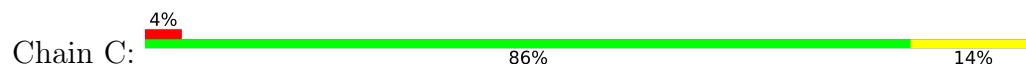


• Molecule 2: ADI-19425 Light Chain





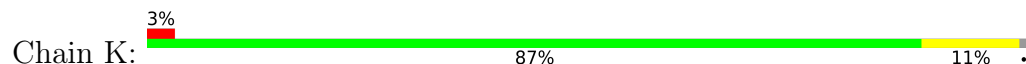
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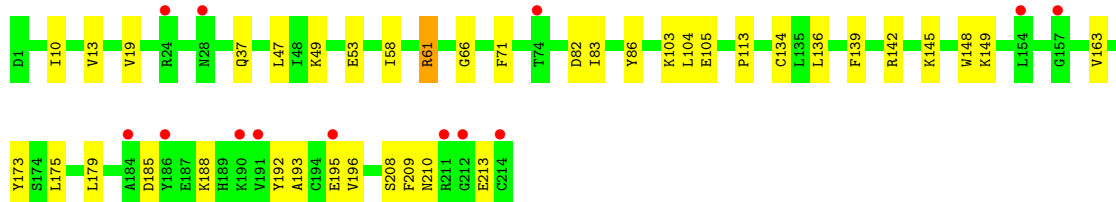
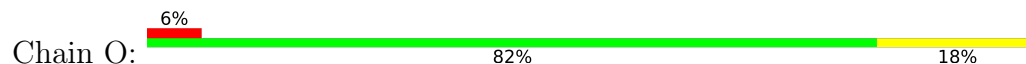
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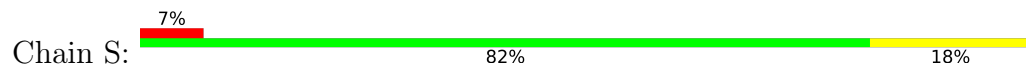
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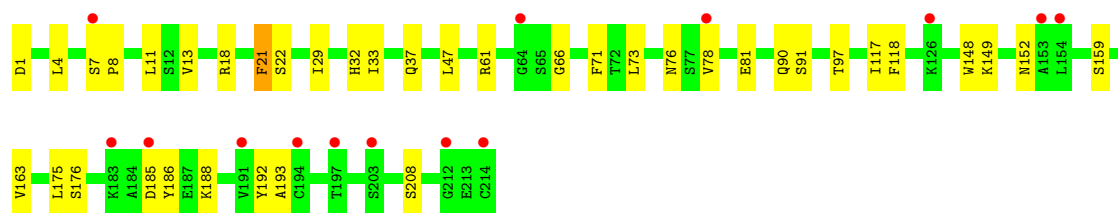


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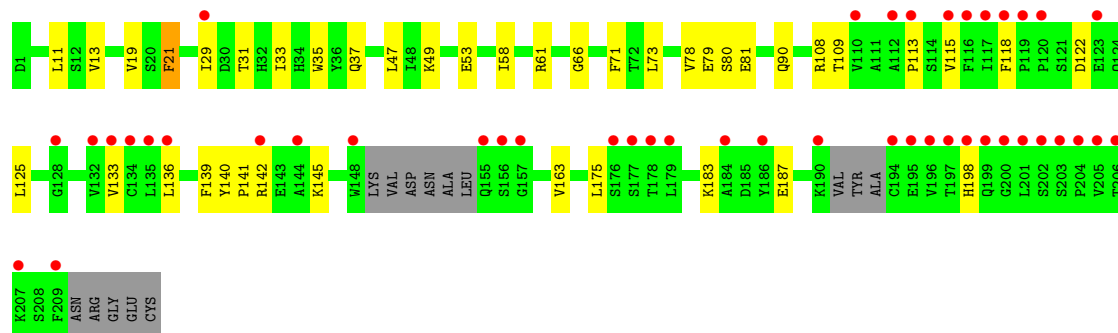
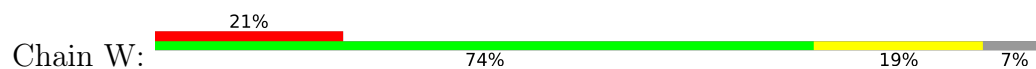


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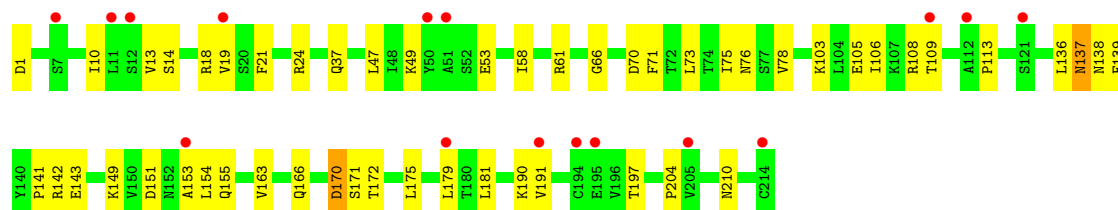
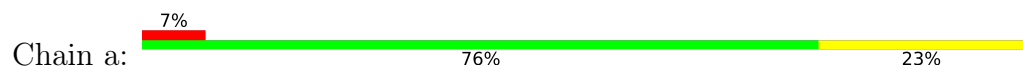




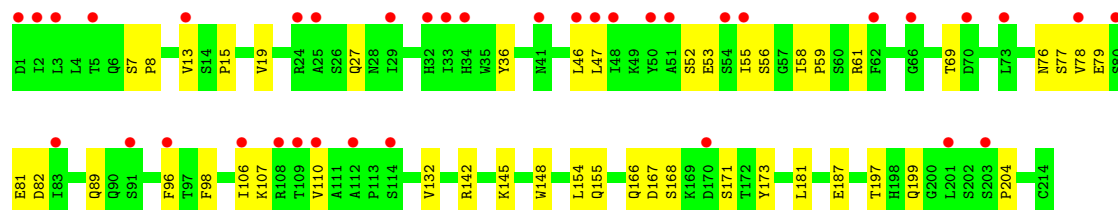
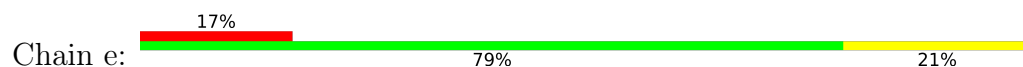
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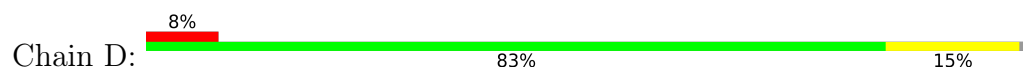
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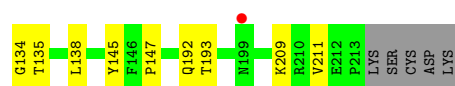


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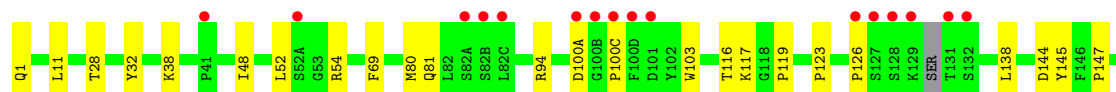
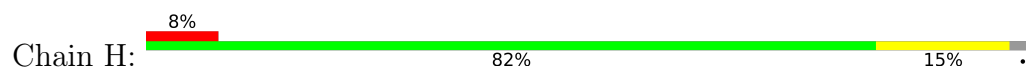


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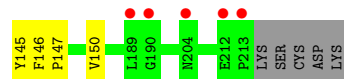
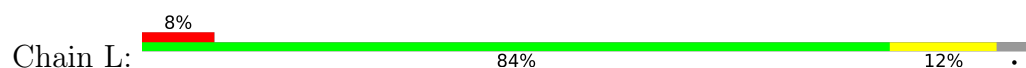




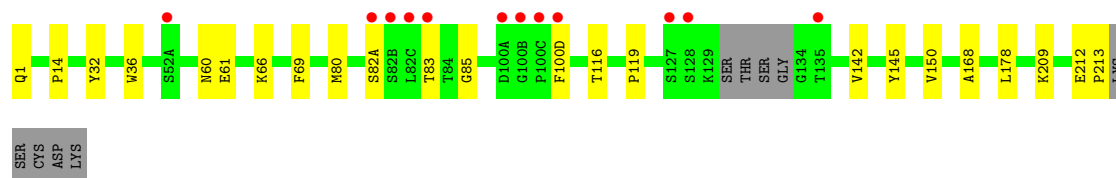
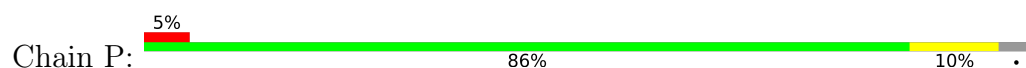
• Molecule 4: 1D3 Heavy Chain



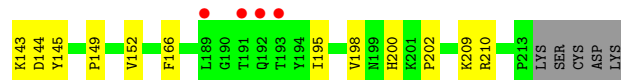
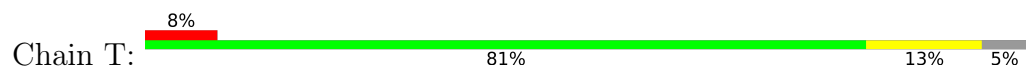
• Molecule 4: 1D3 Heavy Chain



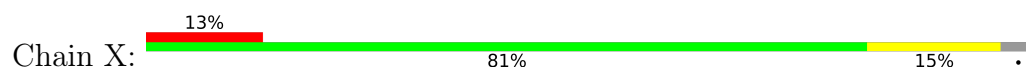
• Molecule 4: 1D3 Heavy Chain

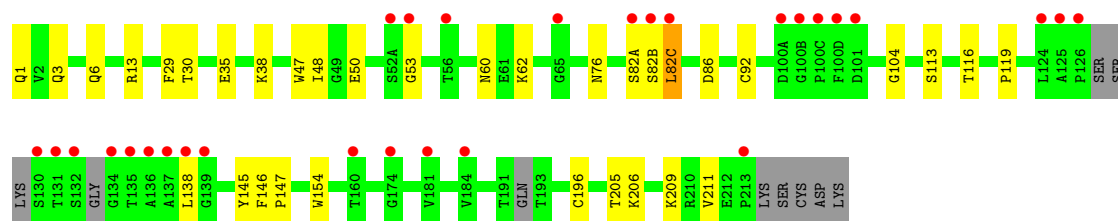


• Molecule 4: 1D3 Heavy Chain

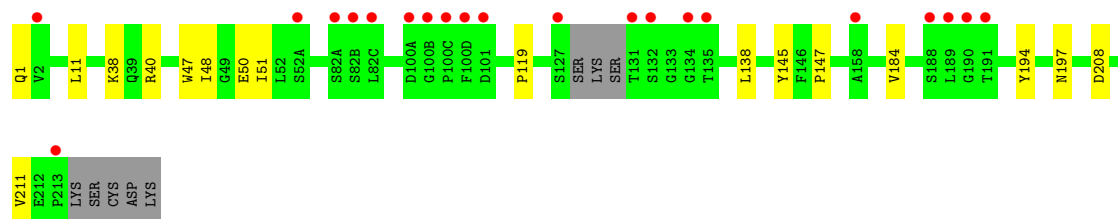
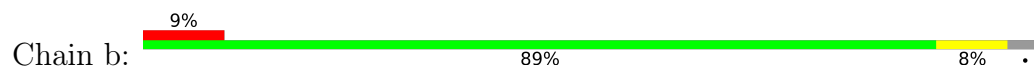


• Molecule 4: 1D3 Heavy Chain

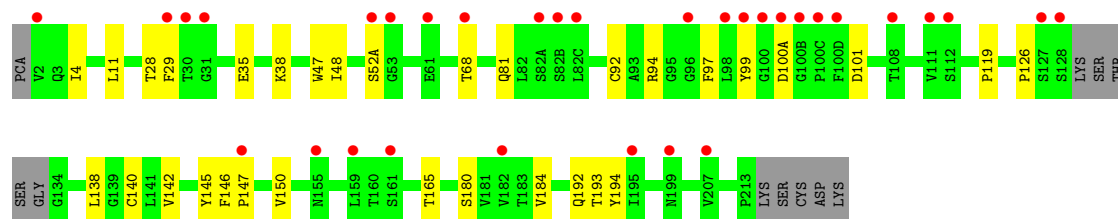
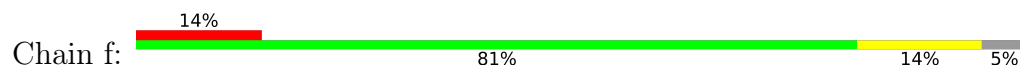




• Molecule 4: 1D3 Heavy Chain



• Molecule 4: 1D3 Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.07Å 149.98Å 164.43Å 83.98° 89.90° 74.61°	Depositor
Resolution (Å)	49.33 – 2.67 49.33 – 2.67	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.33-2.67) 92.5 (49.33-2.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.231 , 0.273 0.233 , 0.275	Depositor DCC
R_{free} test set	11502 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	45030	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: PCA

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	0.12	0/1548	0.31	0/2105
1	E	0.23	0/1584	0.38	0/2153
1	I	0.09	0/941	0.28	0/1272
1	M	0.12	0/1614	0.31	0/2195
1	Q	0.10	0/961	0.29	0/1301
1	U	0.23	0/1377	0.41	0/1863
1	Y	0.09	0/941	0.27	0/1272
1	c	0.21	0/757	0.41	0/1010
2	B	0.17	0/1609	0.35	0/2201
2	F	0.11	0/1621	0.29	0/2218
2	J	0.09	0/822	0.29	0/1121
2	N	0.12	0/1615	0.33	0/2211
2	R	0.10	0/825	0.28	0/1123
2	V	0.19	0/1512	0.36	0/2064
2	Z	0.09	0/811	0.26	0/1106
2	d	0.19	0/610	0.36	0/820
3	C	0.18	0/1685	0.37	0/2288
3	G	0.11	0/1685	0.32	0/2288
3	K	0.10	0/1677	0.32	0/2277
3	O	0.11	0/1693	0.30	0/2297
3	S	0.11	0/1683	0.30	0/2286
3	W	0.11	0/1582	0.33	0/2145
3	a	0.15	0/1681	0.36	0/2285
3	e	0.18	0/1671	0.35	0/2273
4	D	0.18	0/1697	0.38	1/2314 (0.0%)
4	H	0.12	0/1684	0.30	0/2296
4	L	0.12	0/1667	0.30	0/2272
4	P	0.19	0/1673	0.38	1/2280 (0.0%)
4	T	0.20	0/1652	0.43	0/2253
4	X	0.12	0/1656	0.31	0/2257
4	b	0.12	0/1675	0.32	0/2284
4	f	0.19	0/1637	0.40	1/2237 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/45846	0.34	3/62367 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	100(A)	ASP	N-CA-C	-5.87	106.10	113.20
4	D	134	GLY	N-CA-C	-5.24	106.80	114.61
4	P	100(D)	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1512	0	1459	21	0
1	E	1547	0	1501	16	0
1	I	920	0	876	13	0
1	M	1576	0	1528	14	0
1	Q	940	0	887	7	0
1	U	1347	0	1301	14	0
1	Y	920	0	876	13	0
1	c	748	0	705	9	0
2	B	1568	0	1502	19	0
2	F	1587	0	1532	22	0
2	J	802	0	761	7	0
2	N	1581	0	1521	21	0
2	R	806	0	766	14	1
2	V	1484	0	1425	18	0
2	Z	792	0	747	15	0
2	d	602	0	555	12	0
3	C	1649	0	1577	17	0
3	G	1649	0	1579	23	0
3	K	1641	0	1583	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1657	0	1594	25	0
3	S	1647	0	1572	20	0
3	W	1549	0	1488	26	0
3	a	1645	0	1561	39	0
3	e	1635	0	1546	29	1
4	D	1660	0	1607	22	0
4	H	1648	0	1590	25	0
4	L	1632	0	1580	16	0
4	P	1637	0	1586	15	0
4	T	1616	0	1563	17	0
4	X	1622	0	1559	25	0
4	b	1639	0	1583	8	0
4	f	1594	0	1512	23	0
5	A	9	0	0	0	0
5	B	7	0	0	0	0
5	C	5	0	0	0	0
5	D	13	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	10	0	0	0	0
5	H	6	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	3	0	0	0	0
5	L	6	0	0	0	0
5	M	14	0	0	0	0
5	N	5	0	0	0	0
5	O	13	0	0	0	0
5	P	2	0	0	0	0
5	Q	6	0	0	0	0
5	S	5	0	0	0	0
5	T	8	0	0	0	0
5	U	5	0	0	0	0
5	V	4	0	0	0	0
5	W	7	0	0	0	0
5	X	6	0	0	0	0
5	Y	3	0	0	0	0
5	Z	1	0	0	0	0
5	a	7	0	0	0	0
5	b	10	0	0	0	0
5	c	2	0	0	0	0
5	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	f	1	0	0	0	0
All	All	45030	0	43022	539	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 6.

All (539) 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:Z:5:THR:HB	2:Z:24:THR:OG1	1.40	1.21
3:a:13:VAL:CG1	3:a:78:VAL:HG21	1.77	1.14
3:a:13:VAL:HG11	3:a:78:VAL:HG21	1.13	1.07
3:G:11:LEU:HD21	3:G:19:VAL:CG2	1.85	1.07
4:H:123:PRO:HB3	4:H:211:VAL:HG22	1.36	1.02
3:G:11:LEU:HD21	3:G:19:VAL:HG21	1.52	0.88
3:e:132:VAL:HG12	3:e:148:TRP:CH2	2.09	0.87
4:X:138:LEU:HD13	4:X:211:VAL:HG21	1.56	0.86
3:C:2:ILE:HG21	3:C:29:ILE:HD11	1.56	0.86
3:a:191:VAL:HG22	3:a:210:ASN:OD1	1.77	0.84
4:H:123:PRO:CB	4:H:211:VAL:HG22	2.10	0.81
2:Z:5:THR:CB	2:Z:24:THR:OG1	2.27	0.79
3:a:13:VAL:HG11	3:a:78:VAL:CG2	2.06	0.78
2:Z:5:THR:HB	2:Z:24:THR:HG1	1.49	0.78
1:Q:87:THR:HG23	1:Q:110:THR:HA	1.64	0.77
2:V:192:SER:CB	2:V:205:THR:HG22	2.15	0.76
4:D:83:THR:HG23	1:I:13:LYS:HD3	1.68	0.75
2:F:135:LEU:HD23	2:F:175:SER:HB3	1.68	0.75
4:D:4:ILE:CD1	4:D:102:TYR:O	2.36	0.74
3:O:66:GLY:HA3	3:O:71:PHE:HA	1.69	0.74
1:Y:87:THR:HG23	1:Y:110:THR:HA	1.70	0.74
2:J:39:LEU:HD23	2:J:84:ALA:HB2	1.70	0.73
1:Q:22:CYS:HB3	1:Q:78:LEU:HB3	1.69	0.73
3:e:132:VAL:HG12	3:e:148:TRP:HH2	1.54	0.73
1:U:87:THR:HG23	1:U:110:THR:HA	1.70	0.73
3:a:13:VAL:HG12	3:a:14:SER:N	2.05	0.71
3:G:2:ILE:HG21	3:G:29:ILE:HD11	1.74	0.69
4:f:184:VAL:HG11	4:f:194:TYR:HE2	1.56	0.69
3:K:46:LEU:HG	3:K:55:ILE:HD13	1.74	0.68
1:Y:51:ILE:HD13	1:Y:71:ARG:HG2	1.74	0.68
4:D:4:ILE:HD12	4:D:102:TYR:O	1.94	0.68
3:a:170:ASP:O	3:a:172:THR:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:68:THR:OG1	4:f:81:GLN:HB3	1.93	0.67
2:F:135:LEU:CD2	2:F:175:SER:HB3	2.23	0.67
3:W:142:ARG:H	3:W:142:ARG:HD3	1.59	0.67
2:V:61:ARG:NH2	2:V:82:ASP:OD2	2.28	0.67
1:I:87:THR:HG23	1:I:110:THR:HA	1.77	0.67
4:H:116:THR:HG22	4:H:147:PRO:HD3	1.77	0.67
3:S:149:LYS:HE2	3:S:152:ASN:HA	1.75	0.67
3:K:37:GLN:HB2	3:K:47:LEU:HD11	1.78	0.66
3:G:11:LEU:HD21	3:G:19:VAL:HG22	1.74	0.66
1:U:51:ILE:HD13	1:U:71:ARG:HG2	1.76	0.66
1:I:55:SER:OG	1:I:56:TYR:CD1	2.49	0.66
4:X:30:THR:HG23	4:X:53:GLY:HA3	1.78	0.66
4:D:119:PRO:HB3	4:D:145:TYR:HB3	1.78	0.65
2:B:18:ARG:HG3	2:B:76:THR:HG22	1.79	0.65
2:Z:32:ASP:OD2	2:Z:51:ASN:ND2	2.29	0.65
1:M:123:PRO:HG3	1:M:209:LYS:HD2	1.77	0.65
2:V:192:SER:OG	2:V:205:THR:HG22	1.97	0.65
2:R:37:GLN:HB2	2:R:47:LEU:HD22	1.79	0.65
3:S:37:GLN:HB2	3:S:47:LEU:HD11	1.78	0.65
2:F:132:LEU:HD12	2:F:178:LEU:HD23	1.79	0.64
2:R:18:ARG:HG3	2:R:76:THR:HG22	1.79	0.64
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.79	0.64
3:G:11:LEU:CD2	3:G:19:VAL:HG21	2.26	0.64
4:f:184:VAL:HG11	4:f:194:TYR:CE2	2.32	0.64
4:T:119:PRO:HB3	4:T:145:TYR:HB3	1.79	0.64
3:e:166:GLN:NE2	3:e:171:SER:OG	2.28	0.64
3:C:66:GLY:HA3	3:C:71:PHE:HA	1.81	0.63
3:a:24:ARG:NH1	3:a:70:ASP:OD1	2.30	0.63
2:F:80:ALA:HA	2:F:106:VAL:HG21	1.80	0.63
3:O:10:ILE:HD13	3:O:103:LYS:HB3	1.81	0.63
3:a:137:ASN:ND2	3:a:138:ASN:OD1	2.31	0.63
3:W:140:TYR:CD1	3:W:141:PRO:HA	2.34	0.63
2:Z:35:TRP:HB2	2:Z:48:ILE:HB	1.81	0.62
3:W:79:GLU:O	3:W:81:GLU:N	2.33	0.62
1:I:55:SER:OG	1:I:56:TYR:CE1	2.52	0.62
1:U:30:SER:HG	3:W:31:THR:HG1	1.44	0.62
4:X:13:ARG:NH2	4:X:113:SER:O	2.33	0.61
2:N:180:LEU:HD11	2:N:191:TYR:CE2	2.36	0.61
4:X:119:PRO:HB3	4:X:145:TYR:HB3	1.82	0.61
1:E:156:SER:H	1:E:197:ASN:HD21	1.47	0.61
3:G:142:ARG:HH11	3:G:142:ARG:HG2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:14:PRO:HG2	1:U:113:SER:HB3	1.83	0.61
3:a:108:ARG:HD2	3:a:171:SER:OG	2.00	0.61
1:A:197:ASN:ND2	1:A:208:ASP:OD1	2.30	0.61
2:N:4:LEU:HB2	2:N:99:GLY:HA2	1.83	0.60
3:W:66:GLY:HA3	3:W:71:PHE:HA	1.81	0.60
4:X:6:GLN:NE2	4:X:92:CYS:H	1.99	0.60
3:a:163:VAL:HG22	3:a:175:LEU:HD12	1.83	0.60
1:M:34:MET:HB3	1:M:78:LEU:HD22	1.83	0.60
3:O:136:LEU:HD11	3:O:196:VAL:HG21	1.84	0.60
2:Z:5:THR:CB	2:Z:24:THR:HG1	2.13	0.60
4:b:38:LYS:HB2	4:b:48:ILE:HD11	1.85	0.59
2:R:80:ALA:HA	2:R:106:VAL:HG11	1.85	0.59
4:b:138:LEU:HD13	4:b:211:VAL:HG21	1.84	0.59
2:B:132:LEU:HD22	2:B:178:LEU:HD23	1.84	0.59
1:E:166:PHE:CE1	2:F:135:LEU:HD13	2.37	0.59
2:V:145:THR:OG1	2:V:196:THR:OG1	2.20	0.59
3:a:13:VAL:CG1	3:a:14:SER:N	2.65	0.59
3:W:47:LEU:HD23	3:W:58:ILE:HD12	1.84	0.58
3:a:191:VAL:CG2	3:a:210:ASN:OD1	2.49	0.58
4:D:38:LYS:HB2	4:D:48:ILE:HD11	1.86	0.58
3:S:18:ARG:HG3	3:S:76:ASN:HA	1.85	0.58
1:A:143:LYS:NZ	2:B:131:THR:OG1	2.37	0.58
1:E:159:LEU:HD21	1:E:182:VAL:HG21	1.85	0.58
4:T:82:LEU:HB3	4:T:82(C):LEU:HD21	1.86	0.58
3:G:11:LEU:CD2	3:G:19:VAL:CG2	2.73	0.58
3:a:66:GLY:HA3	3:a:71:PHE:HA	1.85	0.58
2:R:19:VAL:HG13	2:R:78:LEU:HD11	1.85	0.57
3:a:37:GLN:HB2	3:a:47:LEU:HD11	1.86	0.57
2:V:18:ARG:HG3	2:V:76:THR:HG22	1.85	0.57
3:W:122:ASP:HA	3:W:125:LEU:HD12	1.86	0.57
3:S:61:ARG:NH2	3:S:81:GLU:OE2	2.29	0.57
4:L:30:THR:HG23	4:L:53:GLY:HA3	1.85	0.57
3:W:113:PRO:HD3	3:W:198:HIS:HD2	1.69	0.57
4:b:119:PRO:HB3	4:b:145:TYR:HB3	1.85	0.57
2:R:47:LEU:HD11	2:R:62:PHE:CD2	2.39	0.57
3:W:163:VAL:HG22	3:W:175:LEU:HD12	1.85	0.57
4:P:14:PRO:HB3	1:Y:13:LYS:HZ1	1.68	0.56
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.88	0.56
1:Y:100:GLY:O	1:Y:100(B):SER:N	2.38	0.56
2:F:135:LEU:HD23	2:F:175:SER:CB	2.36	0.56
3:e:79:GLU:O	3:e:81:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:126:PRO:HG3	4:H:138:LEU:HB3	1.89	0.55
1:E:20:LEU:HG	1:E:82:MET:HE2	1.87	0.55
2:N:69:THR:OG1	2:V:70:SER:OG	2.24	0.55
1:Y:37:VAL:HG22	1:Y:47:TRP:HA	1.89	0.55
3:G:126:LYS:N	3:G:126:LYS:HD2	2.21	0.55
4:P:83:THR:O	4:P:85:GLY:N	2.33	0.55
4:P:119:PRO:HB3	4:P:145:TYR:HB3	1.88	0.55
2:V:39:LEU:HD23	2:V:84:ALA:HB2	1.88	0.55
4:f:68:THR:HG1	4:f:81:GLN:HB3	1.71	0.55
3:S:21:PHE:HE2	3:S:73:LEU:HD23	1.71	0.55
3:a:49:LYS:HG3	3:a:53:GLU:HB2	1.89	0.55
3:a:106:ILE:H	3:a:166:GLN:HE22	1.55	0.55
3:S:66:GLY:HA3	3:S:71:PHE:HA	1.89	0.55
1:Y:101:ASP:HA	2:Z:46:LEU:HD13	1.88	0.54
4:T:7:SER:HB3	4:T:21:SER:HB2	1.90	0.54
3:a:108:ARG:CD	3:a:171:SER:OG	2.55	0.54
3:e:15:PRO:HD3	3:e:106:ILE:HG23	1.88	0.54
4:H:203:SER:HA	4:P:116:THR:HG22	1.88	0.54
4:P:212:GLU:HG3	4:P:213:PRO:HD2	1.89	0.54
1:M:150:VAL:HG12	1:M:178:LEU:HD21	1.89	0.54
4:f:4:ILE:HD11	4:f:94:ARG:HB2	1.89	0.54
3:W:108:ARG:HH11	3:W:108:ARG:HG2	1.73	0.54
3:W:113:PRO:HD3	3:W:198:HIS:CD2	2.43	0.54
3:e:55:ILE:HG22	3:e:56:SER:N	2.23	0.54
3:W:108:ARG:HD3	3:W:109:THR:O	2.08	0.53
1:Q:100(A):GLY:N	4:T:32:TYR:OH	2.38	0.53
4:D:30:THR:HG23	4:D:53:GLY:HA3	1.89	0.53
2:F:39:LEU:HD13	2:F:84:ALA:HB2	1.89	0.53
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.89	0.53
3:K:66:GLY:HA3	3:K:71:PHE:HA	1.89	0.53
4:f:165:THR:HG23	4:f:180:SER:HB2	1.90	0.53
4:H:119:PRO:HB3	4:H:145:TYR:HB3	1.89	0.53
3:O:149:LYS:NZ	3:O:195:GLU:OE1	2.33	0.53
3:a:108:ARG:NH2	3:a:109:THR:OG1	2.41	0.53
2:N:149:LYS:HD3	2:N:154:PRO:HA	1.91	0.53
4:X:38:LYS:HB2	4:X:48:ILE:HD11	1.90	0.53
4:X:82(A):SER:O	4:X:82(C):LEU:N	2.40	0.53
2:Z:46:LEU:HD23	2:Z:55:PRO:HG3	1.90	0.53
3:K:124:GLN:HE22	3:K:131:SER:HB2	1.74	0.53
2:N:39:LEU:HD23	2:N:84:ALA:HB2	1.90	0.53
3:O:13:VAL:HG12	3:O:19:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:35:TRP:HB2	2:V:48:ILE:HB	1.90	0.53
3:K:163:VAL:HG22	3:K:175:LEU:HD12	1.89	0.53
2:N:81:GLU:CD	2:N:81:GLU:H	2.17	0.53
3:e:197:THR:HG22	3:e:204:PRO:HB3	1.90	0.53
2:F:196:THR:OG1	2:F:201:THR:OG1	2.24	0.52
4:X:47:TRP:HZ2	4:X:50:GLU:HG2	1.74	0.52
4:L:53:GLY:HA2	4:L:73:THR:HG22	1.91	0.52
2:F:184:GLN:O	2:F:191:TYR:OH	2.27	0.52
3:W:37:GLN:HB2	3:W:47:LEU:HD11	1.91	0.52
3:a:143:GLU:CD	3:a:143:GLU:H	2.17	0.52
1:I:36:TRP:HD1	1:I:69:ILE:HD12	1.75	0.52
3:W:108:ARG:NH1	3:W:109:THR:OG1	2.43	0.51
4:X:60:ASN:OD1	4:X:62:LYS:HG2	2.09	0.51
1:A:124:LEU:HD12	2:B:118:PHE:HB3	1.93	0.51
3:O:193:ALA:HB2	3:O:208:SER:HB3	1.91	0.51
2:N:180:LEU:HD11	2:N:191:TYR:CZ	2.46	0.51
3:O:142:ARG:HH11	3:O:163:VAL:HG11	1.76	0.51
3:K:21:PHE:HE1	3:K:73:LEU:HD23	1.76	0.51
2:R:47:LEU:HD12	2:R:58:VAL:CG2	2.41	0.51
3:e:132:VAL:CG1	3:e:148:TRP:CH2	2.88	0.51
3:C:4:LEU:HD11	3:C:90:GLN:HB3	1.92	0.51
4:D:11:LEU:HD22	4:D:147:PRO:HG3	1.92	0.51
2:F:31:TYR:CZ	4:H:28:THR:HG21	2.46	0.51
4:H:117:LYS:NZ	4:H:144:ASP:O	2.44	0.51
3:W:13:VAL:HG21	3:W:78:VAL:HG21	1.92	0.51
3:C:193:ALA:HB2	3:C:208:SER:HB3	1.92	0.51
4:b:47:TRP:HZ2	4:b:50:GLU:HG2	1.75	0.51
4:H:191:THR:OG1	4:H:192:GLN:N	2.42	0.50
3:S:4:LEU:HD11	3:S:90:GLN:HB3	1.92	0.50
1:A:170:LEU:HD11	1:A:174:GLY:HA2	1.92	0.50
2:R:39:LEU:HD12	2:R:84:ALA:HB2	1.93	0.50
4:T:152:VAL:HG22	4:T:198:VAL:HG22	1.93	0.50
1:Q:15:GLY:N	1:Q:82(C):LEU:O	2.41	0.50
3:e:36:TYR:HE1	3:e:89:GLN:HB3	1.76	0.50
3:G:142:ARG:HG2	3:G:142:ARG:NH1	2.23	0.50
4:T:200:HIS:NE2	4:T:202:PRO:HG2	2.27	0.50
4:L:119:PRO:HB3	4:L:145:TYR:HB3	1.94	0.50
3:e:46:LEU:HD22	4:f:101:ASP:HA	1.94	0.50
1:E:19:ARG:NH1	4:T:61:GLU:OE2	2.44	0.50
1:A:20:LEU:HG	1:A:82:MET:HE2	1.92	0.50
2:F:35:TRP:HB2	2:F:48:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:36:TRP:NE1	1:Q:80:LEU:HB2	2.27	0.50
3:S:13:VAL:HG21	3:S:78:VAL:HG11	1.93	0.50
4:D:138:LEU:HD13	4:D:211:VAL:HG21	1.94	0.50
2:N:95:LEU:HD23	2:N:95(A):SER:H	1.76	0.50
3:W:11:LEU:HD11	3:W:19:VAL:HG21	1.93	0.49
2:d:31:TYR:CD1	4:f:28:THR:HG21	2.46	0.49
3:S:163:VAL:HG22	3:S:175:LEU:HD12	1.94	0.49
2:V:192:SER:HB3	2:V:205:THR:HG22	1.92	0.49
3:C:155:GLN:HB3	3:C:158:ASN:HD21	1.75	0.49
1:E:40:ALA:HB3	1:E:43:LYS:HB2	1.95	0.49
1:Q:39:GLN:HB2	1:Q:45:LEU:HD23	1.93	0.49
2:R:14:ALA:HB3	2:R:17:GLN:HE22	1.76	0.49
1:U:82:MET:HB3	1:U:82(C):LEU:HD21	1.94	0.49
3:e:78:VAL:HG13	3:e:82:ASP:HB2	1.93	0.49
3:e:76:ASN:OD1	3:e:77:SER:N	2.45	0.49
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.94	0.49
4:f:192:GLN:HB3	4:f:194:TYR:HE1	1.77	0.49
3:O:148:TRP:CE2	3:O:179:LEU:HB2	2.47	0.49
2:F:117:LEU:HD13	2:F:134:CYS:HB2	1.95	0.49
4:H:69:PHE:CE1	4:H:80:MET:HG3	2.48	0.49
4:X:6:GLN:NE2	4:X:92:CYS:SG	2.86	0.49
1:I:59:TYR:HB2	1:I:64:LYS:HB2	1.95	0.48
3:O:142:ARG:HG3	3:O:173:TYR:CG	2.48	0.48
3:O:185:ASP:HA	3:O:188:LYS:HE2	1.95	0.48
1:U:123:PRO:HG2	2:V:121:SER:HB2	1.95	0.48
3:W:118:PHE:HB2	3:W:133:VAL:HB	1.95	0.48
2:F:95(B):GLY:N	4:H:54:ARG:HH21	2.10	0.48
2:V:138:ASP:HA	2:V:171:LYS:HE3	1.93	0.48
1:E:171:GLN:HE21	1:E:175:LEU:HB2	1.78	0.48
3:e:55:ILE:CG2	3:e:56:SER:N	2.76	0.48
3:G:25:ALA:HB1	3:G:29:ILE:HD12	1.95	0.48
1:Q:34:MET:SD	1:Q:94:ARG:HG3	2.53	0.48
2:V:4:LEU:HB2	2:V:99:GLY:HA2	1.95	0.48
3:S:29:ILE:HD11	3:S:33:ILE:HG12	1.96	0.48
4:X:138:LEU:C	4:X:138:LEU:HD12	2.39	0.48
1:c:97:TYR:HE2	3:e:53:GLU:HG2	1.79	0.48
2:d:46:LEU:HD21	2:d:49:TYR:HB3	1.95	0.48
2:N:181:THR:HG23	2:N:184:GLN:H	1.77	0.48
1:E:94:ARG:NH2	1:E:101:ASP:OD2	2.34	0.48
4:X:116:THR:HG22	4:X:147:PRO:HD3	1.96	0.48
3:a:142:ARG:HG2	3:a:142:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:SER:HB3	1:E:56:TYR:HB2	1.94	0.48
4:H:163:VAL:HG22	4:H:182:VAL:HB	1.96	0.48
4:f:119:PRO:HB3	4:f:145:TYR:HB3	1.95	0.48
4:L:47:TRP:HZ2	4:L:50:GLU:HG2	1.79	0.48
3:O:37:GLN:HB2	3:O:47:LEU:HD11	1.95	0.48
1:U:32:TYR:O	1:U:71:ARG:NH2	2.44	0.48
1:M:141:LEU:HD21	1:M:143:LYS:HD3	1.95	0.47
1:c:39:GLN:HB2	1:c:45:LEU:HD23	1.96	0.47
1:M:122:PHE:HD2	1:M:141:LEU:HD22	1.79	0.47
3:a:105:GLU:HG2	3:a:166:GLN:NE2	2.29	0.47
4:f:138:LEU:HD11	4:f:194:TYR:HD2	1.79	0.47
4:H:52:LEU:HD13	4:H:54:ARG:HB2	1.95	0.47
1:A:31:SER:OG	3:C:31:THR:OG1	2.27	0.47
4:D:4:ILE:HD12	4:D:102:TYR:C	2.40	0.47
2:N:132:LEU:HB2	2:N:178:LEU:HB3	1.95	0.47
2:R:47:LEU:HD12	2:R:58:VAL:HG21	1.96	0.47
3:e:154:LEU:HD12	3:e:155:GLN:H	1.80	0.47
4:f:126:PRO:HD3	4:f:138:LEU:HB3	1.96	0.47
4:H:159:LEU:HD11	4:H:182:VAL:HG21	1.97	0.47
3:a:197:THR:HG22	3:a:204:PRO:HB3	1.97	0.47
2:d:31:TYR:HE2	2:d:91:TYR:HD2	1.61	0.47
2:J:61:ARG:HB3	2:J:76:THR:O	2.15	0.47
4:L:38:LYS:HB2	4:L:48:ILE:HD11	1.95	0.47
1:A:142:VAL:HG11	1:A:150:VAL:HG11	1.97	0.47
1:A:148:GLU:HG2	1:A:176:TYR:CD2	2.50	0.47
4:D:209:LYS:HA	4:D:209:LYS:HD3	1.69	0.47
1:E:144:ASP:OD1	1:E:171:GLN:NE2	2.47	0.47
3:K:36:TYR:CE1	4:L:100(D):PHE:HB2	2.49	0.47
4:T:195:ILE:HD11	4:T:210:ARG:HD2	1.96	0.47
2:V:181:THR:N	2:V:184:GLN:OE1	2.47	0.47
2:V:197:HIS:O	2:V:199:GLY:N	2.46	0.47
4:X:6:GLN:NE2	4:X:104:GLY:HA3	2.30	0.47
3:a:13:VAL:CG1	3:a:14:SER:H	2.27	0.47
3:G:122:ASP:O	3:G:125:LEU:N	2.47	0.47
4:L:72:ASP:OD1	4:L:75:SER:OG	2.31	0.47
3:K:142:ARG:HG2	3:K:142:ARG:HH11	1.80	0.47
1:M:169:VAL:HG23	2:N:162:THR:HG22	1.97	0.47
2:d:31:TYR:HD1	4:f:28:THR:HG21	1.80	0.47
3:G:49:LYS:HB2	4:H:100(C):PRO:HG3	1.97	0.47
1:c:67:PHE:HB3	1:c:80:LEU:HD21	1.96	0.47
2:V:169:ASN:HD21	2:V:171:LYS:NZ	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:113:PRO:HB3	3:W:139:PHE:HB3	1.97	0.46
4:T:69:PHE:CE1	4:T:80:MET:HG3	2.50	0.46
3:G:44:PRO:HG2	4:H:103:TRP:CE3	2.50	0.46
4:P:142:VAL:HG11	4:P:150:VAL:HG11	1.98	0.46
3:W:11:LEU:HD11	3:W:19:VAL:CG2	2.46	0.46
2:Z:26:SER:OG	2:Z:27(B):ASN:ND2	2.48	0.46
4:L:32:TYR:O	4:L:52(A):SER:OG	2.22	0.46
3:O:136:LEU:HD23	3:O:175:LEU:HD22	1.98	0.46
4:b:184:VAL:HG11	4:b:194:TYR:CE2	2.51	0.46
1:c:75:LYS:HE2	1:c:75:LYS:HB2	1.79	0.46
1:A:124:LEU:HD21	1:A:141:LEU:HB2	1.97	0.46
1:A:169:VAL:HB	2:B:162:THR:HG22	1.96	0.46
2:F:95:LEU:HB2	2:F:95(C):PHE:HE2	1.80	0.46
4:H:32:TYR:CD1	4:H:94:ARG:HD3	2.51	0.46
1:M:141:LEU:HD12	2:N:133:VAL:HG21	1.96	0.46
2:N:180:LEU:CD1	2:N:191:TYR:CZ	2.99	0.46
3:S:148:TRP:CD1	3:S:159:SER:HG	2.34	0.46
1:c:48:VAL:HG13	1:c:63:VAL:HG21	1.96	0.46
1:A:166:PHE:CZ	2:B:135:LEU:HB3	2.51	0.46
4:T:38:LYS:HB2	4:T:48:ILE:HD11	1.98	0.46
2:Z:90:SER:OG	2:Z:91:TYR:N	2.45	0.46
3:C:61:ARG:CZ	3:C:79:GLU:HG3	2.46	0.46
4:D:69:PHE:CE1	4:D:80:MET:HG3	2.51	0.46
3:a:142:ARG:HG2	3:a:142:ARG:NH1	2.31	0.46
1:E:75:LYS:HE2	1:E:75:LYS:HB2	1.63	0.45
3:K:2:ILE:HD13	3:K:29:ILE:HD11	1.99	0.45
3:O:47:LEU:HA	3:O:58:ILE:HG13	1.97	0.45
2:R:60:ASP:OD1	2:R:60:ASP:N	2.49	0.45
3:a:61:ARG:O	3:a:75:ILE:HA	2.16	0.45
2:d:27(C):ILE:N	2:d:27(C):ILE:HD12	2.31	0.45
2:B:2:PRO:HG2	2:B:95(C):PHE:HZ	1.82	0.45
2:F:11:VAL:HG12	2:F:104:LEU:HD23	1.98	0.45
3:G:21:PHE:HE1	3:G:73:LEU:HD23	1.82	0.45
4:H:203:SER:HA	4:P:116:THR:CG2	2.46	0.45
2:Z:78:LEU:HD12	2:Z:79:GLN:H	1.81	0.45
2:F:4:LEU:HB2	2:F:99:GLY:HA2	1.98	0.45
3:K:21:PHE:CE1	3:K:73:LEU:HD23	2.51	0.45
4:P:36:TRP:CE3	4:P:80:MET:HE2	2.51	0.45
4:T:70:THR:OG1	4:T:79:TYR:HB2	2.16	0.45
3:e:89:GLN:HB2	3:e:98:PHE:CD2	2.52	0.45
3:G:4:LEU:HD11	3:G:90:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2:PRO:HG2	2:J:95(C):PHE:CZ	2.50	0.45
1:U:119:PRO:HB3	1:U:145:TYR:HB3	1.99	0.45
3:W:21:PHE:CE1	3:W:73:LEU:HB3	2.51	0.45
4:X:6:GLN:HE22	4:X:92:CYS:H	1.61	0.45
3:K:169:LYS:NZ	2:d:27:SER:O	2.47	0.45
2:N:35:TRP:HB2	2:N:48:ILE:HB	1.97	0.45
4:T:143:LYS:HG3	4:T:144:ASP:OD1	2.16	0.45
3:a:13:VAL:CG1	3:a:78:VAL:CG2	2.71	0.45
4:D:13:ARG:HH21	4:X:205:THR:HA	1.80	0.45
4:L:53:GLY:HA2	4:L:73:THR:CG2	2.47	0.45
3:S:32:HIS:HB3	3:S:91:SER:OG	2.17	0.45
2:d:27(B):ASN:HB2	2:d:27(C):ILE:HD12	1.99	0.45
4:L:142:VAL:HG11	4:L:150:VAL:HG11	1.99	0.45
2:N:166:LYS:HE2	2:N:166:LYS:HB2	1.68	0.45
1:A:13:LYS:H	1:A:13:LYS:HD2	1.82	0.45
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.99	0.45
1:E:166:PHE:CZ	2:F:135:LEU:HB3	2.52	0.45
1:I:61:ASP:HA	1:I:64:LYS:HE2	1.98	0.45
3:O:145:LYS:HA	3:O:145:LYS:HD3	1.73	0.45
3:a:179:LEU:HD21	3:a:181:LEU:HD11	1.99	0.45
4:H:11:LEU:HD22	4:H:147:PRO:HG3	1.99	0.45
4:P:209:LYS:HA	4:P:209:LYS:HD3	1.77	0.45
2:d:31:TYR:CE2	2:d:91:TYR:HD2	2.34	0.45
1:A:117:LYS:HD3	1:A:118:GLY:O	2.17	0.45
3:C:142:ARG:HD2	3:C:173:TYR:CE1	2.52	0.45
4:T:54:ARG:H	4:T:54:ARG:HG2	1.59	0.45
2:Z:61:ARG:HB3	2:Z:76:THR:O	2.17	0.45
1:I:36:TRP:CG	1:I:80:LEU:HD22	2.52	0.44
2:R:35:TRP:HB2	2:R:48:ILE:HB	1.99	0.44
3:S:7:SER:O	3:S:22:SER:OG	2.29	0.44
4:b:40:ARG:HG3	4:b:40:ARG:HH11	1.82	0.44
2:F:9:SER:HB2	2:F:143:ALA:HB3	2.00	0.44
4:L:6:GLN:H	4:L:105:GLN:HE22	1.66	0.44
3:S:185:ASP:HA	3:S:188:LYS:HD3	2.00	0.44
1:Y:69:ILE:HD11	1:Y:78:LEU:HD11	1.99	0.44
1:E:119:PRO:HB3	1:E:145:TYR:HB3	2.00	0.44
3:O:49:LYS:HG3	3:O:53:GLU:HB2	2.00	0.44
3:e:96:PHE:HB2	4:f:47:TRP:CD2	2.53	0.44
1:A:148:GLU:HG2	1:A:176:TYR:CE2	2.53	0.44
2:B:53:ASN:OD1	2:N:60:ASP:HB3	2.18	0.44
4:D:133:GLY:C	4:D:135:THR:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:LEU:HD13	2:F:106:VAL:HG12	2.00	0.44
1:I:82:MET:HE1	1:I:109:VAL:HG21	1.99	0.44
2:R:13:GLY:O	2:R:106:VAL:HA	2.17	0.44
4:T:33:TRP:HE3	4:T:50:GLU:HB2	1.82	0.44
1:E:170:LEU:HD13	1:E:176:TYR:CZ	2.53	0.44
2:J:60:ASP:OD1	2:J:60:ASP:N	2.50	0.44
2:N:19:VAL:HG22	2:N:78:LEU:HD21	2.00	0.44
3:O:210:ASN:HB2	3:O:213:GLU:HB2	1.99	0.44
1:I:29:PHE:HB3	1:I:76:ASN:OD1	2.17	0.44
1:U:34:MET:HG2	1:U:71:ARG:NH2	2.33	0.44
2:V:61:ARG:HB3	2:V:76:THR:O	2.18	0.44
2:V:161:THR:HG22	2:V:176:SER:OG	2.18	0.44
2:d:55:PRO:HD2	2:d:58:VAL:HG21	1.99	0.44
4:L:33:TRP:CE2	4:L:52:LEU:HD13	2.53	0.44
3:O:86:TYR:HE2	3:O:104:LEU:HD22	1.83	0.44
3:a:58:ILE:HD13	3:a:58:ILE:HA	1.85	0.44
3:e:59:PRO:HB2	3:e:61:ARG:HD3	2.00	0.44
4:L:94:ARG:HE	4:L:94:ARG:HB3	1.69	0.43
3:S:176:SER:HB3	4:T:166:PHE:CZ	2.53	0.43
1:Y:36:TRP:NE1	1:Y:80:LEU:HB2	2.33	0.43
2:Z:21:ILE:HD11	2:Z:104:LEU:HD13	2.00	0.43
1:c:36:TRP:CD1	1:c:80:LEU:HD12	2.53	0.43
1:I:100(D):HIS:HB3	2:J:34:HIS:CG	2.53	0.43
1:M:163:VAL:HA	1:M:182:VAL:HG22	2.00	0.43
3:W:115:VAL:HG22	3:W:136:LEU:HD22	1.99	0.43
4:H:154:TRP:HB3	4:H:159:LEU:HD23	1.99	0.43
4:T:200:HIS:CE1	4:T:202:PRO:HG2	2.53	0.43
4:H:80:MET:HE2	4:H:80:MET:HB3	1.81	0.43
3:K:142:ARG:HG2	3:K:142:ARG:NH1	2.33	0.43
3:O:148:TRP:CG	3:O:179:LEU:HD13	2.54	0.43
4:P:83:THR:HA	1:Y:13:LYS:HE3	1.99	0.43
3:K:145:LYS:HA	3:K:145:LYS:HD2	1.76	0.43
1:Y:89:VAL:HG22	1:Y:108:LEU:HD13	2.01	0.43
3:e:145:LYS:HB3	3:e:197:THR:OG1	2.18	0.43
3:e:154:LEU:HD12	3:e:155:GLN:N	2.33	0.43
3:O:61:ARG:NH2	3:O:82:ASP:OD1	2.51	0.43
3:e:110:VAL:HG21	3:e:199:GLN:NE2	2.33	0.43
4:f:94:ARG:HB3	4:f:101:ASP:OD1	2.19	0.43
3:C:46:LEU:HG	3:C:55:ILE:HG13	2.01	0.43
3:C:126:LYS:HB2	3:C:126:LYS:HE3	1.76	0.43
2:N:108:GLN:HE22	2:N:171:LYS:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:209:LYS:HA	4:X:209:LYS:HD3	1.54	0.43
3:a:10:ILE:HG13	3:a:103:LYS:HB3	2.00	0.43
4:f:193:THR:C	4:f:194:TYR:HD1	2.27	0.43
3:C:116:PHE:HE1	4:D:132:SER:OG	2.01	0.43
1:U:39:GLN:HB2	1:U:45:LEU:HD23	2.00	0.43
4:X:47:TRP:CZ2	4:X:50:GLU:HG2	2.52	0.43
3:e:13:VAL:HG11	3:e:19:VAL:HB	2.00	0.43
4:D:6:GLN:H	4:D:105:GLN:HE22	1.67	0.43
3:K:8:PRO:HG2	3:K:10:ILE:O	2.18	0.43
2:N:151:ASP:OD2	2:N:188:HIS:ND1	2.32	0.43
3:O:142:ARG:HH12	3:O:163:VAL:HG21	1.84	0.43
3:a:151:ASP:C	3:a:153:ALA:H	2.27	0.43
3:C:54:SER:O	3:C:55:ILE:HD13	2.19	0.43
4:D:192:GLN:OE1	4:D:193:THR:N	2.46	0.43
3:K:190:LYS:HB2	3:K:190:LYS:HE2	1.78	0.43
3:e:167:ASP:OD1	3:e:168:SER:N	2.51	0.43
2:B:14:ALA:HB3	2:B:17:GLN:HG3	2.01	0.42
2:B:166:LYS:HE2	2:B:166:LYS:H	1.83	0.42
1:M:209:LYS:HE2	1:M:209:LYS:HB2	1.80	0.42
4:P:66:LYS:NZ	4:P:82(A):SER:O	2.40	0.42
4:D:13:ARG:HE	4:X:206:LYS:H	1.66	0.42
3:G:119:PRO:HB3	3:G:209:PHE:CE2	2.55	0.42
3:O:192:TYR:HB2	3:O:209:PHE:CE1	2.54	0.42
3:W:29:ILE:HD11	3:W:90:GLN:HB2	2.01	0.42
3:C:13:VAL:HG22	3:C:105:GLU:O	2.20	0.42
4:D:83:THR:HG22	4:D:85:GLY:H	1.84	0.42
4:D:12:MET:HE3	4:D:12:MET:HB3	1.82	0.42
3:K:86:TYR:CE1	3:K:104:LEU:HD12	2.55	0.42
4:T:123:PRO:HD3	4:T:209:LYS:HE2	2.01	0.42
1:c:97:TYR:CE2	3:e:53:GLU:HG2	2.55	0.42
4:f:38:LYS:HB2	4:f:48:ILE:HD11	2.01	0.42
4:f:146:PHE:HA	4:f:147:PRO:HA	1.83	0.42
3:a:149:LYS:HA	3:a:154:LEU:HA	2.01	0.42
1:U:196:CYS:HB3	1:U:209:LYS:O	2.18	0.42
1:Y:61:ASP:N	1:Y:61:ASP:OD1	2.52	0.42
2:Z:36:TYR:HE1	2:Z:89:GLN:HB3	1.84	0.42
4:f:35:GLU:O	4:f:92:CYS:HA	2.19	0.42
2:B:132:LEU:HB2	2:B:178:LEU:HB3	2.01	0.42
2:B:2:PRO:HG2	2:B:95(C):PHE:CZ	2.54	0.42
3:C:2:ILE:HG12	3:C:27:GLN:HG2	2.01	0.42
4:D:97:PHE:CD2	4:D:98:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:140:TYR:CG	3:G:141:PRO:HA	2.55	0.42
4:H:38:LYS:HB2	4:H:48:ILE:HD11	2.01	0.42
3:S:186:TYR:O	3:S:192:TYR:OH	2.35	0.42
3:W:49:LYS:HG3	3:W:53:GLU:HB2	2.02	0.42
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.55	0.42
4:H:100(A):ASP:OD1	4:H:100(A):ASP:N	2.53	0.42
1:M:61:ASP:OD2	2:N:95:LEU:HD21	2.20	0.42
2:R:61:ARG:HB3	2:R:76:THR:O	2.19	0.42
1:A:199:ASN:HD22	1:A:206:LYS:HG2	1.85	0.42
4:D:33:TRP:CE2	4:D:52:LEU:HD13	2.54	0.42
2:F:83:GLU:HB2	2:F:106:VAL:HG22	2.02	0.42
1:M:124:LEU:HD21	1:M:141:LEU:HB2	2.02	0.42
3:W:35:TRP:CG	3:W:73:LEU:HD12	2.55	0.42
3:W:145:LYS:HA	3:W:145:LYS:HD2	1.81	0.42
3:W:183:LYS:O	3:W:187:GLU:HG3	2.19	0.42
4:X:154:TRP:CZ3	4:X:196:CYS:HB3	2.54	0.42
3:C:13:VAL:HG21	3:C:78:VAL:HG11	2.01	0.41
3:G:20:SER:HB2	3:G:74:THR:HG22	2.02	0.41
3:G:44:PRO:HG2	4:H:103:TRP:CZ3	2.55	0.41
4:P:60:ASN:OD1	4:P:61:GLU:N	2.53	0.41
4:f:97:PHE:C	4:f:99:TYR:H	2.27	0.41
1:A:52:SER:HB3	1:A:56:TYR:HB2	2.01	0.41
2:B:142:GLY:HA3	2:B:172:TYR:CD2	2.55	0.41
3:G:108:ARG:NH1	3:G:109:THR:OG1	2.52	0.41
2:V:192:SER:OG	2:V:205:THR:CG2	2.68	0.41
4:X:138:LEU:HD12	4:X:138:LEU:O	2.20	0.41
4:X:146:PHE:HA	4:X:147:PRO:HA	1.79	0.41
1:c:82(C):LEU:HB3	1:c:111:VAL:HG21	2.02	0.41
1:A:13:LYS:HD2	1:A:13:LYS:N	2.35	0.41
1:E:152:VAL:HA	1:E:197:ASN:O	2.20	0.41
1:I:6:GLU:OE2	1:I:92:CYS:N	2.39	0.41
1:U:146:PHE:HA	1:U:147:PRO:HA	1.86	0.41
4:b:11:LEU:HD22	4:b:147:PRO:HG3	2.01	0.41
4:b:197:ASN:ND2	4:b:208:ASP:OD1	2.32	0.41
2:J:78:LEU:HD12	2:J:78:LEU:HA	1.84	0.41
4:P:168:ALA:HB2	4:P:178:LEU:HD12	2.01	0.41
3:S:8:PRO:HG2	3:S:11:LEU:HD22	2.02	0.41
4:X:38:LYS:NZ	4:X:86:ASP:HA	2.35	0.41
1:Y:13:LYS:HZ2	1:Y:13:LYS:HG2	1.70	0.41
1:Y:82:MET:HB3	1:Y:82(C):LEU:HD21	2.01	0.41
3:a:18:ARG:HG2	3:a:76:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:7:SER:HA	3:e:8:PRO:HA	1.89	0.41
3:S:193:ALA:HB2	3:S:208:SER:HB2	2.03	0.41
3:a:21:PHE:HE1	3:a:73:LEU:HD23	1.86	0.41
3:e:142:ARG:HB2	3:e:173:TYR:CE2	2.55	0.41
2:F:61:ARG:HB3	2:F:76:THR:O	2.20	0.41
3:O:86:TYR:CE2	3:O:104:LEU:HD22	2.55	0.41
1:I:40:ALA:HB3	1:I:43:LYS:HB2	2.03	0.41
4:L:146:PHE:HA	4:L:147:PRO:HA	1.85	0.41
1:M:100(A):GLY:N	4:P:32:TYR:OH	2.53	0.41
3:O:113:PRO:HB3	3:O:139:PHE:HB3	2.02	0.41
3:O:134:CYS:HB2	3:O:148:TRP:CH2	2.56	0.41
3:S:90:GLN:HG3	3:S:97:THR:H	1.85	0.41
3:S:117:ILE:HD12	3:S:118:PHE:H	1.85	0.41
1:c:3:GLN:OE1	1:c:25:SER:N	2.53	0.41
3:e:47:LEU:HD22	3:e:58:ILE:HD11	2.03	0.41
4:f:29:PHE:CE2	4:f:52(A):SER:HB2	2.56	0.41
1:A:36:TRP:HD1	1:A:69:ILE:HD12	1.85	0.41
2:B:58:VAL:HA	2:B:59:PRO:HD3	1.95	0.41
2:B:105:THR:HG21	2:B:141:PRO:HB3	2.02	0.41
2:B:134:CYS:HB2	2:B:148:TRP:CZ2	2.56	0.41
4:X:29:PHE:HB2	4:X:76:ASN:OD1	2.21	0.41
2:Z:80:ALA:HA	2:Z:106:VAL:HG21	2.02	0.41
3:a:141:PRO:HB2	3:a:143:GLU:OE1	2.21	0.41
2:d:27:SER:HA	2:d:28:GLY:HA3	2.03	0.41
3:e:27:GLN:O	3:e:69:THR:HG22	2.20	0.41
4:f:11:LEU:HD22	4:f:147:PRO:HD3	2.02	0.41
4:D:13:ARG:NH2	4:X:205:THR:HA	2.36	0.41
4:H:200:HIS:NE2	4:H:202:PRO:HG2	2.36	0.41
1:A:22:CYS:HB3	1:A:78:LEU:HB3	2.02	0.40
1:A:121:VAL:HA	1:A:141:LEU:O	2.21	0.40
3:G:146:VAL:HG22	3:G:196:VAL:HG22	2.03	0.40
2:J:27(B):ASN:OD1	2:J:27(C):ILE:N	2.42	0.40
3:O:83:ILE:HD13	3:O:83:ILE:HA	1.89	0.40
4:P:69:PHE:CE1	4:P:80:MET:HG3	2.56	0.40
2:R:66:LYS:HA	2:R:71:ALA:HA	2.03	0.40
2:d:4:LEU:O	2:d:100:THR:HG23	2.21	0.40
3:e:110:VAL:HG21	3:e:199:GLN:HE21	1.86	0.40
4:L:35:GLU:HG3	4:L:100(D):PHE:CE1	2.56	0.40
1:M:14:PRO:HD2	1:M:113:SER:HB3	2.03	0.40
2:N:7:PRO:HA	2:N:8:PRO:HD3	1.96	0.40
4:X:35:GLU:O	4:X:92:CYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:17:SER:OG	4:L:82(A):SER:O	2.35	0.40
1:M:119:PRO:HB3	1:M:145:TYR:HB3	2.04	0.40
3:a:13:VAL:HG12	3:a:78:VAL:HG21	1.85	0.40
2:d:4:LEU:HD21	2:d:27(C):ILE:CD1	2.52	0.40
4:f:142:VAL:HG11	4:f:150:VAL:HG11	2.02	0.40
2:B:156:LYS:HD3	2:B:156:LYS:HA	1.90	0.40
1:E:184:VAL:HG11	1:E:194:TYR:CZ	2.57	0.40
3:G:198:HIS:CD2	3:G:200:GLY:H	2.39	0.40
1:U:11:LEU:HD12	1:U:12:VAL:H	1.86	0.40
3:a:136:LEU:HD22	3:a:175:LEU:HD22	2.03	0.40
3:G:25:ALA:HB3	3:G:69:THR:HA	2.04	0.40
1:U:38:ARG:HG2	1:U:48:VAL:HG23	2.02	0.40
3:a:19:VAL:HG12	3:a:75:ILE:HB	2.03	0.40
3:a:113:PRO:HB3	3:a:139:PHE:CD2	2.56	0.40
3:a:190:LYS:HG3	3:a:210:ASN:OD1	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)
2:R:54:ARG:NH2	3:e:187:GLU:O[1_454]	2.19	0.01

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	197/227 (87%)	183 (93%)	12 (6%)	2 (1%)	12	28
1	E	200/227 (88%)	193 (96%)	6 (3%)	1 (0%)	24	45
1	I	119/227 (52%)	114 (96%)	4 (3%)	1 (1%)	16	34
1	M	204/227 (90%)	197 (97%)	6 (3%)	1 (0%)	24	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	123/227 (54%)	119 (97%)	2 (2%)	2 (2%)	7	18
1	U	170/227 (75%)	155 (91%)	13 (8%)	2 (1%)	10	24
1	Y	119/227 (52%)	113 (95%)	4 (3%)	2 (2%)	7	17
1	c	78/227 (34%)	72 (92%)	6 (8%)	0	100	100
2	B	211/218 (97%)	197 (93%)	14 (7%)	0	100	100
2	F	212/218 (97%)	200 (94%)	12 (6%)	0	100	100
2	J	108/218 (50%)	99 (92%)	8 (7%)	1 (1%)	14	31
2	N	212/218 (97%)	198 (93%)	14 (7%)	0	100	100
2	R	106/218 (49%)	96 (91%)	10 (9%)	0	100	100
2	V	191/218 (88%)	176 (92%)	14 (7%)	1 (0%)	24	45
2	Z	104/218 (48%)	96 (92%)	8 (8%)	0	100	100
2	d	63/218 (29%)	55 (87%)	8 (13%)	0	100	100
3	C	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	G	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	K	210/214 (98%)	199 (95%)	10 (5%)	1 (0%)	24	45
3	O	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	S	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	W	194/214 (91%)	178 (92%)	15 (8%)	1 (0%)	24	45
3	a	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
3	e	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	24	45
4	D	219/226 (97%)	210 (96%)	8 (4%)	1 (0%)	24	45
4	H	216/226 (96%)	205 (95%)	11 (5%)	0	100	100
4	L	214/226 (95%)	205 (96%)	8 (4%)	1 (0%)	24	45
4	P	213/226 (94%)	203 (95%)	10 (5%)	0	100	100
4	T	210/226 (93%)	197 (94%)	12 (6%)	1 (0%)	24	45
4	X	208/226 (92%)	198 (95%)	8 (4%)	2 (1%)	12	28
4	b	214/226 (95%)	200 (94%)	14 (6%)	0	100	100
4	f	211/226 (93%)	200 (95%)	11 (5%)	0	100	100
All	All	5798/7080 (82%)	5460 (94%)	317 (6%)	21 (0%)	30	51

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	100(A)	GLY
1	Q	115	SER
1	U	113	SER
1	A	100(B)	SER
1	A	114	ALA
1	E	100(B)	SER
4	L	101	ASP
1	Q	100(B)	SER
1	U	100(B)	SER
2	V	199	GLY
1	Y	100(B)	SER
4	D	82(B)	SER
1	I	100(B)	SER
1	M	100(B)	SER
4	X	82(C)	LEU
3	K	76	ASN
3	W	80	SER
4	X	82(B)	SER
2	J	95(B)	GLY
3	e	52	SER
4	T	149	PRO

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	167/191 (87%)	166 (99%)	1 (1%)	78	90
1	E	173/191 (91%)	167 (96%)	6 (4%)	32	58
1	I	99/191 (52%)	99 (100%)	0	100	100
1	M	177/191 (93%)	176 (99%)	1 (1%)	78	90
1	Q	101/191 (53%)	100 (99%)	1 (1%)	68	84
1	U	151/191 (79%)	150 (99%)	1 (1%)	76	89
1	Y	99/191 (52%)	97 (98%)	2 (2%)	48	74
1	c	80/191 (42%)	79 (99%)	1 (1%)	61	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	174/181 (96%)	173 (99%)	1 (1%)	78	90
2	F	177/181 (98%)	176 (99%)	1 (1%)	78	90
2	J	88/181 (49%)	87 (99%)	1 (1%)	65	83
2	N	176/181 (97%)	176 (100%)	0	100	100
2	R	89/181 (49%)	89 (100%)	0	100	100
2	V	165/181 (91%)	164 (99%)	1 (1%)	78	90
2	Z	87/181 (48%)	86 (99%)	1 (1%)	65	83
2	d	66/181 (36%)	66 (100%)	0	100	100
3	C	189/191 (99%)	188 (100%)	1 (0%)	81	91
3	G	189/191 (99%)	188 (100%)	1 (0%)	81	91
3	K	189/191 (99%)	187 (99%)	2 (1%)	65	83
3	O	191/191 (100%)	189 (99%)	2 (1%)	68	84
3	S	189/191 (99%)	187 (99%)	2 (1%)	65	83
3	W	180/191 (94%)	177 (98%)	3 (2%)	53	77
3	a	188/191 (98%)	184 (98%)	4 (2%)	47	73
3	e	186/191 (97%)	184 (99%)	2 (1%)	65	83
4	D	181/186 (97%)	180 (99%)	1 (1%)	78	90
4	H	179/186 (96%)	178 (99%)	1 (1%)	78	90
4	L	177/186 (95%)	175 (99%)	2 (1%)	65	83
4	P	178/186 (96%)	178 (100%)	0	100	100
4	T	175/186 (94%)	173 (99%)	2 (1%)	65	83
4	X	176/186 (95%)	175 (99%)	1 (1%)	78	90
4	b	178/186 (96%)	177 (99%)	1 (1%)	78	90
4	f	171/186 (92%)	170 (99%)	1 (1%)	78	90
All	All	4985/5992 (83%)	4941 (99%)	44 (1%)	70	86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	160	GLU
3	C	190	LYS
4	D	64	LYS
1	E	35	ASN

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Mol	Chain	Res	Type
1	E	92	CYS
1	E	115	SER
1	E	116	THR
1	E	140	CYS
1	E	197	ASN
2	F	204	LYS
3	G	21	PHE
4	H	81	GLN
2	J	60	ASP
3	K	21	PHE
3	K	107	LYS
4	L	61	GLU
4	L	94	ARG
1	M	210	ARG
3	O	61	ARG
3	O	105	GLU
1	Q	83	ARG
3	S	1	ASP
3	S	21	PHE
4	T	54	ARG
4	T	66	LYS
1	U	140	CYS
2	V	3	VAL
3	W	21	PHE
3	W	33	ILE
3	W	61	ARG
4	X	3	GLN
1	Y	13	LYS
1	Y	92	CYS
2	Z	85	ASP
3	a	1	ASP
3	a	137	ASN
3	a	155	GLN
3	a	170	ASP
4	b	51	ILE
1	c	92	CYS
3	e	107	LYS
3	e	181	LEU
4	f	140	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	171	GLN
1	A	199	ASN
2	B	38	GLN
2	B	108	GLN
3	C	92	ASN
3	C	124	GLN
3	C	210	ASN
4	D	76	ASN
1	E	197	ASN
2	F	79	GLN
3	G	38	GLN
3	G	92	ASN
3	G	152	ASN
3	G	198	HIS
4	H	39	GLN
1	I	39	GLN
2	J	38	GLN
2	J	79	GLN
1	M	81	GLN
1	M	171	GLN
2	N	108	GLN
3	O	32	HIS
3	O	92	ASN
4	P	58	ASN
1	Q	3	GLN
2	V	37	GLN
2	V	169	ASN
3	W	92	ASN
3	W	198	HIS
4	X	6	GLN
2	Z	17	GLN
3	a	92	ASN
3	a	124	GLN
3	a	137	ASN
4	b	5	GLN
4	b	76	ASN
2	d	38	GLN
3	e	28	ASN
3	e	166	GLN
3	e	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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	PCA	H	1	4	7,8,9	0.59	0	9,10,12	1.02	1 (11%)
4	PCA	L	1	4	7,8,9	0.45	0	9,10,12	0.79	1 (11%)
4	PCA	X	1	4	7,8,9	0.61	0	9,10,12	0.82	1 (11%)
2	PCA	N	1	2	7,8,9	0.48	0	9,10,12	1.24	1 (11%)
2	PCA	F	1	2	7,8,9	0.47	0	9,10,12	0.88	1 (11%)
2	PCA	V	1	2	7,8,9	0.46	0	9,10,12	1.27	1 (11%)
4	PCA	T	1	4	7,8,9	0.51	0	9,10,12	0.98	1 (11%)
4	PCA	b	1	4	7,8,9	0.60	0	9,10,12	1.19	1 (11%)
4	PCA	D	1	4	7,8,9	0.55	0	9,10,12	0.87	1 (11%)
4	PCA	P	1	4	7,8,9	0.52	0	9,10,12	0.91	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCA	H	1	4	-	0/0/11/13	0/1/1/1
4	PCA	L	1	4	-	0/0/11/13	0/1/1/1
4	PCA	X	1	4	-	0/0/11/13	0/1/1/1
2	PCA	N	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	PCA	V	1	2	-	0/0/11/13	0/1/1/1
4	PCA	T	1	4	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCA	b	1	4	-	0/0/11/13	0/1/1/1
4	PCA	D	1	4	-	0/0/11/13	0/1/1/1
4	PCA	P	1	4	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	1	PCA	O-C-CA	-3.70	115.26	124.77
2	N	1	PCA	O-C-CA	-3.28	116.33	124.77
4	b	1	PCA	O-C-CA	-3.20	116.53	124.77
4	T	1	PCA	O-C-CA	-2.86	117.41	124.77
4	H	1	PCA	O-C-CA	-2.44	118.49	124.77
4	P	1	PCA	O-C-CA	-2.43	118.53	124.77
4	D	1	PCA	O-C-CA	-2.37	118.67	124.77
2	F	1	PCA	O-C-CA	-2.34	118.75	124.77
4	X	1	PCA	O-C-CA	-2.17	119.18	124.77
4	L	1	PCA	O-C-CA	-2.17	119.19	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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	203/227 (89%)	0.47	22 (10%) 11 9	24, 40, 88, 103	0
1	E	206/227 (90%)	0.22	4 (1%) 66 63	24, 41, 75, 88	0
1	I	121/227 (53%)	0.21	4 (3%) 49 44	29, 45, 63, 83	0
1	M	210/227 (92%)	0.32	12 (5%) 29 25	26, 43, 73, 87	0
1	Q	125/227 (55%)	0.30	6 (4%) 35 31	29, 48, 68, 85	0
1	U	178/227 (78%)	0.80	25 (14%) 6 5	34, 52, 93, 109	0
1	Y	121/227 (53%)	0.90	12 (9%) 13 10	34, 56, 77, 89	0
1	c	98/227 (43%)	2.47	61 (62%) 0 0	83, 102, 112, 124	0
2	B	213/218 (97%)	0.48	15 (7%) 22 19	26, 49, 95, 103	1 (0%)
2	F	213/218 (97%)	0.21	4 (1%) 66 63	26, 47, 74, 95	1 (0%)
2	J	110/218 (50%)	0.75	9 (8%) 17 14	43, 58, 75, 83	0
2	N	213/218 (97%)	0.31	7 (3%) 49 44	26, 46, 73, 99	1 (0%)
2	R	110/218 (50%)	0.83	9 (8%) 17 14	45, 61, 84, 145	0
2	V	200/218 (91%)	1.03	46 (23%) 2 1	29, 58, 117, 131	0
2	Z	108/218 (49%)	1.65	31 (28%) 1 1	60, 82, 98, 107	0
2	d	81/218 (37%)	2.46	47 (58%) 0 0	81, 104, 116, 119	0
3	C	214/214 (100%)	0.31	8 (3%) 45 40	27, 48, 70, 105	0
3	G	214/214 (100%)	0.25	1 (0%) 87 86	29, 49, 70, 91	0
3	K	212/214 (99%)	0.27	6 (2%) 55 51	27, 49, 67, 79	0
3	O	214/214 (100%)	0.57	13 (6%) 27 23	29, 50, 81, 102	0
3	S	214/214 (100%)	0.64	14 (6%) 25 21	35, 57, 78, 110	0
3	W	200/214 (93%)	1.33	45 (22%) 2 1	36, 66, 98, 109	0
3	a	214/214 (100%)	0.77	16 (7%) 20 17	33, 61, 89, 110	0
3	e	214/214 (100%)	1.17	37 (17%) 4 3	49, 73, 92, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
4	D	220/226 (97%)	0.39	19 (8%)	16	13	27, 43, 87, 141	5 (2%)
4	H	219/226 (96%)	0.35	18 (8%)	17	14	26, 43, 88, 137	0
4	L	217/226 (96%)	0.64	19 (8%)	15	13	29, 47, 82, 180	1 (0%)
4	P	216/226 (95%)	0.40	12 (5%)	30	26	26, 43, 79, 141	2 (0%)
4	T	213/226 (94%)	0.52	17 (7%)	18	15	29, 43, 76, 174	1 (0%)
4	X	215/226 (95%)	0.92	29 (13%)	7	6	29, 51, 101, 187	0
4	b	217/226 (96%)	0.61	21 (9%)	13	11	30, 45, 77, 171	2 (0%)
4	f	215/226 (95%)	1.27	32 (14%)	5	4	46, 70, 104, 155	5 (2%)
All	All	5938/7080 (83%)	0.67	621 (10%)	11	9	24, 52, 97, 187	19 (0%)

All (621) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	X	100(B)	GLY	10.1
4	L	100(C)	PRO	9.9
4	b	52(A)	SER	9.4
4	f	100(B)	GLY	9.1
4	b	100(D)	PHE	8.6
4	L	52(A)	SER	8.4
4	H	82(C)	LEU	8.4
4	L	100(D)	PHE	8.3
4	L	82(B)	SER	8.2
4	b	82(B)	SER	8.2
4	T	100(C)	PRO	8.2
4	f	82(A)	SER	8.0
4	b	100(A)	ASP	8.0
4	X	100(A)	ASP	7.8
4	L	100(B)	GLY	7.5
4	X	100(C)	PRO	7.4
4	P	82(B)	SER	7.4
4	D	52(A)	SER	7.4
4	T	82(B)	SER	7.4
4	b	82(A)	SER	7.4
4	D	100(B)	GLY	7.3
4	f	100(D)	PHE	7.3
2	F	106(A)	LEU	6.9
3	W	194	CYS	6.9
2	B	106(A)	LEU	6.8
4	T	52(A)	SER	6.7

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Mol	Chain	Res	Type	RSRZ
4	D	100(C)	PRO	6.7
4	X	100(D)	PHE	6.7
4	D	100(D)	PHE	6.6
4	P	100(C)	PRO	6.4
4	L	82(A)	SER	6.4
4	f	100(C)	PRO	6.3
4	H	52(A)	SER	6.2
1	c	29	PHE	6.2
2	V	106(A)	LEU	6.2
4	T	100(D)	PHE	6.1
4	P	52(A)	SER	6.1
4	L	82(C)	LEU	6.0
4	f	82(B)	SER	5.9
2	d	33	VAL	5.8
4	H	100(D)	PHE	5.7
2	Z	95(C)	PHE	5.6
4	T	100(A)	ASP	5.6
4	X	82(C)	LEU	5.6
4	X	82(B)	SER	5.6
4	P	100(A)	ASP	5.5
4	b	100(C)	PRO	5.4
3	W	177	SER	5.4
4	X	130	SER	5.3
4	P	82(C)	LEU	5.3
1	c	98	CYS	5.2
2	Z	77	GLY	5.2
2	N	106(A)	LEU	5.0
2	Z	106	VAL	5.0
4	L	100(A)	ASP	5.0
4	T	82(A)	SER	5.0
4	f	52(A)	SER	5.0
2	d	71	ALA	5.0
4	T	82(C)	LEU	4.9
2	R	14	ALA	4.9
1	I	100(A)	GLY	4.9
2	R	106(A)	LEU	4.9
3	W	144	ALA	4.9
4	H	82(A)	SER	4.8
1	M	100(A)	GLY	4.8
4	T	100(B)	GLY	4.8
4	f	98	LEU	4.8
2	d	75	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
4	P	82(A)	SER	4.8
2	d	96	TYR	4.7
2	d	86	TYR	4.7
2	d	91	TYR	4.7
2	R	95(A)	SER	4.6
1	U	181	VAL	4.6
2	d	47	LEU	4.6
4	f	100(A)	ASP	4.5
4	X	52(A)	SER	4.5
1	c	109	VAL	4.5
1	c	102	TYR	4.5
2	d	36	TYR	4.4
4	f	82(C)	LEU	4.4
3	e	51	ALA	4.4
1	I	100	GLY	4.4
1	M	170	LEU	4.4
1	c	58	TYR	4.4
4	T	101	ASP	4.3
3	O	154	LEU	4.3
1	c	106	GLY	4.3
4	H	100(B)	GLY	4.3
3	K	212	GLY	4.3
1	c	110	THR	4.3
2	d	78	LEU	4.3
4	D	100(A)	ASP	4.3
1	Q	116	THR	4.2
3	W	148	TRP	4.2
4	X	137	ALA	4.2
1	Q	100(A)	GLY	4.2
3	e	55	ILE	4.2
1	c	45	LEU	4.2
4	H	82(B)	SER	4.1
2	V	208	PRO	4.1
4	H	100(A)	ASP	4.1
2	V	149	LYS	4.1
4	b	131	THR	4.1
1	Y	100	GLY	4.0
2	d	59	PRO	4.0
3	W	134	CYS	4.0
3	W	200	GLY	4.0
1	c	103	TRP	4.0
4	f	128	SER	3.9

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Mol	Chain	Res	Type	RSRZ
4	f	29	PHE	3.9
2	V	131	THR	3.9
2	V	207	ALA	3.9
3	W	205	VAL	3.9
3	e	78	VAL	3.9
4	X	213	PRO	3.9
2	d	44	PRO	3.8
2	V	202	VAL	3.8
2	R	2	PRO	3.8
3	S	7	SER	3.8
4	P	128	SER	3.8
1	E	100(A)	GLY	3.8
4	P	100(B)	GLY	3.8
4	X	184	VAL	3.8
1	c	35	ASN	3.7
1	A	159	LEU	3.7
3	e	50	TYR	3.7
2	J	95(A)	SER	3.7
4	f	100	GLY	3.7
3	W	118	PHE	3.7
2	d	37	GLN	3.7
2	V	95	LEU	3.7
4	f	31	GLY	3.7
1	c	14	PRO	3.7
2	d	46	LEU	3.7
1	U	165	THR	3.7
3	W	132	VAL	3.7
2	Z	101	GLY	3.6
2	B	200	SER	3.6
4	D	82(B)	SER	3.6
4	X	126	PRO	3.6
4	H	101	ASP	3.6
2	d	35	TRP	3.6
1	M	135	THR	3.6
1	c	44	GLY	3.6
4	L	101	ASP	3.6
4	L	127	SER	3.6
1	Q	100	GLY	3.5
1	U	209	LYS	3.5
3	W	209	PHE	3.5
3	W	201	LEU	3.5
1	c	52(A)	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	Z	76	THR	3.5
2	B	119	PRO	3.5
1	A	99	SER	3.5
1	c	82	MET	3.5
3	W	184	ALA	3.5
4	X	138	LEU	3.5
2	Z	96	TYR	3.5
1	I	99	SER	3.5
2	V	116	THR	3.5
3	e	3	LEU	3.5
4	H	211	VAL	3.5
2	J	2	PRO	3.4
3	W	195	GLU	3.4
2	B	206	VAL	3.4
1	c	47	TRP	3.4
1	Y	28	THR	3.4
1	c	75	LYS	3.4
1	A	100	GLY	3.4
2	Z	95(B)	GLY	3.4
1	c	27	PHE	3.4
3	W	196	VAL	3.4
2	Z	24	THR	3.4
4	H	131	THR	3.4
1	U	112	SER	3.4
3	W	197	THR	3.4
3	W	204	PRO	3.4
2	Z	95	LEU	3.4
2	d	80	ALA	3.4
3	W	207	LYS	3.3
1	M	210	ARG	3.3
1	c	95	LEU	3.3
3	W	179	LEU	3.3
1	c	93	ALA	3.3
2	V	130	ALA	3.3
1	c	57	ILE	3.3
1	U	210	ARG	3.3
3	e	29	ILE	3.3
1	c	20	LEU	3.3
1	A	100(A)	GLY	3.3
1	c	15	GLY	3.3
4	D	133	GLY	3.3
2	d	97	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	U	113	SER	3.3
1	Y	112	SER	3.3
4	D	132	SER	3.3
1	Y	100(A)	GLY	3.3
2	d	101	GLY	3.3
3	W	133	VAL	3.3
1	A	126	PRO	3.2
2	d	42	THR	3.2
4	D	130	SER	3.2
4	b	132	SER	3.2
1	c	48	VAL	3.2
3	K	152	ASN	3.2
2	V	178	LEU	3.2
1	Q	100(B)	SER	3.2
1	Y	99	SER	3.2
3	S	154	LEU	3.2
3	W	206	THR	3.2
4	X	131	THR	3.2
2	d	99	GLY	3.2
2	V	127	ALA	3.2
4	X	132	SER	3.2
2	R	95(C)	PHE	3.2
4	f	199	ASN	3.2
4	f	53	GLY	3.2
1	c	111	VAL	3.2
4	f	2	VAL	3.2
2	J	95	LEU	3.1
1	U	123	PRO	3.1
4	H	126	PRO	3.1
4	X	134	GLY	3.1
4	X	125	ALA	3.1
1	U	120	SER	3.1
3	W	202	SER	3.1
2	B	156	LYS	3.1
4	D	129	LYS	3.1
1	c	28	THR	3.1
2	d	68	GLY	3.1
4	P	127	SER	3.1
4	X	82(A)	SER	3.1
3	W	186	TYR	3.1
4	H	213	PRO	3.1
4	b	158	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	c	54	SER	3.1
3	W	110	VAL	3.1
4	D	82(C)	LEU	3.1
3	W	155	GLN	3.1
4	b	100(B)	GLY	3.1
3	e	25	ALA	3.1
1	c	100(C)	CYS	3.1
2	V	206	VAL	3.1
2	d	27(C)	ILE	3.0
1	c	12	VAL	3.0
2	V	95(A)	SER	3.0
1	c	32	TYR	3.0
2	V	182	PRO	3.0
2	d	40	PRO	3.0
3	O	24	ARG	3.0
1	c	84	ALA	3.0
2	d	43	ALA	3.0
2	J	95(C)	PHE	3.0
3	O	214	CYS	3.0
4	b	127	SER	3.0
2	Z	17	GLN	3.0
1	c	96	GLY	3.0
3	W	157	GLY	3.0
3	e	48	ILE	3.0
1	c	2	VAL	3.0
2	V	179	SER	3.0
4	f	155	ASN	3.0
2	d	98	PHE	3.0
3	K	7	SER	2.9
3	e	114	SER	2.9
1	c	3	GLN	2.9
3	e	106	ILE	2.9
3	a	51	ALA	2.9
3	O	190	LYS	2.9
2	d	55	PRO	2.9
4	X	135	THR	2.9
4	D	127	SER	2.9
2	Z	91	TYR	2.9
2	d	64	GLY	2.9
3	e	109	THR	2.9
2	Z	3	VAL	2.9
1	M	212	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	Z	95(A)	SER	2.9
3	C	7	SER	2.9
2	V	136	ILE	2.9
4	D	101	ASP	2.9
4	T	74	TYR	2.9
2	d	3	VAL	2.9
1	c	50	SER	2.8
1	c	80	LEU	2.8
3	W	198	HIS	2.8
1	c	51	ILE	2.8
1	c	69	ILE	2.8
1	c	82(B)	SER	2.8
1	U	100(A)	GLY	2.8
2	V	95(B)	GLY	2.8
2	V	158	GLY	2.8
4	X	101	ASP	2.8
4	X	139	GLY	2.8
3	W	178	THR	2.8
3	a	205	VAL	2.8
3	W	119	PRO	2.8
1	A	115	SER	2.8
1	Q	99	SER	2.8
2	d	94	SER	2.8
3	a	12	SER	2.8
3	e	54	SER	2.8
4	H	127	SER	2.8
2	V	117	LEU	2.8
4	T	52	LEU	2.8
3	K	188	LYS	2.8
2	J	48	ILE	2.8
1	c	100(B)	SER	2.8
1	U	139	GLY	2.8
1	U	142	VAL	2.8
1	c	85	GLU	2.8
2	d	19	VAL	2.8
1	E	127	SER	2.7
4	D	128	SER	2.7
1	A	125	ALA	2.7
2	B	205	THR	2.7
2	J	106	VAL	2.7
3	e	13	VAL	2.7
4	X	160	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	b	101	ASP	2.7
2	B	2	PRO	2.7
1	U	196	CYS	2.7
1	E	99	SER	2.7
2	d	29	ALA	2.7
1	A	122	PHE	2.7
1	Y	89	VAL	2.7
2	d	58	VAL	2.7
4	P	135	THR	2.7
3	C	204	PRO	2.7
4	f	147	PRO	2.7
2	R	95(B)	GLY	2.7
2	V	200	SER	2.7
1	U	121	VAL	2.7
1	c	67	PHE	2.7
2	Z	2	PRO	2.7
1	c	105	GLN	2.7
1	Q	115	SER	2.7
3	e	91	SER	2.7
1	A	211	VAL	2.7
2	V	112	ALA	2.7
2	Z	14	ALA	2.7
2	Z	71	ALA	2.7
3	S	197	THR	2.7
3	a	153	ALA	2.7
4	b	2	VAL	2.7
2	d	24	THR	2.7
2	d	82	ASP	2.7
3	S	185	ASP	2.7
1	A	140	CYS	2.6
1	c	4	LEU	2.6
2	N	95	LEU	2.6
3	O	211	ARG	2.6
4	L	212	GLU	2.6
2	V	187	SER	2.6
2	N	2	PRO	2.6
2	Z	15	PRO	2.6
2	d	48	ILE	2.6
1	M	100	GLY	2.6
2	V	199	GLY	2.6
1	U	166	PHE	2.6
3	S	194	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	V	2	PRO	2.6
2	V	173	ALA	2.6
2	Z	11	VAL	2.6
2	Z	62	PHE	2.6
3	W	176	SER	2.6
3	W	29	ILE	2.6
2	V	125	LEU	2.6
2	V	129	LYS	2.6
3	W	112	ALA	2.6
4	P	100(D)	PHE	2.6
1	c	70	SER	2.5
4	f	127	SER	2.5
2	d	31	TYR	2.5
1	E	100	GLY	2.5
2	B	155	VAL	2.5
2	V	181	THR	2.5
2	V	192	SER	2.5
4	H	132	SER	2.5
2	Z	47	LEU	2.5
2	d	4	LEU	2.5
4	b	82(C)	LEU	2.5
2	J	91	TYR	2.5
2	Z	25	GLY	2.5
3	O	212	GLY	2.5
4	L	213	PRO	2.5
1	c	88	ALA	2.5
2	V	168	SER	2.5
2	d	87	TYR	2.5
2	F	199	GLY	2.5
1	c	41	PRO	2.5
2	V	195	VAL	2.5
2	Z	19	VAL	2.5
4	X	136	ALA	2.5
4	P	83	THR	2.5
2	B	125	LEU	2.5
3	W	142	ARG	2.5
3	e	201	LEU	2.5
3	a	50	TYR	2.5
4	f	111	VAL	2.5
3	W	117	ILE	2.4
3	e	46	LEU	2.4
1	Y	100(B)	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	95(A)	SER	2.4
3	e	203	SER	2.4
2	V	123	GLU	2.4
1	A	163	VAL	2.4
2	V	95(C)	PHE	2.4
2	V	111	ALA	2.4
2	d	62	PHE	2.4
3	e	5	THR	2.4
3	W	136	LEU	2.4
1	U	180	SER	2.4
2	N	95(A)	SER	2.4
3	C	65	SER	2.4
1	c	36	TRP	2.4
3	e	170	ASP	2.4
1	M	213	PRO	2.4
2	B	182	PRO	2.4
2	N	95(B)	GLY	2.4
4	T	100	GLY	2.4
1	A	198	VAL	2.4
1	U	150	VAL	2.4
1	c	78	LEU	2.4
1	c	87	THR	2.4
4	D	199	ASN	2.4
1	c	49	SER	2.4
3	e	80	SER	2.4
2	R	81	GLU	2.4
3	S	214	CYS	2.4
4	H	100(C)	PRO	2.4
1	U	151	THR	2.4
4	X	56	THR	2.4
4	f	108	THR	2.4
2	V	188	HIS	2.4
1	M	127	SER	2.4
3	a	7	SER	2.4
1	A	184	VAL	2.4
3	K	191	VAL	2.4
3	e	24	ARG	2.4
4	f	182	VAL	2.4
1	c	23	ALA	2.4
3	a	112	ALA	2.4
1	c	91	TYR	2.3
1	A	183	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	197	ASN	2.3
4	L	204	ASN	2.3
2	N	166	LYS	2.3
3	W	156	SER	2.3
4	X	53	GLY	2.3
4	X	181	VAL	2.3
2	B	157	ALA	2.3
3	O	184	ALA	2.3
4	L	71	ALA	2.3
1	A	151	THR	2.3
3	W	123	GLU	2.3
1	A	147	PRO	2.3
2	Z	99	GLY	2.3
3	S	212	GLY	2.3
1	Y	93	ALA	2.3
2	d	73	LEU	2.3
3	e	83	ILE	2.3
1	c	56	TYR	2.3
4	T	191	THR	2.3
1	U	197	ASN	2.3
1	Y	96	GLY	2.3
2	V	16	GLY	2.3
4	D	53	GLY	2.3
4	b	190	GLY	2.3
3	S	191	VAL	2.3
3	e	73	LEU	2.3
3	e	96	PHE	2.3
4	f	159	LEU	2.3
3	e	112	ALA	2.3
2	Z	42	THR	2.3
2	Z	105	THR	2.3
2	d	45	LYS	2.3
4	f	99	TYR	2.3
3	G	213	GLU	2.3
4	f	61	GLU	2.3
1	I	112	SER	2.3
1	U	100(B)	SER	2.3
2	J	60	ASP	2.3
2	V	119	PRO	2.3
4	H	128	SER	2.3
4	b	213	PRO	2.3
4	f	112	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	V	126	GLN	2.3
2	N	199	GLY	2.3
2	d	28	GLY	2.3
1	U	18	LEU	2.3
3	a	214	CYS	2.2
3	e	34	HIS	2.2
1	U	204	ASN	2.2
1	c	82(A)	ASN	2.2
3	O	28	ASN	2.2
3	e	41	ASN	2.2
2	Z	40	PRO	2.2
2	V	184	GLN	2.2
3	e	1	ASP	2.2
4	D	82(A)	SER	2.2
1	c	42	GLY	2.2
2	B	107	GLY	2.2
3	O	191	VAL	2.2
3	e	47	LEU	2.2
3	e	110	VAL	2.2
2	J	14	ALA	2.2
3	S	153	ALA	2.2
4	f	195	ILE	2.2
2	d	100	THR	2.2
3	a	109	THR	2.2
4	f	30	THR	2.2
2	R	91	TYR	2.2
2	V	169	ASN	2.2
2	B	187	SER	2.2
2	d	57	GLY	2.2
3	C	203	SER	2.2
3	a	121	SER	2.2
4	f	161	SER	2.2
1	U	141	LEU	2.2
3	W	135	LEU	2.2
3	S	183	LYS	2.2
3	W	115	VAL	2.2
1	Y	100(E)	PHE	2.2
3	e	32	HIS	2.2
2	d	49	TYR	2.2
3	W	113	PRO	2.2
3	W	120	PRO	2.2
1	M	192	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	170	LEU	2.2
2	Z	16	GLY	2.2
2	Z	63	SER	2.2
2	Z	73	LEU	2.2
3	a	11	LEU	2.2
4	b	189	LEU	2.2
1	c	63	VAL	2.2
2	Z	69	THR	2.2
4	f	68	THR	2.2
1	c	94	ARG	2.2
3	C	8	PRO	2.2
4	T	192	GLN	2.2
2	B	199	GLY	2.2
4	L	100	GLY	2.2
4	X	124	LEU	2.2
1	A	112	SER	2.2
2	B	168	SER	2.2
3	C	197	THR	2.1
4	b	135	THR	2.1
1	c	92	CYS	2.1
1	Y	64	LYS	2.1
1	c	79	TYR	2.1
4	H	129	LYS	2.1
4	L	129	LYS	2.1
1	A	174	GLY	2.1
1	A	152	VAL	2.1
3	a	191	VAL	2.1
3	e	70	ASP	2.1
4	D	72	ASP	2.1
1	M	161	SER	2.1
4	b	188	SER	2.1
2	V	147	ALA	2.1
3	O	195	GLU	2.1
2	R	103	LYS	2.1
4	H	41	PRO	2.1
1	c	76	ASN	2.1
3	O	186	TYR	2.1
3	e	66	GLY	2.1
4	D	42	GLY	2.1
4	f	96	GLY	2.1
3	W	116	PHE	2.1
1	A	160	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	c	81	GLN	2.1
3	a	194	CYS	2.1
4	L	53	GLY	2.1
4	T	43	HIS	2.1
2	V	106	VAL	2.1
3	C	29	ILE	2.1
3	e	2	ILE	2.1
2	d	26	SER	2.1
3	W	203	SER	2.1
3	e	108	ARG	2.1
2	V	145	THR	2.1
4	b	191	THR	2.1
2	V	113	PRO	2.1
2	V	128	ASN	2.1
3	O	157	GLY	2.1
4	L	190	GLY	2.1
4	X	174	GLY	2.1
1	A	194	TYR	2.1
2	d	21	ILE	2.1
1	U	152	VAL	2.1
3	S	78	VAL	2.1
4	f	207	VAL	2.1
3	e	62	PHE	2.1
3	a	195	GLU	2.0
3	S	203	SER	2.0
2	V	163	THR	2.0
2	d	38	GLN	2.0
3	a	179	LEU	2.0
3	C	66	GLY	2.0
3	S	64	GLY	2.0
3	W	128	GLY	2.0
3	e	33	ILE	2.0
1	U	198	VAL	2.0
3	a	19	VAL	2.0
2	F	160	GLU	2.0
2	Z	45	LYS	2.0
3	S	126	LYS	2.0
3	W	190	LYS	2.0
3	K	100	SER	2.0
3	O	74	THR	2.0
4	T	193	THR	2.0
1	Y	11	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	W	199	GLN	2.0
4	L	189	LEU	2.0
4	T	189	LEU	2.0
4	X	65	GLY	2.0
4	b	134	GLY	2.0
1	M	198	VAL	2.0
1	U	12	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
4	PCA	b	1	8/9	0.50	0.33	20,20,20,20	0
4	PCA	T	1	8/9	0.56	0.30	20,20,20,20	0
4	PCA	L	1	8/9	0.67	0.26	20,20,20,20	0
2	PCA	F	1	8/9	0.68	0.27	20,20,20,20	0
2	PCA	V	1	8/9	0.71	0.36	20,20,20,20	0
2	PCA	N	1	8/9	0.79	0.32	20,20,20,20	0
4	PCA	P	1	8/9	0.85	0.23	20,20,20,20	0
4	PCA	H	1	8/9	0.88	0.22	20,20,20,20	0
4	PCA	X	1	8/9	0.89	0.19	20,20,20,20	0
4	PCA	D	1	8/9	0.90	0.16	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.