Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2022 – 12:24 am GMT

PDB ID	:	7PI3
Title	:	PfCyRPA bound to Fab fragments from monoclonal antibodies Cy.003, Cy.004 and Cy.007
Authors	:	Ragotte, R.J.; Higgins, M.K.
Deposited on	:	2021-08-19
Resolution	:	3.27 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:

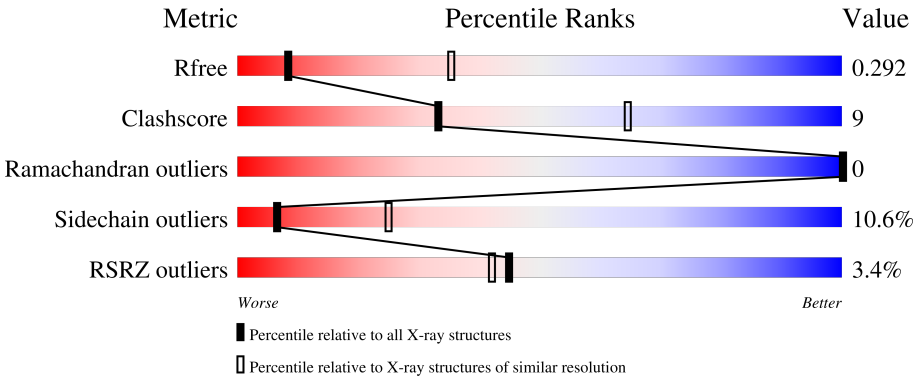
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	343	55% 36% 6%
1	H	343	60% 29% 6%
1	O	343	61% 32% 5%
1	V	343	60% 30% 5%
2	B	230	72% 23%

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Mol	Chain	Length	Quality of chain
2	I	230	2% 76% 18%
2	P	230	2% 80% 14%
2	W	230	3% 73% 20% 5%
3	C	210	% 77% 20%
3	J	210	2% 79% 19%
3	Q	210	5% 86% 12%
3	X	210	2% 72% 24%
4	D	230	4% 78% 15%
4	K	230	% 78% 16%
4	R	230	2% 76% 18%
4	Y	230	8% 79% 15%
5	E	209	% 85% 12%
5	L	209	3% 85% 11%
5	S	209	3% 84% 11%
5	Z	209	6% 83% 13%
6	F	321	% 60% 10% 31%
6	M	321	2% 56% 13% 31%
6	T	321	% 58% 10% 32%
6	a	321	% 64% 32%
7	G	209	% 87% 12%
7	N	209	4% 88% 11%
7	U	209	3% 85% 14%
7	b	209	3% 89% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 48847 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2730	1755	439	523	13			
1	H	321	Total	C	N	O	S	0	0	0
			2675	1723	429	510	13			
1	O	327	Total	C	N	O	S	0	0	0
			2722	1751	438	520	13			
1	V	325	Total	C	N	O	S	0	0	0
			2705	1741	435	516	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
H	147	ALA	SER	conflict	UNP Q8IFM8
H	324	ALA	THR	conflict	UNP Q8IFM8
H	340	ALA	THR	conflict	UNP Q8IFM8
H	363	GLY	-	expression tag	UNP Q8IFM8
H	364	GLY	-	expression tag	UNP Q8IFM8
H	365	GLY	-	expression tag	UNP Q8IFM8
H	366	GLY	-	expression tag	UNP Q8IFM8
H	367	SER	-	expression tag	UNP Q8IFM8
H	368	GLU	-	expression tag	UNP Q8IFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	369	PRO	-	expression tag	UNP Q8IFM8
H	370	GLU	-	expression tag	UNP Q8IFM8
H	371	ALA	-	expression tag	UNP Q8IFM8
O	147	ALA	SER	conflict	UNP Q8IFM8
O	324	ALA	THR	conflict	UNP Q8IFM8
O	340	ALA	THR	conflict	UNP Q8IFM8
O	363	GLY	-	expression tag	UNP Q8IFM8
O	364	GLY	-	expression tag	UNP Q8IFM8
O	365	GLY	-	expression tag	UNP Q8IFM8
O	366	GLY	-	expression tag	UNP Q8IFM8
O	367	SER	-	expression tag	UNP Q8IFM8
O	368	GLU	-	expression tag	UNP Q8IFM8
O	369	PRO	-	expression tag	UNP Q8IFM8
O	370	GLU	-	expression tag	UNP Q8IFM8
O	371	ALA	-	expression tag	UNP Q8IFM8
V	147	ALA	SER	conflict	UNP Q8IFM8
V	324	ALA	THR	conflict	UNP Q8IFM8
V	340	ALA	THR	conflict	UNP Q8IFM8
V	363	GLY	-	expression tag	UNP Q8IFM8
V	364	GLY	-	expression tag	UNP Q8IFM8
V	365	GLY	-	expression tag	UNP Q8IFM8
V	366	GLY	-	expression tag	UNP Q8IFM8
V	367	SER	-	expression tag	UNP Q8IFM8
V	368	GLU	-	expression tag	UNP Q8IFM8
V	369	PRO	-	expression tag	UNP Q8IFM8
V	370	GLU	-	expression tag	UNP Q8IFM8
V	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.003 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1611	1009	276	319	7			
2	I	221	Total	C	N	O	S	132	0	0
			1611	1009	276	319	7			
2	P	221	Total	C	N	O	S	442	0	0
			1611	1009	276	319	7			
2	W	218	Total	C	N	O	S	0	0	0
			1597	1002	273	315	7			

- Molecule 3 is a protein called Monoclonal antibody Cy.003 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1552	963	263	322	4			
3	J	207	Total	C	N	O	S	102	0	0
			1552	963	263	322	4			
3	Q	207	Total	C	N	O	S	580	0	0
			1552	963	263	322	4			
3	X	206	Total	C	N	O	S	0	0	0
			1547	960	262	321	4			

- Molecule 4 is a protein called Monoclonal antibody Cy.007 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			
4	K	220	Total	C	N	O	S	690	0	0
			1614	1010	271	326	7			
4	R	221	Total	C	N	O	S	690	0	0
			1619	1013	272	327	7			
4	Y	221	Total	C	N	O	S	621	0	0
			1619	1013	272	327	7			

- Molecule 5 is a protein called Monoclonal antibody Cy.007 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	204	Total	C	N	O	S	777	0	0
			1541	957	262	318	4			
5	L	203	Total	C	N	O	S	777	0	0
			1536	954	261	317	4			
5	S	200	Total	C	N	O	S	796	0	0
			1517	942	258	313	4			
5	Z	203	Total	C	N	O	S	777	0	0
			1537	955	261	317	4			

- Molecule 6 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	223	Total	C	N	O	S	685	0	0
			1634	1023	277	329	5			
6	M	223	Total	C	N	O	S	493	0	0
			1634	1023	277	329	5			
6	T	218	Total	C	N	O	S	533	0	0
			1603	1005	271	322	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	a	219	Total	C	N	O	S	660	0	0
			1604	1004	272	323	5			

- Molecule 7 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	209	Total	C	N	O	S	834	0	0
			1577	978	265	329	5			
7	N	209	Total	C	N	O	S	30	0	0
			1577	978	265	329	5			
7	U	208	Total	C	N	O	S	359	0	0
			1572	975	264	328	5			
7	b	208	Total	C	N	O	S	535	0	0
			1571	975	264	328	4			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

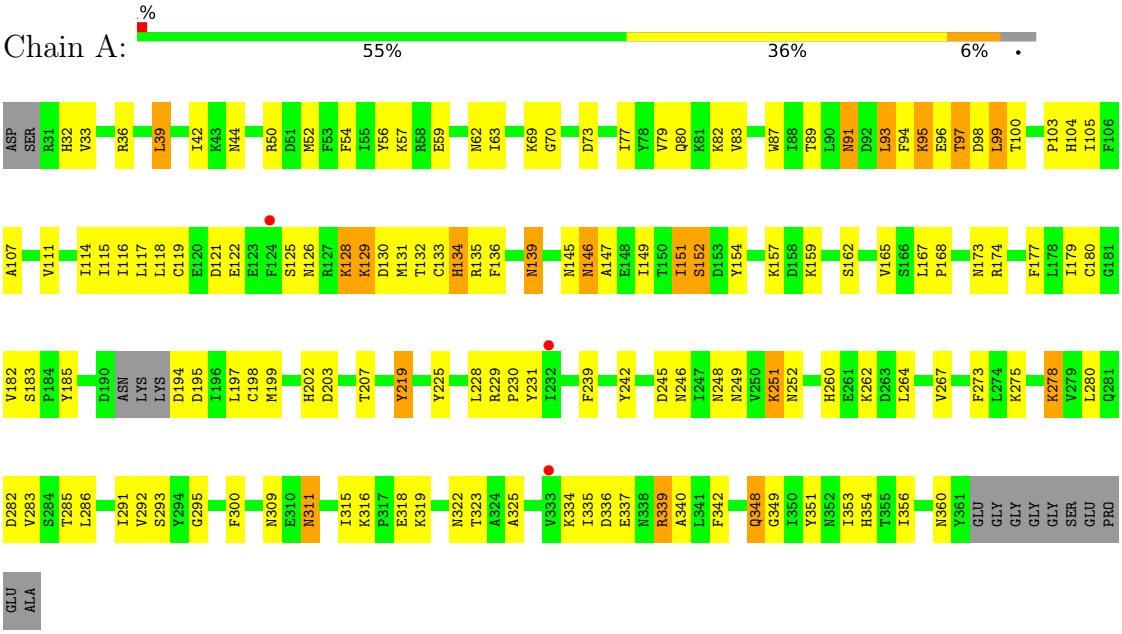
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	2	Total	Ca	2	0
			2	2		
8	H	1	Total	Ca	1	0
			1	1		
8	M	1	Total	Ca	1	0
			1	1		
8	T	2	Total	Ca	2	0
			2	2		
8	a	2	Total	Ca	2	0
			2	2		

3 Residue-property plots (i)

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

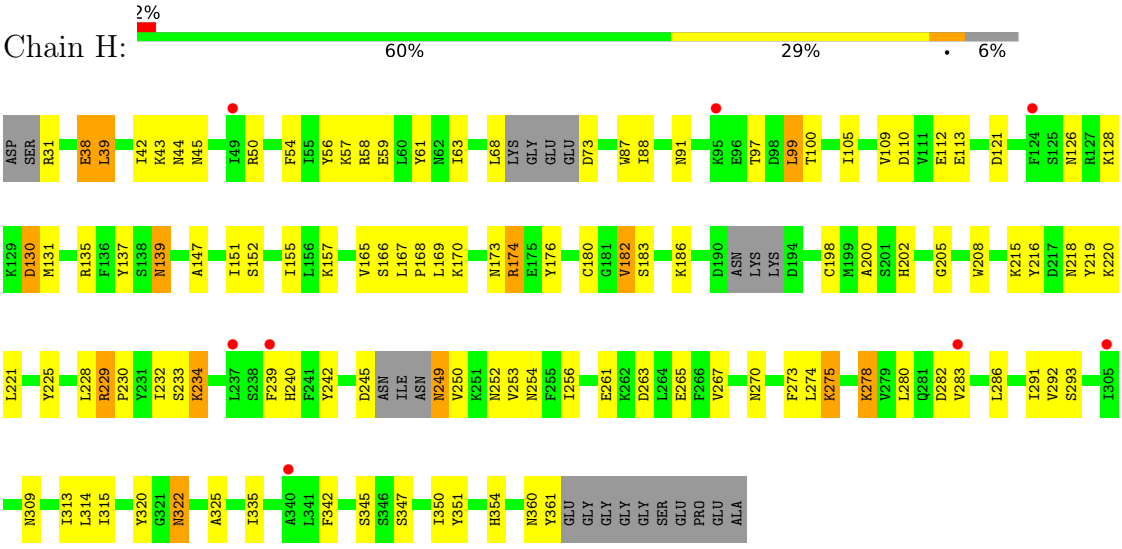
• Molecule 1: Cysteine-rich protective antigen

Chain A:



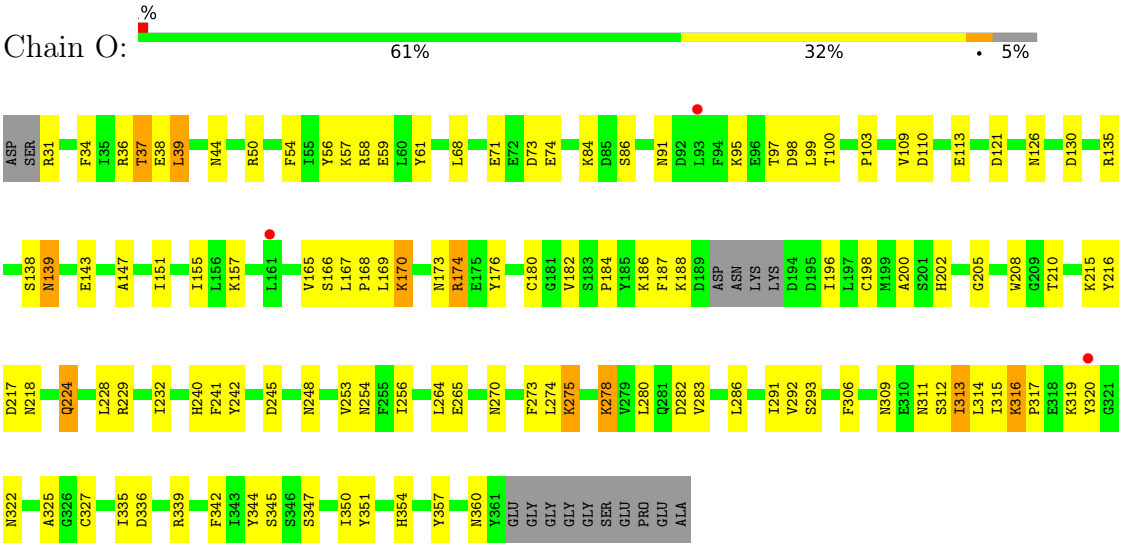
• Molecule 1: Cysteine-rich protective antigen

Chain H:



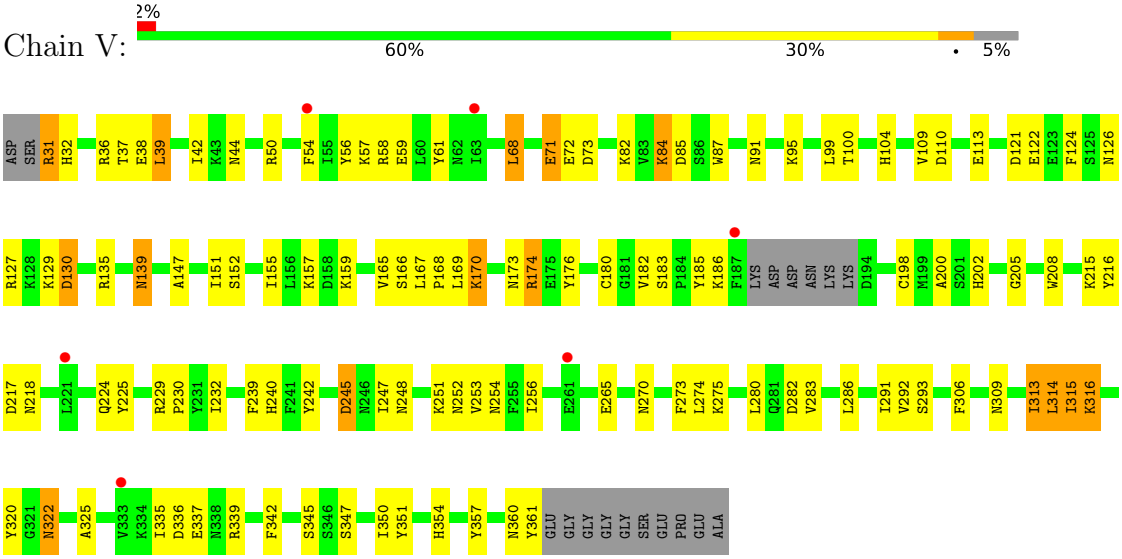
• Molecule 1: Cysteine-rich protective antigen

Chain O:



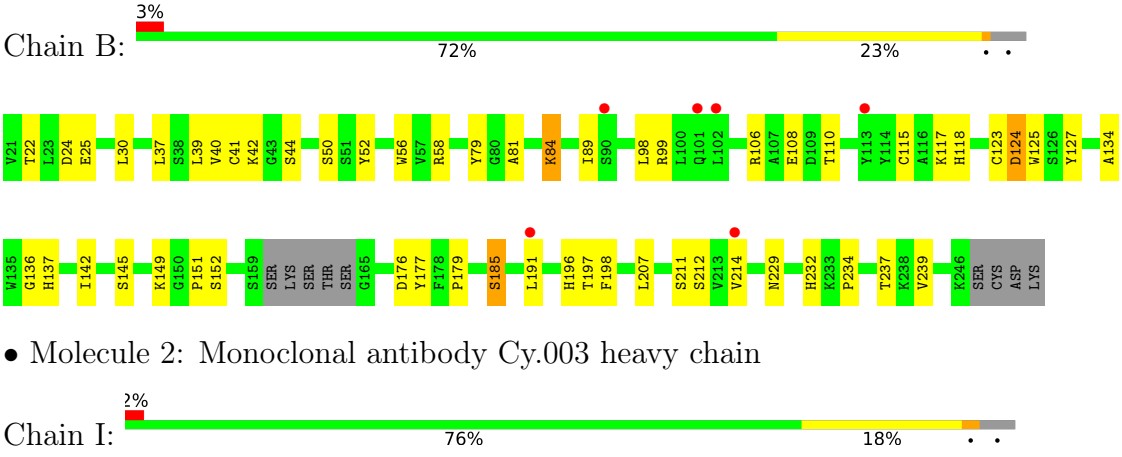
• Molecule 1: Cysteine-rich protective antigen

Chain V:



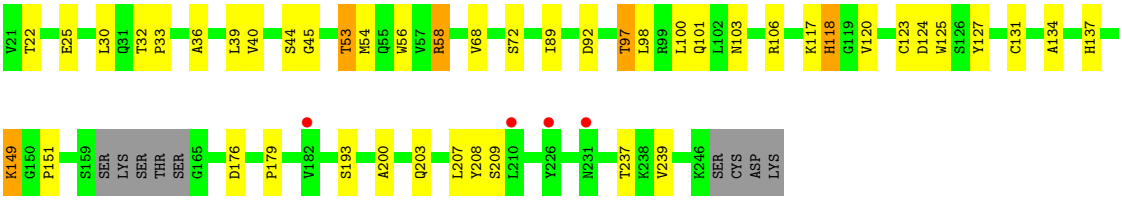
• Molecule 2: Monoclonal antibody Cy.003 heavy chain

Chain B:

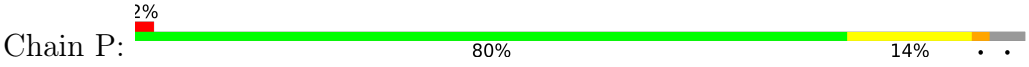


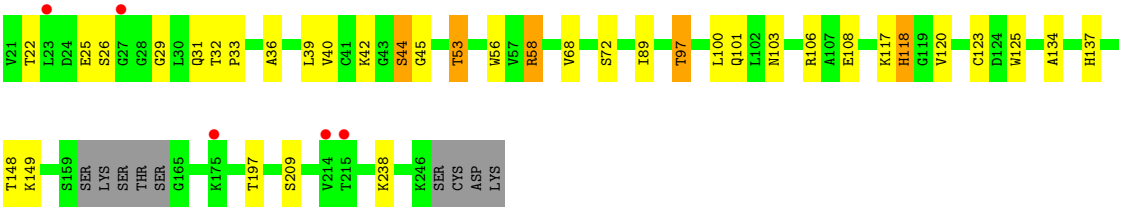
• Molecule 2: Monoclonal antibody Cy.003 heavy chain

Chain I:

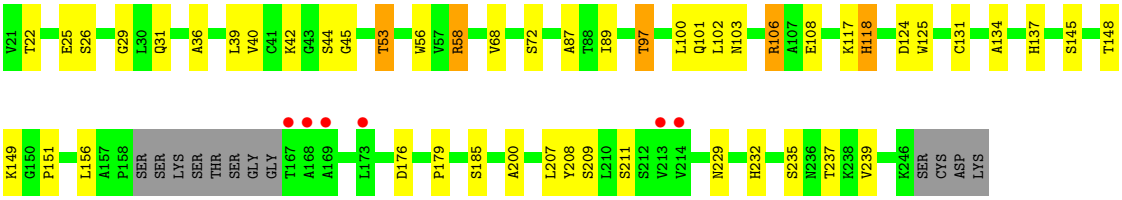


• Molecule 2: Monoclonal antibody Cy.003 heavy chain

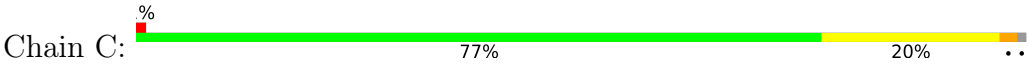


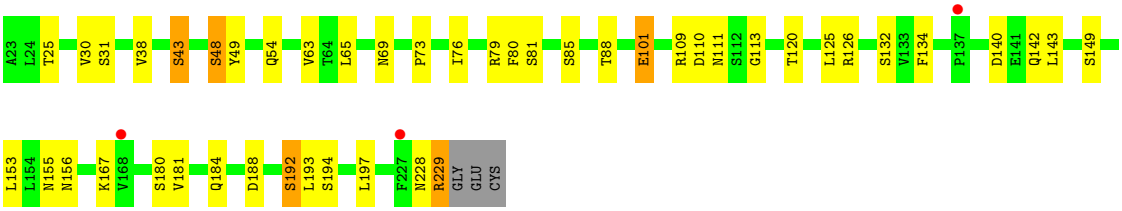


• Molecule 2: Monoclonal antibody Cy.003 heavy chain

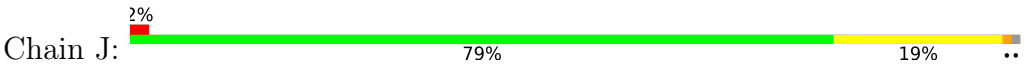


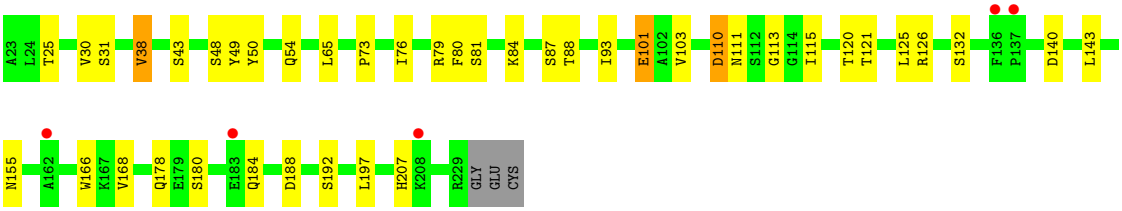
• Molecule 3: Monoclonal antibody Cy.003 light chain





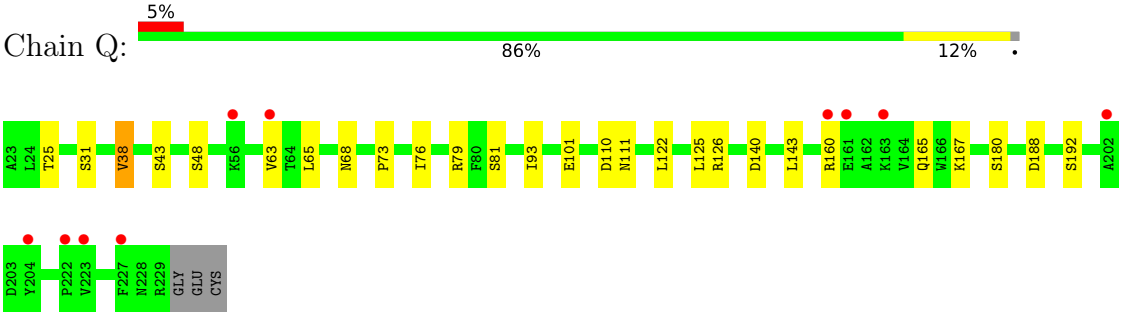
• Molecule 3: Monoclonal antibody Cy.003 light chain





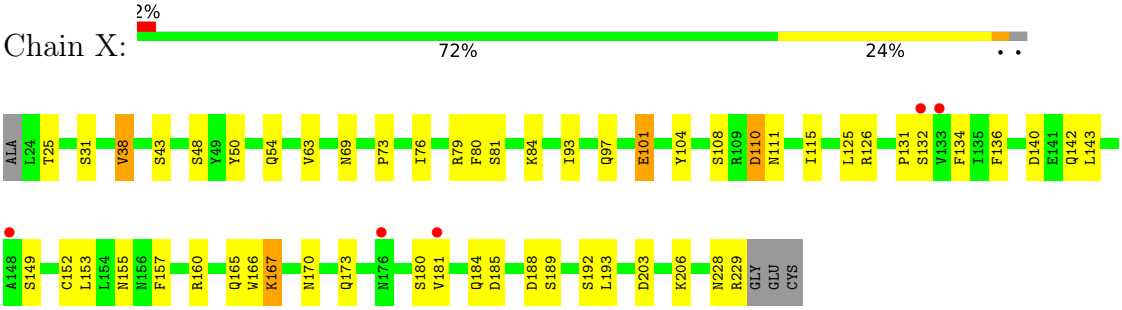
• Molecule 3: Monoclonal antibody Cy.003 light chain

Chain Q:



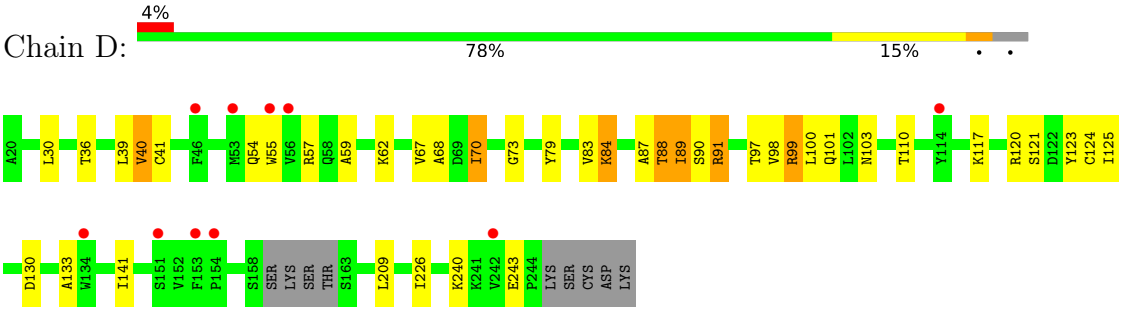
• Molecule 3: Monoclonal antibody Cy.003 light chain

Chain X:



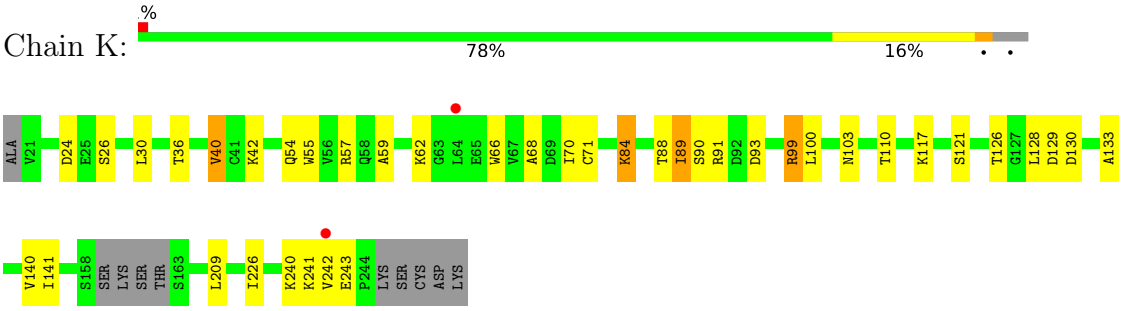
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

Chain D:



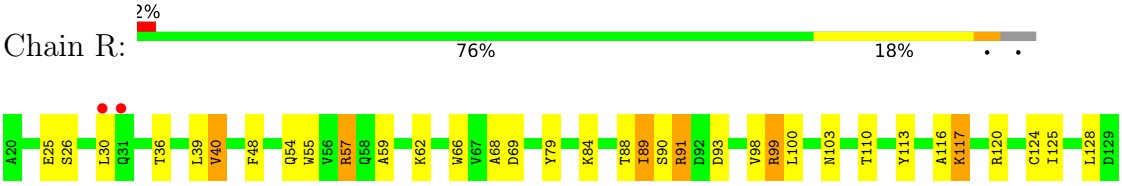
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

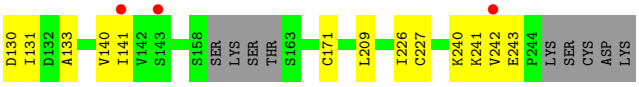
Chain K:



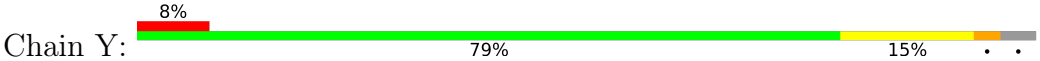
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

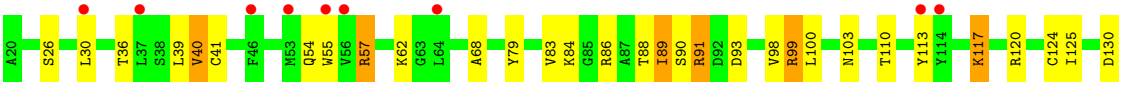
Chain R:

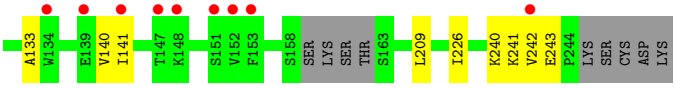




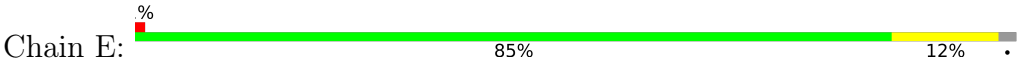
• Molecule 4: Monoclonal antibody Cy.007 heavy chain

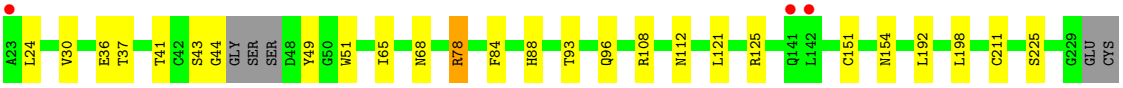




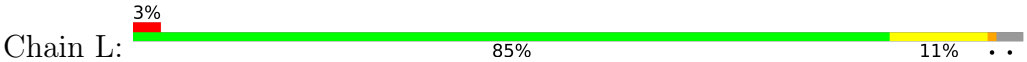


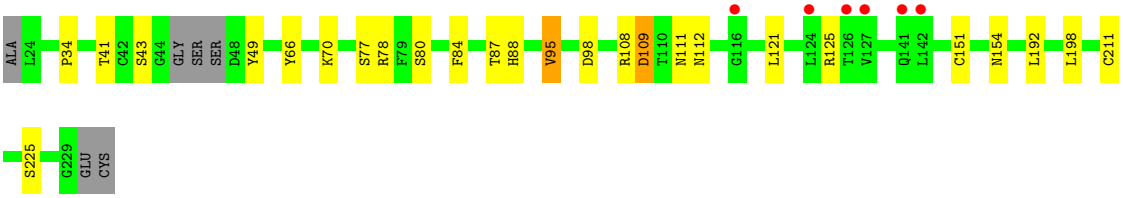
• Molecule 5: Monoclonal antibody Cy.007 light chain



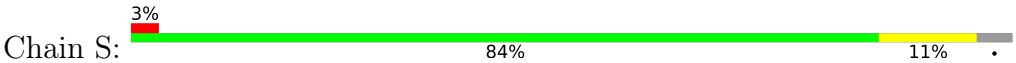


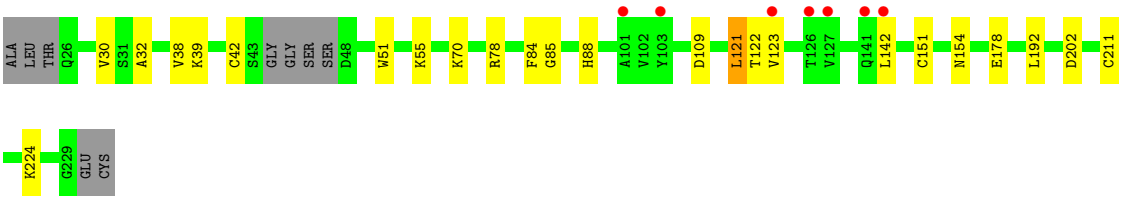
• Molecule 5: Monoclonal antibody Cy.007 light chain



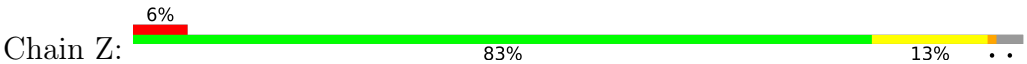


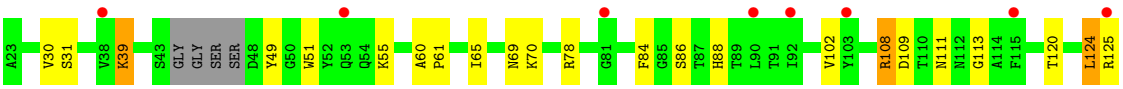
• Molecule 5: Monoclonal antibody Cy.007 light chain





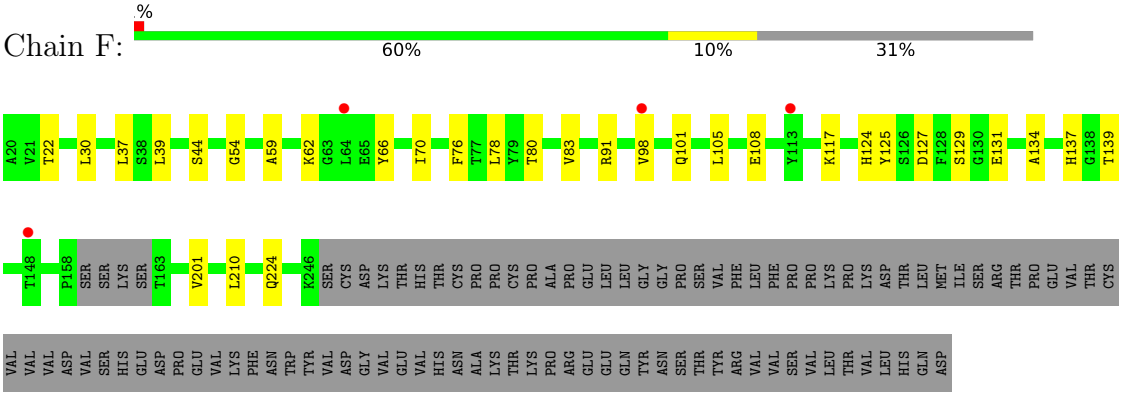
• Molecule 5: Monoclonal antibody Cy.007 light chain





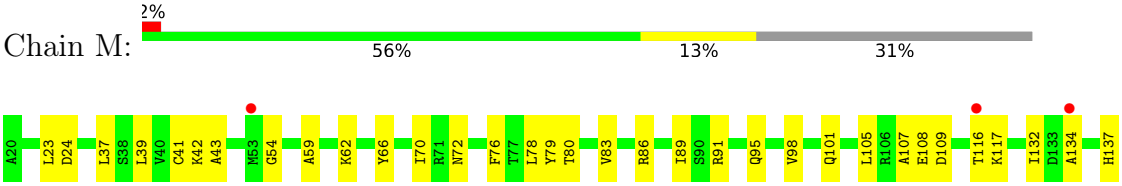
• Molecule 6: Monoclonal antibody Cy.004 heavy chain

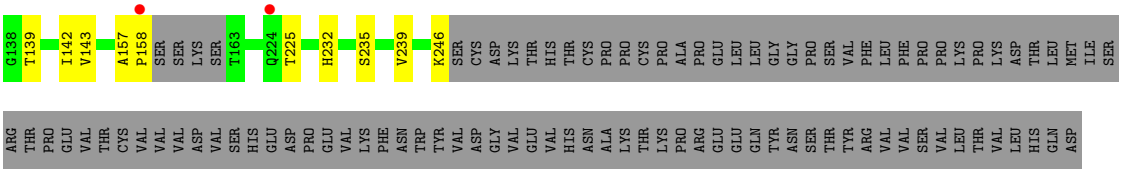
Chain F:



• Molecule 6: Monoclonal antibody Cy.004 heavy chain

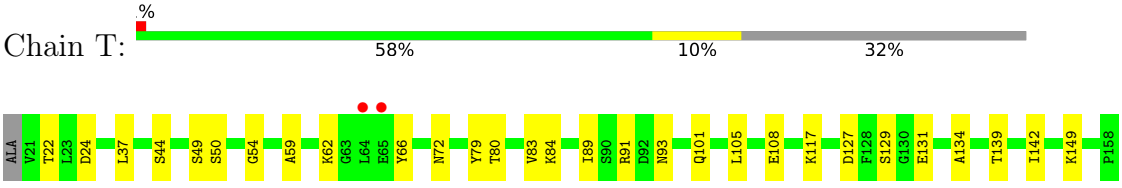
Chain M:

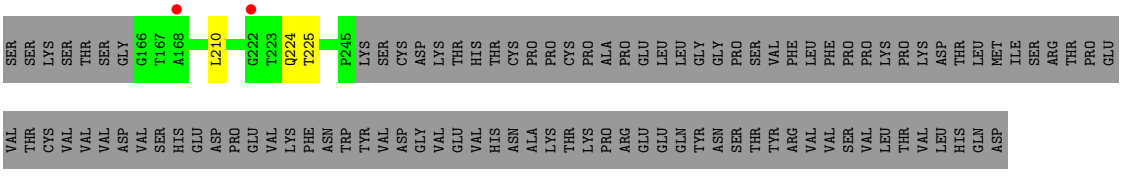




• Molecule 6: Monoclonal antibody Cy.004 heavy chain

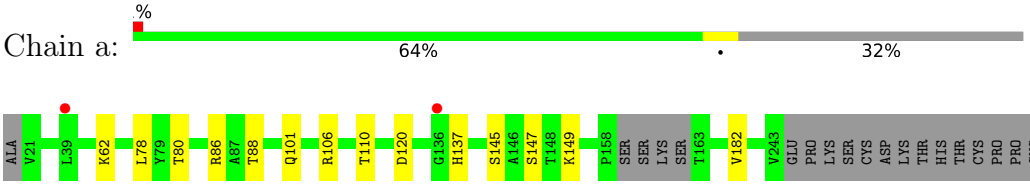
Chain T:





• Molecule 6: Monoclonal antibody Cy.004 heavy chain

Chain a:

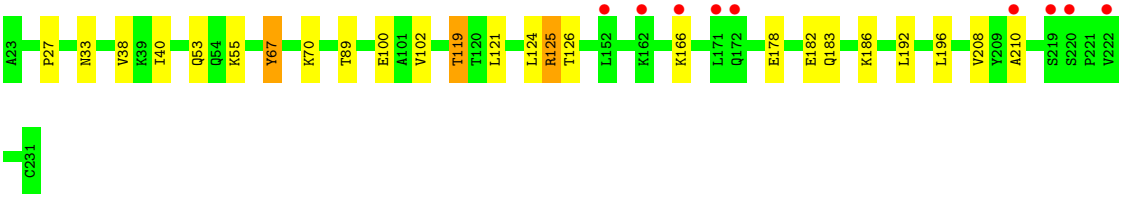


• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain G:

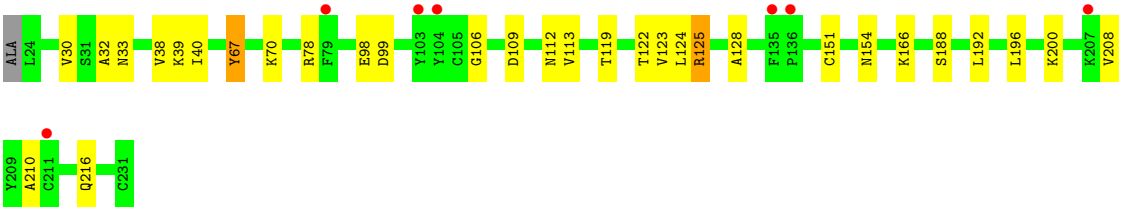
• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain N:



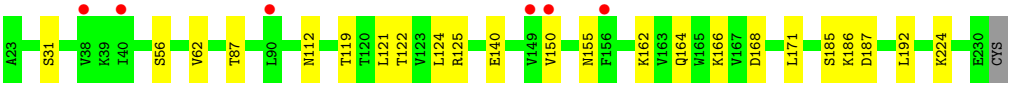
• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain U:



• Molecule 7: Monoclonal antibody Cy.004 light chain

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	164.84Å 164.84Å 382.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 3.27 47.64 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.64-3.27) 99.9 (47.64-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.285 , 0.298 0.280 , 0.292	Depositor DCC
R_{free} test set	7806 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	113.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	48847	wwPDB-VP
Average B, all atoms (Å^2)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA

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	0.54	0/2793	0.73	0/3772
1	H	0.37	0/2736	0.62	0/3693
1	O	0.37	0/2785	0.63	0/3761
1	V	0.35	0/2768	0.60	0/3739
2	B	0.35	0/1648	0.64	0/2243
2	I	0.29	0/1648	0.54	0/2243
2	P	0.28	0/1648	0.53	0/2243
2	W	0.31	0/1634	0.55	0/2225
3	C	0.32	0/1584	0.54	0/2153
3	J	0.30	0/1584	0.52	0/2153
3	Q	0.28	0/1584	0.51	0/2153
3	X	0.31	0/1579	0.53	0/2146
4	D	0.25	0/1654	0.46	0/2254
4	K	0.26	0/1649	0.46	0/2247
4	R	0.25	0/1654	0.46	0/2254
4	Y	0.25	0/1654	0.45	0/2254
5	E	0.27	0/1573	0.45	0/2139
5	L	0.26	0/1568	0.44	0/2132
5	S	0.26	0/1549	0.44	0/2106
5	Z	0.26	0/1569	0.44	0/2134
6	F	0.25	0/1670	0.46	0/2273
6	M	0.29	0/1670	0.51	0/2273
6	T	0.26	0/1639	0.46	0/2232
6	a	0.27	0/1639	0.48	0/2231
7	G	0.27	0/1610	0.49	0/2192
7	N	0.29	0/1610	0.51	0/2192
7	U	0.27	0/1605	0.49	0/2185
7	b	0.29	0/1604	0.51	0/2184
All	All	0.31	0/49908	0.53	0/67806

There are no bond length outliers.

There are no bond angle outliers.

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	2730	0	2615	101	0
1	H	2675	0	2562	65	0
1	O	2722	0	2611	67	0
1	V	2705	0	2594	71	0
2	B	1611	0	1561	43	0
2	I	1611	0	1561	28	0
2	P	1611	0	1561	21	0
2	W	1597	0	1550	29	0
3	C	1552	0	1499	26	0
3	J	1552	0	1499	22	0
3	Q	1552	0	1499	6	0
3	X	1547	0	1494	23	0
4	D	1619	0	1570	20	0
4	K	1614	0	1565	19	0
4	R	1619	0	1570	17	0
4	Y	1619	0	1570	13	0
5	E	1541	0	1479	7	0
5	L	1536	0	1474	7	0
5	S	1517	0	1453	6	0
5	Z	1537	0	1476	8	0
6	F	1634	0	1582	14	0
6	M	1634	0	1582	16	0
6	T	1603	0	1549	15	0
6	a	1604	0	1551	0	0
7	G	1577	0	1513	11	0
7	N	1577	0	1513	8	0
7	U	1572	0	1508	12	0
7	b	1571	0	1508	0	0
8	F	2	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	2	0	0	0	0
8	a	2	0	0	0	0
All	All	48847	0	47069	619	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 9.

All (619) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:130:ASP:HB3	1:V:152:SER:HA	1.19	1.15
7:U:40:ILE:HG21	7:U:119:THR:HG21	1.47	0.95
1:V:68:LEU:HB2	1:V:73:ASP:HB3	1.49	0.91
1:A:130:ASP:HB3	1:A:152:SER:HA	1.53	0.91
1:A:130:ASP:CB	1:A:152:SER:HA	2.05	0.86
4:D:88:THR:HG23	4:D:101:GLN:HB2	1.55	0.85
4:Y:55:TRP:HE1	4:Y:98:VAL:HG12	1.44	0.82
4:K:55:TRP:CD1	4:K:100:LEU:HD23	2.14	0.81
1:A:79:VAL:HG23	1:A:93:LEU:HD11	1.63	0.80
1:A:131:MET:HB3	1:A:151:ILE:HG13	1.63	0.79
4:Y:55:TRP:HE1	4:Y:98:VAL:CG1	1.96	0.77
1:H:39:LEU:HG	1:H:354:HIS:CE1	2.20	0.77
1:V:39:LEU:HG	1:V:354:HIS:CE1	2.19	0.77
1:O:39:LEU:HG	1:O:354:HIS:CE1	2.19	0.76
3:C:79:ARG:NH1	3:C:80:PHE:HE1	1.85	0.75
2:B:56:TRP:HD1	2:B:89:ILE:HD12	1.51	0.75
3:C:79:ARG:HH11	3:C:80:PHE:HE1	1.32	0.75
2:B:185:SER:O	2:B:229:ASN:HB2	1.87	0.74
2:I:92:ASP:HB3	2:I:97:THR:HG23	1.69	0.74
1:A:315:ILE:HB	1:A:354:HIS:HE1	1.52	0.74
1:H:174:ARG:NH1	1:H:202:HIS:HD2	1.86	0.74
3:J:79:ARG:NH1	3:J:80:PHE:HE1	1.87	0.73
1:O:174:ARG:NH1	1:O:202:HIS:HD2	1.86	0.72
1:A:315:ILE:HB	1:A:354:HIS:CE1	2.24	0.72
1:O:151:ILE:CD1	1:O:208:TRP:HD1	2.04	0.71
3:J:79:ARG:HH11	3:J:80:PHE:HE1	1.38	0.71
1:V:130:ASP:CB	1:V:152:SER:HA	2.10	0.71
1:V:174:ARG:NH1	1:V:202:HIS:HD2	1.88	0.71
1:A:39:LEU:HD21	1:A:354:HIS:CD2	2.26	0.70
1:V:37:THR:HG21	1:V:313:ILE:HD13	1.72	0.70
1:V:283:VAL:HG22	1:V:292:VAL:HG12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:ILE:CD1	1:H:208:TRP:HD1	2.04	0.70
2:W:185:SER:HB2	2:W:229:ASN:HB2	1.74	0.70
1:O:283:VAL:HG22	1:O:292:VAL:HG12	1.74	0.69
1:O:286:LEU:HB2	1:O:291:ILE:HD11	1.74	0.69
1:V:151:ILE:CD1	1:V:208:TRP:HD1	2.05	0.69
6:M:117:LYS:HB3	6:M:134:ALA:HB3	1.75	0.69
1:A:342:PHE:HB3	1:A:354:HIS:HB2	1.75	0.69
6:T:117:LYS:HB3	6:T:134:ALA:HB3	1.74	0.69
1:A:122:GLU:HA	1:A:126:ASN:HB2	1.74	0.68
1:V:286:LEU:HB2	1:V:291:ILE:HD11	1.75	0.68
1:H:283:VAL:HG22	1:H:292:VAL:HG12	1.75	0.67
1:A:80:GLN:HG2	1:A:89:THR:HA	1.76	0.67
1:A:322:ASN:HB3	1:A:325:ALA:HB2	1.77	0.67
3:C:31:SER:HB3	3:C:125:LEU:HD21	1.76	0.67
1:H:286:LEU:HB2	1:H:291:ILE:HD11	1.77	0.67
3:C:101:GLU:HG3	3:C:184:GLN:HB3	1.76	0.67
4:R:57:ARG:NH1	4:R:113:TYR:OH	2.27	0.67
1:A:39:LEU:HD21	1:A:354:HIS:NE2	2.10	0.67
1:H:240:HIS:HE2	1:H:253:VAL:HG11	1.59	0.66
1:A:117:LEU:HD21	1:A:149:ILE:HD11	1.77	0.66
1:V:240:HIS:HE2	1:V:253:VAL:HG11	1.60	0.66
3:Q:31:SER:HB3	3:Q:125:LEU:HD21	1.78	0.66
3:X:31:SER:HB3	3:X:125:LEU:HD21	1.78	0.66
4:D:68:ALA:HB1	4:D:89:ILE:HD13	1.76	0.66
5:Z:51:TRP:HE1	5:Z:88:HIS:CE1	2.13	0.66
2:I:25:GLU:O	2:I:137:HIS:HE1	1.78	0.66
3:J:101:GLU:HG3	3:J:184:GLN:HB3	1.77	0.66
3:X:101:GLU:HG3	3:X:184:GLN:HB3	1.78	0.66
1:V:322:ASN:HB3	1:V:325:ALA:HB2	1.78	0.66
1:A:93:LEU:O	1:A:96:GLU:HG2	1.97	0.65
1:H:322:ASN:HB3	1:H:325:ALA:HB2	1.77	0.65
3:J:31:SER:HB3	3:J:125:LEU:HD21	1.78	0.65
1:A:286:LEU:HD12	1:A:291:ILE:HG12	1.78	0.65
1:O:240:HIS:HE2	1:O:253:VAL:HG11	1.61	0.65
2:P:25:GLU:O	2:P:137:HIS:HE1	1.79	0.65
3:X:167:LYS:HG3	3:X:170:ASN:HA	1.77	0.65
4:Y:57:ARG:NH1	4:Y:113:TYR:OH	2.29	0.65
5:E:51:TRP:HE1	5:E:88:HIS:CE1	2.15	0.64
4:K:130:ASP:HA	5:L:66:TYR:HB2	1.79	0.64
3:X:132:SER:HB2	3:X:155:ASN:HB3	1.78	0.64
2:B:40:VAL:HG22	2:B:99:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:HIS:HE1	3:C:156:ASN:HD21	1.43	0.64
1:O:151:ILE:HD11	1:O:208:TRP:HD1	1.61	0.64
1:A:203:ASP:OD2	1:A:207:THR:HG23	1.98	0.64
4:Y:68:ALA:HB1	4:Y:89:ILE:HD13	1.78	0.64
3:X:79:ARG:NH1	3:X:80:PHE:HE2	1.95	0.64
4:R:68:ALA:HB1	4:R:89:ILE:HD13	1.78	0.64
6:F:117:LYS:HB3	6:F:134:ALA:HB3	1.80	0.63
1:H:170:LYS:NZ	1:H:173:ASN:H	1.95	0.63
1:O:54:PHE:HB3	1:O:165:VAL:HG11	1.80	0.63
1:A:42:ILE:HD12	1:A:353:ILE:HD11	1.80	0.63
1:H:151:ILE:HD11	1:H:208:TRP:HD1	1.63	0.63
2:B:191:LEU:HD21	2:B:214:VAL:HG21	1.81	0.63
1:O:97:THR:HG22	1:O:99:LEU:H	1.63	0.63
2:W:25:GLU:O	2:W:137:HIS:HE1	1.80	0.63
2:B:25:GLU:HA	2:B:41:CYS:HA	1.80	0.63
3:J:132:SER:HB2	3:J:155:ASN:HB3	1.81	0.63
3:X:134:PHE:HB2	3:X:153:LEU:HB3	1.80	0.63
1:V:182:VAL:HG21	1:V:225:TYR:HB2	1.82	0.62
1:H:176:TYR:HB3	1:H:200:ALA:HB1	1.82	0.62
1:V:139:ASN:H	1:V:139:ASN:HD22	1.48	0.62
1:A:130:ASP:HB2	1:A:152:SER:HA	1.81	0.62
3:C:134:PHE:HB2	3:C:153:LEU:HB3	1.81	0.62
5:S:51:TRP:HE1	5:S:88:HIS:CE1	2.18	0.62
3:X:181:VAL:HG22	3:X:193:LEU:HD12	1.81	0.62
1:H:54:PHE:HB3	1:H:165:VAL:HG11	1.82	0.62
3:C:54:GLN:HB2	3:C:65:LEU:HD11	1.82	0.61
1:O:139:ASN:H	1:O:139:ASN:HD22	1.48	0.61
2:P:36:ALA:HA	2:P:103:ASN:HA	1.83	0.61
1:O:176:TYR:HB3	1:O:200:ALA:HB1	1.81	0.61
4:K:68:ALA:HB1	4:K:89:ILE:HD13	1.81	0.61
2:P:39:LEU:HD12	2:P:100:LEU:HD23	1.83	0.61
1:V:54:PHE:HB3	1:V:165:VAL:HG11	1.83	0.61
1:A:147:ALA:HB2	3:C:109:ARG:NH2	2.15	0.61
1:H:139:ASN:HD22	1:H:139:ASN:H	1.48	0.61
1:O:169:LEU:HB2	1:O:232:ILE:HD13	1.83	0.61
2:I:200:ALA:HB1	2:I:208:TYR:HB3	1.82	0.61
7:G:67:TYR:HB3	7:G:70:LYS:HG3	1.82	0.61
4:D:117:LYS:HB3	4:D:133:ALA:HB3	1.83	0.60
2:W:39:LEU:HD12	2:W:100:LEU:HD23	1.83	0.60
2:B:79:TYR:HB2	2:B:84:LYS:HG3	1.83	0.60
1:V:151:ILE:HD11	1:V:208:TRP:HD1	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:215:LYS:NZ	1:V:265:GLU:HB3	2.16	0.60
1:A:316:LYS:HE2	1:A:318:GLU:HB2	1.83	0.60
2:I:39:LEU:HD12	2:I:100:LEU:HD23	1.82	0.60
3:C:181:VAL:HG22	3:C:193:LEU:HD12	1.82	0.60
2:W:200:ALA:HB1	2:W:208:TYR:HB3	1.83	0.60
6:T:59:ALA:HB3	6:T:62:LYS:HB2	1.83	0.60
2:W:36:ALA:HA	2:W:103:ASN:HA	1.83	0.60
1:H:97:THR:HG22	1:H:99:LEU:H	1.67	0.60
1:V:169:LEU:HB2	1:V:232:ILE:HD13	1.84	0.59
2:I:36:ALA:HA	2:I:103:ASN:HA	1.83	0.59
1:V:147:ALA:HB3	2:W:125:TRP:CH2	2.38	0.59
4:R:48:PHE:CE1	4:R:91:ARG:NH2	2.70	0.59
2:I:56:TRP:HD1	2:I:89:ILE:CD1	2.16	0.59
4:R:117:LYS:HB3	4:R:133:ALA:HB3	1.85	0.59
6:T:91:ARG:HH11	6:T:93:ASN:HD21	1.51	0.59
1:O:170:LYS:HD2	1:O:173:ASN:HA	1.85	0.59
1:O:110:ASP:HB3	1:O:113:GLU:HG3	1.85	0.59
5:E:24:LEU:HA	5:E:44:GLY:HA3	1.84	0.58
1:A:147:ALA:HB3	2:B:125:TRP:CH2	2.38	0.58
1:A:147:ALA:HB2	3:C:109:ARG:HH22	1.68	0.58
2:W:156:LEU:HD22	3:X:136:PHE:HB3	1.86	0.58
2:P:56:TRP:HD1	2:P:89:ILE:CD1	2.17	0.58
2:W:56:TRP:HD1	2:W:89:ILE:CD1	2.16	0.58
2:B:56:TRP:HD1	2:B:89:ILE:CD1	2.15	0.58
1:V:176:TYR:HB3	1:V:200:ALA:HB1	1.86	0.57
1:H:169:LEU:HB2	1:H:232:ILE:HD13	1.85	0.57
1:H:182:VAL:HG21	1:H:225:TYR:HB2	1.87	0.57
4:R:110:THR:HG23	4:R:141:ILE:HA	1.87	0.56
1:V:314:LEU:HG	1:V:316:LYS:NZ	2.20	0.56
1:O:31:ARG:HD2	1:O:360:ASN:HD21	1.70	0.56
2:B:79:TYR:CE1	2:B:89:ILE:HG22	2.40	0.56
7:G:24:LEU:HD21	7:G:45:SER:HB2	1.88	0.56
1:H:38:GLU:HB3	1:V:32:HIS:HD2	1.70	0.56
1:H:42:ILE:HG22	1:H:87:TRP:CD1	2.41	0.56
7:N:67:TYR:HB3	7:N:70:LYS:HG3	1.87	0.56
7:U:67:TYR:HB3	7:U:70:LYS:HG3	1.87	0.56
1:H:31:ARG:HD2	1:H:360:ASN:HD21	1.71	0.56
6:M:23:LEU:HD23	6:M:43:ALA:HB2	1.87	0.56
1:V:42:ILE:HG22	1:V:87:TRP:CD1	2.40	0.56
1:A:139:ASN:HD22	1:A:139:ASN:H	1.51	0.56
2:B:127:TYR:CD1	3:C:113:GLY:HA2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:SER:HB2	3:C:155:ASN:HB3	1.86	0.56
1:O:336:ASP:HB3	1:O:339:ARG:H	1.70	0.56
3:J:166:TRP:CD1	3:J:197:LEU:HD13	2.41	0.56
4:D:70:ILE:HB	4:D:89:ILE:HD12	1.87	0.56
6:F:127:ASP:OD1	6:F:131:GLU:OE2	2.24	0.56
1:H:240:HIS:HE2	1:H:253:VAL:CG1	2.19	0.55
1:O:147:ALA:HB3	2:P:125:TRP:CH2	2.41	0.55
6:T:54:GLY:HA3	6:T:66:TYR:OH	2.06	0.55
6:T:91:ARG:HH11	6:T:93:ASN:ND2	2.02	0.55
6:T:37:LEU:HD23	6:T:105:LEU:HD21	1.89	0.55
1:V:336:ASP:HB3	1:V:339:ARG:H	1.71	0.55
1:A:122:GLU:HA	1:A:126:ASN:CB	2.37	0.55
6:F:37:LEU:HD23	6:F:105:LEU:HD21	1.88	0.55
1:O:215:LYS:NZ	1:O:265:GLU:HB3	2.21	0.55
1:H:230:PRO:HB3	1:H:239:PHE:CE1	2.42	0.55
1:A:132:THR:HG21	6:F:124:HIS:CE1	2.42	0.55
2:B:56:TRP:CD1	2:B:89:ILE:HD12	2.39	0.55
5:L:34:PRO:HA	5:L:95:VAL:HG12	1.89	0.55
1:A:134:HIS:HD2	1:A:136:PHE:CZ	2.25	0.55
3:X:50:TYR:HE1	3:X:84:LYS:HE2	1.73	0.55
7:G:53:GLN:HG3	7:G:101:ALA:CB	2.36	0.54
1:V:36:ARG:HH11	1:V:38:GLU:HG3	1.71	0.54
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.42	0.54
1:A:245:ASP:O	1:A:248:ASN:O	2.25	0.54
3:C:49:TYR:HA	3:C:69:ASN:HD21	1.72	0.54
4:D:40:VAL:HG23	4:D:99:ARG:HG3	1.89	0.54
6:F:80:THR:HG22	6:F:83:VAL:HG22	1.90	0.54
1:V:230:PRO:HB3	1:V:239:PHE:CE1	2.43	0.54
1:A:315:ILE:HG21	1:A:354:HIS:ND1	2.23	0.54
1:H:216:TYR:CZ	1:H:218:ASN:HB3	2.42	0.54
7:N:38:VAL:HG11	7:N:121:LEU:HD21	1.90	0.54
1:A:56:TYR:CD2	1:A:114:ILE:HD11	2.43	0.54
4:K:126:THR:HG23	5:L:108:ARG:HE	1.73	0.54
1:O:240:HIS:HE2	1:O:253:VAL:CG1	2.20	0.53
2:B:81:ALA:HA	2:B:84:LYS:HE3	1.90	0.53
2:B:117:LYS:HB3	2:B:134:ALA:HB3	1.89	0.53
2:B:237:THR:HG22	2:B:239:VAL:HG23	1.91	0.53
6:T:127:ASP:OD1	6:T:131:GLU:OE2	2.26	0.53
3:C:43:SER:HB3	3:C:88:THR:HG22	1.89	0.53
6:M:54:GLY:HA3	6:M:66:TYR:OH	2.08	0.53
4:R:26:SER:HB3	4:R:40:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ASN:ND2	6:T:72:ASN:HD21	2.06	0.53
6:F:54:GLY:HA3	6:F:66:TYR:OH	2.09	0.53
1:H:249:ASN:HD22	1:H:250:VAL:HG23	1.73	0.53
2:P:45:GLY:HA3	3:X:63:VAL:HG21	1.90	0.53
1:A:77:ILE:HD13	1:A:105:ILE:HD11	1.90	0.53
1:V:82:LYS:NZ	1:V:85:ASP:H	2.06	0.53
1:V:240:HIS:HE2	1:V:253:VAL:CG1	2.20	0.53
1:A:219:TYR:HA	1:A:225:TYR:OH	2.09	0.52
1:O:173:ASN:OD1	3:X:97:GLN:OE1	2.28	0.52
1:A:282:ASP:H	1:A:293:SER:HB3	1.74	0.52
1:V:31:ARG:NH1	1:V:360:ASN:HD21	2.06	0.52
1:V:44:ASN:HB2	1:V:351:TYR:HE2	1.75	0.52
1:H:151:ILE:HD12	1:H:208:TRP:HD1	1.74	0.52
1:H:130:ASP:HB3	1:H:152:SER:HA	1.90	0.52
1:A:119:CYS:HB3	1:A:131:MET:SD	2.50	0.52
1:H:240:HIS:NE2	1:H:253:VAL:HG11	2.23	0.52
6:M:37:LEU:HD13	6:M:39:LEU:HG	1.92	0.52
7:U:78:ARG:NH2	7:U:99:ASP:OD1	2.42	0.52
6:T:80:THR:HG22	6:T:83:VAL:HG22	1.92	0.52
2:B:56:TRP:CD1	2:B:89:ILE:CD1	2.93	0.52
1:H:45:ASN:ND2	4:K:121:SER:OG	2.43	0.52
7:N:100:GLU:HG3	7:N:183:GLN:HB3	1.91	0.52
1:H:31:ARG:HH11	1:H:360:ASN:HD21	1.57	0.51
1:H:147:ALA:HB3	2:I:125:TRP:CH2	2.45	0.51
1:A:182:VAL:HG21	1:A:225:TYR:HB2	1.92	0.51
4:D:110:THR:HG23	4:D:141:ILE:HA	1.92	0.51
1:H:44:ASN:HB2	1:H:351:TYR:HE2	1.75	0.51
1:O:44:ASN:HB2	1:O:351:TYR:HE2	1.75	0.51
2:B:232:HIS:CD2	2:B:234:PRO:HD2	2.45	0.51
4:K:110:THR:HG23	4:K:141:ILE:HA	1.92	0.51
1:O:99:LEU:HD23	1:O:103:PRO:HB3	1.92	0.51
1:V:314:LEU:HG	1:V:316:LYS:HZ1	1.75	0.51
5:E:49:TYR:H	5:E:68:ASN:ND2	2.08	0.51
1:V:110:ASP:HB3	1:V:113:GLU:HG3	1.93	0.51
1:V:215:LYS:HZ2	1:V:265:GLU:HB3	1.76	0.51
1:O:256:ILE:HG22	1:O:270:ASN:HA	1.93	0.51
2:B:41:CYS:HB3	2:B:98:LEU:HB3	1.91	0.51
2:B:176:ASP:HB3	2:B:207:LEU:HD22	1.91	0.51
3:J:88:THR:CG2	4:K:84:LYS:HD2	2.41	0.51
6:M:80:THR:HG22	6:M:83:VAL:HG22	1.92	0.51
1:A:107:ALA:HB2	1:A:116:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:HB3	1:A:339:ARG:H	1.76	0.51
1:H:151:ILE:HD11	1:H:208:TRP:CD1	2.45	0.51
1:V:84:LYS:O	1:V:85:ASP:HB2	2.11	0.51
3:X:131:PRO:HB3	3:X:157:PHE:HB3	1.93	0.51
5:E:108:ARG:HG2	5:E:112:ASN:O	2.11	0.51
7:G:53:GLN:HB2	7:G:103:TYR:CE2	2.46	0.51
2:B:30:LEU:HD22	2:B:179:PRO:HG3	1.92	0.50
1:A:54:PHE:HB3	1:A:165:VAL:HG11	1.93	0.50
1:A:56:TYR:CD2	1:A:57:LYS:HG2	2.46	0.50
3:J:38:VAL:HG12	3:J:93:ILE:HB	1.93	0.50
2:P:123:CYS:SG	3:Q:68:ASN:ND2	2.84	0.50
1:V:240:HIS:NE2	1:V:253:VAL:HG11	2.25	0.50
2:B:52:TYR:HE2	2:B:117:LYS:HZ3	1.57	0.50
1:V:151:ILE:HD12	1:V:208:TRP:HD1	1.77	0.50
2:B:24:ASP:HB3	2:B:42:LYS:HB3	1.92	0.50
1:A:97:THR:HB	1:A:99:LEU:HB2	1.93	0.50
5:L:109:ASP:OD1	5:L:109:ASP:O	2.29	0.50
1:O:31:ARG:HH11	1:O:360:ASN:HD21	1.59	0.50
1:V:135:ARG:HB3	2:W:125:TRP:HH2	1.77	0.50
2:B:196:HIS:HE1	3:C:156:ASN:ND2	2.08	0.50
1:V:342:PHE:HB3	1:V:354:HIS:HB2	1.94	0.50
3:X:79:ARG:NH1	3:X:80:PHE:CE2	2.76	0.50
3:J:54:GLN:HB2	3:J:65:LEU:HD11	1.94	0.50
1:V:245:ASP:O	1:V:248:ASN:O	2.30	0.50
2:I:203:GLN:HA	3:J:178:GLN:HE22	1.76	0.50
1:V:68:LEU:HB2	1:V:73:ASP:CB	2.34	0.50
1:O:68:LEU:HB2	1:O:73:ASP:HB3	1.93	0.49
1:V:256:ILE:HG22	1:V:270:ASN:HA	1.94	0.49
1:H:135:ARG:HB3	2:I:125:TRP:HH2	1.77	0.49
2:W:179:PRO:O	2:W:232:HIS:HE1	1.95	0.49
4:D:90:SER:HB3	4:D:99:ARG:HB2	1.94	0.49
1:H:170:LYS:HZ2	1:H:173:ASN:H	1.58	0.49
6:M:86:ARG:NH2	6:M:109:ASP:OD2	2.30	0.49
1:A:135:ARG:HB3	2:B:125:TRP:CH2	2.48	0.49
3:X:38:VAL:HG12	3:X:93:ILE:HB	1.95	0.49
1:H:240:HIS:NE2	1:H:253:VAL:CG1	2.76	0.49
1:V:122:GLU:HG2	1:V:126:ASN:HB2	1.95	0.49
1:A:117:LEU:CD2	1:A:149:ILE:HD11	2.43	0.49
1:H:110:ASP:HB3	1:H:113:GLU:HG2	1.95	0.49
4:R:59:ALA:HB3	4:R:62:LYS:HB2	1.94	0.49
5:S:109:ASP:OD1	5:S:109:ASP:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HB	1:A:94:PHE:HB2	1.94	0.49
1:A:129:LYS:HB2	1:A:157:LYS:NZ	2.28	0.49
1:A:136:PHE:CD2	1:A:146:ASN:HB3	2.48	0.49
1:O:184:PRO:O	1:O:224:GLN:HA	2.12	0.49
1:O:240:HIS:NE2	1:O:253:VAL:HG11	2.25	0.49
1:A:195:ASP:HB3	1:A:219:TYR:CD2	2.47	0.48
1:A:229:ARG:HH12	1:A:231:TYR:HB2	1.77	0.48
2:I:117:LYS:HB3	2:I:134:ALA:HB3	1.94	0.48
1:O:342:PHE:HB3	1:O:354:HIS:HB2	1.94	0.48
1:V:240:HIS:NE2	1:V:253:VAL:CG1	2.76	0.48
1:H:240:HIS:CD2	1:H:253:VAL:CG1	2.96	0.48
3:Q:38:VAL:HG12	3:Q:93:ILE:HB	1.96	0.48
3:X:69:ASN:HD21	3:X:84:LYS:HD2	1.79	0.48
1:H:167:LEU:HB2	1:H:168:PRO:HD2	1.95	0.48
1:O:167:LEU:HB2	1:O:168:PRO:HD2	1.95	0.48
1:V:135:ARG:HB3	2:W:125:TRP:CH2	2.47	0.48
1:A:115:ILE:HD13	1:A:177:PHE:CE2	2.49	0.48
1:A:132:THR:CG2	6:F:124:HIS:CE1	2.97	0.48
3:C:85:SER:HB3	4:D:84:LYS:HD3	1.96	0.48
4:D:59:ALA:HB3	4:D:62:LYS:HB2	1.95	0.48
2:W:151:PRO:HD2	2:W:237:THR:HG21	1.94	0.48
4:Y:110:THR:HG23	4:Y:141:ILE:HA	1.94	0.48
3:J:103:VAL:HG22	3:J:121:THR:HG22	1.95	0.48
4:K:59:ALA:HB3	4:K:62:LYS:HB2	1.95	0.48
4:K:117:LYS:HB3	4:K:133:ALA:HB3	1.96	0.48
4:K:90:SER:HB3	4:K:99:ARG:HB2	1.96	0.48
1:A:70:GLY:H	1:A:73:ASP:HB2	1.78	0.48
1:H:256:ILE:HG22	1:H:270:ASN:HA	1.95	0.48
1:O:151:ILE:HD12	1:O:208:TRP:HD1	1.77	0.48
4:R:69:ASP:OD1	4:R:69:ASP:O	2.31	0.48
4:Y:90:SER:HB3	4:Y:99:ARG:HB2	1.95	0.48
1:H:174:ARG:NH1	1:H:202:HIS:CD2	2.75	0.48
1:H:261:GLU:HB2	1:H:267:VAL:HG12	1.95	0.48
5:Z:49:TYR:OH	5:Z:86:SER:O	2.31	0.48
1:A:36:ARG:HG3	1:O:34:PHE:CD1	2.48	0.48
1:A:99:LEU:HD12	1:A:103:PRO:HB3	1.96	0.48
2:B:25:GLU:O	2:B:25:GLU:HG2	2.13	0.48
4:D:55:TRP:HE1	4:D:98:VAL:HG12	1.79	0.48
1:V:167:LEU:HB2	1:V:168:PRO:HD2	1.95	0.48
1:A:283:VAL:HG22	1:A:292:VAL:HG12	1.95	0.47
6:F:59:ALA:HB3	6:F:62:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:240:HIS:CD2	1:O:253:VAL:CG1	2.97	0.47
2:B:108:GLU:CD	2:B:108:GLU:H	2.18	0.47
4:R:90:SER:HB3	4:R:99:ARG:HB2	1.95	0.47
1:V:42:ILE:CG2	1:V:87:TRP:CD1	2.96	0.47
1:A:295:GLY:HA3	1:A:300:PHE:CD1	2.49	0.47
1:H:126:ASN:HD21	6:M:72:ASN:HD21	1.60	0.47
1:H:151:ILE:CD1	1:H:208:TRP:CD1	2.92	0.47
6:M:232:HIS:ND1	6:M:235:SER:OG	2.44	0.47
1:O:205:GLY:HA2	1:O:208:TRP:CZ2	2.49	0.47
1:O:240:HIS:NE2	1:O:253:VAL:CG1	2.77	0.47
1:V:205:GLY:HA2	1:V:208:TRP:CZ2	2.50	0.47
5:E:37:THR:HG22	5:E:93:THR:HA	1.95	0.47
2:W:117:LYS:HB3	2:W:134:ALA:HB3	1.96	0.47
3:X:73:PRO:HG2	3:X:76:ILE:HG13	1.97	0.47
1:H:42:ILE:CG2	1:H:87:TRP:CD1	2.97	0.47
6:M:107:ALA:HA	6:M:143:VAL:HG21	1.95	0.47
1:V:56:TYR:HB3	1:V:61:TYR:CE2	2.50	0.47
1:A:42:ILE:CG2	1:A:87:TRP:CD1	2.97	0.47
1:H:342:PHE:HB3	1:H:354:HIS:HB2	1.96	0.47
1:O:182:VAL:HG23	1:O:196:ILE:HG12	1.97	0.47
3:J:88:THR:HG21	4:K:84:LYS:HD2	1.95	0.47
1:A:147:ALA:HB3	2:B:125:TRP:CZ2	2.50	0.47
2:B:79:TYR:HE1	2:B:89:ILE:HG22	1.80	0.47
1:H:135:ARG:HB3	2:I:125:TRP:CH2	2.50	0.47
1:O:282:ASP:H	1:O:293:SER:HB3	1.79	0.47
4:R:91:ARG:HD3	4:R:93:ASP:OD1	2.15	0.47
3:X:54:GLN:HG3	3:X:104:TYR:CE2	2.50	0.47
1:A:315:ILE:CG2	1:A:354:HIS:ND1	2.78	0.47
6:M:59:ALA:HB3	6:M:62:LYS:HB2	1.97	0.47
1:O:37:THR:HG21	1:O:313:ILE:HD13	1.98	0.47
1:O:273:PHE:HB2	1:O:280:LEU:HD22	1.96	0.47
2:P:36:ALA:HB1	2:P:101:GLN:HE22	1.79	0.47
1:V:240:HIS:CD2	1:V:253:VAL:CG1	2.97	0.47
1:A:42:ILE:HB	1:A:351:TYR:HB2	1.97	0.46
1:A:134:HIS:CD2	1:A:136:PHE:CZ	3.04	0.46
2:B:196:HIS:CE1	3:C:156:ASN:HD21	2.29	0.46
4:K:26:SER:HB3	4:K:40:VAL:HG12	1.97	0.46
1:O:56:TYR:HB3	1:O:61:TYR:CE2	2.50	0.46
2:P:117:LYS:HB3	2:P:134:ALA:HB3	1.97	0.46
2:I:36:ALA:HB1	2:I:101:GLN:HE22	1.80	0.46
2:I:176:ASP:HB3	2:I:207:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:39:LYS:HB2	5:Z:39:LYS:HE2	1.77	0.46
5:Z:102:VAL:HG22	5:Z:120:THR:HG23	1.98	0.46
4:R:55:TRP:HE1	4:R:98:VAL:HG12	1.80	0.46
2:I:149:LYS:HE2	2:I:207:LEU:HD21	1.98	0.46
1:H:56:TYR:HB3	1:H:61:TYR:CE2	2.51	0.46
3:J:73:PRO:HG2	3:J:76:ILE:HG13	1.97	0.46
1:O:275:LYS:HG2	1:O:278:LYS:NZ	2.31	0.46
1:V:151:ILE:HD11	1:V:208:TRP:CD1	2.46	0.46
4:D:70:ILE:HG12	4:D:91:ARG:HG2	1.98	0.46
1:O:151:ILE:HD11	1:O:208:TRP:CD1	2.44	0.46
1:O:228:LEU:HA	1:O:241:PHE:HB3	1.98	0.46
2:P:42:LYS:HD2	2:P:97:THR:HG23	1.98	0.46
1:V:282:ASP:H	1:V:293:SER:HB3	1.81	0.46
6:F:70:ILE:HG23	6:F:91:ARG:HH21	1.79	0.46
6:F:129:SER:O	7:G:106:GLY:HA3	2.16	0.46
2:W:176:ASP:HB3	2:W:207:LEU:HD22	1.97	0.46
2:B:197:THR:HG23	2:B:212:SER:HB2	1.98	0.46
1:H:282:ASP:H	1:H:293:SER:HB3	1.81	0.46
2:W:53:THR:HG23	2:W:118:HIS:CB	2.46	0.46
2:B:84:LYS:HE3	2:B:84:LYS:HB2	1.72	0.46
2:I:203:GLN:NE2	2:I:209:SER:HB3	2.31	0.46
4:K:91:ARG:HD3	4:K:93:ASP:OD1	2.16	0.46
1:O:174:ARG:NH1	1:O:202:HIS:CD2	2.76	0.46
3:X:142:GLN:HE22	3:X:149:SER:HB2	1.80	0.46
3:C:228:ASN:O	3:C:229:ARG:HD3	2.16	0.45
1:H:205:GLY:HA2	1:H:208:TRP:CZ2	2.51	0.45
1:H:275:LYS:HG2	1:H:278:LYS:NZ	2.31	0.45
1:O:151:ILE:CD1	1:O:208:TRP:CD1	2.93	0.45
1:V:253:VAL:HG12	1:V:254:ASN:H	1.82	0.45
2:I:56:TRP:HD1	2:I:89:ILE:HD12	1.81	0.45
3:J:166:TRP:CG	3:J:197:LEU:HD13	2.51	0.45
4:K:70:ILE:HB	4:K:89:ILE:HD12	1.99	0.45
6:M:76:PHE:HE2	6:M:78:LEU:HD23	1.81	0.45
2:B:25:GLU:O	2:B:137:HIS:CE1	2.69	0.45
1:A:97:THR:C	1:A:99:LEU:H	2.19	0.45
1:A:174:ARG:CZ	1:A:202:HIS:HD2	2.30	0.45
1:A:311:ASN:HA	1:O:312:SER:O	2.15	0.45
4:D:40:VAL:HG22	4:D:97:THR:HB	1.99	0.45
3:Q:63:VAL:HG21	2:W:45:GLY:HA3	1.98	0.45
1:V:273:PHE:HB2	1:V:280:LEU:HD22	1.97	0.45
3:C:73:PRO:HG2	3:C:76:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:GLY:O	7:G:94:GLY:HA2	2.17	0.45
1:V:315:ILE:HG21	1:V:354:HIS:CD2	2.52	0.45
2:W:42:LYS:HD2	2:W:97:THR:HG23	1.99	0.45
2:B:137:HIS:H	2:B:137:HIS:CD2	2.34	0.45
2:B:197:THR:HA	2:B:212:SER:HA	1.99	0.45
1:H:273:PHE:HB2	1:H:280:LEU:HD22	1.99	0.45
2:I:53:THR:HG23	2:I:118:HIS:CB	2.47	0.45
2:I:58:ARG:HG2	2:I:68:VAL:CG2	2.46	0.45
1:A:39:LEU:HD21	1:A:354:HIS:CE1	2.51	0.45
3:J:50:TYR:HE1	3:J:84:LYS:HE2	1.82	0.45
3:J:87:SER:OG	5:L:112:ASN:ND2	2.50	0.45
4:K:36:THR:HG22	4:K:103:ASN:HB3	1.99	0.45
1:V:82:LYS:HZ2	1:V:85:ASP:H	1.65	0.45
1:A:230:PRO:HB3	1:A:239:PHE:CE1	2.52	0.45
1:O:215:LYS:HZ2	1:O:265:GLU:HB3	1.81	0.45
1:V:104:HIS:NE2	1:V:121:ASP:OD1	2.50	0.45
4:Y:117:LYS:HB3	4:Y:133:ALA:HB3	1.99	0.45
2:B:198:PHE:CZ	3:C:192:SER:HB3	2.51	0.44
5:E:78:ARG:HH21	5:E:96:GLN:HE22	1.65	0.44
1:H:253:VAL:HG12	1:H:254:ASN:H	1.82	0.44
1:H:322:ASN:HB3	1:H:325:ALA:CB	2.46	0.44
1:V:170:LYS:HE2	1:V:173:ASN:HA	1.99	0.44
4:Y:91:ARG:HD3	4:Y:93:ASP:OD1	2.17	0.44
1:A:295:GLY:HA3	1:A:300:PHE:HD1	1.82	0.44
1:A:348:GLN:HE21	1:A:349:GLY:H	1.64	0.44
4:D:83:VAL:HB	4:D:87:ALA:HB2	1.99	0.44
5:L:49:TYR:CD2	5:L:88:HIS:HB2	2.51	0.44
1:A:242:TYR:HB3	1:A:251:LYS:HB2	2.00	0.44
2:B:24:ASP:HA	2:B:137:HIS:NE2	2.32	0.44
4:K:126:THR:CG2	5:L:108:ARG:HE	2.29	0.44
1:O:135:ARG:HB3	2:P:125:TRP:HH2	1.82	0.44
1:O:322:ASN:HB3	1:O:325:ALA:HB2	1.99	0.44
2:P:53:THR:HG23	2:P:118:HIS:CB	2.47	0.44
3:Q:73:PRO:HG2	3:Q:76:ILE:HG13	1.98	0.44
6:T:129:SER:O	7:U:106:GLY:HA3	2.16	0.44
2:W:58:ARG:HG2	2:W:68:VAL:CG2	2.47	0.44
2:B:185:SER:O	2:B:229:ASN:CB	2.63	0.44
1:H:233:SER:C	1:H:234:LYS:HG3	2.37	0.44
1:H:253:VAL:HG12	1:H:254:ASN:N	2.33	0.44
4:R:79:TYR:HE1	4:R:89:ILE:HG12	1.83	0.44
1:V:71:GLU:H	1:V:71:GLU:HG3	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:106:ARG:HD3	2:W:108:GLU:HB2	1.99	0.44
1:A:97:THR:C	1:A:99:LEU:N	2.71	0.44
1:A:97:THR:HG23	1:A:134:HIS:CD2	2.52	0.44
6:T:129:SER:HB3	7:U:113:VAL:CG1	2.48	0.44
1:V:216:TYR:CE1	1:V:218:ASN:HB2	2.53	0.44
2:W:36:ALA:HB1	2:W:101:GLN:HE22	1.83	0.44
1:A:89:THR:HB	4:D:123:TYR:HA	2.00	0.44
1:O:245:ASP:O	1:O:248:ASN:O	2.36	0.44
1:A:39:LEU:CD2	1:A:354:HIS:CD2	2.97	0.44
3:C:63:VAL:HG21	2:I:45:GLY:HA3	1.98	0.44
4:D:36:THR:HG22	4:D:103:ASN:HB3	2.00	0.44
4:D:67:VAL:HG13	4:D:83:VAL:HG21	2.00	0.44
1:V:31:ARG:HH11	1:V:360:ASN:HD21	1.65	0.44
1:A:174:ARG:HD2	1:A:202:HIS:HB2	2.00	0.44
3:C:142:GLN:HE22	3:C:149:SER:HB2	1.82	0.44
1:H:39:LEU:HG	1:H:354:HIS:HE1	1.78	0.44
4:K:40:VAL:HG23	4:K:99:ARG:HG3	1.99	0.44
1:O:138:SER:OG	1:O:143:GLU:O	2.29	0.44
7:U:78:ARG:HH21	7:U:99:ASP:CG	2.21	0.44
1:A:42:ILE:HD11	1:A:82:LYS:HD2	2.00	0.43
6:F:76:PHE:HE2	6:F:78:LEU:HD23	1.83	0.43
1:O:316:LYS:O	1:O:319:LYS:HG2	2.18	0.43
4:R:36:THR:HG22	4:R:103:ASN:HB3	1.99	0.43
4:Y:36:THR:HG22	4:Y:103:ASN:HB3	2.00	0.43
1:A:273:PHE:HB2	1:A:280:LEU:HD22	1.99	0.43
4:D:39:LEU:HB2	4:D:100:LEU:HB3	2.00	0.43
7:G:100:GLU:O	7:G:101:ALA:HB2	2.18	0.43
1:O:253:VAL:HG12	1:O:254:ASN:N	2.34	0.43
1:A:260:HIS:HE1	1:A:264:LEU:H	1.66	0.43
1:H:137:TYR:OH	3:J:49:TYR:OH	2.30	0.43
1:H:347:SER:HB3	1:H:350:ILE:HB	2.01	0.43
4:K:66:TRP:HB2	4:K:128:LEU:HD11	2.00	0.43
1:V:253:VAL:HG12	1:V:254:ASN:N	2.32	0.43
2:B:25:GLU:OE2	2:B:136:GLY:HA3	2.18	0.43
2:I:22:THR:HB	2:I:44:SER:HB2	2.01	0.43
1:O:253:VAL:HG12	1:O:254:ASN:H	1.83	0.43
6:T:49:SER:HA	6:T:93:ASN:HD22	1.82	0.43
1:A:122:GLU:CA	1:A:126:ASN:HB2	2.43	0.43
1:A:126:ASN:HD22	1:A:126:ASN:HA	1.78	0.43
2:B:151:PRO:HB3	2:B:177:TYR:HB3	2.01	0.43
3:C:65:LEU:O	3:C:73:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:22:THR:OG1	6:F:44:SER:OG	2.37	0.43
1:V:151:ILE:CD1	1:V:208:TRP:CD1	2.94	0.43
1:A:151:ILE:HD12	1:A:199:MET:CE	2.48	0.43
1:O:316:LYS:HE2	1:O:316:LYS:HB2	1.57	0.43
1:A:91:ASN:OD1	1:A:93:LEU:HG	2.18	0.43
1:A:99:LEU:O	7:G:111:ARG:NH1	2.52	0.43
1:A:104:HIS:O	1:A:118:LEU:HA	2.18	0.43
1:A:117:LEU:HG	1:A:134:HIS:O	2.19	0.43
2:I:53:THR:HB	2:I:72:SER:HA	2.01	0.43
2:P:22:THR:HB	2:P:44:SER:HB2	2.01	0.43
4:R:39:LEU:HB2	4:R:100:LEU:HB3	2.00	0.43
2:W:56:TRP:HD1	2:W:89:ILE:HD11	1.84	0.43
1:A:340:ALA:O	1:A:356:ILE:HB	2.18	0.43
2:P:53:THR:HB	2:P:72:SER:HA	2.01	0.43
1:V:36:ARG:HB3	1:V:357:TYR:HB3	2.00	0.43
1:A:167:LEU:HB2	1:A:168:PRO:HD2	2.01	0.42
4:D:41:CYS:SG	4:D:55:TRP:CZ2	3.12	0.42
1:H:218:ASN:HA	1:H:220:LYS:NZ	2.34	0.42
3:Q:65:LEU:O	3:Q:73:PRO:HD2	2.18	0.42
6:T:22:THR:OG1	6:T:44:SER:OG	2.37	0.42
4:Y:26:SER:HB3	4:Y:40:VAL:HG12	2.01	0.42
5:Z:108:ARG:HA	5:Z:113:GLY:HA2	2.01	0.42
1:A:95:LYS:O	1:A:95:LYS:CG	2.66	0.42
7:U:32:ALA:HB3	7:U:38:VAL:HG22	2.01	0.42
2:W:22:THR:HB	2:W:44:SER:HB2	2.01	0.42
1:H:88:ILE:HG21	4:K:71:CYS:SG	2.59	0.42
1:V:292:VAL:HG23	1:V:306:PHE:HB2	2.01	0.42
5:Z:51:TRP:NE1	5:Z:88:HIS:CE1	2.85	0.42
5:S:42:CYS:HB2	5:S:51:TRP:CZ2	2.54	0.42
4:Y:79:TYR:HE1	4:Y:89:ILE:HG12	1.84	0.42
1:A:115:ILE:HD13	1:A:177:PHE:CZ	2.54	0.42
4:Y:39:LEU:HB2	4:Y:100:LEU:HB3	2.00	0.42
5:Z:60:ALA:HA	5:Z:61:PRO:HD3	1.94	0.42
7:N:33:ASN:HA	7:N:124:LEU:HB2	2.01	0.42
7:N:166:LYS:HB2	7:N:210:ALA:HB3	2.01	0.42
1:O:39:LEU:HG	1:O:354:HIS:HE1	1.79	0.42
1:V:315:ILE:CG2	1:V:354:HIS:CE1	3.03	0.42
1:A:319:LYS:HD3	1:A:319:LYS:HA	1.88	0.42
2:I:237:THR:HG22	2:I:239:VAL:HG23	2.01	0.42
2:P:56:TRP:HD1	2:P:89:ILE:HD12	1.83	0.42
7:U:125:ARG:CD	7:U:188:SER:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:53:THR:HB	2:W:72:SER:HA	2.02	0.42
1:A:103:PRO:HB2	1:A:118:LEU:HB3	2.02	0.42
1:A:128:LYS:HE2	1:A:128:LYS:HB3	1.71	0.42
1:H:215:LYS:NZ	1:H:265:GLU:HB3	2.35	0.42
3:J:79:ARG:NH1	3:J:80:PHE:CE1	2.74	0.42
7:N:40:ILE:O	7:N:89:THR:HA	2.20	0.42
2:W:56:TRP:HD1	2:W:89:ILE:HD12	1.82	0.42
1:O:36:ARG:HB3	1:O:357:TYR:HB3	2.02	0.42
1:O:135:ARG:HB3	2:P:125:TRP:CH2	2.54	0.42
7:U:125:ARG:HH21	7:U:128:ALA:HB2	1.85	0.42
1:A:44:ASN:HB2	1:A:87:TRP:HD1	1.84	0.41
3:J:168:VAL:CG1	3:J:207:HIS:ND1	2.83	0.41
3:C:49:TYR:HA	3:C:69:ASN:ND2	2.34	0.41
4:R:116:ALA:HB1	4:R:131:ILE:HG23	2.01	0.41
7:U:33:ASN:HA	7:U:124:LEU:HB2	2.02	0.41
4:D:79:TYR:HE1	4:D:89:ILE:HG12	1.85	0.41
1:O:210:THR:HG23	1:O:264:LEU:HD21	2.03	0.41
2:P:29:GLY:O	2:P:31:GLN:HG2	2.20	0.41
4:R:66:TRP:HB2	4:R:128:LEU:HD11	2.01	0.41
6:T:91:ARG:NH1	6:T:93:ASN:HD21	2.15	0.41
1:A:278:LYS:NZ	1:A:278:LYS:HB2	2.35	0.41
3:C:30:VAL:HG12	3:C:120:THR:HG22	2.03	0.41
5:S:32:ALA:HB3	5:S:38:VAL:HG22	2.01	0.41
1:V:159:LYS:HE2	1:V:183:SER:HB2	2.03	0.41
2:I:56:TRP:CD1	2:I:89:ILE:HD11	2.56	0.41
1:O:347:SER:HB3	1:O:350:ILE:HB	2.02	0.41
7:U:166:LYS:HB2	7:U:210:ALA:HB3	2.02	0.41
2:B:25:GLU:HB3	2:B:115:CYS:HB2	2.02	0.41
5:E:51:TRP:NE1	5:E:88:HIS:CE1	2.86	0.41
1:H:186:LYS:HG3	1:H:221:LEU:CD2	2.50	0.41
1:H:229:ARG:HA	1:H:230:PRO:HD3	1.91	0.41
2:I:54:MET:HB3	2:I:98:LEU:HD22	2.02	0.41
6:M:157:ALA:HA	6:M:158:PRO:HD3	1.96	0.41
7:N:125:ARG:HD2	7:N:126:THR:H	1.86	0.41
5:S:85:GLY:HA2	7:U:109:ASP:O	2.20	0.41
2:W:29:GLY:O	2:W:31:GLN:HG2	2.21	0.41
2:W:124:ASP:HB3	3:X:48:SER:HB2	2.02	0.41
3:X:152:CYS:HB2	3:X:166:TRP:CH2	2.55	0.41
7:G:45:SER:OG	7:G:108:SER:O	2.36	0.41
7:G:64:VAL:HG12	7:G:65:ILE:HG12	2.03	0.41
3:X:110:ASP:HB2	3:X:115:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:H	1:A:151:ILE:HG12	1.56	0.41
2:B:179:PRO:HD2	2:B:234:PRO:HG2	2.01	0.41
6:M:37:LEU:HD23	6:M:105:LEU:HD21	2.03	0.41
2:P:56:TRP:CD1	2:P:89:ILE:HD11	2.56	0.41
2:P:106:ARG:HE	2:P:108:GLU:HB2	1.86	0.41
5:S:38:VAL:HG11	5:S:121:LEU:CD1	2.50	0.41
2:W:87:ALA:HB2	2:W:102:LEU:HD13	2.03	0.41
5:Z:31:SER:HB2	5:Z:124:LEU:HD13	2.03	0.41
1:A:52:MET:O	1:A:62:ASN:HA	2.20	0.41
2:B:110:THR:HG23	2:B:142:ILE:HA	2.03	0.41
2:I:151:PRO:HD2	2:I:237:THR:HG21	2.02	0.41
3:J:30:VAL:HG12	3:J:120:THR:HG22	2.03	0.41
6:M:79:TYR:CE1	6:M:89:ILE:HG22	2.56	0.41
1:O:97:THR:HG22	1:O:98:ASP:N	2.36	0.41
1:O:242:TYR:CE2	1:O:253:VAL:HG22	2.55	0.41
1:O:292:VAL:HG23	1:O:306:PHE:HB2	2.02	0.41
2:P:32:THR:HA	2:P:33:PRO:HD3	1.96	0.41
4:R:48:PHE:CD1	4:R:91:ARG:NH2	2.87	0.41
1:V:322:ASN:HB3	1:V:325:ALA:CB	2.45	0.41
1:V:347:SER:HB3	1:V:350:ILE:HB	2.01	0.41
2:W:56:TRP:CD1	2:W:89:ILE:HD11	2.55	0.41
3:X:203:ASP:HA	3:X:206:LYS:HE3	2.02	0.41
1:A:32:HIS:HD2	1:O:38:GLU:HB3	1.86	0.41
1:A:79:VAL:CG2	1:A:93:LEU:HD21	2.51	0.41
1:A:99:LEU:CD1	1:A:103:PRO:HB3	2.51	0.41
1:H:228:LEU:HD21	1:H:239:PHE:CD1	2.55	0.41
2:I:32:THR:HA	2:I:33:PRO:HD3	1.97	0.41
6:M:70:ILE:HG23	6:M:91:ARG:HH21	1.86	0.41
6:M:116:THR:HB	6:M:132:ILE:HG21	2.02	0.41
1:H:63:ILE:HG21	1:H:105:ILE:HG21	2.03	0.40
2:I:127:TYR:CD1	3:J:113:GLY:HA2	2.57	0.40
1:A:98:ASP:OD1	6:F:125:TYR:HB2	2.20	0.40
7:G:23:ALA:HA	7:G:109:ASP:OD2	2.21	0.40
7:N:27:PRO:O	7:N:119:THR:OG1	2.34	0.40
1:O:216:TYR:CE1	1:O:218:ASN:HB2	2.56	0.40
1:H:242:TYR:CE2	1:H:253:VAL:HG22	2.56	0.40
3:J:110:ASP:HB2	3:J:115:ILE:CG2	2.51	0.40
1:O:316:LYS:HA	1:O:317:PRO:HD3	1.90	0.40
1:O:327:CYS:HA	1:O:344:TYR:CD2	2.56	0.40
1:V:39:LEU:HG	1:V:354:HIS:HE1	1.79	0.40
1:A:83:VAL:HG11	4:D:73:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:CG2	6:F:124:HIS:NE2	2.84	0.40
1:A:285:THR:O	1:A:334:LYS:HD2	2.21	0.40
6:T:79:TYR:CE1	6:T:89:ILE:HG22	2.56	0.40
1:V:242:TYR:CE2	1:V:253:VAL:HG22	2.56	0.40
1:V:251:LYS:HB2	1:V:251:LYS:HE3	1.92	0.40
3:X:166:TRP:HB2	3:X:173:GLN:HB2	2.03	0.40
4:Y:83:VAL:HA	4:Y:86:ARG:HH11	1.86	0.40
1:A:179:ILE:HD12	1:A:199:MET:HE2	2.04	0.40
2:B:124:ASP:HB3	3:C:48:SER:HB2	2.03	0.40
1:H:218:ASN:HA	1:H:220:LYS:HZ1	1.86	0.40
2:I:30:LEU:HD22	2:I:179:PRO:HG3	2.03	0.40
2:P:58:ARG:HG2	2:P:68:VAL:CG2	2.52	0.40
1:V:315:ILE:HG22	1:V:354:HIS:CE1	2.57	0.40
2:W:148:THR:HG22	2:W:235:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/343 (94%)	267 (82%)	57 (18%)	0	100	100
1	H	313/343 (91%)	283 (90%)	30 (10%)	0	100	100
1	O	323/343 (94%)	295 (91%)	28 (9%)	0	100	100
1	V	321/343 (94%)	289 (90%)	32 (10%)	0	100	100
2	B	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	I	217/230 (94%)	198 (91%)	19 (9%)	0	100	100
2	P	217/230 (94%)	202 (93%)	15 (7%)	0	100	100
2	W	214/230 (93%)	193 (90%)	21 (10%)	0	100	100
3	C	205/210 (98%)	189 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	205/210 (98%)	191 (93%)	14 (7%)	0	100	100
3	Q	205/210 (98%)	189 (92%)	16 (8%)	0	100	100
3	X	204/210 (97%)	190 (93%)	14 (7%)	0	100	100
4	D	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
4	K	216/230 (94%)	207 (96%)	9 (4%)	0	100	100
4	R	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
4	Y	217/230 (94%)	210 (97%)	7 (3%)	0	100	100
5	E	200/209 (96%)	190 (95%)	10 (5%)	0	100	100
5	L	199/209 (95%)	191 (96%)	8 (4%)	0	100	100
5	S	196/209 (94%)	187 (95%)	9 (5%)	0	100	100
5	Z	199/209 (95%)	190 (96%)	9 (4%)	0	100	100
6	F	219/321 (68%)	205 (94%)	14 (6%)	0	100	100
6	M	219/321 (68%)	203 (93%)	16 (7%)	0	100	100
6	T	214/321 (67%)	201 (94%)	13 (6%)	0	100	100
6	a	215/321 (67%)	195 (91%)	20 (9%)	0	100	100
7	G	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	N	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	U	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
7	b	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
All	All	6319/7008 (90%)	5874 (93%)	445 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/316 (97%)	254 (83%)	52 (17%)	2	9
1	H	300/316 (95%)	254 (85%)	46 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	305/316 (96%)	263 (86%)	42 (14%)	3 16
1	V	303/316 (96%)	255 (84%)	48 (16%)	2 11
2	B	177/186 (95%)	161 (91%)	16 (9%)	9 32
2	I	177/186 (95%)	165 (93%)	12 (7%)	16 44
2	P	177/186 (95%)	164 (93%)	13 (7%)	14 40
2	W	176/186 (95%)	163 (93%)	13 (7%)	13 40
3	C	177/179 (99%)	159 (90%)	18 (10%)	7 27
3	J	177/179 (99%)	163 (92%)	14 (8%)	12 37
3	Q	177/179 (99%)	158 (89%)	19 (11%)	6 25
3	X	177/179 (99%)	156 (88%)	21 (12%)	5 20
4	D	179/188 (95%)	160 (89%)	19 (11%)	6 25
4	K	179/188 (95%)	161 (90%)	18 (10%)	7 27
4	R	179/188 (95%)	155 (87%)	24 (13%)	4 16
4	Y	179/188 (95%)	156 (87%)	23 (13%)	4 18
5	E	175/179 (98%)	160 (91%)	15 (9%)	10 34
5	L	175/179 (98%)	155 (89%)	20 (11%)	5 22
5	S	173/179 (97%)	156 (90%)	17 (10%)	8 29
5	Z	175/179 (98%)	155 (89%)	20 (11%)	5 22
6	F	179/272 (66%)	169 (94%)	10 (6%)	21 52
6	M	179/272 (66%)	166 (93%)	13 (7%)	14 40
6	T	176/272 (65%)	165 (94%)	11 (6%)	18 47
6	a	176/272 (65%)	162 (92%)	14 (8%)	12 37
7	G	180/180 (100%)	169 (94%)	11 (6%)	18 49
7	N	180/180 (100%)	168 (93%)	12 (7%)	16 45
7	U	180/180 (100%)	165 (92%)	15 (8%)	11 36
7	b	179/180 (99%)	156 (87%)	23 (13%)	4 18
All	All	5472/6000 (91%)	4893 (89%)	579 (11%)	6 25

All (579) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	50	ARG
1	A	59	GLU
1	A	63	ILE
1	A	69	LYS
1	A	91	ASN
1	A	93	LEU
1	A	95	LYS
1	A	97	THR
1	A	99	LEU
1	A	100	THR
1	A	111	VAL
1	A	121	ASP
1	A	125	SER
1	A	128	LYS
1	A	129	LYS
1	A	133	CYS
1	A	134	HIS
1	A	139	ASN
1	A	145	ASN
1	A	146	ASN
1	A	151	ILE
1	A	152	SER
1	A	154	TYR
1	A	159	LYS
1	A	162	SER
1	A	173	ASN
1	A	180	CYS
1	A	183	SER
1	A	185	TYR
1	A	194	ASP
1	A	197	LEU
1	A	198	CYS
1	A	219	TYR
1	A	228	LEU
1	A	246	ASN
1	A	249	ASN
1	A	251	LYS
1	A	252	ASN
1	A	262	LYS
1	A	267	VAL
1	A	275	LYS
1	A	278	LYS

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Mol	Chain	Res	Type
1	A	309	ASN
1	A	311	ASN
1	A	323	THR
1	A	335	ILE
1	A	337	GLU
1	A	339	ARG
1	A	348	GLN
1	A	360	ASN
2	B	22	THR
2	B	37	LEU
2	B	39	LEU
2	B	44	SER
2	B	50	SER
2	B	58	ARG
2	B	84	LYS
2	B	106	ARG
2	B	118	HIS
2	B	123	CYS
2	B	124	ASP
2	B	145	SER
2	B	149	LYS
2	B	152	SER
2	B	185	SER
2	B	211	SER
3	C	25	THR
3	C	38	VAL
3	C	43	SER
3	C	48	SER
3	C	81	SER
3	C	101	GLU
3	C	110	ASP
3	C	111	ASN
3	C	126	ARG
3	C	140	ASP
3	C	143	LEU
3	C	167	LYS
3	C	180	SER
3	C	188	ASP
3	C	192	SER
3	C	194	SER
3	C	197	LEU
3	C	229	ARG

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Mol	Chain	Res	Type
4	D	30	LEU
4	D	40	VAL
4	D	54	GLN
4	D	57	ARG
4	D	70	ILE
4	D	84	LYS
4	D	88	THR
4	D	89	ILE
4	D	91	ARG
4	D	99	ARG
4	D	120	ARG
4	D	121	SER
4	D	124	CYS
4	D	125	ILE
4	D	130	ASP
4	D	209	LEU
4	D	226	ILE
4	D	240	LYS
4	D	243	GLU
5	E	30	VAL
5	E	36	GLU
5	E	41	THR
5	E	43	SER
5	E	65	ILE
5	E	78	ARG
5	E	84	PHE
5	E	121	LEU
5	E	125	ARG
5	E	151	CYS
5	E	154	ASN
5	E	192	LEU
5	E	198	LEU
5	E	211	CYS
5	E	225	SER
6	F	30	LEU
6	F	39	LEU
6	F	98	VAL
6	F	101	GLN
6	F	108	GLU
6	F	137	HIS
6	F	139	THR
6	F	201	VAL

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Mol	Chain	Res	Type
6	F	210	LEU
6	F	224	GLN
7	G	30	VAL
7	G	67	TYR
7	G	121	LEU
7	G	122	THR
7	G	148	SER
7	G	151	CYS
7	G	154	ASN
7	G	192	LEU
7	G	196	LEU
7	G	208	VAL
7	G	225	SER
1	H	38	GLU
1	H	39	LEU
1	H	43	LYS
1	H	50	ARG
1	H	57	LYS
1	H	58	ARG
1	H	59	GLU
1	H	68	LEU
1	H	73	ASP
1	H	91	ASN
1	H	99	LEU
1	H	100	THR
1	H	109	VAL
1	H	112	GLU
1	H	121	ASP
1	H	128	LYS
1	H	130	ASP
1	H	131	MET
1	H	139	ASN
1	H	155	ILE
1	H	157	LYS
1	H	166	SER
1	H	174	ARG
1	H	180	CYS
1	H	182	VAL
1	H	183	SER
1	H	198	CYS
1	H	219	TYR
1	H	229	ARG

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Mol	Chain	Res	Type
1	H	234	LYS
1	H	245	ASP
1	H	249	ASN
1	H	252	ASN
1	H	263	ASP
1	H	274	LEU
1	H	275	LYS
1	H	278	LYS
1	H	309	ASN
1	H	313	ILE
1	H	314	LEU
1	H	315	ILE
1	H	320	TYR
1	H	322	ASN
1	H	335	ILE
1	H	345	SER
1	H	361	TYR
2	I	40	VAL
2	I	53	THR
2	I	58	ARG
2	I	97	THR
2	I	106	ARG
2	I	118	HIS
2	I	120	VAL
2	I	123	CYS
2	I	124	ASP
2	I	131	CYS
2	I	149	LYS
2	I	193	SER
3	J	25	THR
3	J	38	VAL
3	J	43	SER
3	J	48	SER
3	J	81	SER
3	J	101	GLU
3	J	110	ASP
3	J	111	ASN
3	J	126	ARG
3	J	140	ASP
3	J	143	LEU
3	J	180	SER
3	J	188	ASP

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Mol	Chain	Res	Type
3	J	192	SER
4	K	24	ASP
4	K	30	LEU
4	K	40	VAL
4	K	42	LYS
4	K	54	GLN
4	K	57	ARG
4	K	84	LYS
4	K	88	THR
4	K	89	ILE
4	K	99	ARG
4	K	129	ASP
4	K	140	VAL
4	K	209	LEU
4	K	226	ILE
4	K	240	LYS
4	K	241	LYS
4	K	242	VAL
4	K	243	GLU
5	L	41	THR
5	L	43	SER
5	L	70	LYS
5	L	77	SER
5	L	78	ARG
5	L	80	SER
5	L	84	PHE
5	L	87	THR
5	L	95	VAL
5	L	98	ASP
5	L	109	ASP
5	L	111	ASN
5	L	121	LEU
5	L	125	ARG
5	L	151	CYS
5	L	154	ASN
5	L	192	LEU
5	L	198	LEU
5	L	211	CYS
5	L	225	SER
6	M	24	ASP
6	M	41	CYS
6	M	42	LYS

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Mol	Chain	Res	Type
6	M	95	GLN
6	M	98	VAL
6	M	101	GLN
6	M	108	GLU
6	M	137	HIS
6	M	139	THR
6	M	142	ILE
6	M	225	THR
6	M	239	VAL
6	M	246	LYS
7	N	53	GLN
7	N	55	LYS
7	N	67	TYR
7	N	102	VAL
7	N	119	THR
7	N	125	ARG
7	N	178	GLU
7	N	182	GLU
7	N	186	LYS
7	N	192	LEU
7	N	196	LEU
7	N	208	VAL
1	O	37	THR
1	O	39	LEU
1	O	50	ARG
1	O	57	LYS
1	O	58	ARG
1	O	59	GLU
1	O	71	GLU
1	O	74	GLU
1	O	84	LYS
1	O	86	SER
1	O	91	ASN
1	O	95	LYS
1	O	100	THR
1	O	109	VAL
1	O	121	ASP
1	O	130	ASP
1	O	139	ASN
1	O	155	ILE
1	O	157	LYS
1	O	166	SER

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Mol	Chain	Res	Type
1	O	170	LYS
1	O	174	ARG
1	O	180	CYS
1	O	186	LYS
1	O	187	PHE
1	O	188	LYS
1	O	198	CYS
1	O	217	ASP
1	O	224	GLN
1	O	229	ARG
1	O	274	LEU
1	O	275	LYS
1	O	278	LYS
1	O	309	ASN
1	O	311	ASN
1	O	313	ILE
1	O	314	LEU
1	O	315	ILE
1	O	316	LYS
1	O	320	TYR
1	O	335	ILE
1	O	345	SER
2	P	26	SER
2	P	40	VAL
2	P	44	SER
2	P	53	THR
2	P	58	ARG
2	P	97	THR
2	P	118	HIS
2	P	120	VAL
2	P	148	THR
2	P	149	LYS
2	P	197	THR
2	P	209	SER
2	P	238	LYS
3	Q	25	THR
3	Q	38	VAL
3	Q	43	SER
3	Q	48	SER
3	Q	79	ARG
3	Q	81	SER
3	Q	101	GLU

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Mol	Chain	Res	Type
3	Q	110	ASP
3	Q	111	ASN
3	Q	122	LEU
3	Q	126	ARG
3	Q	140	ASP
3	Q	143	LEU
3	Q	160	ARG
3	Q	165	GLN
3	Q	167	LYS
3	Q	180	SER
3	Q	188	ASP
3	Q	192	SER
4	R	25	GLU
4	R	30	LEU
4	R	40	VAL
4	R	54	GLN
4	R	57	ARG
4	R	84	LYS
4	R	88	THR
4	R	89	ILE
4	R	91	ARG
4	R	99	ARG
4	R	117	LYS
4	R	120	ARG
4	R	124	CYS
4	R	125	ILE
4	R	130	ASP
4	R	140	VAL
4	R	171	CYS
4	R	209	LEU
4	R	226	ILE
4	R	227	CYS
4	R	240	LYS
4	R	241	LYS
4	R	242	VAL
4	R	243	GLU
5	S	30	VAL
5	S	39	LYS
5	S	55	LYS
5	S	70	LYS
5	S	78	ARG
5	S	84	PHE

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Mol	Chain	Res	Type
5	S	121	LEU
5	S	122	THR
5	S	123	VAL
5	S	142	LEU
5	S	151	CYS
5	S	154	ASN
5	S	178	GLU
5	S	192	LEU
5	S	202	ASP
5	S	211	CYS
5	S	224	LYS
6	T	24	ASP
6	T	50	SER
6	T	84	LYS
6	T	101	GLN
6	T	108	GLU
6	T	139	THR
6	T	142	ILE
6	T	149	LYS
6	T	210	LEU
6	T	224	GLN
6	T	225	THR
7	U	30	VAL
7	U	39	LYS
7	U	67	TYR
7	U	98	GLU
7	U	112	ASN
7	U	122	THR
7	U	123	VAL
7	U	125	ARG
7	U	151	CYS
7	U	154	ASN
7	U	192	LEU
7	U	196	LEU
7	U	200	LYS
7	U	208	VAL
7	U	216	GLN
1	V	31	ARG
1	V	39	LEU
1	V	50	ARG
1	V	57	LYS
1	V	58	ARG

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Mol	Chain	Res	Type
1	V	59	GLU
1	V	68	LEU
1	V	71	GLU
1	V	72	GLU
1	V	84	LYS
1	V	91	ASN
1	V	95	LYS
1	V	99	LEU
1	V	100	THR
1	V	109	VAL
1	V	124	PHE
1	V	127	ARG
1	V	129	LYS
1	V	130	ASP
1	V	139	ASN
1	V	155	ILE
1	V	157	LYS
1	V	166	SER
1	V	170	LYS
1	V	174	ARG
1	V	180	CYS
1	V	185	TYR
1	V	186	LYS
1	V	198	CYS
1	V	217	ASP
1	V	224	GLN
1	V	229	ARG
1	V	245	ASP
1	V	247	ILE
1	V	252	ASN
1	V	274	LEU
1	V	275	LYS
1	V	309	ASN
1	V	313	ILE
1	V	314	LEU
1	V	315	ILE
1	V	316	LYS
1	V	320	TYR
1	V	322	ASN
1	V	335	ILE
1	V	337	GLU
1	V	345	SER

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Mol	Chain	Res	Type
1	V	361	TYR
2	W	26	SER
2	W	40	VAL
2	W	53	THR
2	W	58	ARG
2	W	97	THR
2	W	106	ARG
2	W	118	HIS
2	W	131	CYS
2	W	145	SER
2	W	149	LYS
2	W	209	SER
2	W	211	SER
2	W	239	VAL
3	X	25	THR
3	X	38	VAL
3	X	43	SER
3	X	81	SER
3	X	101	GLU
3	X	108	SER
3	X	110	ASP
3	X	111	ASN
3	X	126	ARG
3	X	140	ASP
3	X	143	LEU
3	X	160	ARG
3	X	165	GLN
3	X	167	LYS
3	X	180	SER
3	X	185	ASP
3	X	188	ASP
3	X	189	SER
3	X	192	SER
3	X	228	ASN
3	X	229	ARG
4	Y	30	LEU
4	Y	40	VAL
4	Y	41	CYS
4	Y	54	GLN
4	Y	57	ARG
4	Y	62	LYS
4	Y	84	LYS

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Mol	Chain	Res	Type
4	Y	88	THR
4	Y	89	ILE
4	Y	91	ARG
4	Y	99	ARG
4	Y	117	LYS
4	Y	120	ARG
4	Y	124	CYS
4	Y	125	ILE
4	Y	130	ASP
4	Y	140	VAL
4	Y	209	LEU
4	Y	226	ILE
4	Y	240	LYS
4	Y	241	LYS
4	Y	242	VAL
4	Y	243	GLU
5	Z	30	VAL
5	Z	39	LYS
5	Z	55	LYS
5	Z	65	ILE
5	Z	69	ASN
5	Z	70	LYS
5	Z	78	ARG
5	Z	84	PHE
5	Z	108	ARG
5	Z	109	ASP
5	Z	111	ASN
5	Z	124	LEU
5	Z	125	ARG
5	Z	151	CYS
5	Z	154	ASN
5	Z	186	LYS
5	Z	192	LEU
5	Z	198	LEU
5	Z	211	CYS
5	Z	225	SER
6	a	62	LYS
6	a	78	LEU
6	a	80	THR
6	a	86	ARG
6	a	88	THR
6	a	101	GLN

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Mol	Chain	Res	Type
6	a	106	ARG
6	a	110	THR
6	a	120	ASP
6	a	137	HIS
6	a	145	SER
6	a	147	SER
6	a	149	LYS
6	a	182	VAL
7	b	31	SER
7	b	56	SER
7	b	62	VAL
7	b	87	THR
7	b	112	ASN
7	b	119	THR
7	b	121	LEU
7	b	122	THR
7	b	124	LEU
7	b	125	ARG
7	b	140	GLU
7	b	150	VAL
7	b	155	ASN
7	b	162	LYS
7	b	164	GLN
7	b	166	LYS
7	b	168	ASP
7	b	171	LEU
7	b	185	SER
7	b	186	LYS
7	b	187	ASP
7	b	192	LEU
7	b	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	76	HIS
1	A	139	ASN
1	A	224	GLN
1	A	260	HIS
1	A	287	ASN
1	A	311	ASN

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Mol	Chain	Res	Type
1	A	348	GLN
2	B	196	HIS
2	B	232	HIS
3	C	142	GLN
3	C	155	ASN
3	C	156	ASN
5	E	68	ASN
5	E	141	GLN
7	G	53	GLN
1	H	45	ASN
1	H	126	ASN
1	H	139	ASN
1	H	146	ASN
1	H	202	HIS
1	H	249	ASN
1	H	254	ASN
1	H	309	ASN
1	H	311	ASN
1	H	348	GLN
1	H	360	ASN
2	I	59	GLN
2	I	101	GLN
2	I	121	ASN
2	I	137	HIS
2	I	203	GLN
2	I	232	HIS
3	J	55	GLN
3	J	178	GLN
5	L	33	ASN
5	L	112	ASN
5	L	141	GLN
7	N	53	GLN
1	O	126	ASN
1	O	139	ASN
1	O	146	ASN
1	O	254	ASN
1	O	309	ASN
1	O	348	GLN
1	O	360	ASN
2	P	101	GLN
2	P	121	ASN
2	P	137	HIS

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Mol	Chain	Res	Type
2	P	232	HIS
3	Q	228	ASN
6	T	93	ASN
6	T	203	GLN
7	U	112	ASN
1	V	32	HIS
1	V	139	ASN
1	V	146	ASN
1	V	224	GLN
1	V	246	ASN
1	V	254	ASN
1	V	309	ASN
1	V	311	ASN
1	V	348	GLN
1	V	354	HIS
1	V	360	ASN
2	W	101	GLN
2	W	232	HIS
3	X	142	GLN
3	X	156	ASN
3	X	165	GLN
5	Z	69	ASN
5	Z	112	ASN
5	Z	141	GLN
7	b	53	GLN
7	b	112	ASN
7	b	141	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	328/343 (95%)	-0.07	3 (0%) 84 84	76, 140, 180, 206	0
1	H	321/343 (93%)	-0.02	8 (2%) 57 53	122, 149, 182, 203	0
1	O	327/343 (95%)	-0.13	3 (0%) 84 84	125, 151, 182, 196	0
1	V	325/343 (94%)	-0.13	6 (1%) 68 65	139, 169, 200, 214	0
2	B	221/230 (96%)	-0.15	6 (2%) 54 51	123, 147, 178, 193	0
2	I	202/230 (87%)	-0.13	4 (1%) 65 63	119, 146, 248, 251	0
2	P	159/230 (69%)	-0.06	5 (3%) 49 47	141, 168, 274, 277	0
2	W	218/230 (94%)	-0.22	6 (2%) 53 50	142, 168, 219, 229	0
3	C	207/210 (98%)	-0.20	3 (1%) 75 74	118, 151, 189, 201	0
3	J	192/210 (91%)	-0.12	5 (2%) 56 52	123, 151, 258, 268	0
3	Q	129/210 (61%)	0.10	10 (7%) 13 12	134, 162, 271, 278	0
3	X	206/210 (98%)	-0.08	5 (2%) 59 55	140, 190, 222, 233	0
4	D	136/230 (59%)	0.27	10 (7%) 14 14	154, 190, 243, 257	1 (0%)
4	K	125/230 (54%)	-0.33	2 (1%) 72 69	159, 189, 212, 216	1 (0%)
4	R	126/230 (54%)	-0.22	5 (3%) 38 35	167, 203, 227, 233	1 (0%)
4	Y	136/230 (59%)	0.38	18 (13%) 3 3	181, 207, 264, 283	1 (0%)
5	E	104/209 (49%)	-0.02	3 (2%) 51 50	157, 185, 199, 283	2 (1%)
5	L	103/209 (49%)	0.01	6 (5%) 23 22	161, 188, 208, 247	2 (1%)
5	S	98/209 (46%)	0.09	7 (7%) 16 15	191, 205, 219, 279	2 (2%)
5	Z	103/209 (49%)	0.32	12 (11%) 4 4	184, 211, 230, 298	2 (1%)
6	F	129/321 (40%)	-0.08	4 (3%) 49 47	143, 181, 202, 205	0
6	M	155/321 (48%)	-0.05	5 (3%) 47 45	133, 153, 203, 252	0
6	T	146/321 (45%)	-0.22	4 (2%) 54 51	170, 194, 241, 251	0
6	a	128/321 (39%)	-0.42	2 (1%) 72 69	181, 203, 209, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	G	101/209 (48%)	-0.18	3 (2%) 50 48	146, 162, 178, 184	0
7	N	206/209 (98%)	-0.18	9 (4%) 34 32	149, 183, 211, 219	0
7	U	160/209 (76%)	-0.08	7 (4%) 34 32	168, 194, 251, 256	0
7	b	139/209 (66%)	-0.21	6 (4%) 35 33	180, 193, 236, 242	0
All	All	4930/7008 (70%)	-0.09	167 (3%) 45 42	76, 172, 228, 298	12 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	141	GLN	27.1
4	Y	242	VAL	16.7
5	S	126	THR	16.1
4	D	242	VAL	15.1
5	Z	142	LEU	12.8
5	Z	141	GLN	11.0
4	D	154	PRO	10.9
5	L	141	GLN	10.1
4	K	242	VAL	9.2
5	E	142	LEU	8.6
5	L	142	LEU	8.5
5	S	142	LEU	8.4
5	Z	126	THR	8.3
7	N	172	GLN	8.1
4	Y	153	PHE	7.6
5	Z	38	VAL	6.8
5	S	127	VAL	6.7
3	X	133	VAL	6.4
4	Y	151	SER	6.3
5	Z	92	ILE	6.3
7	b	149	VAL	6.1
4	Y	148	LYS	5.8
6	T	222	GLY	5.7
2	I	226	TYR	5.7
5	Z	125	ARG	5.6
5	L	127	VAL	5.6
3	Q	204	TYR	5.5
4	Y	152	VAL	5.2
2	W	169	ALA	5.0
5	S	123	VAL	5.0
7	U	103	TYR	4.7
4	D	153	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
5	Z	103	TYR	4.5
1	O	320	TYR	4.5
4	Y	147	THR	4.4
1	V	187	PHE	4.4
4	D	55	TRP	4.2
2	I	182	VAL	4.2
7	U	211	CYS	4.1
4	Y	56	VAL	4.1
4	R	242	VAL	4.0
6	T	64	LEU	3.9
1	H	340	ALA	3.8
2	W	213	VAL	3.8
7	b	90	LEU	3.8
2	W	167	THR	3.7
4	Y	114	TYR	3.7
3	Q	161	GLU	3.7
7	b	40	ILE	3.6
2	B	102	LEU	3.6
6	a	136	GLY	3.6
7	N	171	LEU	3.6
3	Q	202	ALA	3.6
2	B	191	LEU	3.5
3	J	136	PHE	3.5
3	Q	63	VAL	3.4
7	N	166	LYS	3.4
4	Y	37	LEU	3.4
4	Y	64	LEU	3.4
5	Z	127	VAL	3.3
4	R	30	LEU	3.3
6	M	158	PRO	3.3
2	I	210	LEU	3.2
3	X	176	ASN	3.2
1	H	239	PHE	3.2
1	A	124	PHE	3.2
3	J	208	LYS	3.2
7	b	156	PHE	3.2
4	D	56	VAL	3.1
4	R	31	GLN	3.1
1	H	283	VAL	3.1
3	Q	163	LYS	3.1
3	Q	223	VAL	3.1
6	a	39	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	305	ILE	3.1
2	P	23	LEU	3.0
6	M	116	THR	3.0
4	D	114	TYR	3.0
4	R	141	ILE	3.0
7	U	136	PRO	3.0
5	L	124	LEU	3.0
7	b	38	VAL	2.9
2	W	168	ALA	2.9
2	B	113	TYR	2.9
2	P	27	GLY	2.9
3	Q	56	LYS	2.9
4	Y	30	LEU	2.9
6	F	98	VAL	2.8
7	G	64	VAL	2.8
3	J	183	GLU	2.8
4	Y	141	ILE	2.8
6	F	113	TYR	2.8
1	V	54	PHE	2.7
3	C	227	PHE	2.7
2	B	101	GLN	2.7
2	P	215	THR	2.7
4	Y	53	MET	2.7
7	b	150	VAL	2.7
4	Y	46	PHE	2.7
6	F	64	LEU	2.7
4	Y	55	TRP	2.7
5	Z	115	PHE	2.6
4	D	53	MET	2.6
6	T	168	ALA	2.6
4	D	151	SER	2.6
4	D	134	TRP	2.6
7	U	104	TYR	2.6
1	V	221	LEU	2.6
5	S	103	TYR	2.6
4	Y	139	GLU	2.6
1	O	161	LEU	2.6
5	Z	53	GLN	2.5
7	N	220	SER	2.5
5	L	126	THR	2.5
3	Q	160	ARG	2.5
3	C	137	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	N	222	VAL	2.4
5	S	101	ALA	2.4
1	H	237	LEU	2.4
5	E	23	ALA	2.4
3	C	168	VAL	2.4
3	X	132	SER	2.3
3	Q	222	PRO	2.3
1	A	232	ILE	2.3
6	M	134	ALA	2.3
4	D	46	PHE	2.3
1	V	261	GLU	2.3
6	M	53	MET	2.3
2	P	214	VAL	2.3
1	V	63	ILE	2.3
7	N	152	LEU	2.3
7	U	207	LYS	2.3
4	Y	134	TRP	2.3
5	S	141	GLN	2.3
7	N	219	SER	2.3
3	X	181	VAL	2.3
4	R	143	SER	2.2
6	M	224	GLN	2.2
4	Y	113	TYR	2.2
7	U	79	PHE	2.2
2	W	173	LEU	2.2
1	H	49	ILE	2.2
7	N	162	LYS	2.2
3	J	137	PRO	2.2
4	K	64	LEU	2.2
2	P	175	LYS	2.2
2	B	214	VAL	2.2
1	H	124	PHE	2.1
1	O	93	LEU	2.1
5	Z	90	LEU	2.1
3	Q	227	PHE	2.1
7	N	210	ALA	2.1
1	A	333	VAL	2.1
1	V	333	VAL	2.1
2	W	214	VAL	2.1
7	U	135	PHE	2.1
7	G	30	VAL	2.1
2	B	90	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	162	ALA	2.1
6	F	148	THR	2.1
3	X	148	ALA	2.1
5	L	116	GLY	2.1
7	G	99	ASP	2.1
1	H	95	LYS	2.0
6	T	65	GLU	2.0
5	Z	81	GLY	2.0
2	I	231	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.