Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2017 – 04:49 AM EST

PDB ID	:	5KOV
Title	:	Crystal structure of the human astrovirus 2 capsid protein spike in complex with a single chain variable fragment of an astrovirus neutralizing antibody at 3.24-A resolution
Authors	:	Bogdanoff, W.A.; DuBois, R.M.
Deposited on	:	2016-07-01
Resolution	:	3.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

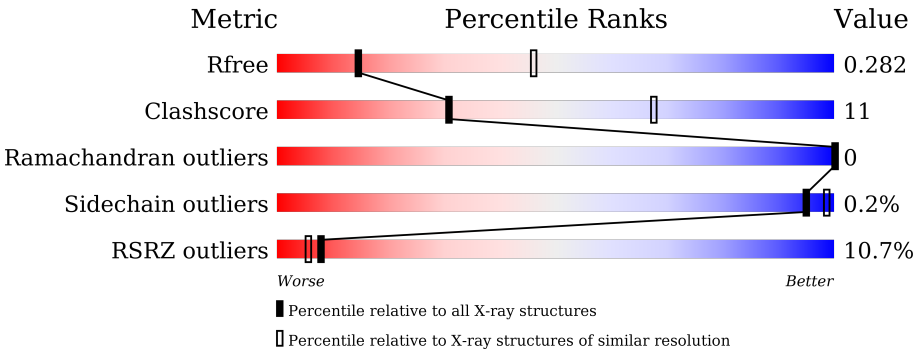
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	228	5% 69% 25% 5%
1	B	228	10% 74% 22% .
1	G	228	13% 68% 28% .
1	H	228	6% 69% 25% 5%
1	M	228	11% 74% 21% 5%
1	N	228	5% 74% 21% 5%

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Mol	Chain	Length	Quality of chain
1	S	228	8% 75% 20%
1	T	228	14% 70% 25% 5%
2	C	251	4% 66% 23% 11%
2	E	251	9% 65% 24% 11%
2	I	251	15% 70% 19% 10%
2	K	251	5% 68% 21% 11%
2	O	251	10% 60% 24% 16%
2	Q	251	8% 29% 8% 63%
2	U	251	10% 67% 22% 12%
2	W	251	14% 30% 12% 58%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25943 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 Capsid polyprotein VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1745	1118	290	328	9			
1	B	218	Total	C	N	O	S	0	0	0
			1756	1125	292	330	9			
1	H	216	Total	C	N	O	S	0	0	0
			1745	1118	290	328	9			
1	G	219	Total	C	N	O	S	0	0	0
			1760	1127	293	331	9			
1	N	217	Total	C	N	O	S	0	0	0
			1750	1121	291	329	9			
1	M	216	Total	C	N	O	S	0	0	0
			1745	1118	290	328	9			
1	S	218	Total	C	N	O	S	0	0	0
			1755	1124	292	330	9			
1	T	216	Total	C	N	O	S	0	0	0
			1745	1118	290	328	9			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	MET	-	initiating methionine	UNP Q82446
A	428	GLY	-	expression tag	UNP Q82446
A	645	ALA	-	expression tag	UNP Q82446
A	646	ALA	-	expression tag	UNP Q82446
A	647	ALA	-	expression tag	UNP Q82446
A	648	GLU	-	expression tag	UNP Q82446
A	649	LEU	-	expression tag	UNP Q82446
A	650	ALA	-	expression tag	UNP Q82446
A	651	LEU	-	expression tag	UNP Q82446
A	652	VAL	-	expression tag	UNP Q82446
A	653	PRO	-	expression tag	UNP Q82446
A	654	ARG	-	expression tag	UNP Q82446
B	427	MET	-	initiating methionine	UNP Q82446

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Chain	Residue	Modelled	Actual	Comment	Reference
B	428	GLY	-	expression tag	UNP Q82446
B	645	ALA	-	expression tag	UNP Q82446
B	646	ALA	-	expression tag	UNP Q82446
B	647	ALA	-	expression tag	UNP Q82446
B	648	GLU	-	expression tag	UNP Q82446
B	649	LEU	-	expression tag	UNP Q82446
B	650	ALA	-	expression tag	UNP Q82446
B	651	LEU	-	expression tag	UNP Q82446
B	652	VAL	-	expression tag	UNP Q82446
B	653	PRO	-	expression tag	UNP Q82446
B	654	ARG	-	expression tag	UNP Q82446
H	427	MET	-	initiating methionine	UNP Q82446
H	428	GLY	-	expression tag	UNP Q82446
H	645	ALA	-	expression tag	UNP Q82446
H	646	ALA	-	expression tag	UNP Q82446
H	647	ALA	-	expression tag	UNP Q82446
H	648	GLU	-	expression tag	UNP Q82446
H	649	LEU	-	expression tag	UNP Q82446
H	650	ALA	-	expression tag	UNP Q82446
H	651	LEU	-	expression tag	UNP Q82446
H	652	VAL	-	expression tag	UNP Q82446
H	653	PRO	-	expression tag	UNP Q82446
H	654	ARG	-	expression tag	UNP Q82446
G	427	MET	-	initiating methionine	UNP Q82446
G	428	GLY	-	expression tag	UNP Q82446
G	645	ALA	-	expression tag	UNP Q82446
G	646	ALA	-	expression tag	UNP Q82446
G	647	ALA	-	expression tag	UNP Q82446
G	648	GLU	-	expression tag	UNP Q82446
G	649	LEU	-	expression tag	UNP Q82446
G	650	ALA	-	expression tag	UNP Q82446
G	651	LEU	-	expression tag	UNP Q82446
G	652	VAL	-	expression tag	UNP Q82446
G	653	PRO	-	expression tag	UNP Q82446
G	654	ARG	-	expression tag	UNP Q82446
N	427	MET	-	initiating methionine	UNP Q82446
N	428	GLY	-	expression tag	UNP Q82446
N	645	ALA	-	expression tag	UNP Q82446
N	646	ALA	-	expression tag	UNP Q82446
N	647	ALA	-	expression tag	UNP Q82446
N	648	GLU	-	expression tag	UNP Q82446
N	649	LEU	-	expression tag	UNP Q82446

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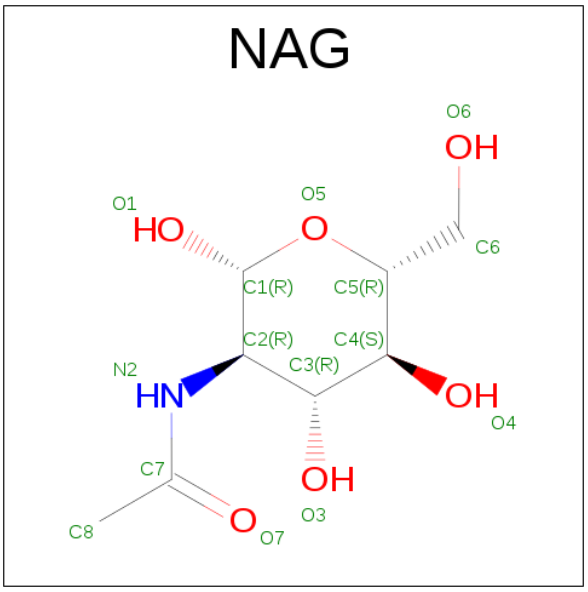
Chain	Residue	Modelled	Actual	Comment	Reference
N	650	ALA	-	expression tag	UNP Q82446
N	651	LEU	-	expression tag	UNP Q82446
N	652	VAL	-	expression tag	UNP Q82446
N	653	PRO	-	expression tag	UNP Q82446
N	654	ARG	-	expression tag	UNP Q82446
M	427	MET	-	initiating methionine	UNP Q82446
M	428	GLY	-	expression tag	UNP Q82446
M	645	ALA	-	expression tag	UNP Q82446
M	646	ALA	-	expression tag	UNP Q82446
M	647	ALA	-	expression tag	UNP Q82446
M	648	GLU	-	expression tag	UNP Q82446
M	649	LEU	-	expression tag	UNP Q82446
M	650	ALA	-	expression tag	UNP Q82446
M	651	LEU	-	expression tag	UNP Q82446
M	652	VAL	-	expression tag	UNP Q82446
M	653	PRO	-	expression tag	UNP Q82446
M	654	ARG	-	expression tag	UNP Q82446
S	427	MET	-	initiating methionine	UNP Q82446
S	428	GLY	-	expression tag	UNP Q82446
S	645	ALA	-	expression tag	UNP Q82446
S	646	ALA	-	expression tag	UNP Q82446
S	647	ALA	-	expression tag	UNP Q82446
S	648	GLU	-	expression tag	UNP Q82446
S	649	LEU	-	expression tag	UNP Q82446
S	650	ALA	-	expression tag	UNP Q82446
S	651	LEU	-	expression tag	UNP Q82446
S	652	VAL	-	expression tag	UNP Q82446
S	653	PRO	-	expression tag	UNP Q82446
S	654	ARG	-	expression tag	UNP Q82446
T	427	MET	-	initiating methionine	UNP Q82446
T	428	GLY	-	expression tag	UNP Q82446
T	645	ALA	-	expression tag	UNP Q82446
T	646	ALA	-	expression tag	UNP Q82446
T	647	ALA	-	expression tag	UNP Q82446
T	648	GLU	-	expression tag	UNP Q82446
T	649	LEU	-	expression tag	UNP Q82446
T	650	ALA	-	expression tag	UNP Q82446
T	651	LEU	-	expression tag	UNP Q82446
T	652	VAL	-	expression tag	UNP Q82446
T	653	PRO	-	expression tag	UNP Q82446
T	654	ARG	-	expression tag	UNP Q82446

- Molecule 2 is a protein called PL-2 scFv chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	E	224	Total	C	N	O	S	0	0	0
			1727	1087	288	345	7			
2	K	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	I	225	Total	C	N	O	S	0	0	0
			1738	1093	292	346	7			
2	Q	93	Total	C	N	O	S	0	0	0
			746	482	122	138	4			
2	O	212	Total	C	N	O	S	0	0	0
			1651	1043	276	325	7			
2	W	105	Total	C	N	O	S	0	0	0
			853	548	141	159	5			
2	U	222	Total	C	N	O	S	0	0	0
			1719	1082	289	341	7			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



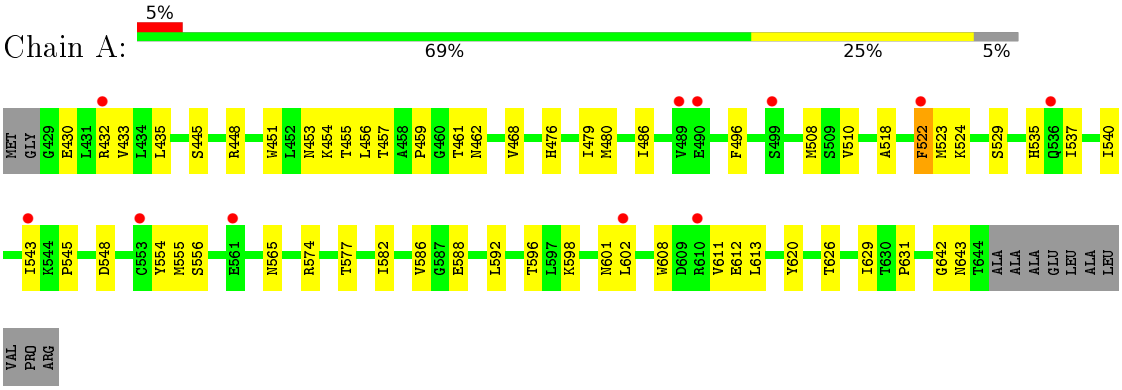
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

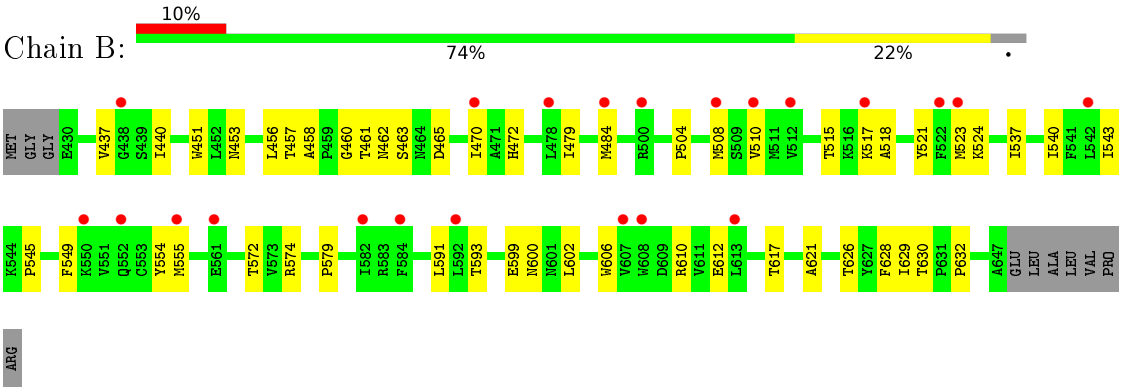
- Molecule 1: Capsid polyprotein VP90

Chain A:



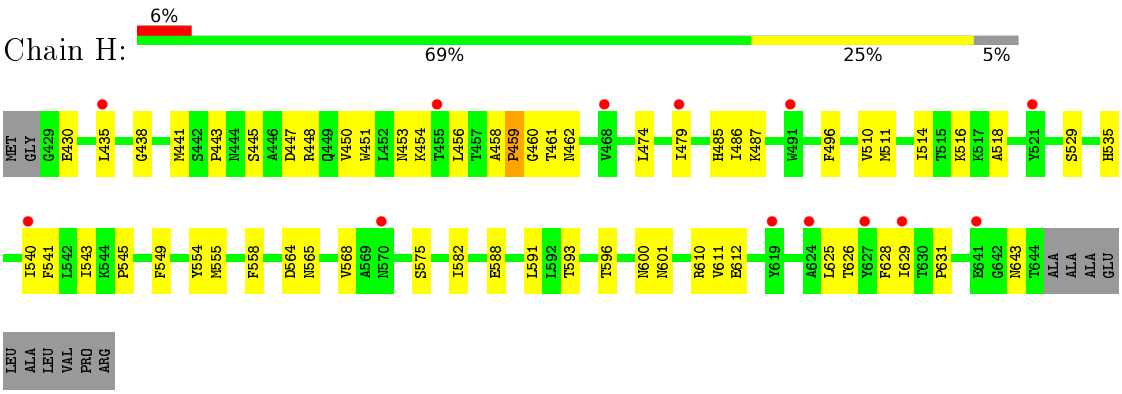
- Molecule 1: Capsid polyprotein VP90

Chain B:



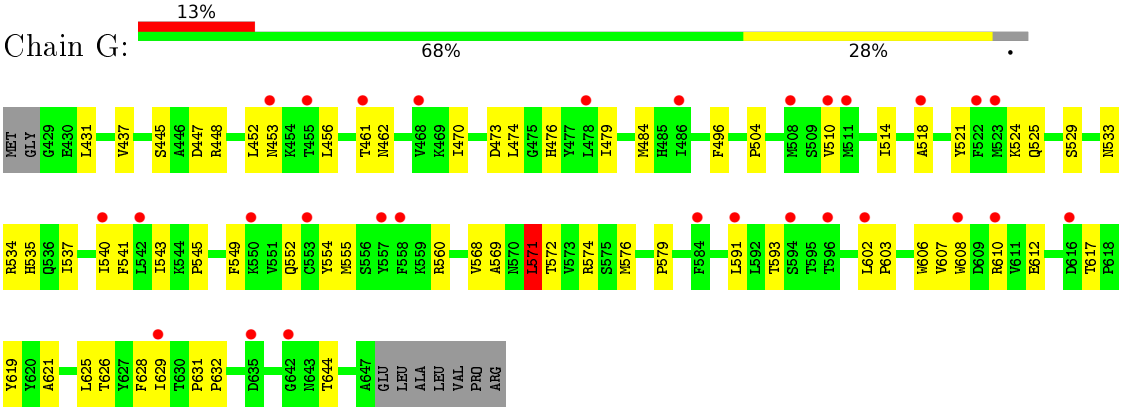
- Molecule 1: Capsid polyprotein VP90

Chain H:



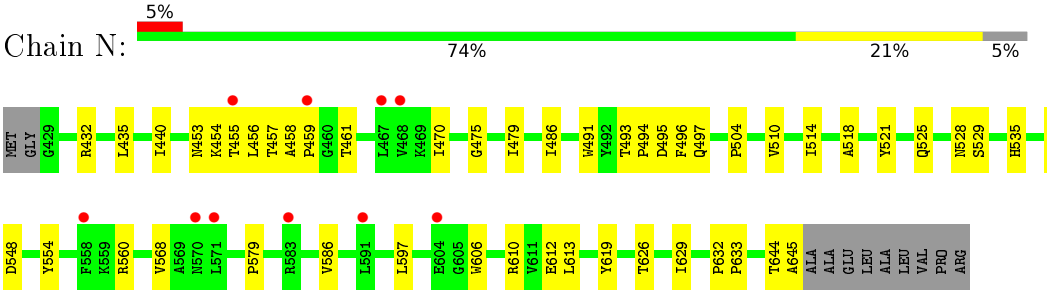
- Molecule 1: Capsid polyprotein VP90

Chain G:



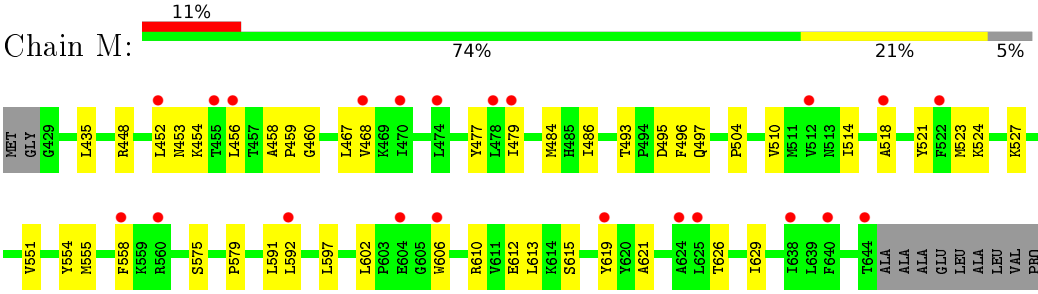
- Molecule 1: Capsid polyprotein VP90

Chain N:



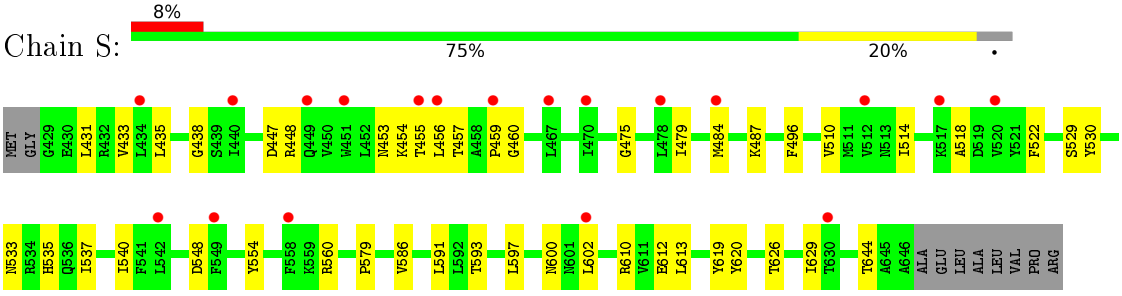
- Molecule 1: Capsid polyprotein VP90

Chain M:



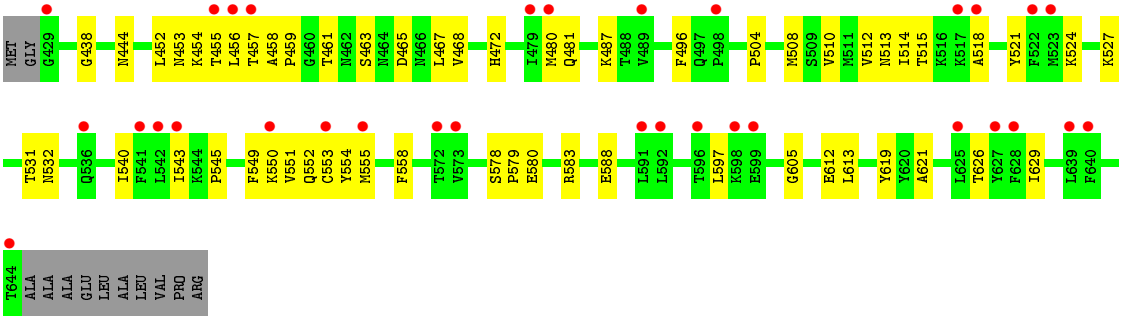
- Molecule 1: Capsid polyprotein VP90

Chain S:



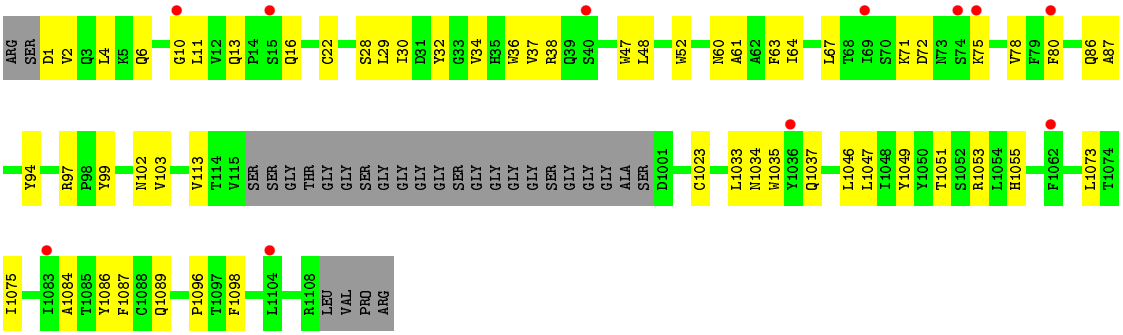
- Molecule 1: Capsid polyprotein VP90

Chain T:



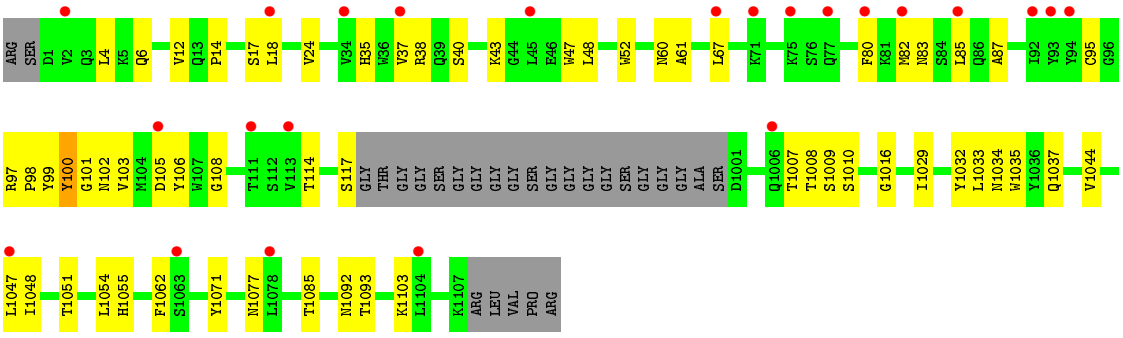
- Molecule 2: PL-2 scFv chain

Chain C:



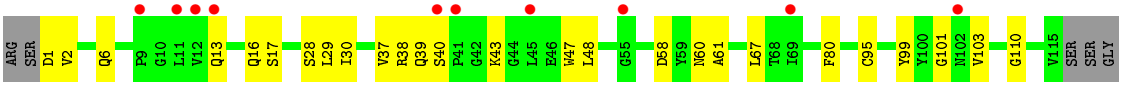
- Molecule 2: PL-2 scFv chain

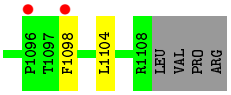
Chain E:



- Molecule 2: PL-2 scFv chain

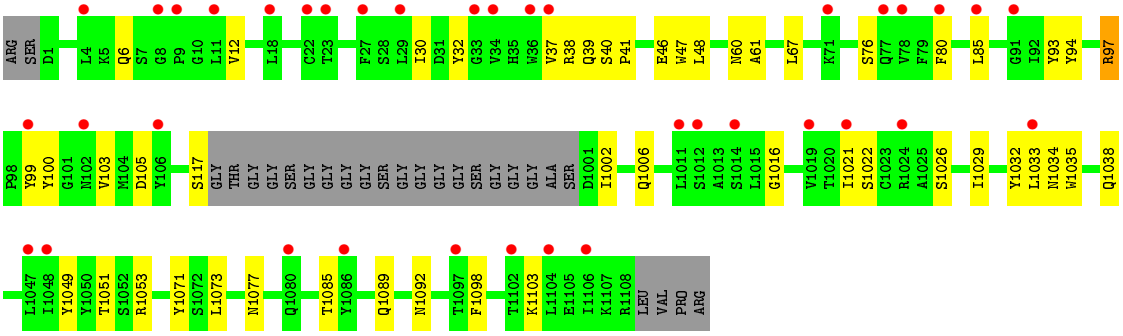
Chain K:





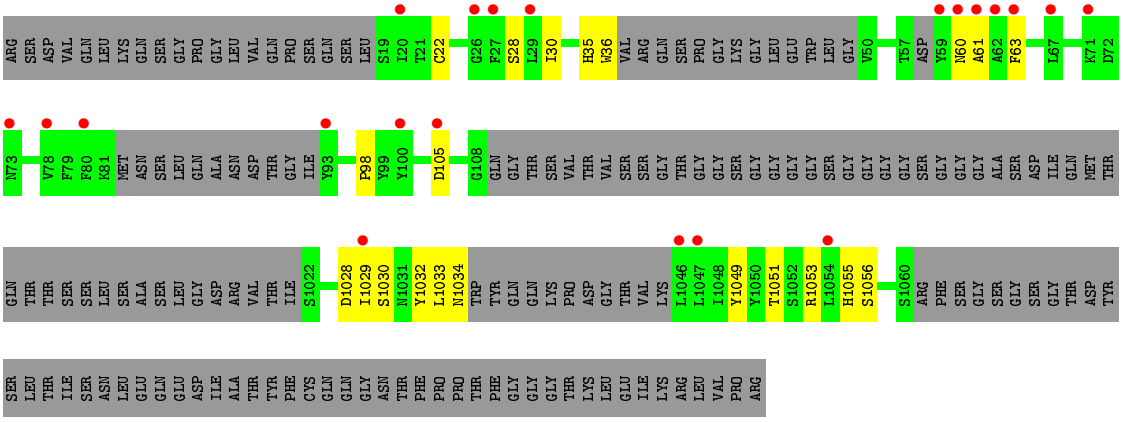
- Molecule 2: PL-2 scFv chain

Chain I:



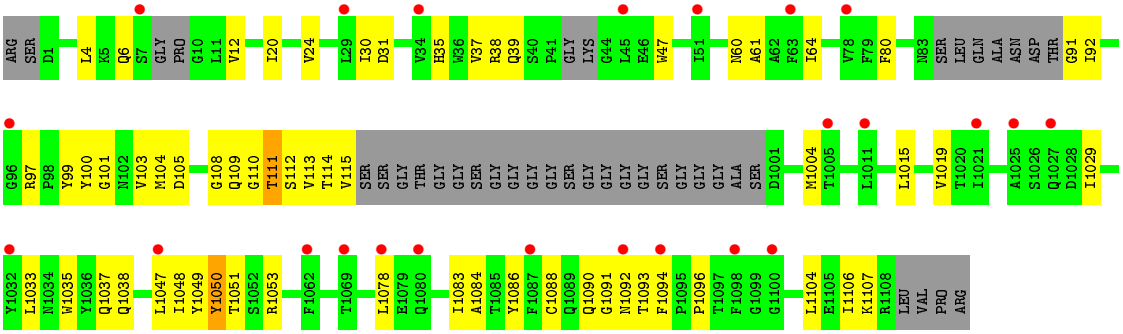
- Molecule 2: PL-2 scFv chain

Chain Q:



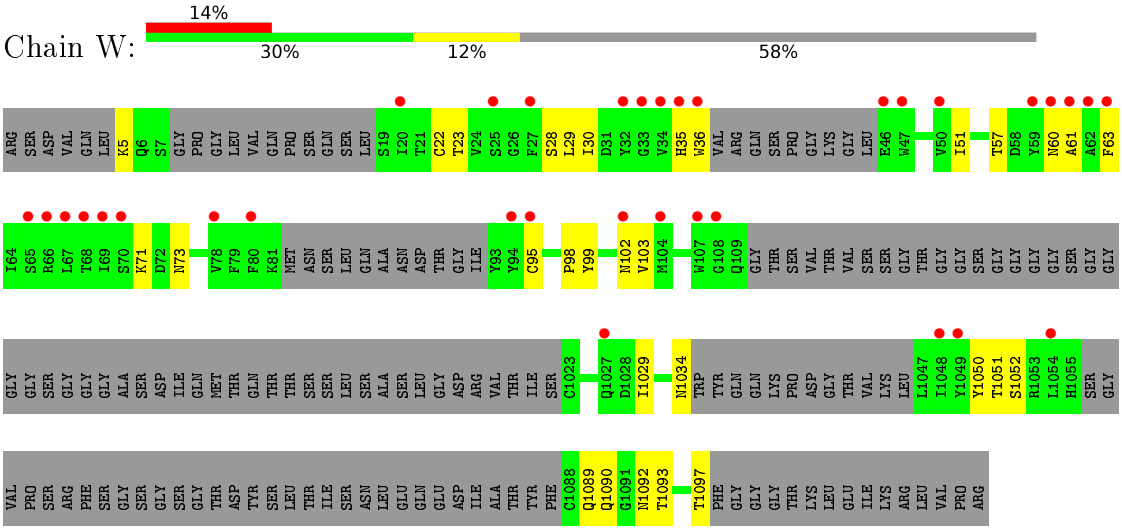
- Molecule 2: PL-2 scFv chain

Chain O:



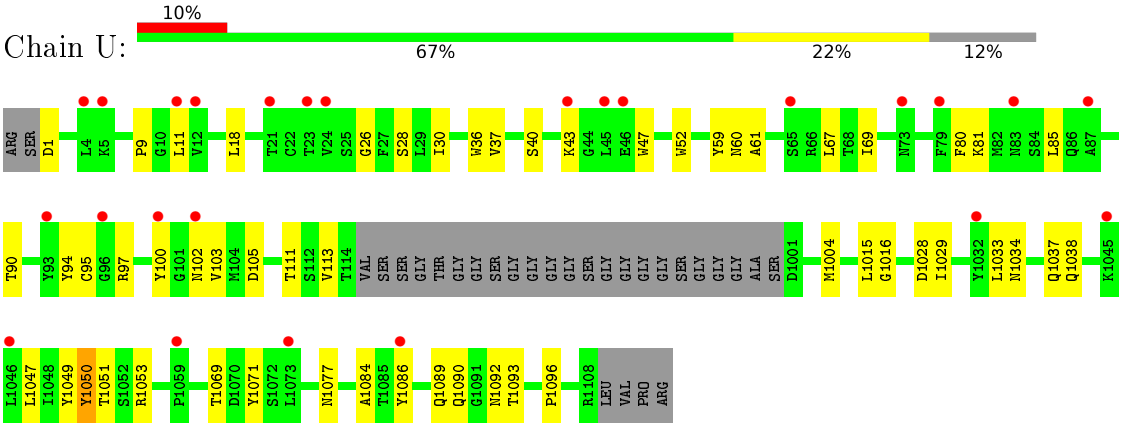
- Molecule 2: PL-2 scFv chain

Chain W:



- Molecule 2: PL-2 scFv chain

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	200.00Å 200.00Å 157.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	88.1 (50.00-3.25) 81.5 (50.00-3.24)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.241 , 0.288 0.236 , 0.282	Depositor DCC
R_{free} test set	3851 reflections (4.82%)	DCC
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25943	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NAG

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	0.28	0/1792	0.54	1/2441 (0.0%)
1	B	0.30	0/1803	0.53	0/2457
1	G	0.30	0/1807	0.55	1/2462 (0.0%)
1	H	0.29	0/1792	0.52	0/2441
1	M	0.27	0/1792	0.53	0/2441
1	N	0.28	0/1797	0.51	0/2448
1	S	0.28	0/1802	0.55	0/2455
1	T	0.29	0/1792	0.53	0/2441
2	C	0.36	1/1765 (0.1%)	0.54	0/2395
2	E	0.27	0/1766	0.52	0/2397
2	I	0.29	0/1777	0.54	1/2411 (0.0%)
2	K	0.30	0/1765	0.53	0/2395
2	O	0.27	0/1686	0.53	0/2283
2	Q	0.24	0/764	0.48	0/1031
2	U	0.27	0/1758	0.52	0/2385
2	W	0.25	0/874	0.47	0/1179
All	All	0.29	1/26532 (0.0%)	0.53	3/36062 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	O	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1087	PHE	CG-CD2	-5.03	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	571	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	601	ASN	C-N-CA	5.64	135.81	121.70
2	I	97	ARG	NE-CZ-NH1	-5.45	117.57	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	459	PRO	Peptide
2	O	111	THR	Peptide

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	1745	0	1709	43	0
1	B	1756	0	1721	34	0
1	G	1760	0	1724	46	0
1	H	1745	0	1709	44	0
1	M	1745	0	1709	36	0
1	N	1750	0	1714	35	0
1	S	1755	0	1719	32	0
1	T	1745	0	1709	52	0
2	C	1726	0	1661	38	0
2	E	1727	0	1658	48	0
2	I	1738	0	1671	34	0
2	K	1726	0	1661	37	0
2	O	1651	0	1587	49	0
2	Q	746	0	701	14	0
2	U	1719	0	1653	45	0
2	W	853	0	788	22	0
3	C	14	0	13	1	0
3	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	14	0	13	0	0
3	K	14	0	13	1	0
All	All	25943	0	25146	555	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 11.

All (555) 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:H:514:ILE:HD11	2:K:30:ILE:HB	1.54	0.90
1:T:554:TYR:HA	1:T:579:PRO:HA	1.55	0.89
1:S:484:MET:HB3	1:S:591:LEU:HB3	1.56	0.88
1:B:461:THR:HG22	1:B:463:SER:H	1.42	0.84
1:G:461:THR:HG22	1:G:462:ASN:H	1.42	0.83
1:T:552:GLN:HE21	1:T:579:PRO:HB2	1.42	0.82
1:T:510:VAL:HB	1:T:518:ALA:HB3	1.64	0.80
1:A:461:THR:HG21	2:C:52:TRP:CZ2	2.19	0.78
1:N:493:THR:HG22	1:N:497:GLN:H	1.49	0.77
1:H:448:ARG:HG2	1:G:568:VAL:HG12	1.65	0.77
1:M:493:THR:HG22	1:M:497:GLN:H	1.51	0.76
1:M:510:VAL:HB	1:M:518:ALA:HB3	1.67	0.76
2:O:37:VAL:HG12	2:O:47:TRP:HA	1.70	0.74
2:E:37:VAL:HG12	2:E:47:TRP:HA	1.69	0.74
2:O:1033:LEU:HD21	2:O:1088:CYS:HB2	1.69	0.73
1:S:510:VAL:HB	1:S:518:ALA:HB3	1.71	0.71
2:U:37:VAL:HG12	2:U:47:TRP:HA	1.72	0.71
2:K:1037:GLN:HB2	2:K:1047:LEU:HD11	1.71	0.71
2:C:102:ASN:ND2	2:C:1096:PRO:HG3	2.06	0.71
1:H:510:VAL:HB	1:H:518:ALA:HB3	1.72	0.71
1:G:484:MET:HB2	1:G:591:LEU:HB3	1.72	0.70
1:T:552:GLN:NE2	1:T:579:PRO:HB2	2.05	0.70
2:U:1050:TYR:CE1	1:T:579:PRO:HD2	2.25	0.70
2:U:67:LEU:HD21	2:U:80:PHE:CE1	2.27	0.70
1:M:456:LEU:HG	1:M:612:GLU:HB3	1.74	0.69
1:T:453:ASN:ND2	1:T:553:CYS:HB3	2.08	0.69
1:N:510:VAL:HB	1:N:518:ALA:HB3	1.75	0.69
1:A:522:PHE:HE2	1:A:642:GLY:HA3	1.58	0.68
1:H:568:VAL:HG12	1:G:448:ARG:HG2	1.73	0.68
1:N:493:THR:HG23	1:N:495:ASP:H	1.56	0.68
2:O:92:ILE:HG23	2:O:112:SER:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:459:PRO:HD3	1:S:554:TYR:CZ	2.29	0.67
1:T:453:ASN:HB3	1:T:481:GLN:HA	1.75	0.67
2:K:6:GLN:NE2	2:K:95:CYS:SG	2.68	0.67
1:H:443:PRO:O	1:H:448:ARG:NH1	2.27	0.67
2:E:14:PRO:HG3	2:E:117:SER:H	1.60	0.67
1:T:468:VAL:HG23	1:T:551:VAL:HG21	1.76	0.67
2:W:29:LEU:HD21	2:W:71:LYS:HD2	1.77	0.66
1:T:458:ALA:HB3	1:T:461:THR:HB	1.77	0.66
2:O:12:VAL:O	2:O:115:VAL:HG11	1.97	0.65
2:U:30:ILE:HD11	1:T:514:ILE:HD11	1.78	0.65
1:B:510:VAL:HB	1:B:518:ALA:HB3	1.78	0.65
1:B:470:ILE:HG12	1:B:510:VAL:HG22	1.79	0.65
2:O:99:TYR:HB3	2:O:103:VAL:HG13	1.77	0.65
2:W:51:ILE:HG13	2:W:57:THR:HG22	1.78	0.65
2:E:105:ASP:OD1	2:E:1055:HIS:NE2	2.30	0.64
2:C:29:LEU:HD13	2:C:71:LYS:HD2	1.79	0.64
1:A:468:VAL:HG21	1:A:480:MET:HE3	1.78	0.64
2:U:103:VAL:HG22	2:U:1034:ASN:HD21	1.63	0.64
2:I:32:TYR:CD2	2:I:97:ARG:HD2	2.32	0.64
1:S:629:ILE:HG13	1:T:629:ILE:HG13	1.80	0.64
1:A:510:VAL:HB	1:A:518:ALA:HB3	1.80	0.63
1:N:629:ILE:HG13	1:M:629:ILE:HG13	1.79	0.63
2:K:6:GLN:HG3	2:K:110:GLY:H	1.63	0.63
2:W:1092:ASN:OD1	2:W:1093:THR:N	2.29	0.63
1:A:461:THR:HG22	1:A:462:ASN:H	1.63	0.63
1:T:458:ALA:HA	1:T:554:TYR:HE2	1.64	0.63
1:A:529:SER:HB3	1:A:535:HIS:CD2	2.34	0.63
2:O:99:TYR:C	2:O:101:GLY:HA2	2.18	0.62
1:T:514:ILE:O	1:T:515:THR:OG1	2.18	0.62
1:B:457:THR:OG1	1:B:458:ALA:N	2.32	0.62
1:T:456:LEU:HG	1:T:612:GLU:HB3	1.80	0.62
2:U:59:TYR:CD2	2:U:67:LEU:HD12	2.35	0.62
2:C:86:GLN:HG3	2:C:87:ALA:H	1.65	0.62
1:N:458:ALA:HB3	1:N:461:THR:HG22	1.81	0.62
1:S:459:PRO:HD3	1:S:554:TYR:CE2	2.36	0.61
2:E:100:TYR:N	2:E:101:GLY:HA2	2.16	0.61
2:K:103:VAL:O	2:K:1036:TYR:OH	2.18	0.61
1:G:456:LEU:HG	1:G:612:GLU:HB3	1.81	0.61
1:A:461:THR:HG21	2:C:52:TRP:HZ2	1.64	0.60
2:K:39:GLN:OE1	2:K:1038:GLN:NE2	2.30	0.60
1:T:527:LYS:NZ	1:T:605:GLY:O	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:GLN:HE22	2:C:94:TYR:HA	1.66	0.60
2:I:1085:THR:HG22	2:I:1103:LYS:HG2	1.84	0.60
2:E:12:VAL:HG11	2:E:85:LEU:HD22	1.84	0.60
2:U:52:TRP:HB3	1:T:465:ASP:OD2	2.01	0.60
1:B:456:LEU:HG	1:B:612:GLU:HB3	1.83	0.59
1:N:455:THR:OG1	1:N:457:THR:O	2.19	0.59
1:N:454:LYS:HG3	1:N:613:LEU:HB2	1.84	0.59
2:I:103:VAL:CG1	2:I:1034:ASN:HD21	2.14	0.59
2:I:30:ILE:HB	1:G:514:ILE:HD11	1.84	0.59
2:O:1015:LEU:O	1:S:475:GLY:HA3	2.02	0.59
1:T:461:THR:HG22	1:T:463:SER:H	1.67	0.59
2:U:1050:TYR:CD1	1:T:579:PRO:HD2	2.37	0.59
2:E:6:GLN:HE22	2:E:108:GLY:HA3	1.67	0.59
2:E:1092:ASN:OD1	2:E:1093:THR:N	2.35	0.59
2:C:37:VAL:HG12	2:C:47:TRP:HA	1.83	0.59
2:I:103:VAL:HG12	2:I:1034:ASN:HD21	1.67	0.59
2:I:37:VAL:HG12	2:I:47:TRP:HA	1.85	0.59
2:K:40:SER:HB2	2:K:43:LYS:HB2	1.83	0.58
1:A:459:PRO:HD3	1:A:554:TYR:CE2	2.39	0.58
2:C:1084:ALA:HB3	2:C:1086:TYR:HE1	1.69	0.58
2:O:91:GLY:N	2:O:114:THR:HG1	2.01	0.58
2:O:100:TYR:N	2:O:101:GLY:HA2	2.19	0.58
2:C:10:GLY:O	2:C:113:VAL:HA	2.04	0.58
1:N:496:PHE:HB3	1:M:496:PHE:HB3	1.84	0.58
2:O:1094:PHE:O	2:O:1096:PRO:HD3	2.04	0.57
1:B:479:ILE:HG12	1:B:610:ARG:HD2	1.86	0.57
2:E:40:SER:HB2	2:E:43:LYS:HB2	1.86	0.57
2:U:103:VAL:HG22	2:U:1034:ASN:ND2	2.19	0.57
1:B:484:MET:HB3	1:B:591:LEU:HB3	1.85	0.57
2:E:38:ARG:NH1	2:E:40:SER:OG	2.38	0.57
1:H:447:ASP:OD1	1:H:448:ARG:N	2.37	0.57
1:S:479:ILE:HG12	1:S:610:ARG:HD2	1.87	0.57
2:E:1029:ILE:HA	2:E:1092:ASN:ND2	2.20	0.57
2:O:1029:ILE:HD13	2:O:1090:GLN:HB2	1.85	0.57
1:S:456:LEU:HG	1:S:612:GLU:HB3	1.87	0.57
2:E:35:HIS:HE2	2:E:102:ASN:HA	1.70	0.56
2:C:99:TYR:O	2:C:103:VAL:HB	2.05	0.56
2:K:37:VAL:HG12	2:K:47:TRP:HA	1.86	0.56
2:I:1002:ILE:HG23	2:I:1026:SER:HB3	1.87	0.56
1:G:484:MET:HG2	1:G:628:PHE:HE1	1.70	0.56
1:B:453:ASN:HA	1:B:554:TYR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1037:GLN:HB3	2:C:1047:LEU:HD11	1.88	0.56
1:G:560:ARG:HB2	1:G:571:LEU:HB3	1.87	0.56
1:H:629:ILE:HG13	1:G:629:ILE:HG13	1.88	0.56
2:E:87:ALA:HB2	2:E:117:SER:HB3	1.88	0.56
1:A:430:GLU:HA	1:A:643:ASN:HA	1.88	0.56
2:O:111:THR:O	2:O:113:VAL:HG23	2.05	0.56
1:S:431:LEU:HD12	1:S:644:THR:HG21	1.87	0.56
1:H:496:PHE:HB3	1:G:496:PHE:HB3	1.88	0.55
1:M:454:LYS:NZ	1:M:615:SER:HB3	2.20	0.55
2:U:1037:GLN:HB2	2:U:1047:LEU:HD11	1.87	0.55
1:S:460:GLY:O	2:W:102:ASN:ND2	2.39	0.55
2:K:1035:TRP:CE2	2:K:1073:LEU:HB2	2.42	0.55
2:I:48:LEU:O	2:I:60:ASN:N	2.39	0.55
2:I:100:TYR:HD1	1:G:552:GLN:HB3	1.71	0.55
1:G:529:SER:HB3	1:G:535:HIS:ND1	2.22	0.55
2:I:6:GLN:HE22	2:I:94:TYR:HA	1.72	0.55
2:E:1016:GLY:HA2	2:E:1077:ASN:HB2	1.88	0.55
1:G:572:THR:HG22	1:G:617:THR:O	2.06	0.55
2:Q:1055:HIS:CD2	2:Q:1056:SER:H	2.24	0.55
2:W:1090:GLN:HE22	2:W:1097:THR:HG22	1.71	0.55
1:A:626:THR:O	1:B:626:THR:OG1	2.24	0.55
1:T:455:THR:OG1	1:T:457:THR:O	2.18	0.55
2:C:1033:LEU:HB3	2:C:1051:THR:HG22	1.89	0.55
1:N:432:ARG:NH1	1:N:494:PRO:O	2.40	0.55
2:O:1004:MET:SD	2:O:1090:GLN:HB3	2.47	0.55
2:O:6:GLN:NE2	2:O:110:GLY:H	2.05	0.55
2:O:38:ARG:HA	2:O:92:ILE:O	2.05	0.55
2:E:99:TYR:C	2:E:101:GLY:HA2	2.27	0.54
1:T:459:PRO:HD3	1:T:554:TYR:CE2	2.42	0.54
1:T:531:THR:HG22	1:T:532:ASN:H	1.72	0.54
1:T:550:LYS:HB3	1:T:583:ARG:HG2	1.89	0.54
1:A:629:ILE:HG13	1:B:629:ILE:HG13	1.88	0.54
2:K:13:GLN:HB3	2:K:16:GLN:HG3	1.89	0.54
1:G:537:ILE:HD11	1:G:602:LEU:HD22	1.88	0.54
1:M:453:ASN:HA	1:M:554:TYR:O	2.07	0.54
2:U:11:LEU:H	2:U:11:LEU:HD12	1.73	0.54
2:C:28:SER:HB3	2:C:30:ILE:HG22	1.87	0.54
1:G:510:VAL:HB	1:G:518:ALA:HB3	1.89	0.54
2:I:1016:GLY:HA2	2:I:1077:ASN:HB2	1.89	0.54
1:N:597:LEU:HD11	1:N:619:TYR:CE1	2.43	0.54
2:O:1037:GLN:HG3	2:O:1086:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:470:ILE:HG12	1:G:510:VAL:HG22	1.89	0.54
2:O:1050:TYR:CE2	1:M:579:PRO:HD2	2.43	0.54
1:A:555:MET:HE1	1:A:582:ILE:HD11	1.90	0.54
1:B:572:THR:HG22	1:B:617:THR:O	2.08	0.54
1:S:453:ASN:HA	1:S:554:TYR:O	2.07	0.54
2:O:30:ILE:HG23	2:O:31:ASP:OD1	2.07	0.53
2:U:1050:TYR:HE1	1:T:579:PRO:HD2	1.70	0.53
2:W:60:ASN:OD1	2:W:61:ALA:N	2.41	0.53
2:O:35:HIS:NE2	2:O:101:GLY:O	2.31	0.53
1:A:620:TYR:HB3	1:B:630:THR:HG21	1.89	0.53
2:E:38:ARG:HH12	2:E:40:SER:HG	1.57	0.53
1:T:458:ALA:HA	1:T:554:TYR:CE2	2.43	0.53
2:U:1050:TYR:O	2:U:1050:TYR:HD2	1.92	0.53
2:E:6:GLN:NE2	2:E:108:GLY:HA3	2.23	0.53
2:U:97:ARG:NH2	2:U:105:ASP:OD2	2.36	0.53
1:B:537:ILE:HD11	1:B:602:LEU:HD22	1.90	0.53
2:O:39:GLN:HB3	2:O:92:ILE:HB	1.90	0.53
2:Q:60:ASN:OD1	2:Q:61:ALA:N	2.42	0.53
1:S:455:THR:OG1	1:S:457:THR:O	2.23	0.53
2:I:38:ARG:NH2	2:I:46:GLU:OE1	2.41	0.53
2:K:1037:GLN:HG3	2:K:1086:TYR:CE1	2.44	0.53
1:S:537:ILE:HD11	1:S:602:LEU:HD22	1.90	0.53
2:W:60:ASN:HB3	2:W:63:PHE:HD2	1.74	0.53
1:N:440:ILE:H	1:N:440:ILE:HD12	1.73	0.53
1:N:456:LEU:HG	1:N:612:GLU:HB3	1.91	0.52
2:I:100:TYR:O	1:G:554:TYR:OH	2.19	0.52
2:W:1051:THR:HG23	2:W:1052:SER:H	1.73	0.52
1:N:470:ILE:HD13	1:N:541:PHE:CD2	2.44	0.52
1:S:529:SER:HB3	1:S:535:HIS:CD2	2.44	0.52
1:H:514:ILE:HD11	2:K:30:ILE:CB	2.35	0.52
2:U:30:ILE:HD11	1:T:514:ILE:CD1	2.40	0.52
2:K:1084:ALA:HB3	2:K:1086:TYR:HE1	1.74	0.52
1:S:454:LYS:HG3	1:S:613:LEU:HB2	1.91	0.52
1:B:440:ILE:HD12	1:B:440:ILE:H	1.73	0.52
2:E:4:LEU:HD22	2:E:24:VAL:HG12	1.92	0.52
1:H:626:THR:O	1:G:626:THR:OG1	2.27	0.52
2:I:1021:ILE:HD11	2:I:1073:LEU:HD23	1.91	0.52
1:S:597:LEU:HD11	1:S:619:TYR:CE1	2.45	0.52
2:U:1:ASP:HA	2:U:26:GLY:HA3	1.90	0.52
1:A:456:LEU:O	1:A:479:ILE:HD13	2.10	0.52
2:E:1029:ILE:HD11	2:E:1071:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:ARG:HE	2:E:106:TYR:HD2	1.56	0.52
2:W:35:HIS:CD2	2:W:98:PRO:HB3	2.45	0.52
1:A:522:PHE:HD2	1:A:523:MET:N	2.07	0.52
2:O:1050:TYR:O	2:O:1051:THR:HG22	2.09	0.52
2:Q:1030:SER:HB2	2:Q:1032:TYR:HD2	1.74	0.52
2:E:35:HIS:NE2	2:E:102:ASN:HA	2.25	0.51
2:E:98:PRO:HB3	2:E:102:ASN:H	1.75	0.51
2:O:35:HIS:HD2	2:O:104:MET:HG2	1.75	0.51
1:A:461:THR:HG22	1:A:462:ASN:N	2.26	0.51
2:K:1050:TYR:O	2:K:1051:THR:HG22	2.11	0.51
1:M:493:THR:HG23	1:M:495:ASP:H	1.75	0.51
2:Q:1033:LEU:HB3	2:Q:1051:THR:HG22	1.92	0.51
2:U:1004:MET:SD	2:U:1090:GLN:HB3	2.51	0.51
1:A:555:MET:CE	1:A:582:ILE:HD11	2.40	0.51
1:S:496:PHE:HB3	1:T:496:PHE:HB3	1.91	0.51
1:S:533:ASN:O	1:S:600:ASN:N	2.42	0.51
1:B:460:GLY:O	1:B:461:THR:OG1	2.27	0.51
1:H:600:ASN:OD1	1:H:601:ASN:N	2.44	0.51
2:Q:105:ASP:HB2	2:Q:1055:HIS:HE1	1.76	0.51
1:S:548:ASP:OD1	1:S:586:VAL:N	2.41	0.51
1:A:456:LEU:HG	1:A:612:GLU:HB3	1.92	0.51
1:B:504:PRO:HG3	1:B:521:TYR:HE1	1.76	0.51
2:I:1033:LEU:HB2	2:I:1051:THR:HG22	1.92	0.51
2:C:1035:TRP:CE2	2:C:1073:LEU:HB2	2.46	0.51
1:G:543:ILE:HD12	1:G:545:PRO:HD3	1.92	0.51
1:A:524:LYS:HB3	1:A:540:ILE:HG12	1.93	0.50
1:M:468:VAL:HG23	1:M:551:VAL:HG11	1.92	0.50
1:N:479:ILE:HG12	1:N:610:ARG:HD2	1.93	0.50
2:O:99:TYR:O	2:O:103:VAL:HG12	2.11	0.50
1:S:530:TYR:CE2	1:S:620:TYR:HB2	2.46	0.50
1:A:453:ASN:HA	1:A:554:TYR:O	2.11	0.50
2:I:1029:ILE:HD11	2:I:1071:TYR:CE2	2.46	0.50
2:C:60:ASN:HB3	2:C:63:PHE:HD2	1.75	0.50
1:G:479:ILE:HG12	1:G:610:ARG:HD2	1.94	0.50
1:H:529:SER:HB3	1:H:535:HIS:ND1	2.25	0.50
1:M:454:LYS:NZ	1:M:575:SER:O	2.44	0.50
1:A:522:PHE:HD2	1:A:523:MET:H	1.59	0.50
2:E:99:TYR:O	2:E:100:TYR:HB2	2.11	0.50
1:M:479:ILE:HG12	1:M:610:ARG:HD2	1.93	0.50
1:N:453:ASN:HA	1:N:554:TYR:O	2.12	0.50
1:H:453:ASN:HA	1:H:554:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:VAL:HG22	2:C:1034:ASN:OD1	2.11	0.50
1:H:510:VAL:HG21	1:H:543:ILE:HG21	1.94	0.50
1:H:445:SER:O	1:H:631:PRO:HG2	2.10	0.50
2:W:99:TYR:O	2:W:103:VAL:HB	2.11	0.50
1:B:543:ILE:HD12	1:B:545:PRO:HD3	1.92	0.50
2:E:1009:SER:O	2:E:1103:LYS:N	2.43	0.50
2:E:17:SER:HA	2:E:83:ASN:HA	1.92	0.50
2:I:1032:TYR:HE1	1:G:579:PRO:HD3	1.77	0.50
1:N:456:LEU:HD13	1:N:610:ARG:HG2	1.94	0.50
2:O:60:ASN:O	2:O:64:ILE:HG23	2.12	0.50
2:C:47:TRP:CD2	2:C:1096:PRO:HD2	2.47	0.49
2:C:67:LEU:HD11	2:C:80:PHE:CE1	2.47	0.49
1:H:462:ASN:HD21	2:K:58:ASP:HB3	1.77	0.49
2:Q:1033:LEU:HD23	2:Q:1034:ASN:N	2.27	0.49
1:T:552:GLN:HG3	1:T:580:GLU:O	2.12	0.49
2:U:40:SER:OG	2:U:43:LYS:HB2	2.12	0.49
2:E:1037:GLN:HB2	2:E:1047:LEU:HD11	1.95	0.49
1:N:491:TRP:HZ3	1:N:644:THR:HG21	1.76	0.49
1:T:545:PRO:HB3	1:T:549:PHE:HE1	1.77	0.49
1:N:475:GLY:HA3	2:U:1015:LEU:O	2.12	0.49
2:U:1016:GLY:HA2	2:U:1077:ASN:HB2	1.94	0.49
1:G:545:PRO:HB3	1:G:549:PHE:HE1	1.78	0.49
1:G:453:ASN:HA	1:G:554:TYR:O	2.12	0.49
2:E:103:VAL:HG22	2:E:1034:ASN:OD1	2.13	0.49
1:N:644:THR:OG1	1:N:645:ALA:N	2.45	0.49
2:U:67:LEU:HD21	2:U:80:PHE:HE1	1.75	0.49
1:N:568:VAL:HG22	1:M:448:ARG:HG2	1.95	0.49
2:Q:1028:ASP:OD1	2:Q:1029:ILE:N	2.46	0.49
1:T:621:ALA:HB1	1:T:626:THR:HA	1.95	0.49
2:O:6:GLN:OE1	2:O:108:GLY:HA3	2.13	0.49
2:I:40:SER:OG	2:I:41:PRO:HD2	2.13	0.49
1:M:454:LYS:HG3	1:M:613:LEU:HB2	1.94	0.49
2:O:1037:GLN:HB2	2:O:1047:LEU:HD11	1.95	0.49
2:C:60:ASN:OD1	2:C:61:ALA:N	2.44	0.48
1:T:543:ILE:HD12	1:T:545:PRO:HD3	1.94	0.48
2:U:1028:ASP:HA	2:U:1069:THR:HG22	1.95	0.48
2:E:6:GLN:HE21	2:E:95:CYS:H	1.60	0.48
1:H:456:LEU:HG	1:H:612:GLU:HB3	1.94	0.48
2:K:67:LEU:HD11	2:K:80:PHE:CE1	2.48	0.48
1:B:515:THR:OG1	1:B:517:LYS:HD3	2.14	0.48
1:T:524:LYS:HB3	1:T:540:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:554:TYR:C	1:T:555:MET:HG2	2.34	0.48
2:I:1035:TRP:CE2	2:I:1073:LEU:HB2	2.49	0.48
1:M:527:LYS:HD3	1:M:602:LEU:HD13	1.96	0.48
1:A:435:LEU:HD13	1:A:486:ILE:HD12	1.96	0.48
2:O:1092:ASN:OD1	2:O:1093:THR:N	2.46	0.48
2:U:1037:GLN:HG3	2:U:1086:TYR:CE1	2.49	0.48
1:A:565:ASN:O	1:B:574:ARG:NH1	2.47	0.48
1:S:514:ILE:HG13	2:W:30:ILE:HD11	1.95	0.48
1:A:445:SER:O	1:A:631:PRO:HG2	2.14	0.48
2:K:99:TYR:C	2:K:101:GLY:H	2.17	0.48
2:U:60:ASN:OD1	2:U:61:ALA:N	2.46	0.48
2:U:1050:TYR:HE1	1:T:578:SER:HA	1.77	0.48
2:W:29:LEU:HD23	2:W:73:ASN:HA	1.94	0.48
1:A:522:PHE:CD2	1:A:523:MET:N	2.82	0.48
1:N:528:ASN:O	1:N:529:SER:OG	2.30	0.48
2:W:103:VAL:HG22	2:W:1034:ASN:ND2	2.29	0.48
1:A:455:THR:OG1	1:A:457:THR:O	2.20	0.47
1:H:555:MET:CE	1:H:582:ILE:HD11	2.44	0.47
1:S:433:VAL:HG22	1:S:435:LEU:HD12	1.95	0.47
1:A:448:ARG:HH12	1:A:451:TRP:HE1	1.61	0.47
1:B:599:GLU:HG3	1:B:600:ASN:H	1.79	0.47
1:G:461:THR:HG22	1:G:462:ASN:N	2.21	0.47
1:S:579:PRO:HD2	2:W:1050:TYR:CE1	2.49	0.47
1:B:463:SER:OG	1:B:465:ASP:OD1	2.32	0.47
2:C:13:GLN:HB3	2:C:16:GLN:HG3	1.96	0.47
1:G:431:LEU:HD12	1:G:644:THR:HG21	1.97	0.47
2:E:114:THR:HG21	1:M:477:TYR:HE1	1.80	0.47
2:C:86:GLN:HG2	3:C:1201:NAG:H61	1.97	0.47
1:H:435:LEU:HD13	1:H:486:ILE:HD12	1.97	0.47
2:Q:35:HIS:NE2	2:Q:98:PRO:HB3	2.30	0.47
1:H:626:THR:OG1	1:G:626:THR:O	2.32	0.47
1:T:454:LYS:HG3	1:T:613:LEU:HB2	1.96	0.47
1:A:522:PHE:CE2	1:A:642:GLY:HA3	2.44	0.47
2:E:99:TYR:N	2:E:103:VAL:O	2.48	0.47
1:H:458:ALA:O	1:H:461:THR:HG22	2.14	0.47
2:U:1033:LEU:HA	2:U:1089:GLN:O	2.14	0.47
2:K:60:ASN:OD1	2:K:61:ALA:N	2.47	0.47
1:N:579:PRO:HD3	2:Q:1032:TYR:CE1	2.50	0.47
1:T:472:HIS:HB2	1:T:508:MET:SD	2.55	0.47
1:T:512:VAL:HG11	1:T:551:VAL:HG12	1.96	0.47
2:U:9:PRO:HB3	2:U:111:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:448:ARG:NH2	1:H:451:TRP:HE1	2.12	0.46
1:M:543:ILE:HD13	1:M:592:LEU:HD11	1.96	0.46
2:O:1106:ILE:HG22	2:O:1107:LYS:N	2.30	0.46
2:U:1033:LEU:HB3	2:U:1051:THR:HG22	1.97	0.46
2:U:85:LEU:HD23	2:U:85:LEU:H	1.80	0.46
1:A:543:ILE:HD13	1:A:592:LEU:HD11	1.97	0.46
2:E:99:TYR:O	2:E:103:VAL:HB	2.15	0.46
1:H:438:GLY:HA2	1:H:487:LYS:HB2	1.97	0.46
1:T:504:PRO:HG3	1:T:521:TYR:CE1	2.50	0.46
1:H:558:PHE:O	1:G:560:ARG:NH2	2.36	0.46
2:O:92:ILE:HA	2:O:112:SER:HB2	1.96	0.46
1:T:597:LEU:HD11	1:T:619:TYR:CE1	2.50	0.46
2:U:59:TYR:CE2	2:U:67:LEU:HD12	2.51	0.46
1:H:462:ASN:N	1:H:462:ASN:OD1	2.46	0.46
2:C:28:SER:CB	2:C:30:ILE:HG22	2.45	0.46
1:G:603:PRO:HG2	1:G:607:VAL:HG22	1.96	0.46
1:G:593:THR:HG21	1:G:628:PHE:HE2	1.81	0.46
2:O:39:GLN:O	2:O:92:ILE:N	2.38	0.46
1:A:598:LYS:HD3	1:A:602:LEU:HD23	1.98	0.46
2:I:97:ARG:NH2	2:I:105:ASP:OD2	2.47	0.46
2:O:30:ILE:HD11	1:M:514:ILE:HG13	1.98	0.46
1:T:513:ASN:OD1	1:T:514:ILE:N	2.49	0.46
2:I:1089:GLN:HB2	2:I:1098:PHE:CD2	2.51	0.46
2:K:38:ARG:HB3	2:K:48:LEU:HD11	1.97	0.46
2:U:1051:THR:HG21	2:U:1071:TYR:CD1	2.51	0.46
2:C:1:ASP:OD1	2:C:2:VAL:N	2.49	0.46
2:E:1032:TYR:HE1	1:B:579:PRO:HD3	1.79	0.46
1:N:529:SER:HB3	1:N:535:HIS:CD2	2.50	0.46
2:K:43:LYS:HE3	3:K:1201:NAG:H81	1.97	0.46
2:O:1029:ILE:HA	2:O:1092:ASN:ND2	2.31	0.46
1:A:545:PRO:HD2	1:A:588:GLU:O	2.16	0.45
2:E:1007:THR:OG1	2:E:1008:THR:N	2.49	0.45
1:G:625:LEU:HD23	1:G:628:PHE:HD2	1.81	0.45
2:K:1038:GLN:HG3	2:K:1044:VAL:HG22	1.98	0.45
2:O:60:ASN:OD1	2:O:61:ALA:N	2.49	0.45
1:T:467:LEU:HD22	1:T:553:CYS:HA	1.98	0.45
2:I:12:VAL:HG21	2:I:85:LEU:HD22	1.98	0.45
1:N:454:LYS:HA	1:N:613:LEU:HD12	1.98	0.45
2:U:1049:TYR:O	2:U:1053:ARG:HB2	2.16	0.45
2:C:1049:TYR:O	2:C:1053:ARG:HB2	2.16	0.45
1:G:437:VAL:HG21	1:G:632:PRO:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1083:ILE:HG23	2:K:1104:LEU:O	2.17	0.45
1:A:598:LYS:HB3	1:A:602:LEU:HD21	1.99	0.45
1:G:525:GLN:HG3	1:G:606:TRP:CH2	2.52	0.45
1:A:454:LYS:HG3	1:A:613:LEU:HB2	1.99	0.45
2:C:32:TYR:CD2	2:C:97:ARG:HD2	2.52	0.45
2:C:72:ASP:OD2	2:C:75:LYS:HE2	2.15	0.45
2:I:1033:LEU:HD12	2:I:1071:TYR:CG	2.51	0.45
2:I:60:ASN:OD1	2:I:61:ALA:N	2.49	0.45
1:M:524:LYS:HB3	1:M:540:ILE:HG12	1.99	0.45
1:N:435:LEU:HD13	1:N:486:ILE:HD12	1.99	0.45
2:O:1019:VAL:HG21	2:O:1078:LEU:HD11	1.99	0.45
2:O:20:ILE:HB	2:O:80:PHE:HB3	1.99	0.45
1:T:554:TYR:CD1	1:T:554:TYR:N	2.82	0.45
2:U:1092:ASN:OD1	2:U:1093:THR:N	2.49	0.45
2:E:1010:SER:HA	2:E:1103:LYS:O	2.16	0.45
2:E:52:TRP:CZ2	1:B:461:THR:HG21	2.51	0.45
1:G:445:SER:O	1:G:631:PRO:HG2	2.16	0.45
1:H:456:LEU:HD13	1:H:610:ARG:HG2	1.98	0.45
2:I:1006:GLN:HG3	2:I:1022:SER:O	2.17	0.45
1:M:597:LEU:HD11	1:M:619:TYR:CE1	2.52	0.45
2:U:59:TYR:HE2	2:U:69:ILE:HG13	1.81	0.45
2:K:6:GLN:HG3	2:K:110:GLY:N	2.30	0.45
1:B:545:PRO:HB3	1:B:549:PHE:HE1	1.82	0.44
2:K:1049:TYR:O	2:K:1053:ARG:HB2	2.17	0.44
2:Q:60:ASN:HB3	2:Q:63:PHE:HD1	1.82	0.44
1:T:613:LEU:HD22	1:T:619:TYR:HE2	1.81	0.44
2:E:1033:LEU:HB3	2:E:1051:THR:CG2	2.48	0.44
1:G:504:PRO:HG3	1:G:521:TYR:CE1	2.52	0.44
1:G:524:LYS:HB3	1:G:540:ILE:HG12	2.00	0.44
2:I:1049:TYR:O	2:I:1053:ARG:HB2	2.17	0.44
2:K:29:LEU:HA	2:K:29:LEU:HD12	1.85	0.44
1:M:621:ALA:HB1	1:M:626:THR:HA	1.99	0.44
2:O:92:ILE:HA	2:O:112:SER:CB	2.48	0.44
1:T:438:GLY:HA2	1:T:487:LYS:HB2	1.99	0.44
2:E:67:LEU:HD11	2:E:80:PHE:CE1	2.52	0.44
1:T:467:LEU:CD2	1:T:553:CYS:HA	2.47	0.44
1:S:560:ARG:HD2	1:T:558:PHE:O	2.18	0.44
1:B:462:ASN:OD1	1:B:462:ASN:N	2.47	0.44
2:I:38:ARG:HG3	2:I:93:TYR:CE1	2.53	0.44
2:E:60:ASN:OD1	2:E:61:ALA:N	2.49	0.44
2:C:4:LEU:HD23	2:C:22:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:ARG:HG2	2:E:48:LEU:HD21	1.99	0.44
1:M:452:LEU:O	1:M:555:MET:HA	2.16	0.44
2:O:99:TYR:O	2:O:100:TYR:HB2	2.18	0.44
2:Q:1049:TYR:CE2	2:Q:1053:ARG:HD2	2.52	0.44
1:A:433:VAL:HG11	1:A:522:PHE:CE1	2.53	0.44
1:G:560:ARG:HD2	1:G:569:ALA:O	2.18	0.44
1:M:467:LEU:HD13	1:M:479:ILE:HG23	2.00	0.44
1:N:560:ARG:HD2	1:M:558:PHE:O	2.17	0.44
2:U:102:ASN:ND2	2:U:1096:PRO:HG3	2.32	0.44
1:M:514:ILE:O	1:M:514:ILE:HG13	2.18	0.44
1:M:613:LEU:HD22	1:M:619:TYR:HE2	1.83	0.44
1:S:626:THR:O	1:T:626:THR:OG1	2.36	0.44
1:B:621:ALA:HB1	1:B:626:THR:HA	2.00	0.43
1:B:593:THR:HG21	1:B:628:PHE:HE2	1.83	0.43
2:W:36:TRP:CZ3	2:W:95:CYS:HB3	2.53	0.43
1:G:473:ASP:O	1:G:474:LEU:HB3	2.18	0.43
1:N:504:PRO:HG3	1:N:521:TYR:CE1	2.53	0.43
2:C:1089:GLN:HB2	2:C:1098:PHE:CE2	2.53	0.43
2:C:11:LEU:O	2:C:11:LEU:HD12	2.18	0.43
2:C:36:TRP:CZ2	2:C:80:PHE:HB2	2.53	0.43
2:E:1037:GLN:O	2:E:1044:VAL:HA	2.18	0.43
1:G:621:ALA:HB1	1:G:626:THR:HA	2.00	0.43
1:M:458:ALA:HA	1:M:554:TYR:CE2	2.53	0.43
2:I:76:SER:O	2:I:76:SER:OG	2.36	0.43
2:U:18:LEU:O	2:U:81:LYS:HA	2.18	0.43
2:W:5:LYS:N	2:W:23:THR:O	2.52	0.43
2:C:38:ARG:HB3	2:C:48:LEU:HD11	2.00	0.43
1:A:548:ASP:OD1	1:A:586:VAL:N	2.49	0.43
1:B:461:THR:HG22	1:B:462:ASN:N	2.33	0.43
1:H:540:ILE:HG22	1:H:593:THR:HG22	2.01	0.43
2:I:39:GLN:OE1	2:I:1038:GLN:NE2	2.43	0.43
2:I:67:LEU:HD11	2:I:80:PHE:CE1	2.54	0.43
2:K:1089:GLN:HG3	2:K:1098:PHE:CE1	2.54	0.43
1:B:451:TRP:CE3	1:B:555:MET:HB3	2.54	0.43
1:G:533:ASN:OD1	1:G:534:ARG:N	2.51	0.43
1:N:493:THR:HG23	1:N:495:ASP:N	2.30	0.43
2:O:1048:ILE:HA	2:O:1053:ARG:O	2.19	0.43
2:Q:22:CYS:HB2	2:Q:36:TRP:CH2	2.54	0.43
1:A:476:HIS:HB3	1:A:608:TRP:CG	2.54	0.43
2:E:1054:LEU:HD21	2:E:1062:PHE:O	2.19	0.43
1:M:459:PRO:HD3	1:M:554:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:SER:OG	1:A:574:ARG:HB3	2.19	0.42
1:B:437:VAL:HG21	1:B:632:PRO:HB2	2.00	0.42
2:C:1046:LEU:HD23	2:C:1055:HIS:CD2	2.54	0.42
2:C:34:VAL:HG21	2:C:78:VAL:HG21	2.01	0.42
1:N:525:GLN:HG3	1:N:606:TRP:CZ3	2.54	0.42
1:G:452:LEU:O	1:G:555:MET:HA	2.18	0.42
1:G:476:HIS:HB3	1:G:608:TRP:CG	2.54	0.42
2:K:1033:LEU:HD13	2:K:1071:TYR:CG	2.54	0.42
1:T:552:GLN:HG3	1:T:580:GLU:C	2.39	0.42
2:U:1033:LEU:HB3	2:U:1051:THR:CG2	2.48	0.42
2:C:1023:CYS:SG	2:C:1033:LEU:HD11	2.60	0.42
2:E:1033:LEU:HD23	2:E:1034:ASN:N	2.33	0.42
2:E:1035:TRP:HD1	2:E:1048:ILE:HB	1.84	0.42
2:I:99:TYR:HB2	2:I:105:ASP:HB3	2.00	0.42
2:K:1:ASP:OD1	2:K:2:VAL:N	2.52	0.42
1:M:504:PRO:HG3	1:M:521:TYR:CE1	2.54	0.42
1:T:452:LEU:O	1:T:555:MET:HA	2.19	0.42
2:U:1038:GLN:O	2:U:1084:ALA:HB1	2.18	0.42
2:W:1051:THR:HG23	2:W:1052:SER:N	2.33	0.42
2:W:1034:ASN:N	2:W:1089:GLN:O	2.35	0.42
2:W:28:SER:HB2	2:W:30:ILE:HG22	2.01	0.42
1:H:441:MET:HG3	1:H:485:HIS:HB2	2.02	0.42
2:K:16:GLN:O	2:K:17:SER:OG	2.27	0.42
2:K:28:SER:OG	2:K:30:ILE:HG12	2.19	0.42
2:U:100:TYR:CD1	1:T:552:GLN:HB3	2.54	0.42
2:E:1085:THR:HG22	2:E:1103:LYS:HA	2.02	0.42
1:N:514:ILE:O	1:N:514:ILE:HG13	2.20	0.42
1:N:632:PRO:HA	1:N:633:PRO:HD3	1.93	0.42
2:O:111:THR:O	2:O:111:THR:HG22	2.19	0.42
2:E:18:LEU:N	2:E:82:MET:O	2.39	0.42
1:H:459:PRO:HA	1:H:460:GLY:HA2	1.67	0.42
1:H:541:PHE:O	1:H:591:LEU:HD12	2.20	0.42
2:K:1018:ARG:NH2	2:K:1074:THR:HG21	2.35	0.42
1:N:458:ALA:HA	1:N:554:TYR:CE2	2.55	0.42
2:O:6:GLN:HE22	2:O:109:GLN:H	1.67	0.42
1:S:447:ASP:OD1	1:S:448:ARG:N	2.52	0.42
1:S:514:ILE:O	1:S:514:ILE:HG13	2.20	0.42
1:T:545:PRO:HD2	1:T:588:GLU:O	2.20	0.42
1:B:472:HIS:HB2	1:B:508:MET:SD	2.59	0.42
2:C:1089:GLN:HB2	2:C:1098:PHE:CD2	2.54	0.42
1:H:474:LEU:HD12	1:H:474:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:114:THR:HG21	1:M:477:TYR:CE1	2.54	0.42
1:A:508:MET:HG3	1:A:523:MET:SD	2.59	0.42
2:C:29:LEU:HD23	2:C:29:LEU:HA	1.76	0.42
1:A:596:THR:HG23	1:A:611:VAL:HB	2.02	0.42
1:G:541:PHE:O	1:G:591:LEU:HD12	2.20	0.42
1:H:430:GLU:HA	1:H:643:ASN:HA	2.02	0.42
1:M:484:MET:HB3	1:M:591:LEU:HB3	2.02	0.42
1:B:523:MET:HB3	1:B:606:TRP:CZ3	2.54	0.42
1:H:511:MET:HG2	1:H:516:LYS:HA	2.00	0.42
2:K:6:GLN:HE22	2:K:95:CYS:N	2.18	0.42
2:O:97:ARG:NH2	2:O:105:ASP:OD2	2.38	0.42
1:S:540:ILE:HG22	1:S:593:THR:HG22	2.02	0.42
1:M:435:LEU:HD13	1:M:486:ILE:HD12	2.02	0.41
1:A:432:ARG:HD3	1:A:496:PHE:CZ	2.55	0.41
2:E:99:TYR:HB2	2:E:105:ASP:HB2	2.01	0.41
1:H:565:ASN:O	1:G:574:ARG:NH1	2.49	0.41
2:I:1089:GLN:HB2	2:I:1098:PHE:CE2	2.55	0.41
2:O:1035:TRP:HD1	2:O:1048:ILE:HB	1.85	0.41
2:O:1038:GLN:O	2:O:1084:ALA:HB1	2.19	0.41
1:H:593:THR:HG1	1:H:628:PHE:HE2	1.67	0.41
1:H:479:ILE:HG12	1:H:610:ARG:HD2	2.01	0.41
1:S:438:GLY:HA2	1:S:487:LYS:HB2	2.01	0.41
1:S:456:LEU:HD13	1:S:610:ARG:HG2	2.02	0.41
2:W:1029:ILE:HD13	2:W:1090:GLN:HB2	2.02	0.41
2:I:1029:ILE:CD1	2:I:1033:LEU:HG	2.50	0.41
2:U:37:VAL:HG23	2:U:94:TYR:HB2	2.02	0.41
1:H:564:ASP:HB3	1:G:576:MET:HE1	2.03	0.41
2:O:1029:ILE:HD11	2:O:1091:GLY:H	1.85	0.41
1:T:551:VAL:HG23	1:T:553:CYS:SG	2.61	0.41
2:U:1049:TYR:CE2	2:U:1053:ARG:HD2	2.55	0.41
2:C:60:ASN:O	2:C:64:ILE:HG13	2.20	0.41
1:G:447:ASP:OD1	1:G:448:ARG:N	2.54	0.41
1:H:596:THR:HG23	1:H:611:VAL:HB	2.03	0.41
1:H:625:LEU:HD23	1:H:628:PHE:HD2	1.86	0.41
2:K:1015:LEU:HA	2:K:1015:LEU:HD23	1.90	0.41
2:O:92:ILE:HG12	2:O:112:SER:OG	2.21	0.41
1:S:522:PHE:HE2	1:S:540:ILE:HD11	1.86	0.41
1:T:453:ASN:HB3	1:T:480:MET:O	2.21	0.41
2:K:58:ASP:OD1	2:K:58:ASP:N	2.54	0.41
1:A:555:MET:O	1:A:577:THR:HA	2.21	0.41
1:G:571:LEU:HD12	1:G:619:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:555:MET:HE3	1:H:582:ILE:HD11	2.01	0.41
2:K:1025:ALA:HB2	2:K:1029:ILE:HD11	2.03	0.41
1:M:468:VAL:HG13	1:M:510:VAL:HG13	2.02	0.41
2:Q:28:SER:OG	2:Q:30:ILE:HG22	2.21	0.41
2:Q:35:HIS:CD2	2:Q:98:PRO:HB3	2.55	0.41
2:U:90:THR:HG23	2:U:113:VAL:O	2.21	0.41
2:W:22:CYS:HB2	2:W:36:TRP:CH2	2.55	0.41
1:N:548:ASP:OD1	1:N:586:VAL:N	2.48	0.41
2:C:1075:ILE:HD11	2:C:1086:TYR:HE2	1.85	0.41
2:E:48:LEU:O	2:E:60:ASN:N	2.52	0.41
1:H:450:VAL:HB	1:H:628:PHE:O	2.20	0.41
1:H:454:LYS:NZ	1:H:575:SER:O	2.54	0.41
1:H:545:PRO:HB3	1:H:549:PHE:HE1	1.86	0.41
1:M:523:MET:HB3	1:M:606:TRP:CZ3	2.56	0.41
2:O:1049:TYR:O	2:O:1053:ARG:HB2	2.21	0.41
2:O:4:LEU:HG	2:O:24:VAL:HG12	2.03	0.41
2:U:1029:ILE:HA	2:U:1092:ASN:ND2	2.36	0.41
1:A:537:ILE:HD11	1:A:602:LEU:HD22	2.03	0.40
2:K:1086:TYR:C	2:K:1087:PHE:HD1	2.24	0.40
1:A:626:THR:OG1	1:B:626:THR:O	2.39	0.40
2:E:6:GLN:NE2	2:E:95:CYS:H	2.19	0.40
1:H:545:PRO:HD2	1:H:588:GLU:O	2.21	0.40
2:O:1091:GLY:O	1:M:460:GLY:HA3	2.21	0.40
1:N:459:PRO:HD3	1:N:554:TYR:CE2	2.57	0.40
2:I:117:SER:OG	2:I:117:SER:O	2.33	0.40
2:K:1062:PHE:CD1	2:K:1062:PHE:N	2.90	0.40
2:U:28:SER:OG	2:U:30:ILE:HG22	2.22	0.40
1:B:524:LYS:HB3	1:B:540:ILE:HG12	2.04	0.40
1:N:626:THR:O	1:M:626:THR:OG1	2.39	0.40
2:O:1083:ILE:HG23	2:O:1104:LEU:O	2.20	0.40
2:U:36:TRP:CZ3	2:U:95:CYS:HB3	2.57	0.40
1:S:514:ILE:CG1	2:W:30:ILE:HD11	2.51	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	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	B	216/228 (95%)	205 (95%)	11 (5%)	0	100	100
1	G	217/228 (95%)	207 (95%)	10 (5%)	0	100	100
1	H	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	M	214/228 (94%)	204 (95%)	10 (5%)	0	100	100
1	N	215/228 (94%)	201 (94%)	14 (6%)	0	100	100
1	S	216/228 (95%)	204 (94%)	12 (6%)	0	100	100
1	T	214/228 (94%)	202 (94%)	12 (6%)	0	100	100
2	C	219/251 (87%)	213 (97%)	6 (3%)	0	100	100
2	E	220/251 (88%)	211 (96%)	9 (4%)	0	100	100
2	I	221/251 (88%)	212 (96%)	9 (4%)	0	100	100
2	K	219/251 (87%)	209 (95%)	10 (5%)	0	100	100
2	O	202/251 (80%)	194 (96%)	8 (4%)	0	100	100
2	Q	81/251 (32%)	69 (85%)	12 (15%)	0	100	100
2	U	218/251 (87%)	209 (96%)	9 (4%)	0	100	100
2	W	91/251 (36%)	84 (92%)	7 (8%)	0	100	100
All	All	3191/3832 (83%)	3036 (95%)	155 (5%)	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	197/204 (97%)	196 (100%)	1 (0%)	92	97
1	B	197/204 (97%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	197/204 (97%)	196 (100%)	1 (0%)	92 97
1	H	197/204 (97%)	197 (100%)	0	100 100
1	M	197/204 (97%)	197 (100%)	0	100 100
1	N	197/204 (97%)	197 (100%)	0	100 100
1	S	197/204 (97%)	197 (100%)	0	100 100
1	T	197/204 (97%)	196 (100%)	1 (0%)	92 97
2	C	193/206 (94%)	193 (100%)	0	100 100
2	E	194/206 (94%)	193 (100%)	1 (0%)	92 97
2	I	195/206 (95%)	194 (100%)	1 (0%)	92 97
2	K	193/206 (94%)	193 (100%)	0	100 100
2	O	185/206 (90%)	184 (100%)	1 (0%)	92 97
2	Q	82/206 (40%)	82 (100%)	0	100 100
2	U	192/206 (93%)	191 (100%)	1 (0%)	92 97
2	W	93/206 (45%)	93 (100%)	0	100 100
All	All	2903/3280 (88%)	2896 (100%)	7 (0%)	95 99

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	PHE
2	E	100	TYR
2	I	1092	ASN
1	G	571	LEU
2	O	1050	TYR
2	U	1050	TYR
1	T	444	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	K	6	GLN
2	I	1034	ASN
1	G	513	ASN
2	O	6	GLN
1	T	552	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 carbohydrates in this entry.

5.6 Ligand geometry

4 ligands 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	$\#\|Z\| > 2$
3	NAG	C	1201	2	14,14,15	0.38	0	15,19,21	0.36	0
3	NAG	E	1201	2	14,14,15	0.32	0	15,19,21	0.51	0
3	NAG	I	1201	2	14,14,15	0.24	0	15,19,21	0.44	0
3	NAG	K	1201	2	14,14,15	0.31	0	15,19,21	0.38	0

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
3	NAG	C	1201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1201	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1201	2	-	0/6/23/26	0/1/1/1
3	NAG	K	1201	2	-	0/6/23/26	0/1/1/1

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1201	NAG	1	0
3	K	1201	NAG	1	0

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	216/228 (94%)	0.62	11 (5%) 32 21	50, 81, 124, 168	0
1	B	218/228 (95%)	0.73	22 (10%) 9 6	59, 106, 136, 152	0
1	G	219/228 (96%)	0.83	29 (13%) 4 3	64, 108, 146, 163	0
1	H	216/228 (94%)	0.59	13 (6%) 25 15	52, 82, 127, 165	0
1	M	216/228 (94%)	0.91	24 (11%) 7 5	66, 103, 135, 151	0
1	N	217/228 (95%)	0.55	11 (5%) 32 21	59, 91, 129, 147	0
1	S	218/228 (95%)	0.60	19 (8%) 13 8	58, 92, 131, 149	0
1	T	216/228 (94%)	0.90	32 (14%) 3 2	70, 103, 138, 164	0
2	C	223/251 (88%)	0.54	11 (4%) 33 22	48, 70, 122, 147	3 (1%)
2	E	224/251 (89%)	0.81	23 (10%) 9 6	86, 121, 149, 166	3 (1%)
2	I	225/251 (89%)	0.90	37 (16%) 2 2	93, 126, 157, 175	3 (1%)
2	K	223/251 (88%)	0.67	12 (5%) 29 19	46, 72, 125, 146	3 (1%)
2	O	212/251 (84%)	0.70	24 (11%) 7 5	97, 131, 155, 167	3 (1%)
2	Q	93/251 (37%)	1.02	21 (22%) 1 1	120, 145, 163, 172	0
2	U	222/251 (88%)	0.83	25 (11%) 7 5	96, 129, 166, 193	3 (1%)
2	W	105/251 (41%)	1.36	34 (32%) 1 1	114, 145, 162, 173	0
All	All	3263/3832 (85%)	0.76	348 (10%) 8 5	46, 107, 151, 193	18 (0%)

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	37	VAL	6.0
2	W	69	ILE	6.0
1	M	468	VAL	5.9
2	W	1027	GLN	5.6
1	B	608	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
2	I	1106	ILE	5.5
2	W	47	TRP	5.5
2	U	11	LEU	5.4
2	Q	80	PHE	5.3
2	W	63	PHE	5.3
2	E	34	VAL	5.2
2	W	33	GLY	5.0
2	U	23	THR	4.9
2	U	96	GLY	4.8
2	E	82	MET	4.7
2	W	67	LEU	4.7
2	W	25	SER	4.7
2	I	1011	LEU	4.6
1	G	596	THR	4.5
2	O	1011	LEU	4.5
2	W	34	VAL	4.5
2	O	1094	PHE	4.5
1	G	522	PHE	4.4
2	W	46	GLU	4.4
2	W	70	SER	4.4
1	T	429	GLY	4.4
2	U	4	LEU	4.3
2	Q	1046	LEU	4.3
2	I	1080	GLN	4.3
2	U	21	THR	4.3
1	M	456	LEU	4.3
2	O	1092	ASN	4.2
2	E	77	GLN	4.2
1	M	452	LEU	4.1
2	U	12	VAL	4.1
1	M	455	THR	4.0
1	B	510	VAL	4.0
2	W	94	TYR	3.9
2	E	75	LYS	3.9
2	E	1104	LEU	3.9
2	Q	93	TYR	3.8
1	N	558	PHE	3.8
2	U	102	ASN	3.8
1	T	598	LYS	3.8
1	G	584	PHE	3.8
1	T	543	ILE	3.8
2	U	73	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	O	1087	PHE	3.8
1	M	644	THR	3.7
1	B	552	GLN	3.7
2	E	85	LEU	3.7
2	I	102	ASN	3.7
2	W	107	TRP	3.7
1	T	522	PHE	3.6
1	M	542	LEU	3.6
2	I	27	PHE	3.6
1	B	582	ILE	3.6
1	T	455	THR	3.6
2	Q	1029	ILE	3.6
1	B	522	PHE	3.6
2	I	1012	SER	3.5
2	Q	100	TYR	3.5
2	O	1100	GLY	3.5
1	M	619	TYR	3.5
1	B	607	VAL	3.5
1	G	608	TRP	3.5
2	E	2	VAL	3.4
1	T	518	ALA	3.4
2	W	102	ASN	3.4
1	M	478	LEU	3.3
1	T	640	PHE	3.3
1	M	474	LEU	3.3
1	T	541	PHE	3.3
2	U	1045	LYS	3.3
1	N	459	PRO	3.3
2	W	95	CYS	3.2
2	E	71	LYS	3.2
2	W	61	ALA	3.2
2	O	63	PHE	3.2
2	Q	59	TYR	3.2
2	W	35	HIS	3.2
2	O	34	VAL	3.2
1	G	602	LEU	3.2
1	G	478	LEU	3.2
2	K	11	LEU	3.2
1	S	630	THR	3.2
1	T	625	LEU	3.1
2	Q	105	ASP	3.1
2	E	105	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	1104	LEU	3.1
1	M	522	PHE	3.1
1	B	508	MET	3.1
1	G	468	VAL	3.1
1	G	511	MET	3.1
1	H	521	TYR	3.1
2	I	29	LEU	3.1
2	I	1104	LEU	3.1
2	U	24	VAL	3.1
2	I	80	PHE	3.1
1	N	468	VAL	3.1
2	Q	67	LEU	3.1
1	H	619	TYR	3.1
1	M	512	VAL	3.1
2	C	74	SER	3.0
2	I	1021	ILE	3.0
1	B	584	PHE	3.0
1	M	624	ALA	3.0
1	G	510	VAL	3.0
2	U	1073	LEU	3.0
1	T	542	LEU	3.0
1	H	624	ALA	3.0
1	H	540	ILE	2.9
1	B	613	LEU	2.9
1	T	639	LEU	2.9
2	W	66	ARG	2.9
2	W	20	ILE	2.9
2	U	87	ALA	2.9
2	E	94	TYR	2.9
2	Q	26	GLY	2.9
2	U	1086	TYR	2.9
1	G	635	ASP	2.8
1	T	523	MET	2.8
1	M	543	ILE	2.8
2	I	1014	SER	2.8
2	E	1063	SER	2.8
2	U	100	TYR	2.8
1	H	629	ILE	2.8
2	E	80	PHE	2.8
1	T	555	MET	2.8
2	I	1047	LEU	2.8
2	U	45	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	604	GLU	2.7
2	I	11	LEU	2.7
1	T	456	LEU	2.7
1	T	599	GLU	2.7
1	N	571	LEU	2.7
1	M	592	LEU	2.7
1	B	542	LEU	2.7
1	B	555	MET	2.7
1	S	451	TRP	2.7
2	E	37	VAL	2.7
2	I	1033	LEU	2.7
2	U	5	LYS	2.7
1	A	543	ILE	2.7
1	B	478	LEU	2.7
1	G	508	MET	2.7
2	C	15	SER	2.7
2	E	67	LEU	2.7
1	T	573	VAL	2.7
2	I	34	VAL	2.7
2	W	65	SER	2.7
1	G	461	THR	2.7
1	T	591	LEU	2.7
2	K	13	GLN	2.7
2	U	65	SER	2.6
1	G	558	PHE	2.6
1	B	470	ILE	2.6
2	I	33	GLY	2.6
1	B	517	LYS	2.6
2	U	1046	LEU	2.6
2	K	40	SER	2.6
2	I	1019	VAL	2.6
1	T	572	THR	2.6
1	G	540	ILE	2.6
2	O	29	LEU	2.6
2	E	1006	GLN	2.6
1	G	591	LEU	2.6
2	E	18	LEU	2.6
2	I	1102	THR	2.6
2	Q	27	PHE	2.6
2	I	71	LYS	2.6
2	Q	29	LEU	2.6
2	W	27	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	U	93	TYR	2.6
2	O	1069	THR	2.6
2	K	12	VAL	2.6
1	G	542	LEU	2.6
2	I	18	LEU	2.6
1	T	489	VAL	2.6
1	B	592	LEU	2.6
1	H	627	TYR	2.6
1	A	489	VAL	2.6
1	A	610	ARG	2.6
2	K	41	PRO	2.6
2	O	1080	GLN	2.6
2	O	1047	LEU	2.6
2	I	1086	TYR	2.5
2	I	1024	ARG	2.5
1	T	628	PHE	2.5
1	M	470	ILE	2.5
1	T	627	TYR	2.5
1	S	456	LEU	2.5
1	T	480	MET	2.5
2	C	1062	PHE	2.5
1	T	596	THR	2.5
1	A	499	SER	2.5
1	G	610	ARG	2.5
1	S	549	PHE	2.5
2	I	106	TYR	2.5
1	M	560	ARG	2.5
2	I	1097	THR	2.5
2	O	1021	ILE	2.5
2	I	1048	ILE	2.4
2	W	78	VAL	2.4
2	E	92	ILE	2.4
1	S	484	MET	2.4
2	U	1032	TYR	2.4
1	T	457	THR	2.4
2	K	9	PRO	2.4
2	U	43	LYS	2.4
2	Q	63	PHE	2.4
2	I	4	LEU	2.4
1	N	604	GLU	2.4
1	A	553	CYS	2.4
1	G	553	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	77	GLN	2.4
1	T	644	THR	2.4
2	E	93	TYR	2.4
2	E	113	VAL	2.4
2	I	8	GLY	2.4
1	G	453	ASN	2.4
1	N	467	LEU	2.4
1	N	591	LEU	2.4
2	C	10	GLY	2.4
2	O	1098	PHE	2.4
1	S	459	PRO	2.4
1	S	602	LEU	2.4
1	M	640	PHE	2.3
2	I	36	TRP	2.3
2	W	104	MET	2.3
2	K	69	ILE	2.3
2	I	99	TYR	2.3
1	G	629	ILE	2.3
2	W	36	TRP	2.3
2	K	102	ASN	2.3
2	Q	73	ASN	2.3
2	W	68	THR	2.3
2	U	83	ASN	2.3
1	G	594	SER	2.3
1	T	517	LYS	2.3
1	H	570	ASN	2.3
1	M	638	ILE	2.3
1	S	467	LEU	2.3
2	O	1027	GLN	2.3
2	W	80	PHE	2.3
1	H	435	LEU	2.3
2	E	45	LEU	2.3
2	E	1047	LEU	2.3
1	M	479	ILE	2.3
2	I	91	GLY	2.3
2	K	1096	PRO	2.3
2	E	111	THR	2.3
2	I	9	PRO	2.3
2	I	85	LEU	2.3
1	T	550	LYS	2.3
1	T	553	CYS	2.2
2	Q	1047	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	U	79	PHE	2.2
1	A	432	ARG	2.2
1	H	641	GLU	2.2
2	O	7	SER	2.2
1	A	522	PHE	2.2
1	B	500	ARG	2.2
2	O	1005	THR	2.2
2	W	1054	LEU	2.2
1	S	558	PHE	2.2
2	W	50	VAL	2.2
1	M	606	TRP	2.2
2	W	108	GLY	2.2
2	O	78	VAL	2.2
1	M	518	ALA	2.2
2	E	1078	LEU	2.2
2	U	1059	PRO	2.2
2	I	23	THR	2.2
1	N	546	LEU	2.2
2	C	1083	ILE	2.2
1	G	550	LYS	2.2
1	S	434	LEU	2.2
1	A	536	GLN	2.2
1	H	479	ILE	2.2
1	S	512	VAL	2.2
1	T	592	LEU	2.1
1	H	468	VAL	2.1
1	S	470	ILE	2.1
2	Q	78	VAL	2.1
1	H	491	TRP	2.1
2	Q	60	ASN	2.1
2	Q	1054	LEU	2.1
2	W	59	TYR	2.1
1	G	616	ASP	2.1
1	G	455	THR	2.1
2	C	75	LYS	2.1
1	S	440	ILE	2.1
2	K	55	GLY	2.1
1	S	517	LYS	2.1
2	U	46	GLU	2.1
1	B	438	GLY	2.1
1	M	625	LEU	2.1
2	K	1098	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	1062	PHE	2.1
1	G	486	ILE	2.1
1	S	449	GLN	2.1
2	W	1048	ILE	2.1
1	S	542	LEU	2.1
2	K	45	LEU	2.1
2	Q	62	ALA	2.1
1	S	520	VAL	2.1
2	Q	20	ILE	2.1
1	G	523	MET	2.1
2	I	78	VAL	2.1
2	W	60	ASN	2.1
1	N	455	THR	2.1
1	G	557	TYR	2.1
2	O	1032	TYR	2.1
1	G	642	GLY	2.1
1	T	536	GLN	2.1
1	M	558	PHE	2.1
2	C	1036	TYR	2.1
2	Q	61	ALA	2.1
2	Q	71	LYS	2.1
2	W	32	TYR	2.1
2	C	80	PHE	2.1
2	O	1078	LEU	2.1
1	A	602	LEU	2.0
1	S	478	LEU	2.0
1	N	583	ARG	2.0
1	G	518	ALA	2.0
2	I	22	CYS	2.0
1	H	455	THR	2.0
2	O	45	LEU	2.0
1	S	455	THR	2.0
2	O	96	GLY	2.0
1	B	561	GLU	2.0
2	C	40	SER	2.0
1	T	479	ILE	2.0
2	C	69	ILE	2.0
2	O	51	ILE	2.0
1	A	561	GLU	2.0
1	B	484	MET	2.0
1	B	523	MET	2.0
2	O	1025	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	W	62	ALA	2.0
2	W	1049	TYR	2.0
1	T	498	PRO	2.0
1	A	490	GLU	2.0
1	B	550	LYS	2.0
1	N	570	ASN	2.0
1	B	512	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	E	1201	14/15	0.84	0.29	-	138,153,158,158	0
3	NAG	C	1201	14/15	0.65	0.42	-	146,163,170,174	0
3	NAG	I	1201	14/15	0.79	0.19	-	133,147,156,157	0
3	NAG	K	1201	14/15	0.65	0.29	-	140,179,188,188	0

6.5 Other polymers (i)

There are no such residues in this entry.