



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:01 AM GMT

PDB ID : 3CSY
Title : Crystal structure of the trimeric prefusion Ebola virus glycoprotein in complex with a neutralizing antibody from a human survivor
Authors : Lee, J.E.; Fusco, M.L.; Hessel, A.J.; Oswald, W.B.; Burton, D.R.; Saphire, E.O.
Deposited on : 2008-04-10
Resolution : 3.40 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

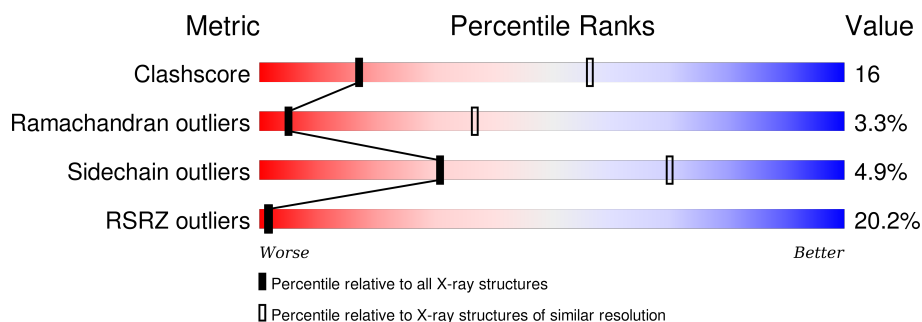
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	<div> <div>20%</div> <div>63%</div> <div>33%</div> <div>.</div> </div>
1	C	226	<div> <div>19%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
1	E	226	<div> <div>17%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	G	226	<div> <div>22%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
2	B	217	<div> <div>33%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
2	D	217	<div> <div>29%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
2	F	217	<div> <div>25%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	217	
3	I	334	
3	K	334	
3	M	334	
3	O	334	
4	J	131	
4	L	131	
4	N	131	
4	P	131	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	K	351	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23539 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 Fab KZ52 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	0	0
			1687	1059	286	334	4	4			
1	C	226	Total	C	N	O	S	Se	0	0	0
			1687	1059	286	334	4	4			
1	E	226	Total	C	N	O	S	Se	0	0	0
			1687	1059	286	334	4	4			
1	G	226	Total	C	N	O	S	Se	0	0	0
			1687	1059	286	334	4	4			

- Molecule 2 is a protein called Fab KZ52 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	Se	0	0	0
			1682	1056	281	340	4	1			
2	D	217	Total	C	N	O	S	Se	0	0	0
			1682	1056	281	340	4	1			
2	F	217	Total	C	N	O	S	Se	0	0	0
			1682	1056	281	340	4	1			
2	H	217	Total	C	N	O	S	Se	0	0	0
			1682	1056	281	340	4	1			

- Molecule 3 is a protein called Envelope glycoprotein GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	236	Total	C	N	O	S	0	0	0
			1707	1085	293	325	4			
3	K	232	Total	C	N	O	S	0	0	0
			1687	1073	289	321	4			
3	M	230	Total	C	N	O	S	0	0	0
			1677	1067	287	319	4			
3	O	225	Total	C	N	O	S	0	0	0
			1651	1052	282	313	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	TYR	-	EXPRESSION TAG	UNP Q05320
I	17	PRO	-	EXPRESSION TAG	UNP Q05320
I	18	TYR	-	EXPRESSION TAG	UNP Q05320
I	19	ASP	-	EXPRESSION TAG	UNP Q05320
I	20	VAL	-	EXPRESSION TAG	UNP Q05320
I	21	PRO	-	EXPRESSION TAG	UNP Q05320
I	22	ASP	-	EXPRESSION TAG	UNP Q05320
I	23	TYR	-	EXPRESSION TAG	UNP Q05320
I	24	ALA	-	EXPRESSION TAG	UNP Q05320
I	25	ILE	-	EXPRESSION TAG	UNP Q05320
I	26	GLU	-	EXPRESSION TAG	UNP Q05320
I	27	GLY	-	EXPRESSION TAG	UNP Q05320
I	28	ARG	-	EXPRESSION TAG	UNP Q05320
I	29	GLY	-	EXPRESSION TAG	UNP Q05320
I	30	ALA	-	EXPRESSION TAG	UNP Q05320
I	31	ARG	-	EXPRESSION TAG	UNP Q05320
I	42	VAL	THR	ENGINEERED	UNP Q05320
I	230	VAL	THR	ENGINEERED	UNP Q05320
K	16	TYR	-	EXPRESSION TAG	UNP Q05320
K	17	PRO	-	EXPRESSION TAG	UNP Q05320
K	18	TYR	-	EXPRESSION TAG	UNP Q05320
K	19	ASP	-	EXPRESSION TAG	UNP Q05320
K	20	VAL	-	EXPRESSION TAG	UNP Q05320
K	21	PRO	-	EXPRESSION TAG	UNP Q05320
K	22	ASP	-	EXPRESSION TAG	UNP Q05320
K	23	TYR	-	EXPRESSION TAG	UNP Q05320
K	24	ALA	-	EXPRESSION TAG	UNP Q05320
K	25	ILE	-	EXPRESSION TAG	UNP Q05320
K	26	GLU	-	EXPRESSION TAG	UNP Q05320
K	27	GLY	-	EXPRESSION TAG	UNP Q05320
K	28	ARG	-	EXPRESSION TAG	UNP Q05320
K	29	GLY	-	EXPRESSION TAG	UNP Q05320
K	30	ALA	-	EXPRESSION TAG	UNP Q05320
K	31	ARG	-	EXPRESSION TAG	UNP Q05320
K	42	VAL	THR	ENGINEERED	UNP Q05320
K	230	VAL	THR	ENGINEERED	UNP Q05320
M	16	TYR	-	EXPRESSION TAG	UNP Q05320
M	17	PRO	-	EXPRESSION TAG	UNP Q05320
M	18	TYR	-	EXPRESSION TAG	UNP Q05320
M	19	ASP	-	EXPRESSION TAG	UNP Q05320
M	20	VAL	-	EXPRESSION TAG	UNP Q05320
M	21	PRO	-	EXPRESSION TAG	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
M	22	ASP	-	EXPRESSION TAG	UNP Q05320
M	23	TYR	-	EXPRESSION TAG	UNP Q05320
M	24	ALA	-	EXPRESSION TAG	UNP Q05320
M	25	ILE	-	EXPRESSION TAG	UNP Q05320
M	26	GLU	-	EXPRESSION TAG	UNP Q05320
M	27	GLY	-	EXPRESSION TAG	UNP Q05320
M	28	ARG	-	EXPRESSION TAG	UNP Q05320
M	29	GLY	-	EXPRESSION TAG	UNP Q05320
M	30	ALA	-	EXPRESSION TAG	UNP Q05320
M	31	ARG	-	EXPRESSION TAG	UNP Q05320
M	42	VAL	THR	ENGINEERED	UNP Q05320
M	230	VAL	THR	ENGINEERED	UNP Q05320
O	16	TYR	-	EXPRESSION TAG	UNP Q05320
O	17	PRO	-	EXPRESSION TAG	UNP Q05320
O	18	TYR	-	EXPRESSION TAG	UNP Q05320
O	19	ASP	-	EXPRESSION TAG	UNP Q05320
O	20	VAL	-	EXPRESSION TAG	UNP Q05320
O	21	PRO	-	EXPRESSION TAG	UNP Q05320
O	22	ASP	-	EXPRESSION TAG	UNP Q05320
O	23	TYR	-	EXPRESSION TAG	UNP Q05320
O	24	ALA	-	EXPRESSION TAG	UNP Q05320
O	25	ILE	-	EXPRESSION TAG	UNP Q05320
O	26	GLU	-	EXPRESSION TAG	UNP Q05320
O	27	GLY	-	EXPRESSION TAG	UNP Q05320
O	28	ARG	-	EXPRESSION TAG	UNP Q05320
O	29	GLY	-	EXPRESSION TAG	UNP Q05320
O	30	ALA	-	EXPRESSION TAG	UNP Q05320
O	31	ARG	-	EXPRESSION TAG	UNP Q05320
O	42	VAL	THR	ENGINEERED	UNP Q05320
O	230	VAL	THR	ENGINEERED	UNP Q05320

- Molecule 4 is a protein called Envelope glycoprotein GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	98	Total	C	N	O	S	0	0	0
			746	477	130	136	3			
4	L	93	Total	C	N	O	S	0	0	0
			727	466	126	132	3			
4	N	95	Total	C	N	O	S	0	0	0
			732	469	128	132	3			
4	P	93	Total	C	N	O	S	0	0	0
			719	462	125	129	3			

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	5	Total	C	N	O	0	0
			61	34	2	25		
6	N	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	2	Total	C	N	O	0	0
			28	16	2	10		

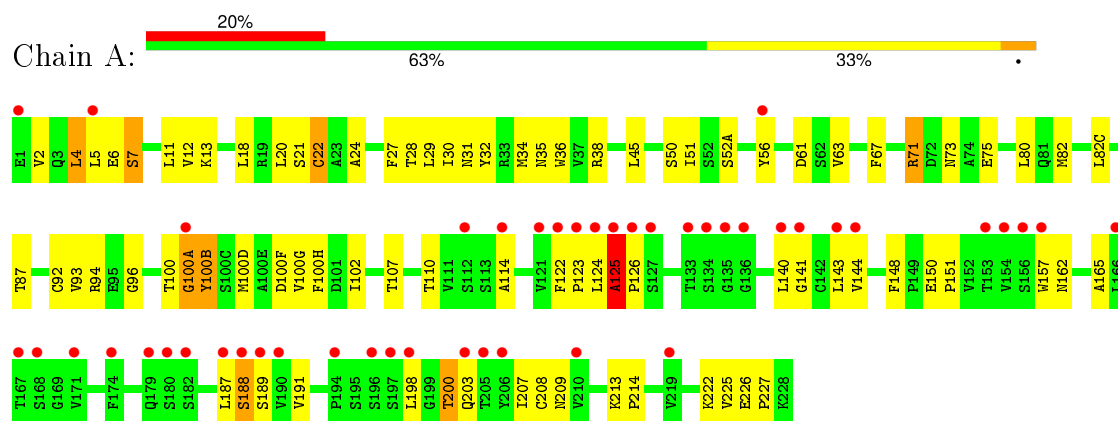
- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	6	Total	C	N	O	0	0
			75	42	3	30		
8	P	6	Total	C	N	O	0	0
			75	42	3	30		

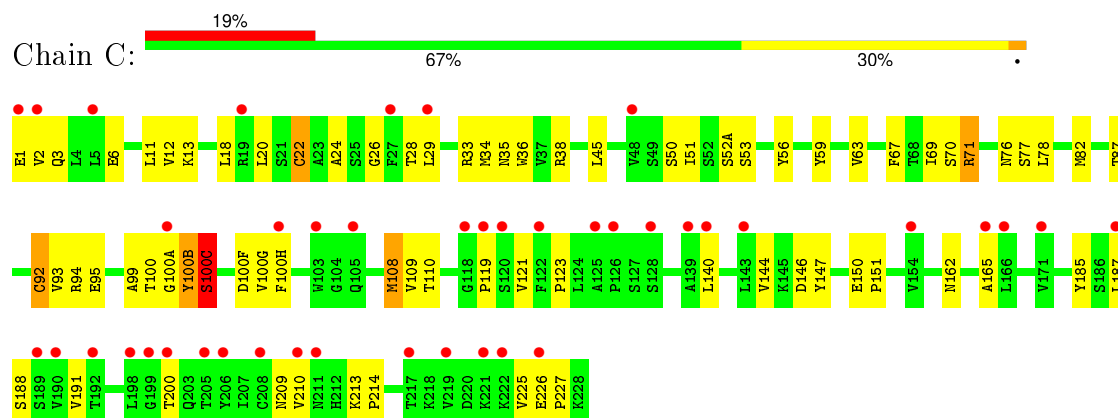
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

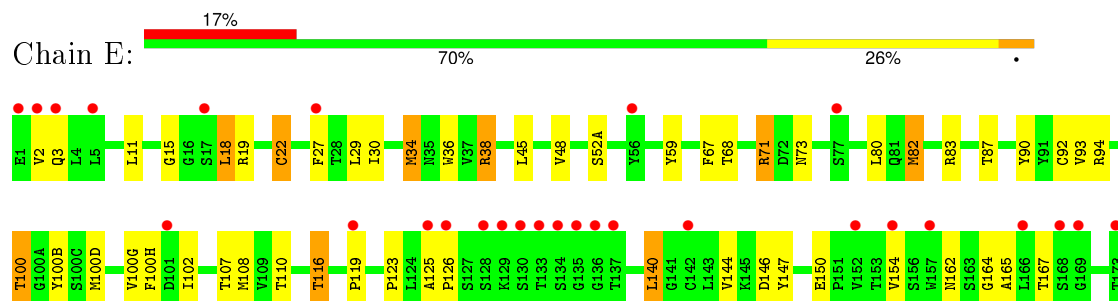
- Molecule 1: Fab KZ52 heavy chain

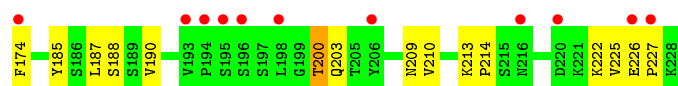


- Molecule 1: Fab KZ52 heavy chain

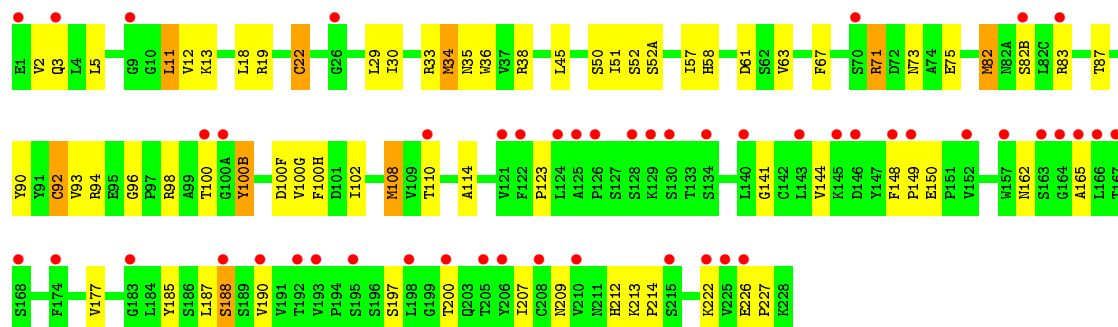


- Molecule 1: Fab KZ52 heavy chain

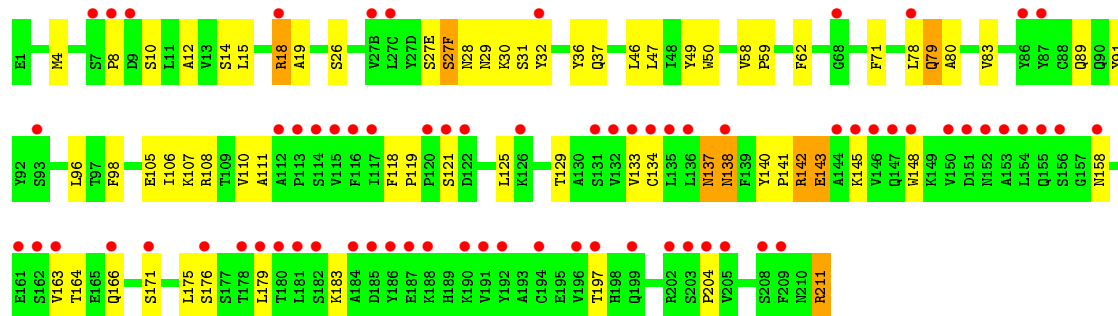




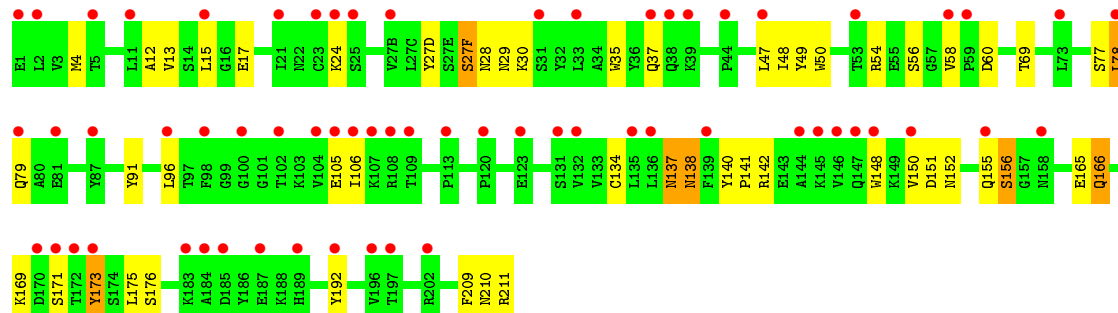
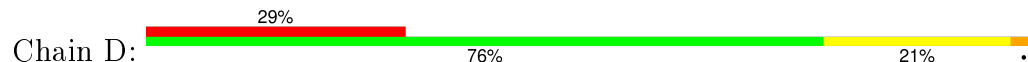
• Molecule 1: Fab KZ52 heavy chain



• Molecule 2: Fab KZ52 light chain

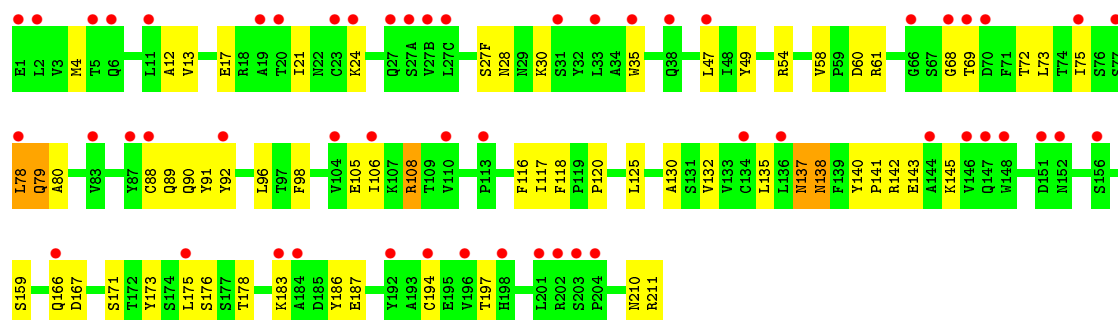


• Molecule 2: Fab KZ52 light chain

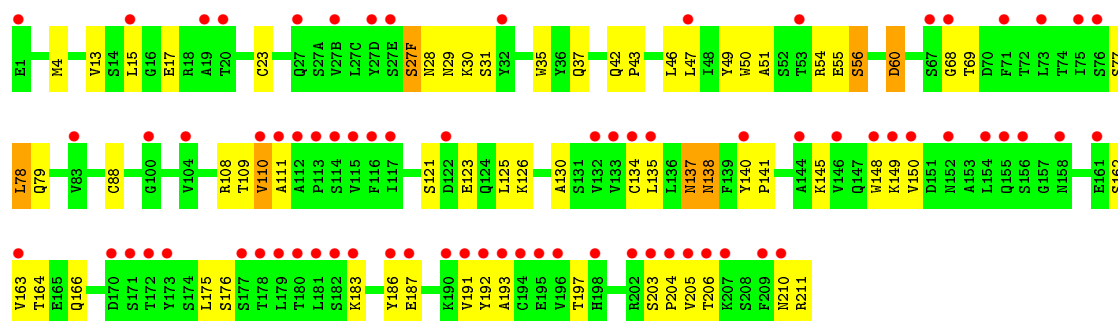


• Molecule 2: Fab KZ52 light chain

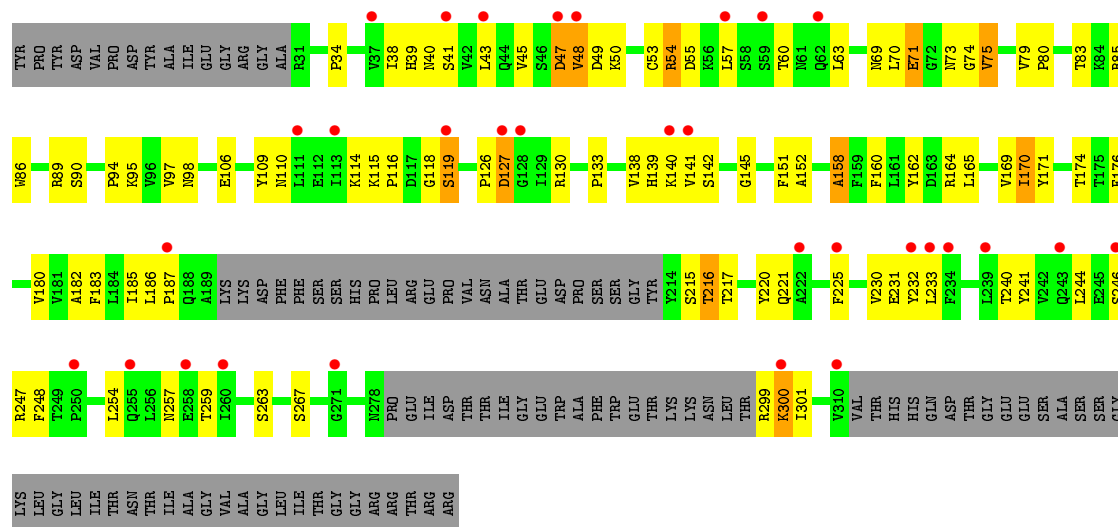




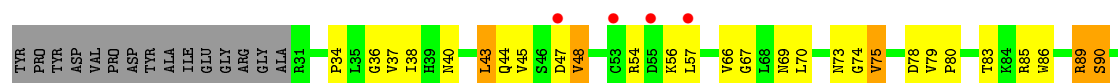
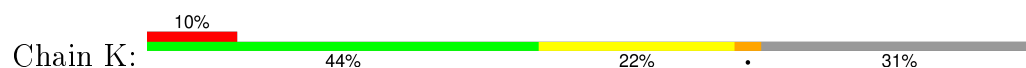
• Molecule 2: Fab KZ52 light chain

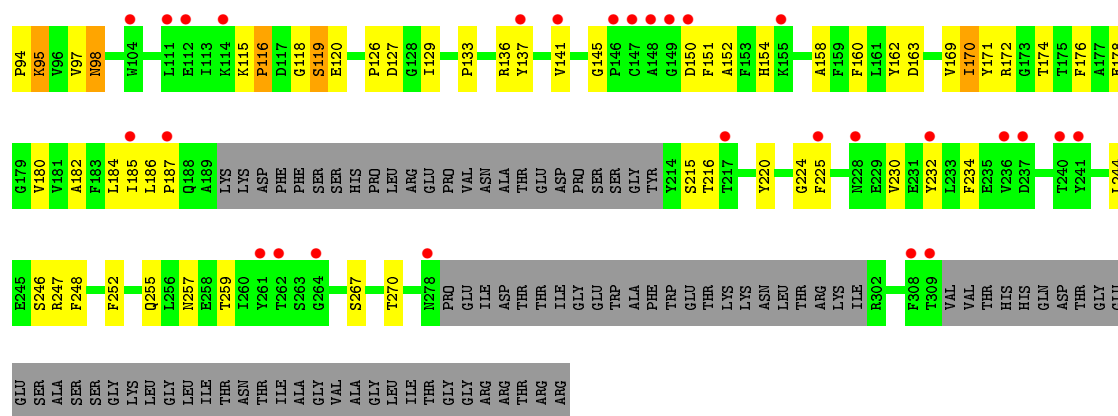


• Molecule 3: Envelope glycoprotein GP1

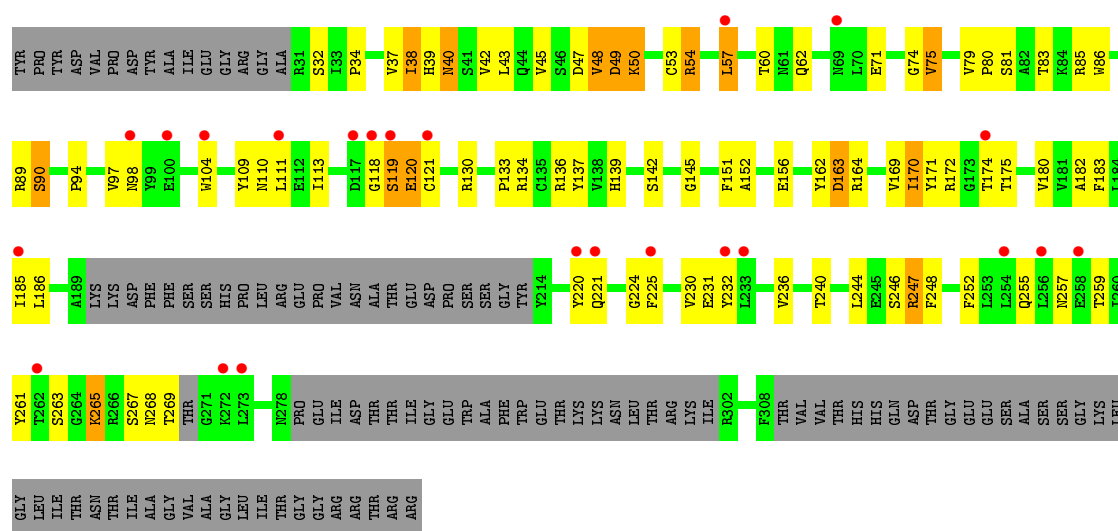


• Molecule 3: Envelope glycoprotein GP1

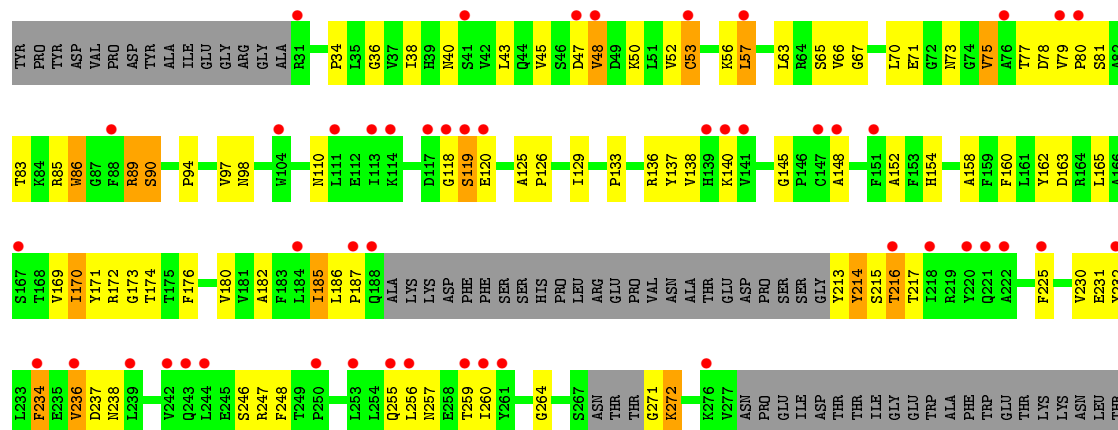




• Molecule 3: Envelope glycoprotein GP1



• Molecule 3: Envelope glycoprotein GP1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	273.71Å 273.71Å 409.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 3.40 48.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.37-3.40) 96.9 (48.37-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.261 , 0.302 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 168.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 151305 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	23539	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.53	0/1721	0.56	0/2333
1	C	0.49	1/1721 (0.1%)	0.50	0/2333
1	E	0.49	1/1721 (0.1%)	0.52	0/2333
1	G	0.48	0/1721	0.52	0/2333
2	B	0.41	0/1718	0.50	0/2331
2	D	0.37	0/1718	0.49	0/2331
2	F	0.42	0/1718	0.49	0/2331
2	H	0.37	0/1718	0.48	0/2331
3	I	0.49	0/1743	0.57	0/2379
3	K	0.44	0/1723	0.54	0/2351
3	M	0.47	0/1712	0.57	1/2334 (0.0%)
3	O	0.41	0/1686	0.53	0/2298
4	J	0.54	0/762	0.60	0/1038
4	L	0.47	0/742	0.56	0/1010
4	N	0.50	0/747	0.61	0/1016
4	P	0.49	0/734	0.61	0/999
All	All	0.46	2/23605 (0.0%)	0.53	1/32081 (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	A	0	1
3	I	0	1
3	K	0	1
4	N	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	MSE	CG-SE	-5.33	1.77	1.95
1	E	34	MSE	CG-SE	-5.19	1.77	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	265	LYS	N-CA-C	5.20	125.03	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ALA	Peptide
3	I	55	ASP	Peptide
3	K	54	ARG	Peptide
4	N	536	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1687	0	1660	78	0
1	C	1687	0	1660	51	0
1	E	1687	0	1660	59	0
1	G	1687	0	1660	53	0
2	B	1682	0	1638	48	0
2	D	1682	0	1638	39	0
2	F	1682	0	1638	38	0
2	H	1682	0	1638	44	0
3	I	1707	0	1548	81	0
3	K	1687	0	1540	73	0
3	M	1677	0	1535	68	0
3	O	1651	0	1520	73	0
4	J	746	0	722	41	0
4	L	727	0	712	44	0
4	N	732	0	716	39	0
4	P	719	0	706	26	0
5	I	39	0	34	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	39	0	34	0	0
5	O	39	0	34	6	0
6	J	61	0	52	2	0
6	N	61	0	52	3	0
7	K	28	0	25	2	0
8	L	75	0	64	3	0
8	P	75	0	64	4	0
All	All	23539	0	22550	750	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 16.

All (750) 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)
4:N:563:ASN:ND2	6:N:701:NAG:C1	1.67	1.54
3:O:257:ASN:HD21	5:O:351:NAG:C1	0.89	1.53
3:I:257:ASN:ND2	5:I:351:NAG:C1	1.68	1.51
3:K:257:ASN:ND2	7:K:351:NAG:C1	1.68	1.50
4:L:563:ASN:ND2	8:L:701:NAG:C1	1.70	1.49
4:P:563:ASN:HD21	8:P:701:NAG:C1	1.25	1.49
3:O:257:ASN:ND2	5:O:351:NAG:C1	1.72	1.44
4:P:563:ASN:ND2	8:P:701:NAG:C1	2.00	1.23
3:I:257:ASN:CG	5:I:351:NAG:C1	2.28	1.02
1:A:125:ALA:HB1	1:A:126:PRO:HD3	1.43	0.99
6:J:703:BMA:H62	6:J:705:MAN:H3	1.44	0.99
1:E:93:VAL:HG11	1:E:100(H):PHE:HB3	1.58	0.86
3:I:257:ASN:ND2	5:I:351:NAG:C2	2.39	0.85
3:I:48:VAL:HG11	4:J:592:PHE:HA	1.62	0.81
4:P:561:LEU:O	4:P:565:THR:HG23	1.82	0.79
3:M:48:VAL:HG11	4:N:592:PHE:HA	1.64	0.79
1:A:35:ASN:OD1	1:A:50:SER:HB3	1.83	0.78
1:A:125:ALA:CB	1:A:126:PRO:HD3	2.14	0.78
4:N:563:ASN:CG	6:N:701:NAG:C1	2.51	0.78
4:N:561:LEU:O	4:N:565:THR:HG23	1.84	0.77
3:M:94:PRO:HB3	3:M:169:VAL:HG21	1.68	0.76
4:L:561:LEU:O	4:L:565:THR:HG23	1.85	0.75
1:A:125:ALA:HB1	1:A:126:PRO:CD	2.17	0.75
4:J:561:LEU:O	4:J:565:THR:HG23	1.86	0.75
3:O:257:ASN:HD21	5:O:351:NAG:C2	1.95	0.74
3:O:257:ASN:CG	5:O:351:NAG:C1	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:563:ASN:CG	8:L:701:NAG:C1	2.55	0.73
3:I:80:PRO:HG2	3:I:246:SER:HA	1.70	0.73
3:I:257:ASN:OD1	5:I:351:NAG:C1	2.36	0.73
1:E:29:LEU:CD2	1:E:34:MSE:SE	2.87	0.72
3:K:89:ARG:HG2	3:K:90:SER:N	2.05	0.70
1:G:29:LEU:CD2	1:G:34:MSE:SE	2.90	0.70
1:A:100(A):GLY:O	1:A:100(B):TYR:HB3	1.93	0.69
4:L:563:ASN:ND2	8:L:701:NAG:C2	2.55	0.69
4:P:563:ASN:CG	8:P:701:NAG:C1	2.61	0.69
3:M:80:PRO:HG2	3:M:246:SER:HA	1.75	0.69
3:K:57:LEU:HD12	3:K:185:ILE:HD11	1.74	0.69
3:K:89:ARG:NH1	4:N:536:GLY:HA3	2.08	0.69
4:J:593:LEU:HD21	4:N:594:LEU:HD23	1.73	0.69
3:K:257:ASN:CG	7:K:351:NAG:C1	2.60	0.68
1:E:100:THR:HG21	1:E:100(B):TYR:CE2	2.28	0.68
3:I:180:VAL:HG23	4:J:562:ALA:HB1	1.73	0.68
4:L:521:GLN:O	4:L:522:ASP:HB2	1.93	0.68
3:M:34:PRO:HG2	4:N:565:THR:HG22	1.77	0.67
1:E:29:LEU:HD22	1:E:34:MSE:SE	2.44	0.67
3:O:34:PRO:HG2	4:P:565:THR:HG22	1.77	0.66
3:I:182:ALA:HB2	4:J:562:ALA:HA	1.77	0.66
1:G:93:VAL:HG11	1:G:100(H):PHE:HB3	1.78	0.66
1:C:100:THR:HG21	1:C:100(B):TYR:CE2	2.31	0.66
4:J:594:LEU:HD23	4:L:593:LEU:HD21	1.78	0.65
3:O:47:ASP:O	3:O:48:VAL:HG23	1.97	0.65
3:O:57:LEU:HD12	3:O:185:ILE:HD11	1.76	0.65
1:C:82:MSE:HE1	1:C:109:VAL:HG21	1.79	0.65
3:M:83:THR:HG21	3:M:232:TYR:OH	1.97	0.64
3:K:34:PRO:HG2	4:L:565:THR:HG22	1.78	0.64
1:E:94:ARG:CZ	1:E:102:ILE:HD12	2.28	0.63
4:J:594:LEU:HD22	3:K:57:LEU:HD22	1.80	0.63
3:O:271:GLY:CA	3:O:272:LYS:CB	2.76	0.63
3:M:97:VAL:CG2	4:N:573:LEU:HD21	2.28	0.63
3:K:97:VAL:HG22	4:L:573:LEU:HD21	1.79	0.63
3:K:83:THR:HG21	3:K:232:TYR:OH	1.99	0.63
1:G:87:THR:HG23	1:G:110:THR:HA	1.81	0.63
1:E:52(A):SER:HA	1:E:71:ARG:CZ	2.29	0.62
1:G:34:MSE:HE3	1:G:94:ARG:HA	1.80	0.62
2:B:28:ASN:HB3	2:B:30:LYS:HG3	1.80	0.62
3:I:152:ALA:HB3	3:I:170:ILE:HG13	1.81	0.62
1:A:87:THR:HG23	1:A:110:THR:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLU:HG2	1:C:185:TYR:CE1	2.35	0.61
1:G:100:THR:HG21	1:G:100(B):TYR:CE2	2.36	0.61
1:G:94:ARG:CZ	1:G:102:ILE:HD12	2.30	0.61
3:M:182:ALA:HB2	4:N:562:ALA:HB2	1.83	0.61
1:A:30:ILE:HG12	1:A:73:ASN:HB3	1.82	0.61
3:I:38:ILE:HD11	3:I:186:LEU:HD23	1.81	0.61
1:C:93:VAL:HG11	1:C:100(H):PHE:HB3	1.82	0.61
2:B:78:LEU:O	2:B:79:GLN:HB2	2.01	0.61
3:M:38:ILE:HD11	3:M:186:LEU:HD23	1.83	0.60
2:H:140:TYR:CD1	2:H:141:PRO:HA	2.36	0.60
3:I:97:VAL:HG22	4:J:573:LEU:HD21	1.83	0.60
1:E:87:THR:HG23	1:E:110:THR:HA	1.82	0.60
3:O:80:PRO:HG2	3:O:246:SER:HA	1.84	0.60
4:L:576:THR:HG23	4:L:578:GLU:HG2	1.83	0.60
3:I:299:ARG:O	3:I:300:LYS:CB	2.50	0.60
3:O:97:VAL:HG22	4:P:573:LEU:HD21	1.83	0.60
3:K:182:ALA:HB2	4:L:562:ALA:HA	1.82	0.60
3:I:97:VAL:HG12	3:I:98:ASN:N	2.17	0.60
3:K:180:VAL:HG23	4:L:562:ALA:HB1	1.82	0.60
2:F:80:ALA:HA	2:F:106:ILE:HD11	1.82	0.60
1:A:123:PRO:HB2	1:A:225:VAL:HG13	1.82	0.60
3:I:34:PRO:HG2	4:J:565:THR:HG22	1.84	0.60
2:F:175:LEU:HD23	2:F:176:SER:N	2.17	0.60
1:E:30:ILE:HG12	1:E:73:ASN:HB3	1.84	0.59
1:A:226:GLU:HB3	1:A:227:PRO:HD2	1.83	0.59
3:K:97:VAL:HG12	3:K:98:ASN:N	2.17	0.59
3:O:70:LEU:HB3	3:O:75:VAL:HG21	1.84	0.59
1:G:11:LEU:HD13	1:G:149:PRO:HG3	1.84	0.59
1:E:100(D):MSE:HE3	2:F:92:TYR:O	2.02	0.59
1:E:36:TRP:O	1:E:48:VAL:HB	2.02	0.59
3:I:83:THR:HG21	3:I:232:TYR:OH	2.02	0.59
3:M:156:GLU:HG2	6:N:702:NAG:H61	1.85	0.59
3:K:79:VAL:HG21	3:K:220:TYR:CZ	2.38	0.59
3:O:215:SER:O	3:O:216:THR:HB	2.03	0.59
3:I:182:ALA:HB2	4:J:562:ALA:CA	2.33	0.58
3:K:47:ASP:O	3:K:48:VAL:HB	2.03	0.58
2:F:78:LEU:O	2:F:79:GLN:HB2	2.04	0.58
3:O:126:PRO:HD2	3:O:129:ILE:HD12	1.84	0.58
2:H:77:SER:O	2:H:78:LEU:HB3	2.04	0.58
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.39	0.58
4:J:509:PRO:O	4:J:510:LYS:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:579:LEU:HD12	4:J:579:LEU:H	1.68	0.58
3:K:74:GLY:O	3:K:75:VAL:C	2.42	0.58
3:I:232:TYR:HB3	3:I:244:LEU:HD12	1.85	0.58
2:B:175:LEU:HD23	2:B:176:SER:N	2.17	0.58
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.85	0.57
4:P:560:GLN:O	4:P:563:ASN:HB3	2.04	0.57
2:D:105:GLU:HB2	2:D:166:GLN:NE2	2.19	0.57
1:A:126:PRO:HD2	1:A:227:PRO:HA	1.86	0.57
3:I:53:CYS:O	3:I:54:ARG:CB	2.52	0.57
3:K:126:PRO:HG2	3:K:129:ILE:HD12	1.87	0.57
3:K:185:ILE:O	3:K:185:ILE:HG23	2.05	0.57
3:M:97:VAL:HG22	4:N:573:LEU:HD21	1.86	0.57
3:I:94:PRO:HB3	3:I:169:VAL:HG21	1.86	0.57
1:A:93:VAL:HG11	1:A:100(H):PHE:HB3	1.85	0.57
2:F:145:LYS:HB3	2:F:197:THR:HB	1.87	0.57
2:H:4:MSE:HE2	2:H:23:CYS:SG	2.45	0.56
1:C:100(G):VAL:HG11	2:D:49:TYR:HB2	1.87	0.56
1:A:20:LEU:HD22	1:A:107:THR:HG21	1.85	0.56
2:F:91:TYR:HA	2:F:96:LEU:HD22	1.88	0.56
2:D:15:LEU:HA	2:D:78:LEU:HD23	1.87	0.56
3:I:160:PHE:CD2	3:I:170:ILE:HG23	2.41	0.56
3:M:48:VAL:HG21	4:N:592:PHE:HB2	1.88	0.56
1:A:100(G):VAL:HG11	2:B:49:TYR:CB	2.36	0.56
2:D:175:LEU:HD23	2:D:176:SER:N	2.21	0.56
1:E:226:GLU:HB3	1:E:227:PRO:HD2	1.87	0.56
3:M:74:GLY:O	3:M:75:VAL:C	2.44	0.56
3:O:180:VAL:HG23	4:P:562:ALA:HB1	1.88	0.56
3:M:230:VAL:HG12	3:M:231:GLU:N	2.20	0.56
2:B:28:ASN:HB3	2:B:30:LYS:CG	2.36	0.55
1:C:226:GLU:HB3	1:C:227:PRO:HD2	1.87	0.55
1:C:150:GLU:OE1	1:C:151:PRO:HA	2.06	0.55
2:F:89:GLN:HB2	2:F:98:PHE:CD2	2.41	0.55
2:D:77:SER:O	2:D:78:LEU:HB3	2.07	0.55
1:C:100:THR:HG23	4:N:552:ASP:HB3	1.89	0.55
2:H:35:TRP:CZ3	2:H:88:CYS:HB3	2.41	0.55
3:K:36:GLY:O	3:K:185:ILE:HG22	2.05	0.55
3:I:185:ILE:HG23	3:I:185:ILE:O	2.07	0.55
1:A:162:ASN:HB2	1:A:165:ALA:HB3	1.87	0.55
3:K:37:VAL:HA	3:K:185:ILE:HG22	1.88	0.55
2:D:134:CYS:HB2	2:D:148:TRP:CH2	2.41	0.55
3:O:215:SER:O	3:O:216:THR:CB	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:VAL:HG21	4:J:504:ILE:HG23	1.89	0.54
2:B:78:LEU:O	2:B:79:GLN:CB	2.55	0.54
1:G:82:MSE:HE1	1:G:90:TYR:CZ	2.42	0.54
1:A:4:LEU:HD11	1:A:102:ILE:HG22	1.89	0.54
3:K:57:LEU:HD23	3:K:57:LEU:C	2.28	0.54
3:I:57:LEU:HD22	4:N:594:LEU:HD22	1.88	0.54
3:K:37:VAL:HA	3:K:185:ILE:CG2	2.37	0.54
1:C:20:LEU:HG	1:C:82:MSE:HE2	1.90	0.54
3:I:74:GLY:O	3:I:75:VAL:C	2.46	0.54
3:K:94:PRO:HB3	3:K:169:VAL:HG21	1.88	0.54
3:O:246:SER:O	3:O:248:PHE:N	2.41	0.54
3:O:97:VAL:HG12	3:O:98:ASN:N	2.22	0.54
3:M:255:GLN:O	3:M:259:THR:HG23	2.07	0.54
3:O:45:VAL:HG21	4:P:504:ILE:HG23	1.90	0.54
3:O:171:TYR:HB2	3:O:174:THR:HG21	1.90	0.54
1:C:52(A):SER:HA	1:C:71:ARG:CZ	2.38	0.54
2:H:140:TYR:CG	2:H:141:PRO:HA	2.44	0.53
3:M:220:TYR:CE2	3:M:244:LEU:HD11	2.42	0.53
1:A:34:MSE:HE3	1:A:93:VAL:O	2.09	0.53
3:M:163:ASP:C	3:M:163:ASP:OD1	2.46	0.53
3:K:47:ASP:O	3:K:48:VAL:CB	2.57	0.53
2:B:108:ARG:CZ	2:B:111:ALA:HB2	2.38	0.53
3:M:180:VAL:HG23	4:N:562:ALA:HB1	1.89	0.53
3:K:160:PHE:CD2	3:K:170:ILE:HG23	2.44	0.53
3:O:94:PRO:HB3	3:O:169:VAL:HG21	1.89	0.53
2:B:108:ARG:NH1	2:B:111:ALA:HB2	2.23	0.53
1:E:190:VAL:HG21	2:F:135:LEU:HD22	1.89	0.53
4:P:563:ASN:OD1	8:P:701:NAG:C1	2.57	0.53
4:L:521:GLN:O	4:L:522:ASP:CB	2.56	0.53
3:M:268:ASN:O	3:M:269:THR:C	2.46	0.53
3:M:142:SER:O	3:M:221:GLN:HA	2.09	0.53
1:E:11:LEU:HB2	1:E:110:THR:O	2.09	0.53
2:H:78:LEU:O	2:H:79:GLN:HB2	2.09	0.53
3:O:169:VAL:HG12	3:O:170:ILE:N	2.24	0.53
4:L:529:LEU:HB3	4:L:532:ILE:HD12	1.90	0.53
2:B:30:LYS:HD2	2:B:50:TRP:CD2	2.43	0.53
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.91	0.53
3:O:216:THR:O	3:O:216:THR:HG23	2.10	0.52
1:E:100(G):VAL:HG11	2:F:49:TYR:HB3	1.91	0.52
3:K:120:GLU:HG2	3:K:172:ARG:HD3	1.91	0.52
1:C:100(B):TYR:CZ	3:M:42:VAL:HG13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ALA:HB1	1:E:126:PRO:CD	2.38	0.52
3:M:130:ARG:O	3:M:162:TYR:HB3	2.09	0.52
1:G:162:ASN:HB2	1:G:165:ALA:HB3	1.90	0.52
1:A:125:ALA:HB2	1:A:225:VAL:HG11	1.91	0.52
1:G:29:LEU:HD22	1:G:34:MSE:SE	2.60	0.52
1:C:144:VAL:HB	1:C:187:LEU:HB3	1.91	0.52
2:H:15:LEU:HA	2:H:78:LEU:HD23	1.92	0.52
4:P:532:ILE:O	4:P:535:PHE:O	2.28	0.52
3:I:182:ALA:HB1	4:J:561:LEU:HD23	1.91	0.52
3:K:152:ALA:HB3	3:K:170:ILE:HG13	1.92	0.52
3:I:240:THR:HG21	3:I:267:SER:H	1.75	0.52
1:C:33:ARG:NE	1:C:95:GLU:OE2	2.43	0.52
1:A:52(A):SER:HA	1:A:71:ARG:CZ	2.40	0.52
4:J:576:THR:HG23	4:J:578:GLU:HG2	1.90	0.52
5:O:351:NAG:O4	5:O:352:NAG:C7	2.58	0.51
1:G:29:LEU:HD21	1:G:34:MSE:SE	2.60	0.51
2:D:30:LYS:HD2	2:D:50:TRP:CD2	2.46	0.51
3:M:89:ARG:HG2	3:M:90:SER:N	2.25	0.51
3:M:169:VAL:HG12	3:M:170:ILE:N	2.25	0.51
3:I:110:ASN:HB3	3:I:140:LYS:HG3	1.92	0.51
3:M:145:GLY:HA3	3:M:225:PHE:H	1.75	0.51
1:C:100(G):VAL:HG11	2:D:49:TYR:CB	2.39	0.51
1:A:100(G):VAL:HG11	2:B:49:TYR:HB3	1.91	0.51
1:G:108:MSE:CE	1:G:150:GLU:HB2	2.39	0.51
3:O:255:GLN:O	3:O:259:THR:HG23	2.10	0.51
1:G:150:GLU:HG2	1:G:185:TYR:CE1	2.46	0.51
3:K:97:VAL:HG12	3:K:98:ASN:H	1.74	0.51
3:K:232:TYR:HB3	3:K:244:LEU:HD12	1.92	0.51
2:F:4:MSE:SE	2:F:90:GLN:HB3	2.60	0.51
3:O:89:ARG:HD3	3:O:90:SER:O	2.10	0.51
3:O:70:LEU:O	3:O:73:ASN:N	2.44	0.51
2:H:134:CYS:HB2	2:H:148:TRP:CH2	2.46	0.51
1:E:162:ASN:HB2	1:E:165:ALA:HB3	1.93	0.51
3:I:48:VAL:C	3:I:50:LYS:H	2.14	0.51
1:C:108:MSE:HE2	1:C:110:THR:OG1	2.11	0.51
2:B:142:ARG:O	2:B:143:GLU:C	2.48	0.51
2:B:27(E):SER:O	2:B:27(F):SER:OG	2.23	0.50
3:I:142:SER:O	3:I:221:GLN:HA	2.11	0.50
2:B:91:TYR:HA	2:B:96:LEU:HD22	1.92	0.50
2:F:210:ASN:O	2:F:211:ARG:HB2	2.11	0.50
1:C:34:MSE:SE	1:C:94:ARG:HG3	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:271:GLY:HA3	3:O:272:LYS:CB	2.40	0.50
3:K:97:VAL:CG2	4:L:573:LEU:HD21	2.42	0.50
3:K:162:TYR:CE2	3:K:176:PHE:HB3	2.47	0.50
2:D:140:TYR:CD1	2:D:141:PRO:HA	2.47	0.50
3:M:133:PRO:HG2	4:N:518:TRP:CH2	2.46	0.50
1:A:125:ALA:CB	1:A:140:LEU:HB2	2.41	0.50
4:N:517:TYR:CZ	4:N:546:GLY:HA3	2.46	0.50
3:I:115:LYS:HG3	3:I:119:SER:HB2	1.93	0.50
3:O:185:ILE:HG23	3:O:185:ILE:O	2.11	0.50
1:A:52(A):SER:O	1:A:71:ARG:HD3	2.12	0.50
1:E:125:ALA:HB1	1:E:126:PRO:HD2	1.93	0.50
2:F:140:TYR:CD1	2:F:141:PRO:HA	2.46	0.50
2:F:54:ARG:HD3	2:F:60:ASP:HA	1.93	0.50
1:E:67:PHE:CZ	1:E:82:MSE:HE2	2.47	0.50
3:M:86:TRP:CZ3	3:M:111:LEU:HD11	2.47	0.50
1:A:56:TYR:CG	1:A:100(A):GLY:O	2.64	0.50
1:G:5:LEU:O	1:G:22:CYS:HA	2.12	0.50
4:J:595:GLN:HA	4:J:595:GLN:HE21	1.77	0.50
3:K:182:ALA:HB2	4:L:562:ALA:CA	2.42	0.50
1:C:87:THR:HG23	1:C:110:THR:HA	1.92	0.50
4:P:576:THR:HG23	4:P:578:GLU:HG2	1.94	0.50
1:A:141:GLY:HA2	1:A:157:TRP:CH2	2.46	0.50
2:B:125:LEU:O	2:B:183:LYS:HD2	2.12	0.50
3:I:171:TYR:O	3:I:174:THR:HG22	2.11	0.49
3:I:114:LYS:HB3	3:I:118:GLY:O	2.12	0.49
3:O:136:ARG:HG2	3:O:137:TYR:CE1	2.47	0.49
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.93	0.49
3:O:234:PHE:CD1	3:O:234:PHE:C	2.86	0.49
3:M:240:THR:HG22	3:M:267:SER:HB3	1.94	0.49
3:O:57:LEU:HD23	3:O:57:LEU:C	2.32	0.49
1:E:100(G):VAL:HG11	2:F:49:TYR:CB	2.42	0.49
3:K:255:GLN:O	3:K:259:THR:HG23	2.11	0.49
1:C:51:ILE:HG23	1:C:51:ILE:O	2.12	0.49
3:I:94:PRO:HD3	3:I:151:PHE:CE1	2.48	0.49
2:F:78:LEU:O	2:F:79:GLN:CB	2.60	0.49
2:H:15:LEU:C	2:H:15:LEU:HD23	2.33	0.49
3:O:145:GLY:HA3	3:O:225:PHE:H	1.77	0.49
3:I:259:THR:O	3:I:263:SER:HB3	2.12	0.49
4:J:593:LEU:HB3	4:L:593:LEU:HD13	1.94	0.49
2:D:54:ARG:HD3	2:D:60:ASP:HA	1.93	0.49
1:G:187:LEU:HG	1:G:188:SER:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:45:VAL:HG22	4:J:561:LEU:HD13	1.95	0.49
1:E:108:MSE:HE2	1:E:110:THR:OG1	2.11	0.49
1:G:67:PHE:CE1	1:G:82:MSE:HB3	2.47	0.49
3:M:120:GLU:HG2	3:M:172:ARG:NE	2.27	0.49
3:K:246:SER:O	3:K:248:PHE:N	2.46	0.49
3:K:38:ILE:HD11	3:K:186:LEU:HD23	1.95	0.49
4:J:577:THR:HG23	4:L:582:PHE:HE2	1.78	0.49
3:I:164:ARG:O	3:I:165:LEU:HD23	2.13	0.49
1:C:187:LEU:HG	1:C:188:SER:N	2.27	0.49
4:J:572:PHE:HE2	4:J:581:THR:HG21	1.78	0.49
2:F:24:LYS:HA	2:F:69:THR:O	2.13	0.49
1:G:50:SER:OG	1:G:58:HIS:HB2	2.13	0.49
3:I:43:LEU:HD13	4:J:504:ILE:HD11	1.95	0.49
2:F:12:ALA:HA	2:F:105:GLU:O	2.12	0.49
1:A:123:PRO:CB	1:A:225:VAL:HG13	2.42	0.49
1:E:11:LEU:HD21	1:E:116:THR:HG22	1.94	0.49
3:K:73:ASN:OD1	4:L:559:ARG:HG2	2.12	0.49
4:J:520:THR:O	4:J:521:GLN:CB	2.60	0.49
2:H:54:ARG:HD3	2:H:60:ASP:HA	1.93	0.49
1:C:100(B):TYR:CD1	1:C:100(C):SER:N	2.81	0.48
1:A:213:LYS:HB2	1:A:214:PRO:HD3	1.95	0.48
3:K:94:PRO:O	3:K:95:LYS:HD2	2.14	0.48
2:F:35:TRP:CZ3	2:F:88:CYS:HB3	2.48	0.48
1:C:213:LYS:HB2	1:C:214:PRO:HD3	1.95	0.48
2:D:142:ARG:HB2	2:D:173:TYR:CE2	2.49	0.48
2:B:12:ALA:HA	2:B:105:GLU:O	2.12	0.48
4:J:532:ILE:O	4:J:535:PHE:O	2.31	0.48
4:N:560:GLN:O	4:N:560:GLN:HG3	2.12	0.48
3:K:267:SER:HB2	3:K:270:THR:O	2.12	0.48
3:K:162:TYR:OH	3:K:170:ILE:HA	2.13	0.48
3:O:162:TYR:OH	3:O:170:ILE:HA	2.14	0.48
1:A:124:LEU:HD11	1:A:143:LEU:HB2	1.95	0.48
3:I:97:VAL:HG12	3:I:98:ASN:H	1.79	0.48
2:D:12:ALA:HA	2:D:105:GLU:O	2.12	0.48
1:A:107:THR:HG23	1:A:107:THR:O	2.13	0.48
3:M:110:ASN:HB2	3:M:175:THR:HG22	1.96	0.48
1:A:187:LEU:HG	1:A:188:SER:H	1.77	0.48
1:G:226:GLU:HB3	1:G:227:PRO:HD2	1.95	0.48
3:M:246:SER:O	3:M:248:PHE:N	2.47	0.48
1:E:100:THR:HG23	4:L:552:ASP:HB3	1.95	0.48
2:F:210:ASN:O	2:F:211:ARG:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:45:VAL:HG21	4:L:504:ILE:HG23	1.96	0.48
2:B:8:PRO:HG2	2:B:10:SER:O	2.12	0.48
2:B:211:ARG:HH21	2:B:211:ARG:CG	2.25	0.48
1:E:52(A):SER:O	1:E:71:ARG:HD3	2.13	0.48
3:I:109:TYR:HB2	3:I:176:PHE:CZ	2.49	0.48
2:F:183:LYS:HE2	2:F:187:GLU:OE1	2.14	0.48
4:L:594:LEU:HD23	4:N:593:LEU:HD21	1.96	0.48
2:D:78:LEU:O	2:D:79:GLN:HB2	2.14	0.48
1:A:144:VAL:HB	1:A:187:LEU:HB3	1.95	0.48
3:O:260:ILE:O	3:O:264:GLY:O	2.31	0.48
3:O:38:ILE:HG22	3:O:43:LEU:HA	1.95	0.48
1:E:34:MSE:HE3	1:E:94:ARG:CA	2.44	0.47
1:G:34:MSE:HE3	1:G:93:VAL:O	2.14	0.47
2:D:78:LEU:HD21	2:D:106:ILE:HG12	1.96	0.47
1:E:222:LYS:HG2	1:E:225:VAL:N	2.29	0.47
3:I:94:PRO:O	3:I:95:LYS:HG2	2.15	0.47
3:K:120:GLU:HG2	3:K:172:ARG:NH2	2.29	0.47
4:J:578:GLU:HB3	4:L:582:PHE:CZ	2.49	0.47
1:G:108:MSE:HE2	1:G:150:GLU:HB2	1.95	0.47
1:C:70:SER:O	1:C:78:LEU:HD12	2.14	0.47
2:B:163:VAL:HG12	2:B:164:THR:O	2.14	0.47
4:N:565:THR:O	4:N:566:THR:C	2.52	0.47
3:I:169:VAL:HG12	3:I:170:ILE:N	2.28	0.47
1:A:71:ARG:HH21	1:A:71:ARG:HG3	1.80	0.47
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.96	0.47
1:E:125:ALA:HB2	1:E:225:VAL:CG1	2.44	0.47
1:G:177:VAL:O	1:G:185:TYR:HA	2.15	0.47
1:A:140:LEU:O	1:A:191:VAL:HG12	2.14	0.47
4:L:594:LEU:HD13	3:M:57:LEU:HD22	1.95	0.47
3:O:57:LEU:HD13	4:P:592:PHE:CD2	2.49	0.47
3:O:129:ILE:HG12	3:O:165:LEU:HD12	1.95	0.47
1:A:67:PHE:CD1	1:A:67:PHE:N	2.79	0.47
1:G:114:ALA:HB3	1:G:148:PHE:CE2	2.50	0.47
1:A:107:THR:CG2	1:A:107:THR:O	2.62	0.47
3:I:115:LYS:HB2	3:I:116:PRO:HD2	1.95	0.47
3:I:138:VAL:HB	3:I:217:THR:HG22	1.96	0.47
1:A:51:ILE:O	1:A:51:ILE:HG23	2.14	0.47
2:B:83:VAL:HG11	2:B:166:GLN:HB3	1.94	0.47
3:I:83:THR:C	3:I:85:ARG:H	2.16	0.47
2:H:77:SER:O	2:H:78:LEU:CB	2.62	0.47
3:O:182:ALA:HB2	4:P:562:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:CD2	1:A:100(A):GLY:O	2.68	0.47
3:O:70:LEU:O	3:O:73:ASN:HB2	2.15	0.47
1:A:63:VAL:HG13	1:A:67:PHE:CG	2.49	0.47
3:O:213:TYR:O	3:O:214:TYR:CB	2.63	0.47
3:M:183:PHE:HD2	4:N:585:LEU:HD21	1.79	0.47
2:H:109:THR:O	2:H:110:VAL:C	2.51	0.47
1:C:100:THR:HG22	1:C:100(A):GLY:H	1.78	0.47
1:C:100:THR:HG22	1:C:100(A):GLY:N	2.30	0.47
1:A:157:TRP:CZ3	1:A:208:CYS:HB3	2.50	0.47
2:H:149:LYS:HB2	2:H:193:ALA:HB3	1.97	0.47
1:A:122:PHE:HB3	2:B:121:SER:OG	2.15	0.47
4:L:517:TYR:CZ	4:L:546:GLY:HA3	2.49	0.47
1:A:126:PRO:HG2	1:A:198:LEU:HD22	1.97	0.47
4:P:566:THR:O	4:P:567:GLN:C	2.54	0.47
1:E:34:MSE:HE3	1:E:94:ARG:HA	1.97	0.47
1:E:71:ARG:NH2	1:E:73:ASN:OD1	2.48	0.47
2:D:28:ASN:O	2:D:29:ASN:HB2	2.14	0.47
3:I:70:LEU:O	3:I:71:GLU:C	2.53	0.47
2:H:31:SER:HB2	2:H:51:ALA:HB2	1.97	0.47
3:M:53:CYS:O	3:M:54:ARG:CB	2.62	0.47
1:A:96:GLY:HA3	1:A:100(F):ASP:OD1	2.15	0.47
1:E:67:PHE:HB3	1:E:80:LEU:HD11	1.96	0.46
3:K:186:LEU:HB3	3:K:187:PRO:CD	2.46	0.46
1:G:100(G):VAL:HG11	2:H:49:TYR:HB3	1.96	0.46
3:O:52:VAL:O	3:O:53:CYS:C	2.52	0.46
3:M:62:GLN:O	3:M:185:ILE:HA	2.15	0.46
3:O:182:ALA:HB2	4:P:562:ALA:CA	2.45	0.46
1:G:177:VAL:CG1	2:H:162:SER:HB2	2.45	0.46
1:A:187:LEU:HG	1:A:188:SER:N	2.30	0.46
3:K:115:LYS:HA	3:K:145:GLY:O	2.15	0.46
3:K:184:LEU:HD11	4:L:558:LEU:HD22	1.97	0.46
3:O:110:ASN:HB3	3:O:140:LYS:HG3	1.97	0.46
2:H:42:GLN:HG2	2:H:43:PRO:HD2	1.97	0.46
3:I:39:HIS:O	3:I:41:SER:N	2.48	0.46
2:D:165:GLU:O	2:D:166:GLN:C	2.54	0.46
3:K:118:GLY:O	3:K:119:SER:O	2.34	0.46
1:E:119:PRO:HB3	1:E:147:TYR:HB3	1.98	0.46
4:N:532:ILE:O	4:N:533:PRO:C	2.52	0.46
1:G:51:ILE:HG13	1:G:57:ILE:HG12	1.98	0.46
3:I:79:VAL:N	3:I:80:PRO:HD2	2.30	0.46
3:O:160:PHE:CD2	3:O:170:ILE:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PHE:CE1	1:E:82:MSE:HB3	2.51	0.46
3:K:38:ILE:HG22	3:K:43:LEU:HA	1.98	0.46
3:I:73:ASN:OD1	4:J:559:ARG:HG2	2.16	0.46
3:M:45:VAL:HG21	4:N:504:ILE:HG23	1.98	0.46
4:N:549:HIS:C	4:N:555:ILE:HD12	2.36	0.46
3:M:136:ARG:HG2	3:M:137:TYR:CE1	2.51	0.46
3:M:152:ALA:HB3	3:M:170:ILE:HG13	1.98	0.46
3:M:38:ILE:HG22	3:M:43:LEU:HA	1.97	0.46
1:A:100(G):VAL:HG11	2:B:49:TYR:HB2	1.98	0.46
3:K:136:ARG:HG2	3:K:137:TYR:CE1	2.51	0.46
2:H:137:ASN:O	2:H:138:ASN:C	2.54	0.46
1:E:154:VAL:HG22	1:E:210:VAL:HA	1.97	0.46
1:A:125:ALA:CB	1:A:126:PRO:CD	2.83	0.46
3:I:38:ILE:O	3:I:187:PRO:HG3	2.15	0.46
3:M:38:ILE:HG22	3:M:42:VAL:O	2.16	0.46
2:B:145:LYS:HB3	2:B:197:THR:HB	1.98	0.46
1:G:213:LYS:HB2	1:G:214:PRO:HD3	1.97	0.46
1:C:63:VAL:HG13	1:C:67:PHE:CG	2.51	0.46
1:G:35:ASN:ND2	1:G:100(H):PHE:CE2	2.85	0.45
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.52	0.45
1:C:123:PRO:HB2	1:C:225:VAL:HG13	1.97	0.45
1:A:6:GLU:HG2	1:A:22:CYS:HB2	1.98	0.45
3:M:118:GLY:O	3:M:119:SER:C	2.55	0.45
2:B:28:ASN:HB2	2:B:30:LYS:H	1.81	0.45
3:O:83:THR:HG23	3:O:225:PHE:CZ	2.51	0.45
1:A:67:PHE:HD1	1:A:67:PHE:N	2.14	0.45
1:G:100(G):VAL:HG11	2:H:49:TYR:CB	2.46	0.45
3:I:48:VAL:HG21	4:J:592:PHE:HB2	1.99	0.45
1:C:22:CYS:SG	1:C:22:CYS:O	2.74	0.45
3:K:79:VAL:HG21	3:K:220:TYR:CE2	2.51	0.45
3:O:83:THR:HG21	3:O:232:TYR:OH	2.17	0.45
3:I:145:GLY:HA3	3:I:225:PHE:H	1.80	0.45
1:A:31:ASN:HB2	1:A:32:TYR:CD2	2.52	0.45
2:H:205:VAL:HG12	2:H:206:THR:N	2.32	0.45
3:I:130:ARG:O	3:I:162:TYR:HB3	2.16	0.45
4:N:532:ILE:O	4:N:535:PHE:O	2.34	0.45
2:F:28:ASN:HB3	2:F:30:LYS:CG	2.47	0.45
2:D:173:TYR:N	2:D:173:TYR:CD1	2.85	0.45
1:A:31:ASN:HB2	1:A:32:TYR:CE2	2.52	0.45
1:G:30:ILE:HG12	1:G:73:ASN:HB3	1.99	0.45
1:E:150:GLU:HG2	1:E:185:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PRO:HB3	1:C:147:TYR:HB3	1.97	0.45
3:I:240:THR:C	3:I:241:TYR:CD1	2.89	0.45
1:A:213:LYS:N	1:A:214:PRO:CD	2.79	0.45
1:G:141:GLY:HA3	1:G:190:VAL:HA	1.99	0.45
3:I:79:VAL:HB	3:I:80:PRO:HD3	1.99	0.45
1:E:100(B):TYR:CD1	1:E:100(B):TYR:C	2.90	0.45
1:E:36:TRP:CZ3	1:E:92:CYS:HB3	2.52	0.45
3:M:259:THR:O	3:M:263:SER:CB	2.65	0.45
3:O:162:TYR:CE2	3:O:176:PHE:HB3	2.51	0.45
3:M:171:TYR:HB2	3:M:174:THR:HG21	1.98	0.45
2:F:142:ARG:O	2:F:143:GLU:C	2.54	0.45
3:K:141:VAL:HA	3:K:220:TYR:HB2	1.99	0.45
2:B:47:LEU:HA	2:B:58:VAL:HG21	1.99	0.45
3:I:215:SER:O	3:I:216:THR:HG23	2.17	0.45
3:O:138:VAL:HB	3:O:217:THR:HG22	1.99	0.45
1:A:100:THR:HG21	4:J:552:ASP:HB3	1.98	0.45
2:H:28:ASN:HB3	2:H:30:LYS:CG	2.47	0.45
2:D:24:LYS:HA	2:D:69:THR:O	2.16	0.45
3:I:141:VAL:HA	3:I:220:TYR:HB2	1.99	0.44
2:D:79:GLN:HA	2:D:79:GLN:OE1	2.17	0.44
1:C:36:TRP:CZ3	1:C:92:CYS:HB3	2.52	0.44
2:D:77:SER:O	2:D:78:LEU:CB	2.64	0.44
1:C:162:ASN:HB2	1:C:165:ALA:HB3	1.99	0.44
1:C:24:ALA:HB3	1:C:76:ASN:ND2	2.32	0.44
1:E:187:LEU:HG	1:E:188:SER:N	2.32	0.44
2:B:71:PHE:N	2:B:71:PHE:CD2	2.85	0.44
3:I:79:VAL:HG21	3:I:220:TYR:CZ	2.52	0.44
1:A:100(A):GLY:O	1:A:100(B):TYR:CB	2.64	0.44
3:O:36:GLY:O	3:O:185:ILE:HG22	2.16	0.44
2:D:91:TYR:HA	2:D:96:LEU:CD2	2.47	0.44
1:G:212:HIS:CD2	1:G:214:PRO:HD2	2.52	0.44
1:G:108:MSE:HG3	1:G:108:MSE:O	2.15	0.44
3:K:115:LYS:HB2	3:K:116:PRO:HD2	1.99	0.44
2:F:47:LEU:HA	2:F:58:VAL:HG21	1.98	0.44
4:J:531:TRP:CG	4:N:567:GLN:HG3	2.53	0.44
4:J:582:PHE:CZ	4:N:578:GLU:HB3	2.53	0.44
1:C:59:TYR:CE2	1:C:69:ILE:HG22	2.52	0.44
1:C:82:MSE:CE	1:C:109:VAL:HG21	2.46	0.44
3:K:48:VAL:HG11	4:L:592:PHE:HA	2.00	0.44
3:M:133:PRO:C	3:M:134:ARG:HD3	2.38	0.44
1:A:5:LEU:O	1:A:22:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:520:THR:HG21	4:L:542:ILE:HD12	1.98	0.44
2:B:14:SER:N	2:B:107:LYS:HB3	2.31	0.44
2:D:13:VAL:CG1	2:D:17:GLU:HB3	2.47	0.44
1:E:100:THR:HG23	4:L:553:GLY:H	1.83	0.44
4:L:551:GLN:O	4:L:552:ASP:HB2	2.17	0.44
3:I:221:GLN:HG3	3:I:241:TYR:HE2	1.82	0.44
3:K:248:PHE:HE1	3:K:252:PHE:CE2	2.35	0.44
3:I:126:PRO:O	3:I:127:ASP:C	2.55	0.44
1:E:213:LYS:N	1:E:214:PRO:CD	2.81	0.44
3:K:224:GLY:O	3:K:230:VAL:HG22	2.17	0.44
2:F:13:VAL:CG1	2:F:17:GLU:HB3	2.48	0.44
3:I:220:TYR:CE2	3:I:244:LEU:HD11	2.52	0.44
3:I:97:VAL:HG23	4:J:573:LEU:HD11	2.00	0.44
1:E:36:TRP:CH2	1:E:92:CYS:HB3	2.52	0.44
3:I:74:GLY:O	3:I:75:VAL:O	2.35	0.44
3:O:230:VAL:HG12	3:O:231:GLU:N	2.33	0.44
3:O:133:PRO:HG2	4:P:518:TRP:CZ3	2.52	0.44
3:O:133:PRO:HG2	4:P:518:TRP:CH2	2.53	0.44
1:E:18:LEU:HD23	1:E:19:ARG:H	1.83	0.44
2:H:123:GLU:HA	2:H:126:LYS:HE2	2.00	0.44
3:O:83:THR:C	3:O:85:ARG:H	2.22	0.44
4:N:576:THR:HG22	4:N:577:THR:N	2.33	0.44
1:A:12:VAL:HG11	1:A:82(C):LEU:HD12	1.99	0.44
1:C:29:LEU:HD21	1:C:34:MSE:HE2	2.00	0.44
1:G:100(G):VAL:HG21	2:H:46:LEU:HD21	2.00	0.44
4:L:574:ARG:HD3	4:N:542:ILE:HG22	2.00	0.44
1:G:52(A):SER:HA	1:G:71:ARG:CZ	2.48	0.44
3:M:246:SER:O	3:M:247:ARG:C	2.56	0.43
3:M:57:LEU:HG	3:M:185:ILE:HD11	2.00	0.43
1:E:38:ARG:HD2	1:E:48:VAL:CG2	2.47	0.43
2:B:18:ARG:HG3	2:B:19:ALA:N	2.33	0.43
2:H:186:TYR:HA	2:H:192:TYR:OH	2.17	0.43
3:K:133:PRO:HG2	4:L:518:TRP:CH2	2.53	0.43
3:O:66:VAL:HG12	3:O:67:GLY:N	2.33	0.43
3:K:90:SER:HB3	3:K:150:ASP:H	1.83	0.43
4:L:592:PHE:O	4:L:595:GLN:HB2	2.18	0.43
2:F:116:PHE:HD1	2:F:135:LEU:HD23	1.83	0.43
2:F:4:MSE:SE	2:F:90:GLN:CG	3.16	0.43
3:K:43:LEU:HD13	4:L:504:ILE:HD11	1.99	0.43
1:E:144:VAL:HB	1:E:187:LEU:HB3	2.00	0.43
3:I:97:VAL:CG2	4:J:573:LEU:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:LEU:O	2:H:79:GLN:CB	2.65	0.43
3:O:186:LEU:HB3	3:O:187:PRO:CD	2.48	0.43
2:F:159:SER:HA	2:F:178:THR:O	2.18	0.43
1:C:12:VAL:HG22	1:C:13:LYS:N	2.33	0.43
1:G:93:VAL:CG1	1:G:100(H):PHE:HB3	2.48	0.43
3:K:79:VAL:HB	3:K:80:PRO:HD3	1.99	0.43
3:O:182:ALA:HB2	4:P:562:ALA:HA	1.99	0.43
2:D:28:ASN:HB3	2:D:30:LYS:CG	2.47	0.43
1:A:124:LEU:HD13	2:B:133:VAL:HG21	2.00	0.43
4:L:554:LEU:O	4:L:558:LEU:HG	2.18	0.43
1:E:213:LYS:HB2	1:E:214:PRO:HD3	2.00	0.43
3:I:133:PRO:HG2	4:J:518:TRP:CZ3	2.54	0.43
2:B:158:ASN:ND2	2:B:179:LEU:HD11	2.34	0.43
3:I:254:LEU:O	3:I:257:ASN:HB3	2.17	0.43
3:M:185:ILE:HG23	3:M:185:ILE:O	2.18	0.43
1:C:100(G):VAL:HG13	2:D:91:TYR:CZ	2.53	0.43
1:A:94:ARG:CZ	1:A:102:ILE:HD12	2.49	0.43
1:A:36:TRP:NE1	1:A:80:LEU:HB2	2.33	0.43
1:G:123:PRO:O	2:H:121:SER:HB3	2.18	0.43
1:G:197:SER:HA	1:G:200:THR:HG22	2.00	0.43
1:C:53:SER:HG	4:N:552:ASP:CG	2.21	0.43
3:O:215:SER:O	3:O:216:THR:HG22	2.17	0.43
3:K:145:GLY:HA3	3:K:225:PHE:H	1.82	0.43
3:O:86:TRP:CD1	3:O:86:TRP:N	2.85	0.43
4:J:553:GLY:O	4:J:554:LEU:C	2.57	0.43
1:C:99:ALA:HB2	1:C:100(F):ASP:N	2.34	0.43
3:O:63:LEU:HB3	4:P:585:LEU:HD13	1.99	0.43
1:E:82:MSE:HE1	1:E:90:TYR:CZ	2.53	0.43
2:F:35:TRP:CD2	2:F:73:LEU:HB2	2.53	0.43
2:B:166:GLN:HG2	2:B:171:SER:HA	2.01	0.43
3:M:183:PHE:CD2	4:N:585:LEU:HD21	2.53	0.43
3:I:158:ALA:HB2	6:J:701:NAG:H81	1.99	0.43
2:H:145:LYS:HB3	2:H:197:THR:HB	2.01	0.43
2:F:137:ASN:O	2:F:138:ASN:C	2.57	0.43
3:I:183:PHE:HB3	4:J:585:LEU:HD21	2.00	0.43
3:O:118:GLY:O	3:O:119:SER:C	2.56	0.43
1:E:100:THR:CG2	4:L:552:ASP:HB3	2.49	0.43
3:M:224:GLY:O	3:M:230:VAL:HG13	2.18	0.43
3:O:125:ALA:HA	3:O:126:PRO:HD3	1.93	0.43
1:A:93:VAL:CG1	1:A:100(H):PHE:HB3	2.49	0.43
1:E:67:PHE:N	1:E:67:PHE:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:TRP:O	2:H:51:ALA:HB3	2.18	0.43
4:L:579:LEU:H	4:L:579:LEU:HD12	1.83	0.43
1:A:125:ALA:CB	1:A:225:VAL:HG11	2.48	0.43
3:K:94:PRO:HD3	3:K:151:PHE:CE1	2.54	0.43
1:A:124:LEU:CD1	1:A:143:LEU:HB2	2.49	0.43
1:G:213:LYS:N	1:G:214:PRO:CD	2.82	0.43
3:O:154:HIS:CD2	3:O:158:ALA:HB3	2.54	0.43
3:I:139:HIS:N	3:I:139:HIS:CD2	2.87	0.43
3:O:152:ALA:HB3	3:O:170:ILE:HG13	2.01	0.43
3:I:230:VAL:HG12	3:I:231:GLU:N	2.34	0.43
1:A:126:PRO:HG3	1:A:140:LEU:HD13	2.01	0.42
3:M:230:VAL:HG11	3:M:232:TYR:CE1	2.53	0.42
3:O:79:VAL:N	3:O:80:PRO:CD	2.81	0.42
1:E:125:ALA:HB2	1:E:225:VAL:HG13	2.01	0.42
1:A:67:PHE:HB3	1:A:80:LEU:HD11	2.01	0.42
4:L:570:GLN:HG2	4:N:533:PRO:HD3	2.01	0.42
4:J:582:PHE:HE2	4:N:577:THR:HG23	1.83	0.42
1:C:121:VAL:HG21	1:C:210:VAL:HG21	2.01	0.42
3:K:215:SER:OG	3:K:216:THR:N	2.52	0.42
2:F:120:PRO:HG3	2:F:186:TYR:CZ	2.54	0.42
1:G:98:ARG:HG2	4:P:506:ASN:HB3	2.01	0.42
1:A:123:PRO:O	2:B:121:SER:HB3	2.20	0.42
3:M:162:TYR:OH	3:M:170:ILE:HA	2.19	0.42
1:A:124:LEU:CD1	2:B:133:VAL:HG21	2.49	0.42
1:G:12:VAL:HG22	1:G:13:LYS:O	2.19	0.42
1:C:2:VAL:HG22	1:C:26:GLY:HA3	2.00	0.42
2:D:150:VAL:HG13	2:D:192:TYR:CE1	2.54	0.42
2:B:28:ASN:OD1	2:B:28:ASN:N	2.48	0.42
3:O:174:THR:HG23	3:O:174:THR:O	2.19	0.42
2:H:30:LYS:HD2	2:H:50:TRP:CD2	2.54	0.42
1:G:51:ILE:O	1:G:51:ILE:HG23	2.19	0.42
1:C:67:PHE:N	1:C:67:PHE:CD1	2.87	0.42
1:E:200:THR:HG23	1:E:203:GLN:H	1.84	0.42
2:D:137:ASN:O	2:D:138:ASN:C	2.58	0.42
1:E:15:GLY:HA3	1:G:19:ARG:HB2	2.00	0.42
4:N:579:LEU:H	4:N:579:LEU:HD12	1.84	0.42
3:K:171:TYR:HB2	3:K:174:THR:HG21	2.01	0.42
4:J:574:ARG:CZ	4:L:537:PRO:HG2	2.49	0.42
3:M:37:VAL:HG22	3:M:185:ILE:CG2	2.49	0.42
3:K:70:LEU:HB3	3:K:75:VAL:HG21	2.00	0.42
3:O:172:ARG:O	3:O:174:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:118:GLY:O	3:I:119:SER:C	2.58	0.42
1:A:141:GLY:HA3	1:A:189:SER:O	2.19	0.42
2:D:151:ASP:O	2:D:152:ASN:HB2	2.19	0.42
1:A:140:LEU:HD23	1:A:191:VAL:HG13	2.02	0.42
3:M:248:PHE:CE1	3:M:252:PHE:CE2	3.07	0.42
2:B:140:TYR:CG	2:B:141:PRO:HA	2.54	0.42
2:D:105:GLU:HB2	2:D:166:GLN:HE22	1.83	0.42
3:I:162:TYR:HE2	3:I:174:THR:HG23	1.85	0.42
2:F:125:LEU:HD23	2:F:130:ALA:HB2	2.02	0.42
3:M:79:VAL:N	3:M:80:PRO:CD	2.82	0.42
2:B:15:LEU:HD23	2:B:15:LEU:C	2.39	0.42
3:K:118:GLY:O	3:K:119:SER:C	2.58	0.42
3:I:63:LEU:HB3	4:J:585:LEU:HD13	2.01	0.42
2:D:210:ASN:O	2:D:211:ARG:HB2	2.19	0.42
2:H:108:ARG:NH2	2:H:111:ALA:HB2	2.33	0.42
1:C:56:TYR:HB2	1:C:100(A):GLY:HA3	2.02	0.42
2:B:91:TYR:HA	2:B:96:LEU:CD2	2.50	0.42
1:E:107:THR:O	1:E:107:THR:HG23	2.19	0.42
2:H:191:VAL:HG22	2:H:210:ASN:OD1	2.20	0.42
3:O:236:VAL:HG12	3:O:237:ASP:N	2.35	0.42
1:G:207:ILE:HG12	1:G:222:LYS:HA	2.02	0.42
1:C:150:GLU:HG2	1:C:185:TYR:CD1	2.55	0.42
3:O:38:ILE:HD11	3:O:186:LEU:CD2	2.50	0.42
1:A:32:TYR:N	1:A:32:TYR:CD2	2.87	0.42
1:A:12:VAL:HG22	1:A:13:LYS:O	2.20	0.42
4:P:509:PRO:O	4:P:510:LYS:HG3	2.20	0.42
1:G:33:ARG:HG3	1:G:52:SER:HA	2.02	0.42
2:D:155:GLN:O	2:D:156:SER:HB3	2.20	0.42
4:J:522:ASP:O	4:J:524:GLY:N	2.52	0.42
3:I:47:ASP:O	3:I:48:VAL:HG23	2.19	0.42
1:C:108:MSE:HG2	1:C:109:VAL:N	2.34	0.42
3:M:97:VAL:HG12	3:M:98:ASN:N	2.35	0.42
1:E:123:PRO:HB3	1:E:225:VAL:HG22	2.02	0.42
2:D:28:ASN:HB2	2:D:30:LYS:H	1.85	0.42
1:G:30:ILE:H	1:G:30:ILE:HG13	1.73	0.42
4:L:575:ALA:O	3:M:164:ARG:NH1	2.53	0.42
1:G:36:TRP:CH2	1:G:92:CYS:HB3	2.54	0.42
3:M:94:PRO:HD3	3:M:151:PHE:CE1	2.55	0.41
2:B:59:PRO:HG2	2:B:62:PHE:CD1	2.54	0.41
1:A:7:SER:HB2	1:A:21:SER:OG	2.20	0.41
1:A:24:ALA:HB1	1:A:27:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:38:ILE:HD11	3:I:186:LEU:CD2	2.46	0.41
1:G:2:VAL:HG11	1:G:102:ILE:CD1	2.50	0.41
3:M:79:VAL:HG21	3:M:220:TYR:CZ	2.54	0.41
3:M:230:VAL:HG12	3:M:231:GLU:H	1.83	0.41
1:A:71:ARG:NH2	1:A:73:ASN:OD1	2.53	0.41
3:K:78:ASP:O	3:K:79:VAL:C	2.58	0.41
3:K:79:VAL:N	3:K:80:PRO:CD	2.83	0.41
3:I:241:TYR:N	3:I:241:TYR:CD1	2.89	0.41
1:A:150:GLU:OE1	1:A:151:PRO:HA	2.20	0.41
2:D:27(D):TYR:CD2	2:D:27(F):SER:HB2	2.55	0.41
3:I:38:ILE:HG22	3:I:43:LEU:HG	2.02	0.41
1:E:27:PHE:HE1	1:E:29:LEU:HD23	1.85	0.41
3:K:97:VAL:HG23	4:L:573:LEU:HD11	2.02	0.41
1:A:28:THR:HG22	1:A:30:ILE:HG13	2.01	0.41
2:D:166:GLN:OE1	2:D:171:SER:HB3	2.20	0.41
2:B:211:ARG:CG	2:B:211:ARG:NH2	2.83	0.41
1:E:213:LYS:N	1:E:214:PRO:HD2	2.36	0.41
2:B:137:ASN:O	2:B:138:ASN:C	2.59	0.41
1:E:59:TYR:OH	1:E:68:THR:HA	2.19	0.41
2:F:61:ARG:O	2:F:75:ILE:HA	2.20	0.41
2:F:167:ASP:O	2:F:171:SER:HA	2.20	0.41
3:I:246:SER:O	3:I:248:PHE:N	2.53	0.41
2:H:79:GLN:OE1	2:H:79:GLN:HA	2.20	0.41
3:M:113:ILE:CD1	3:M:225:PHE:CD2	3.03	0.41
2:B:80:ALA:HA	2:B:106:ILE:HD11	2.02	0.41
2:B:36:TYR:CE2	2:B:46:LEU:HD13	2.55	0.41
1:E:164:GLY:O	1:E:167:THR:HG23	2.20	0.41
2:H:55:GLU:O	2:H:56:SER:C	2.59	0.41
3:M:47:ASP:O	3:M:48:VAL:HG23	2.20	0.41
3:I:232:TYR:O	3:I:233:LEU:HD23	2.20	0.41
1:C:1:GLU:HB3	1:C:2:VAL:H	1.65	0.41
2:H:13:VAL:CG1	2:H:17:GLU:HB3	2.50	0.41
2:D:35:TRP:HB2	2:D:48:ILE:HB	2.03	0.41
3:M:37:VAL:HG22	3:M:185:ILE:HG21	2.02	0.41
3:M:83:THR:C	3:M:85:ARG:H	2.24	0.41
3:M:97:VAL:HG23	4:N:573:LEU:HD11	2.02	0.41
2:D:138:ASN:H	2:D:138:ASN:HD22	1.68	0.41
1:E:2:VAL:O	1:E:3:GLN:CB	2.69	0.41
4:L:590:ILE:O	4:L:591:ASP:C	2.58	0.41
1:A:200:THR:HG23	1:A:203:GLN:H	1.86	0.41
4:P:565:THR:O	4:P:566:THR:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:529:LEU:HB3	4:J:532:ILE:HD12	2.03	0.41
3:I:215:SER:OG	3:I:216:THR:N	2.53	0.41
2:B:89:GLN:HB2	2:B:98:PHE:CD2	2.56	0.41
2:H:175:LEU:HD23	2:H:176:SER:N	2.35	0.41
3:M:49:ASP:O	3:M:50:LYS:CB	2.68	0.41
2:H:183:LYS:O	2:H:187:GLU:HG3	2.21	0.41
1:C:35:ASN:OD1	1:C:50:SER:CB	2.69	0.41
2:F:173:TYR:N	2:F:173:TYR:CD1	2.89	0.41
1:A:100(D):MSE:HE3	1:A:100(D):MSE:HB3	1.96	0.41
3:K:78:ASP:C	3:K:80:PRO:HD2	2.41	0.41
1:C:34:MSE:SE	1:C:94:ARG:HA	2.70	0.41
1:G:144:VAL:HB	1:G:187:LEU:HB3	2.02	0.41
1:G:82(B):SER:OG	1:G:83:ARG:NH2	2.53	0.41
1:G:96:GLY:HA3	1:G:100(F):ASP:OD1	2.20	0.41
3:O:257:ASN:ND2	5:O:351:NAG:C2	2.68	0.41
4:L:593:LEU:HB3	4:N:593:LEU:HD13	2.03	0.41
4:L:578:GLU:HB3	4:N:582:PHE:CZ	2.56	0.41
2:F:91:TYR:HA	2:F:96:LEU:CD2	2.50	0.41
3:O:182:ALA:HB2	4:P:562:ALA:CB	2.51	0.41
3:K:120:GLU:HG2	3:K:172:ARG:CD	2.50	0.41
3:O:38:ILE:HD11	3:O:186:LEU:HD23	2.03	0.41
1:C:6:GLU:HG2	1:C:22:CYS:HB2	2.02	0.41
3:O:66:VAL:CG1	3:O:67:GLY:N	2.84	0.41
1:C:140:LEU:O	1:C:191:VAL:HG12	2.21	0.41
1:A:207:ILE:HG12	1:A:222:LYS:HB2	2.02	0.41
3:M:104:TRP:HE1	4:N:545:GLU:HG3	1.86	0.41
4:P:525:ALA:O	4:P:530:ALA:HB3	2.21	0.41
4:N:573:LEU:HD23	4:N:573:LEU:HA	1.88	0.41
2:B:28:ASN:O	2:B:29:ASN:HB2	2.21	0.41
2:H:28:ASN:O	2:H:29:ASN:HB2	2.21	0.41
3:K:171:TYR:O	3:K:174:THR:HG22	2.21	0.41
1:C:35:ASN:OD1	1:C:50:SER:HB3	2.20	0.41
2:F:117:ILE:HG13	2:F:118:PHE:N	2.36	0.41
1:G:94:ARG:CZ	1:G:102:ILE:CD1	2.98	0.40
3:O:45:VAL:HG21	4:P:504:ILE:CG2	2.49	0.40
2:D:173:TYR:HD1	2:D:173:TYR:N	2.19	0.40
1:G:190:VAL:HG21	2:H:135:LEU:HD22	2.03	0.40
2:F:21:ILE:O	2:F:72:THR:HA	2.20	0.40
4:J:557:GLY:O	4:J:560:GLN:HB3	2.21	0.40
3:I:79:VAL:N	3:I:80:PRO:CD	2.84	0.40
1:G:63:VAL:HG13	1:G:67:PHE:CG	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:205:VAL:CG1	2:H:206:THR:N	2.84	0.40
2:H:150:VAL:HG13	2:H:192:TYR:CE1	2.56	0.40
2:H:163:VAL:HG12	2:H:164:THR:O	2.22	0.40
1:E:22:CYS:SG	1:E:22:CYS:O	2.78	0.40
1:E:140:LEU:H	1:E:140:LEU:HD23	1.86	0.40
3:M:113:ILE:O	3:M:121:CYS:HB2	2.21	0.40
2:H:54:ARG:CD	2:H:60:ASP:HA	2.52	0.40
3:O:256:LEU:O	3:O:260:ILE:HG13	2.21	0.40
3:K:154:HIS:CD2	3:K:158:ALA:HB3	2.56	0.40
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.88	0.40
3:I:60:THR:HG22	4:N:591:ASP:OD1	2.21	0.40
1:A:125:ALA:HB1	1:A:140:LEU:HB2	2.02	0.40
4:J:594:LEU:HD13	3:K:57:LEU:HD21	2.02	0.40
2:B:15:LEU:HA	2:B:78:LEU:HD23	2.02	0.40
1:A:29:LEU:CD2	1:A:34:MSE:SE	3.19	0.40
1:A:2:VAL:HG11	1:A:102:ILE:HD13	2.03	0.40
1:C:67:PHE:N	1:C:67:PHE:HD1	2.19	0.40
3:M:257:ASN:O	3:M:261:TYR:HD1	2.04	0.40
3:K:66:VAL:CG1	3:K:67:GLY:N	2.83	0.40
3:K:85:ARG:HD2	3:K:178:GLU:OE2	2.21	0.40
1:A:114:ALA:HB3	1:A:148:PHE:CE2	2.56	0.40
2:H:125:LEU:HD23	2:H:130:ALA:HB2	2.03	0.40
1:E:174:PHE:HE2	1:E:190:VAL:HG22	1.85	0.40
2:D:192:TYR:HB2	2:D:209:PHE:CE1	2.57	0.40
2:F:108:ARG:HD3	2:F:171:SER:O	2.22	0.40
3:M:109:TYR:HD2	3:M:139:HIS:HB2	1.87	0.40
3:K:44:GLN:HA	4:L:503:ALA:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/226 (99%)	192 (86%)	29 (13%)	3 (1%)	15	57
1	C	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	15	57
1	E	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	21	65
1	G	224/226 (99%)	202 (90%)	21 (9%)	1 (0%)	39	79
2	B	215/217 (99%)	181 (84%)	25 (12%)	9 (4%)	3	29
2	D	215/217 (99%)	183 (85%)	25 (12%)	7 (3%)	5	37
2	F	215/217 (99%)	183 (85%)	26 (12%)	6 (3%)	6	41
2	H	215/217 (99%)	179 (83%)	27 (13%)	9 (4%)	3	29
3	I	230/334 (69%)	184 (80%)	33 (14%)	13 (6%)	2	20
3	K	226/334 (68%)	184 (81%)	33 (15%)	9 (4%)	4	31
3	M	222/334 (66%)	181 (82%)	29 (13%)	12 (5%)	2	22
3	O	217/334 (65%)	171 (79%)	26 (12%)	20 (9%)	1	9
4	J	96/131 (73%)	80 (83%)	14 (15%)	2 (2%)	9	47
4	L	89/131 (68%)	79 (89%)	8 (9%)	2 (2%)	8	46
4	N	91/131 (70%)	80 (88%)	10 (11%)	1 (1%)	17	61
4	P	89/131 (68%)	74 (83%)	13 (15%)	2 (2%)	8	46
All	All	3016/3632 (83%)	2543 (84%)	372 (12%)	101 (3%)	5	37

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100(B)	TYR
2	B	110	VAL
2	D	27(F)	SER
2	D	78	LEU
2	D	169	LYS
2	F	27(F)	SER
2	H	27(F)	SER
2	H	110	VAL
2	H	138	ASN
3	I	54	ARG
3	I	71	GLU
3	I	119	SER
3	I	247	ARG
3	I	300	LYS
4	J	521	GLN
3	K	48	VAL

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Mol	Chain	Res	Type
3	K	119	SER
3	K	163	ASP
3	K	247	ARG
3	M	49	ASP
3	M	50	LYS
3	M	54	ARG
3	M	163	ASP
3	M	247	ARG
3	M	265	LYS
3	O	48	VAL
3	O	50	LYS
3	O	56	LYS
3	O	119	SER
3	O	214	TYR
3	O	216	THR
3	O	238	ASN
3	O	247	ARG
3	O	272	LYS
2	B	27(F)	SER
2	B	138	ASN
1	C	100(C)	SER
2	D	138	ASN
2	D	156	SER
2	F	138	ASN
2	H	78	LEU
3	I	40	ASN
3	I	49	ASP
3	I	75	VAL
3	K	56	LYS
3	K	75	VAL
3	M	75	VAL
3	O	71	GLU
3	O	173	GLY
2	B	79	GLN
2	B	142	ARG
2	B	143	GLU
2	D	56	SER
2	D	166	GLN
2	F	79	GLN
2	F	166	GLN
3	I	47	ASP
3	I	158	ALA

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Mol	Chain	Res	Type
3	I	301	ILE
3	M	119	SER
3	O	40	ASN
3	O	53	CYS
3	O	305	GLU
4	P	579	LEU
2	B	26	SER
2	B	32	TYR
1	C	100(B)	TYR
2	F	78	LEU
1	G	100(B)	TYR
2	H	56	SER
2	H	204	PRO
3	M	40	ASN
4	N	512	ASN
3	O	163	ASP
1	A	125	ALA
2	B	204	PRO
1	C	146	ASP
1	E	116	THR
1	E	146	ASP
2	H	166	GLN
4	J	523	GLU
3	K	40	ASN
3	K	127	ASP
4	L	591	ASP
3	M	71	GLU
2	F	68	GLY
3	I	127	ASP
3	O	57	LEU
3	O	75	VAL
3	O	148	ALA
2	H	68	GLY
3	I	48	VAL
4	L	512	ASN
3	M	48	VAL
4	P	584	ILE
3	K	116	PRO
3	O	236	VAL
2	H	203	SER
3	M	236	VAL
3	O	185	ILE

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Mol	Chain	Res	Type
1	A	100(A)	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/186 (102%)	175 (92%)	15 (8%)	15	52
1	C	190/186 (102%)	177 (93%)	13 (7%)	20	60
1	E	190/186 (102%)	179 (94%)	11 (6%)	25	65
1	G	190/186 (102%)	175 (92%)	15 (8%)	15	52
2	B	191/190 (100%)	185 (97%)	6 (3%)	47	81
2	D	191/190 (100%)	188 (98%)	3 (2%)	70	89
2	F	191/190 (100%)	187 (98%)	4 (2%)	61	86
2	H	191/190 (100%)	186 (97%)	5 (3%)	54	84
3	I	163/282 (58%)	156 (96%)	7 (4%)	35	74
3	K	163/282 (58%)	154 (94%)	9 (6%)	27	66
3	M	163/282 (58%)	153 (94%)	10 (6%)	23	63
3	O	162/282 (57%)	152 (94%)	10 (6%)	23	63
4	J	73/110 (66%)	69 (94%)	4 (6%)	27	66
4	L	74/110 (67%)	71 (96%)	3 (4%)	37	75
4	N	73/110 (66%)	70 (96%)	3 (4%)	37	75
4	P	72/110 (66%)	69 (96%)	3 (4%)	36	74
All	All	2467/3072 (80%)	2346 (95%)	121 (5%)	31	70

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	SER
1	A	11	LEU

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	22	CYS
1	A	38	ARG
1	A	45	LEU
1	A	61	ASP
1	A	71	ARG
1	A	75	GLU
1	A	82	MSE
1	A	92	CYS
1	A	188	SER
1	A	200	THR
1	A	209	ASN
2	B	4	MSE
2	B	18	ARG
2	B	31	SER
2	B	129	THR
2	B	137	ASN
2	B	211	ARG
1	C	3	GLN
1	C	11	LEU
1	C	18	LEU
1	C	22	CYS
1	C	28	THR
1	C	38	ARG
1	C	45	LEU
1	C	71	ARG
1	C	77	SER
1	C	92	CYS
1	C	100(C)	SER
1	C	200	THR
1	C	209	ASN
2	D	4	MSE
2	D	137	ASN
2	D	173	TYR
1	E	18	LEU
1	E	22	CYS
1	E	38	ARG
1	E	45	LEU
1	E	71	ARG
1	E	82	MSE
1	E	83	ARG
1	E	100	THR

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Mol	Chain	Res	Type
1	E	140	LEU
1	E	200	THR
1	E	209	ASN
2	F	108	ARG
2	F	132	VAL
2	F	137	ASN
2	F	194	CYS
1	G	3	GLN
1	G	11	LEU
1	G	18	LEU
1	G	22	CYS
1	G	34	MSE
1	G	38	ARG
1	G	45	LEU
1	G	61	ASP
1	G	71	ARG
1	G	75	GLU
1	G	82	MSE
1	G	92	CYS
1	G	108	MSE
1	G	188	SER
1	G	209	ASN
2	H	27(F)	SER
2	H	60	ASP
2	H	69	THR
2	H	137	ASN
2	H	211	ARG
3	I	69	ASN
3	I	86	TRP
3	I	89	ARG
3	I	90	SER
3	I	106	GLU
3	I	170	ILE
3	I	216	THR
4	J	523	GLU
4	J	579	LEU
4	J	591	ASP
4	J	595	GLN
3	K	43	LEU
3	K	69	ASN
3	K	86	TRP
3	K	89	ARG

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Mol	Chain	Res	Type
3	K	90	SER
3	K	95	LYS
3	K	98	ASN
3	K	170	ILE
3	K	234	PHE
4	L	516	HIS
4	L	579	LEU
4	L	591	ASP
3	M	32	SER
3	M	38	ILE
3	M	39	HIS
3	M	40	ASN
3	M	57	LEU
3	M	60	THR
3	M	81	SER
3	M	90	SER
3	M	120	GLU
3	M	170	ILE
4	N	579	LEU
4	N	586	ASN
4	N	587	ARG
3	O	65	SER
3	O	77	THR
3	O	78	ASP
3	O	81	SER
3	O	86	TRP
3	O	89	ARG
3	O	90	SER
3	O	120	GLU
3	O	170	ILE
3	O	234	PHE
4	P	579	LEU
4	P	587	ARG
4	P	595	GLN

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

Mol	Chain	Res	Type
2	B	155	GLN
3	I	110	ASN
4	J	595	GLN
3	O	257	ASN

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Mol	Chain	Res	Type
4	P	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

33 carbohydrates 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$
5	NAG	I	351	5	14,14,15	0.73	0	15,19,21	2.23	3 (20%)
5	NAG	I	352	5	14,14,15	0.80	0	15,19,21	1.12	1 (6%)
5	BMA	I	353	5	11,11,12	1.41	1 (9%)	14,15,17	2.11	4 (28%)
6	NAG	J	701	6	14,14,15	0.93	1 (7%)	15,19,21	1.20	2 (13%)
6	NAG	J	702	6	14,14,15	0.70	0	15,19,21	2.05	4 (26%)
6	BMA	J	703	6	11,11,12	1.12	1 (9%)	14,15,17	2.25	2 (14%)
6	MAN	J	704	6	11,11,12	0.77	0	14,15,17	1.65	3 (21%)
6	MAN	J	705	6	11,11,12	0.68	0	14,15,17	1.57	2 (14%)
7	NAG	K	351	7	14,14,15	0.75	0	15,19,21	1.80	2 (13%)
7	NAG	K	352	7	14,14,15	0.65	0	15,19,21	1.50	2 (13%)
8	NAG	L	701	8	14,14,15	0.99	1 (7%)	15,19,21	2.45	4 (26%)
8	NAG	L	702	8	14,14,15	0.52	0	15,19,21	1.63	2 (13%)
8	BMA	L	703	8	11,11,12	1.38	2 (18%)	14,15,17	1.92	3 (21%)
8	MAN	L	704	8	11,11,12	0.98	1 (9%)	14,15,17	1.44	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	L	705	8	11,11,12	0.84	1 (9%)	14,15,17	1.73	3 (21%)
8	NAG	L	706	8	14,14,15	0.68	0	15,19,21	1.61	2 (13%)
5	NAG	M	351	5	14,14,15	0.87	0	15,19,21	2.34	3 (20%)
5	NAG	M	352	5	14,14,15	0.56	0	15,19,21	1.54	3 (20%)
5	BMA	M	353	5	11,11,12	1.13	0	14,15,17	1.27	2 (14%)
6	NAG	N	701	6	14,14,15	0.89	1 (7%)	15,19,21	1.91	2 (13%)
6	NAG	N	702	6	14,14,15	0.97	1 (7%)	15,19,21	1.52	4 (26%)
6	BMA	N	703	6	11,11,12	1.20	1 (9%)	14,15,17	2.02	1 (7%)
6	MAN	N	704	6	11,11,12	0.86	1 (9%)	14,15,17	1.52	2 (14%)
6	MAN	N	705	6	11,11,12	0.52	0	14,15,17	1.25	1 (7%)
5	NAG	O	351	5	14,14,15	0.72	0	15,19,21	2.21	2 (13%)
5	NAG	O	352	5	14,14,15	0.86	0	15,19,21	1.35	2 (13%)
5	BMA	O	353	5	11,11,12	1.66	2 (18%)	14,15,17	1.84	1 (7%)
8	NAG	P	701	8	14,14,15	0.90	1 (7%)	15,19,21	1.94	5 (33%)
8	NAG	P	702	8	14,14,15	0.70	0	15,19,21	1.73	3 (20%)
8	BMA	P	703	8	11,11,12	1.21	1 (9%)	14,15,17	1.64	3 (21%)
8	MAN	P	704	8	11,11,12	1.17	2 (18%)	14,15,17	1.28	2 (14%)
8	MAN	P	705	8	11,11,12	0.65	0	14,15,17	1.28	2 (14%)
8	NAG	P	706	8	14,14,15	0.59	0	15,19,21	1.97	1 (6%)

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
5	NAG	I	351	5	-	0/6/23/26	0/1/1/1
5	NAG	I	352	5	-	0/6/23/26	0/1/1/1
5	BMA	I	353	5	-	0/2/19/22	0/1/1/1
6	NAG	J	701	6	-	0/6/23/26	0/1/1/1
6	NAG	J	702	6	-	0/6/23/26	0/1/1/1
6	BMA	J	703	6	-	0/2/19/22	0/1/1/1
6	MAN	J	704	6	-	0/2/19/22	0/1/1/1
6	MAN	J	705	6	-	0/2/19/22	0/1/1/1
7	NAG	K	351	7	-	0/6/23/26	0/1/1/1
7	NAG	K	352	7	-	0/6/23/26	0/1/1/1
8	NAG	L	701	8	-	0/6/23/26	0/1/1/1
8	NAG	L	702	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	L	703	8	-	0/2/19/22	0/1/1/1
8	MAN	L	704	8	-	0/2/19/22	0/1/1/1
8	MAN	L	705	8	-	0/2/19/22	0/1/1/1
8	NAG	L	706	8	-	0/6/23/26	0/1/1/1
5	NAG	M	351	5	-	0/6/23/26	0/1/1/1
5	NAG	M	352	5	-	0/6/23/26	0/1/1/1
5	BMA	M	353	5	-	0/2/19/22	0/1/1/1
6	NAG	N	701	6	-	0/6/23/26	0/1/1/1
6	NAG	N	702	6	-	0/6/23/26	0/1/1/1
6	BMA	N	703	6	-	0/2/19/22	0/1/1/1
6	MAN	N	704	6	-	0/2/19/22	0/1/1/1
6	MAN	N	705	6	-	0/2/19/22	0/1/1/1
5	NAG	O	351	5	-	0/6/23/26	0/1/1/1
5	NAG	O	352	5	-	1/6/23/26	0/1/1/1
5	BMA	O	353	5	-	0/2/19/22	0/1/1/1
8	NAG	P	701	8	-	0/6/23/26	0/1/1/1
8	NAG	P	702	8	-	0/6/23/26	0/1/1/1
8	BMA	P	703	8	-	0/2/19/22	0/1/1/1
8	MAN	P	704	8	-	0/2/19/22	0/1/1/1
8	MAN	P	705	8	-	0/2/19/22	0/1/1/1
8	NAG	P	706	8	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	NAG	O5-C1	-2.72	1.39	1.43
6	N	701	NAG	O5-C1	-2.59	1.39	1.43
8	P	704	MAN	O5-C1	-2.56	1.39	1.43
6	J	701	NAG	O5-C1	-2.49	1.39	1.43
8	P	701	NAG	O5-C1	-2.34	1.39	1.43
6	N	704	MAN	O5-C1	-2.20	1.40	1.43
8	L	704	MAN	O5-C1	-2.11	1.40	1.43
6	N	702	NAG	O5-C1	-2.09	1.40	1.43
5	O	353	BMA	C4-C3	2.08	1.57	1.52
6	J	703	BMA	C6-C5	2.20	1.59	1.51
6	N	703	BMA	C2-C3	2.30	1.55	1.52
8	P	704	MAN	C2-C3	2.33	1.55	1.52
8	L	703	BMA	C4-C3	2.36	1.58	1.52
8	P	703	BMA	C2-C3	2.44	1.55	1.52
8	L	705	MAN	C2-C3	2.48	1.55	1.52
8	L	703	BMA	C2-C3	3.17	1.56	1.52
5	I	353	BMA	C2-C3	3.23	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	353	BMA	C2-C3	3.86	1.57	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	701	NAG	C2-N2-C7	-6.32	114.92	123.04
8	L	701	NAG	C2-N2-C7	-5.33	116.19	123.04
6	J	702	NAG	C2-N2-C7	-4.53	117.22	123.04
5	M	352	NAG	O4-C4-C3	-4.33	100.59	110.34
6	J	703	BMA	C1-C2-C3	-4.20	104.58	109.54
6	N	702	NAG	C3-C2-N2	-3.56	102.02	110.56
6	J	702	NAG	C3-C2-N2	-3.52	102.13	110.56
8	P	702	NAG	C3-C2-N2	-3.31	102.64	110.56
6	J	702	NAG	O3-C3-C2	-3.23	102.71	109.11
8	L	701	NAG	C6-C5-C4	-3.13	105.30	113.02
8	P	701	NAG	C4-C3-C2	-2.99	106.58	111.23
8	P	701	NAG	C2-N2-C7	-2.84	119.39	123.04
8	P	703	BMA	O5-C1-C2	-2.58	106.67	110.86
8	P	701	NAG	C6-C5-C4	-2.55	106.72	113.02
6	N	702	NAG	C2-N2-C7	-2.54	119.78	123.04
8	L	702	NAG	C3-C2-N2	-2.48	104.62	110.56
6	N	702	NAG	O3-C3-C2	-2.47	104.21	109.11
8	P	701	NAG	O6-C6-C5	-2.39	103.44	111.33
6	J	701	NAG	C2-N2-C7	-2.20	120.21	123.04
5	M	352	NAG	C2-N2-C7	-2.14	120.29	123.04
8	P	702	NAG	C2-N2-C7	-2.10	120.34	123.04
8	L	704	MAN	C1-C2-C3	-2.09	107.07	109.54
5	M	353	BMA	C1-C2-C3	-2.09	107.07	109.54
5	I	353	BMA	O5-C5-C6	2.00	111.68	107.35
6	J	704	MAN	O5-C1-C2	2.03	114.14	110.86
6	J	702	NAG	C3-C4-C5	2.04	113.75	110.20
5	M	351	NAG	O3-C3-C2	2.05	113.16	109.11
5	I	351	NAG	O6-C6-C5	2.05	118.11	111.33
7	K	352	NAG	O3-C3-C2	2.10	113.27	109.11
8	P	705	MAN	O5-C5-C6	2.12	111.94	107.35
6	N	701	NAG	C1-O5-C5	2.14	114.97	112.25
5	O	352	NAG	C3-C4-C5	2.15	113.95	110.20
6	N	704	MAN	C3-C4-C5	2.16	113.97	110.20
8	L	704	MAN	O2-C2-C1	2.20	113.62	109.21
5	M	352	NAG	C1-O5-C5	2.23	115.08	112.25
8	P	703	BMA	C2-C3-C4	2.24	114.85	111.04
5	I	353	BMA	O5-C1-C2	2.29	114.57	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	704	MAN	C1-C2-C3	2.35	112.32	109.54
8	P	704	MAN	O2-C2-C1	2.37	113.96	109.21
6	N	702	NAG	O5-C5-C6	2.39	112.52	107.35
5	I	352	NAG	C3-C4-C5	2.49	114.54	110.20
8	P	705	MAN	O2-C2-C1	2.49	114.20	109.21
5	M	353	BMA	O5-C5-C6	2.52	112.81	107.35
8	L	701	NAG	C3-C4-C5	2.54	114.63	110.20
6	J	701	NAG	C1-O5-C5	2.62	115.57	112.25
6	J	705	MAN	O5-C5-C6	2.67	113.12	107.35
6	N	705	MAN	C1-O5-C5	2.69	115.67	112.25
5	M	351	NAG	O5-C5-C6	2.73	113.26	107.35
5	O	352	NAG	C1-O5-C5	2.75	115.73	112.25
7	K	351	NAG	O5-C5-C6	2.76	113.31	107.35
8	L	702	NAG	C1-O5-C5	2.78	115.78	112.25
8	L	705	MAN	C1-C2-C3	2.86	112.92	109.54
8	P	704	MAN	C1-C2-C3	2.87	112.94	109.54
5	O	351	NAG	C3-C4-C5	2.88	115.22	110.20
8	L	706	NAG	O3-C3-C2	2.91	114.87	109.11
8	L	705	MAN	O3-C3-C2	2.97	115.37	110.00
5	I	351	NAG	O5-C5-C6	3.21	114.30	107.35
8	L	703	BMA	O3-C3-C4	3.41	118.01	110.34
8	P	702	NAG	C1-O5-C5	3.48	116.67	112.25
6	J	704	MAN	O2-C2-C1	3.53	116.29	109.21
8	L	705	MAN	C1-O5-C5	3.60	116.81	112.25
8	P	703	BMA	C1-O5-C5	3.64	116.87	112.25
8	L	703	BMA	C1-O5-C5	3.75	117.01	112.25
6	N	704	MAN	O2-C2-C1	3.99	117.21	109.21
8	L	703	BMA	C2-C3-C4	4.03	117.88	111.04
6	J	705	MAN	C1-O5-C5	4.10	117.45	112.25
8	P	701	NAG	C1-O5-C5	4.18	117.55	112.25
7	K	352	NAG	C1-O5-C5	4.37	117.79	112.25
5	I	353	BMA	C1-O5-C5	4.74	118.26	112.25
5	I	353	BMA	C1-C2-C3	4.80	115.22	109.54
8	L	706	NAG	C1-O5-C5	4.90	118.46	112.25
6	J	703	BMA	C1-O5-C5	5.31	118.99	112.25
7	K	351	NAG	C1-O5-C5	5.66	119.43	112.25
5	O	353	BMA	C1-O5-C5	5.72	119.51	112.25
8	L	701	NAG	C1-O5-C5	5.84	119.67	112.25
6	N	703	BMA	C1-O5-C5	6.50	120.50	112.25
5	I	351	NAG	C1-O5-C5	6.65	120.69	112.25
5	O	351	NAG	C1-O5-C5	7.01	121.15	112.25
8	P	706	NAG	C1-O5-C5	7.22	121.41	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	351	NAG	C1-O5-C5	7.61	121.91	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	352	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	351	NAG	4	0
6	J	701	NAG	1	0
6	J	703	BMA	1	0
6	J	705	MAN	1	0
7	K	351	NAG	2	0
8	L	701	NAG	3	0
6	N	701	NAG	2	0
6	N	702	NAG	1	0
5	O	351	NAG	6	0
5	O	352	NAG	1	0
8	P	701	NAG	4	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/226 (98%)	1.27	46 (20%) 1 1	73, 105, 211, 230	0
1	C	222/226 (98%)	1.20	42 (18%) 2 2	85, 116, 174, 196	0
1	E	222/226 (98%)	1.12	39 (17%) 2 2	87, 110, 158, 187	0
1	G	222/226 (98%)	1.38	50 (22%) 1 1	90, 116, 186, 207	0
2	B	216/217 (99%)	1.74	71 (32%) 0 1	87, 137, 195, 219	0
2	D	216/217 (99%)	1.44	64 (29%) 1 1	100, 140, 162, 194	0
2	F	216/217 (99%)	1.32	54 (25%) 1 1	104, 123, 156, 176	0
2	H	216/217 (99%)	1.88	75 (34%) 0 1	101, 140, 203, 234	0
3	I	236/334 (70%)	0.86	31 (13%) 5 4	79, 104, 139, 161	0
3	K	232/334 (69%)	1.03	32 (13%) 4 4	85, 118, 157, 184	0
3	M	230/334 (68%)	0.84	23 (10%) 9 9	84, 108, 144, 172	0
3	O	225/334 (67%)	1.23	50 (22%) 1 1	94, 122, 159, 182	0
4	J	98/131 (74%)	0.82	6 (6%) 25 23	70, 98, 155, 186	0
4	L	93/131 (70%)	1.04	13 (13%) 4 4	76, 106, 138, 177	0
4	N	95/131 (72%)	1.02	10 (10%) 8 8	69, 98, 141, 183	0
4	P	93/131 (70%)	1.12	12 (12%) 5 4	80, 105, 135, 163	0
All	All	3054/3632 (84%)	1.23	618 (20%) 1 1	69, 116, 179, 234	0

All (618) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	SER	13.4
1	A	126	PRO	12.5
1	A	135	GLY	11.9
1	A	140	LEU	9.4
1	G	126	PRO	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	113	PRO	9.1
1	E	136	GLY	9.0
1	G	140	LEU	8.8
2	H	144	ALA	8.4
2	H	186	TYR	7.5
4	P	521	GLN	7.5
2	H	134	CYS	7.4
2	H	112	ALA	7.3
2	H	111	ALA	7.3
2	H	192	TYR	7.1
1	A	205	THR	7.1
2	H	194	CYS	6.9
2	D	146	VAL	6.9
2	D	106	ILE	6.8
3	K	261	TYR	6.8
2	H	181	LEU	6.6
2	B	121	SER	6.6
2	H	133	VAL	6.5
1	G	205	THR	6.5
2	B	209	PHE	6.3
2	H	110	VAL	6.3
1	A	123	PRO	6.1
1	C	126	PRO	6.1
4	L	526	ALA	6.1
1	C	219	VAL	6.1
2	H	115	VAL	6.0
2	B	191	VAL	5.9
1	G	122	PHE	5.9
1	A	166	LEU	5.9
1	E	194	PRO	5.8
3	O	234	PHE	5.7
2	B	146	VAL	5.7
1	C	208	CYS	5.7
2	H	150	VAL	5.7
2	H	161	GLU	5.6
3	I	310	VAL	5.6
2	B	133	VAL	5.5
3	I	258	GLU	5.5
2	B	192	TYR	5.4
2	H	209	PHE	5.4
1	G	129	LYS	5.3
1	A	206	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	140	LEU	5.3
1	G	206	TYR	5.2
2	H	191	VAL	5.2
3	O	225	PHE	5.2
4	J	524	GLY	5.2
3	O	261	TYR	5.2
3	O	119	SER	5.2
2	B	152	ASN	5.2
2	D	139	PHE	5.2
2	H	135	LEU	5.1
1	E	130	SER	5.1
2	F	201	LEU	5.0
1	C	166	LEU	5.0
2	H	152	ASN	5.0
3	O	232	TYR	4.9
2	B	145	LYS	4.9
2	B	196	VAL	4.9
1	E	198	LEU	4.9
2	B	117	ILE	4.9
2	B	162	SER	4.9
2	H	178	THR	4.8
2	B	131	SER	4.8
3	M	258	GLU	4.8
2	B	190	LYS	4.8
2	B	187	GLU	4.8
2	B	184	ALA	4.8
1	A	122	PHE	4.8
2	B	176	SER	4.8
2	F	69	THR	4.7
2	H	68	GLY	4.7
1	A	196	SER	4.7
2	B	147	GLN	4.7
2	F	156	SER	4.7
3	K	236	VAL	4.7
1	E	195	SER	4.6
2	H	146	VAL	4.6
1	G	1	GLU	4.6
2	B	122	ASP	4.6
1	G	143	LEU	4.6
2	B	120	PRO	4.6
2	H	190	LYS	4.6
2	F	77	SER	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	110	VAL	4.6
2	B	154	LEU	4.6
1	A	154	VAL	4.5
2	F	33	LEU	4.5
2	D	78	LEU	4.5
4	N	583	SER	4.5
1	A	198	LEU	4.4
2	B	181	LEU	4.4
2	F	146	VAL	4.4
2	H	205	VAL	4.4
2	B	182	SER	4.3
2	B	203	SER	4.3
2	D	189	HIS	4.3
4	J	525	ALA	4.3
2	D	132	VAL	4.3
3	I	127	ASP	4.3
2	H	171	SER	4.2
2	D	145	LYS	4.2
2	B	116	PHE	4.2
2	D	108	ARG	4.2
3	M	57	LEU	4.2
1	E	226	GLU	4.2
1	G	121	VAL	4.1
1	A	197	SER	4.1
2	H	116	PHE	4.1
1	A	134	SER	4.1
3	O	255	GLN	4.1
2	D	31	SER	4.1
2	D	123	GLU	4.1
2	B	153	ALA	4.1
3	K	225	PHE	4.1
3	O	236	VAL	4.1
2	H	182	SER	4.0
2	D	21	ILE	4.0
4	P	525	ALA	4.0
1	E	206	TYR	4.0
1	A	194	PRO	4.0
1	A	203	GLN	4.0
2	H	113	PRO	4.0
3	M	273	LEU	3.9
1	G	168	SER	3.9
1	G	174	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	78	LEU	3.9
1	C	1	GLU	3.9
3	O	242	VAL	3.9
1	E	168	SER	3.9
2	H	202	ARG	3.9
2	D	147	GLN	3.8
3	O	221	GLN	3.8
2	H	122	ASP	3.8
3	I	59	SER	3.8
2	D	192	TYR	3.8
2	B	155	GLN	3.8
1	A	153	THR	3.8
1	E	126	PRO	3.8
2	H	155	GLN	3.8
3	O	276	LYS	3.8
1	G	70	SER	3.8
2	H	206	THR	3.8
3	K	232	TYR	3.8
4	N	544	THR	3.8
4	L	525	ALA	3.8
2	D	183	LYS	3.8
2	B	151	ASP	3.8
2	F	148	TRP	3.8
4	J	504	ILE	3.8
1	G	167	THR	3.8
3	O	253	LEU	3.7
2	B	178	THR	3.7
1	G	198	LEU	3.7
3	M	272	LYS	3.7
2	D	15	LEU	3.7
4	N	578	GLU	3.7
2	B	171	SER	3.7
3	O	120	GLU	3.7
1	A	167	THR	3.7
2	F	166	GLN	3.7
2	F	19	ALA	3.7
2	D	197	THR	3.7
2	D	144	ALA	3.7
2	H	132	VAL	3.7
3	K	147	CYS	3.7
1	G	200	THR	3.7
2	H	73	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	112	SER	3.6
3	O	256	LEU	3.6
3	I	41	SER	3.6
2	H	193	ALA	3.6
2	B	115	VAL	3.6
3	I	225	PHE	3.6
1	C	226	GLU	3.5
2	D	87	TYR	3.5
2	H	154	LEU	3.5
3	K	57	LEU	3.5
2	B	186	TYR	3.5
2	H	156	SER	3.5
1	E	154	VAL	3.5
4	P	578	GLU	3.5
1	E	129	LYS	3.5
2	F	24	LYS	3.5
2	D	202	ARG	3.5
1	C	189	SER	3.5
2	H	179	LEU	3.5
2	H	158	ASN	3.4
1	A	5	LEU	3.4
3	K	308	PHE	3.4
3	I	141	VAL	3.4
2	B	208	SER	3.4
2	H	196	VAL	3.4
3	I	243	GLN	3.4
1	G	130	SER	3.4
3	K	228	ASN	3.4
1	C	100(H)	PHE	3.4
1	C	198	LEU	3.4
2	B	199	GLN	3.4
1	E	27	PHE	3.3
1	E	133	THR	3.3
2	H	67	SER	3.3
3	I	232	TYR	3.3
4	N	529	LEU	3.3
2	B	148	TRP	3.3
2	F	183	LYS	3.3
2	B	158	ASN	3.3
4	L	520	THR	3.3
1	G	3	GLN	3.3
2	B	114	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	190	VAL	3.3
4	N	527	ILE	3.3
2	B	27(B)	VAL	3.2
2	B	150	VAL	3.2
1	A	219	VAL	3.2
1	G	225	VAL	3.2
2	D	113	PRO	3.2
1	G	146	ASP	3.2
2	F	144	ALA	3.2
1	E	193	VAL	3.2
2	D	109	THR	3.2
1	C	27	PHE	3.2
1	E	135	GLY	3.2
3	O	88	PHE	3.2
2	H	1	GLU	3.2
2	H	207	LYS	3.2
2	F	6	GLN	3.2
2	B	180	THR	3.1
2	F	87	TYR	3.1
3	K	111	LEU	3.1
1	E	220	ASP	3.1
3	M	262	THR	3.1
1	G	134	SER	3.1
1	E	216	ASN	3.1
1	E	3	GLN	3.1
1	C	5	LEU	3.1
3	O	57	LEU	3.1
1	E	196	SER	3.1
1	G	82(B)	SER	3.1
1	G	165	ALA	3.1
3	K	309	THR	3.1
2	F	151	ASP	3.1
1	G	192	THR	3.0
2	B	197	THR	3.0
4	J	523	GLU	3.0
3	O	53	CYS	3.0
3	O	167	SER	3.0
1	C	222	LYS	3.0
2	F	5	THR	3.0
2	B	156	SER	3.0
1	G	124	LEU	3.0
2	H	104	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	131	SER	3.0
2	F	194	CYS	3.0
3	O	47	ASP	3.0
1	G	128	SER	3.0
2	B	7	SER	3.0
2	D	150	VAL	3.0
2	B	87	TYR	3.0
1	A	168	SER	3.0
3	O	41	SER	3.0
3	M	111	LEU	3.0
4	P	535	PHE	3.0
1	C	125	ALA	3.0
2	F	204	PRO	3.0
4	L	527	ILE	3.0
2	D	155	GLN	3.0
3	K	104	TRP	3.0
4	P	547	LEU	3.0
2	B	132	VAL	3.0
2	B	8	PRO	3.0
2	H	117	ILE	3.0
2	F	152	ASN	3.0
3	M	117	ASP	3.0
3	M	225	PHE	3.0
1	A	121	VAL	3.0
2	D	100	GLY	3.0
2	H	204	PRO	3.0
1	C	206	TYR	3.0
3	O	307	SER	3.0
1	G	166	LEU	3.0
3	I	57	LEU	3.0
3	O	104	TRP	2.9
1	A	156	SER	2.9
2	H	149	LYS	2.9
3	O	48	VAL	2.9
2	F	2	LEU	2.9
2	D	136	LEU	2.9
2	D	27(B)	VAL	2.9
4	L	583	SER	2.9
3	O	239	LEU	2.9
1	A	1	GLU	2.9
2	F	47	LEU	2.9
3	O	113	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	187	LEU	2.9
3	I	43	LEU	2.9
3	O	31	ARG	2.9
3	M	221	GLN	2.9
2	F	147	GLN	2.8
3	O	111	LEU	2.8
2	H	180	THR	2.8
1	E	227	PRO	2.8
2	H	140	TYR	2.8
3	O	259	THR	2.8
2	F	113	PRO	2.8
3	I	233	LEU	2.8
2	D	105	GLU	2.8
2	H	195	GLU	2.8
3	O	147	CYS	2.8
1	G	26	GLY	2.8
2	D	39	LYS	2.8
3	O	148	ALA	2.8
1	G	157	TRP	2.8
2	B	126	LYS	2.8
2	B	134	CYS	2.8
3	O	117	ASP	2.8
1	A	182	SER	2.8
4	P	583	SER	2.8
2	B	204	PRO	2.8
3	K	187	PRO	2.8
3	O	76	ALA	2.8
1	A	124	LEU	2.7
4	N	594	LEU	2.7
2	D	104	VAL	2.7
2	B	138	ASN	2.7
1	C	221	LYS	2.7
2	F	184	ALA	2.7
2	F	104	VAL	2.7
2	F	11	LEU	2.7
2	H	15	LEU	2.7
3	M	118	GLY	2.7
1	A	56	TYR	2.7
2	H	53	THR	2.7
2	D	96	LEU	2.7
1	C	165	ALA	2.7
1	A	141	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	27	GLN	2.7
1	C	103	TRP	2.7
1	C	119	PRO	2.7
2	D	102	THR	2.7
2	B	32	TYR	2.7
2	H	198	HIS	2.7
3	O	220	TYR	2.7
3	I	239	LEU	2.7
1	A	189	SER	2.7
2	H	27	GLN	2.7
1	C	100(A)	GLY	2.7
3	M	100	GLU	2.7
2	D	59	PRO	2.7
2	H	27(E)	SER	2.7
2	H	177	SER	2.7
3	I	119	SER	2.7
1	C	2	VAL	2.7
1	C	105	GLN	2.7
2	F	92	TYR	2.7
3	O	222	ALA	2.7
2	D	5	THR	2.7
2	H	32	TYR	2.6
3	K	185	ILE	2.6
1	A	171	VAL	2.6
1	G	163	SER	2.6
1	G	210	VAL	2.6
1	A	143	LEU	2.6
4	L	504	ILE	2.6
4	L	542	ILE	2.6
1	C	48	VAL	2.6
1	E	152	VAL	2.6
3	K	240	THR	2.6
3	I	234	PHE	2.6
1	C	211	ASN	2.6
1	A	210	VAL	2.6
2	B	166	GLN	2.6
2	F	20	THR	2.6
2	H	20	THR	2.6
1	G	152	VAL	2.6
2	F	27(A)	SER	2.6
2	F	75	ILE	2.6
2	F	196	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	136	LEU	2.6
3	O	140	LYS	2.6
1	C	210	VAL	2.6
4	L	537	PRO	2.6
1	C	122	PHE	2.6
1	G	222	LYS	2.6
3	M	232	TYR	2.6
2	H	19	ALA	2.5
1	A	136	GLY	2.5
1	A	157	TRP	2.5
1	E	157	TRP	2.5
2	D	158	ASN	2.5
3	O	260	ILE	2.5
2	D	187	GLU	2.5
1	G	100	THR	2.5
3	K	217	THR	2.5
4	L	578	GLU	2.5
1	C	29	LEU	2.5
2	F	27(C)	LEU	2.5
3	O	141	VAL	2.5
4	P	526	ALA	2.5
4	N	577	THR	2.5
3	K	278	ASN	2.5
3	I	47	ASP	2.5
2	D	185	ASP	2.5
2	F	192	TYR	2.5
4	L	586	ASN	2.5
3	K	53	CYS	2.5
1	C	118	GLY	2.5
2	B	188	LYS	2.5
3	I	300	LYS	2.5
1	E	5	LEU	2.5
1	G	193	VAL	2.5
2	B	144	ALA	2.5
2	H	27(D)	TYR	2.5
3	K	137	TYR	2.5
2	F	175	LEU	2.5
3	I	271	GLY	2.4
2	F	203	SER	2.4
2	H	172	THR	2.4
3	K	55	ASP	2.4
1	C	192	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	110	THR	2.4
2	D	2	LEU	2.4
3	I	48	VAL	2.4
2	H	210	ASN	2.4
2	B	18	ARG	2.4
2	D	98	PHE	2.4
2	H	27(B)	VAL	2.4
3	K	262	THR	2.4
4	P	520	THR	2.4
3	I	37	VAL	2.4
2	H	47	LEU	2.4
3	M	119	SER	2.4
2	D	81	GLU	2.4
3	I	113	ILE	2.4
2	F	23	CYS	2.4
2	B	202	ARG	2.4
2	B	161	GLU	2.4
1	E	174	PHE	2.4
3	M	220	TYR	2.4
2	D	47	LEU	2.4
2	D	73	LEU	2.4
4	J	529	LEU	2.4
4	L	529	LEU	2.4
3	I	187	PRO	2.4
2	F	88	CYS	2.4
2	D	33	LEU	2.4
2	F	202	ARG	2.4
2	F	31	SER	2.4
3	M	256	LEU	2.4
1	G	83	ARG	2.4
1	E	134	SER	2.3
3	M	121	CYS	2.3
2	D	1	GLU	2.3
1	A	187	LEU	2.3
3	O	139	HIS	2.3
2	D	173	TYR	2.3
3	O	243	GLN	2.3
1	E	169	GLY	2.3
3	K	149	GLY	2.3
3	O	80	PRO	2.3
2	B	27(C)	LEU	2.3
2	D	24	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	112	GLU	2.3
1	A	188	SER	2.3
1	G	100(A)	GLY	2.3
2	D	11	LEU	2.3
2	F	68	GLY	2.3
2	H	170	ASP	2.3
1	E	2	VAL	2.3
2	H	76	SER	2.3
2	D	184	ALA	2.3
2	F	70	ASP	2.3
1	G	208	CYS	2.3
3	O	250	PRO	2.3
2	D	25	SER	2.3
3	I	140	LYS	2.3
1	E	166	LEU	2.3
2	H	163	VAL	2.3
4	L	503	ALA	2.3
3	O	114	LYS	2.3
2	B	9	ASP	2.3
4	J	545	GLU	2.3
2	F	66	GLY	2.3
3	K	114	LYS	2.3
2	F	38	GLN	2.3
2	F	1	GLU	2.2
2	B	112	ALA	2.2
2	H	203	SER	2.2
4	N	576	THR	2.2
1	A	100(A)	GLY	2.2
3	M	254	LEU	2.2
2	F	83	VAL	2.2
2	H	114	SER	2.2
3	K	148	ALA	2.2
1	E	142	CYS	2.2
2	B	194	CYS	2.2
2	B	86	TYR	2.2
2	H	71	PHE	2.2
2	F	198	HIS	2.2
1	G	188	SER	2.2
2	H	75	ILE	2.2
1	C	217	THR	2.2
3	O	244	LEU	2.2
1	A	125	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	185	ASP	2.2
3	O	187	PRO	2.2
2	D	148	TRP	2.2
2	B	68	GLY	2.2
4	N	524	GLY	2.2
1	A	144	VAL	2.2
1	E	137	THR	2.2
4	N	519	THR	2.2
3	K	150	ASP	2.2
2	F	134	CYS	2.2
3	I	128	GLY	2.2
1	C	154	VAL	2.2
3	O	188	GLN	2.2
2	B	179	LEU	2.2
2	D	23	CYS	2.2
3	M	104	TRP	2.2
3	O	118	GLY	2.2
3	K	237	ASP	2.2
3	O	151	PHE	2.2
2	D	171	SER	2.2
1	G	149	PRO	2.2
1	E	128	SER	2.2
2	D	172	THR	2.2
1	G	215	SER	2.1
1	E	119	PRO	2.1
1	G	164	GLY	2.1
2	D	53	THR	2.1
3	I	250	PRO	2.1
2	B	163	VAL	2.1
1	G	145	LYS	2.1
1	C	143	LEU	2.1
1	E	17	SER	2.1
1	C	205	THR	2.1
1	E	101	ASP	2.1
3	M	69	ASN	2.1
2	D	37	GLN	2.1
1	C	171	VAL	2.1
2	B	205	VAL	2.1
2	D	107	LYS	2.1
3	K	155	LYS	2.1
1	A	133	THR	2.1
3	I	62	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	27(B)	VAL	2.1
1	A	180	SER	2.1
2	D	44	PRO	2.1
1	C	200	THR	2.1
2	B	135	LEU	2.1
4	L	512	ASN	2.1
2	H	183	LYS	2.1
2	D	38	GLN	2.1
2	H	100	GLY	2.1
4	P	576	THR	2.1
1	C	190	VAL	2.1
2	B	93	SER	2.1
3	I	111	LEU	2.1
1	G	125	ALA	2.1
3	M	174	THR	2.1
2	F	106	ILE	2.1
1	C	128	SER	2.1
1	G	9	GLY	2.1
1	A	179	GLN	2.1
2	D	196	VAL	2.1
4	P	519	THR	2.1
2	H	148	TRP	2.1
1	A	114	ALA	2.1
1	G	226	GLU	2.1
3	I	255	GLN	2.1
3	M	185	ILE	2.1
2	D	135	LEU	2.1
3	O	184	LEU	2.1
2	H	173	TYR	2.1
3	K	241	TYR	2.1
1	E	1	GLU	2.1
2	D	79	GLN	2.1
2	F	35	TRP	2.1
1	E	56	TYR	2.1
2	D	120	PRO	2.1
3	I	222	ALA	2.1
3	O	218	ILE	2.0
3	M	233	LEU	2.0
4	P	552	ASP	2.0
1	G	183	GLY	2.0
1	A	190	VAL	2.0
3	K	146	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	77	SER	2.0
3	I	246	SER	2.0
3	K	47	ASP	2.0
1	E	173	THR	2.0
4	P	540	GLU	2.0
1	C	139	ALA	2.0
1	E	125	ALA	2.0
2	D	58	VAL	2.0
2	D	170	ASP	2.0
3	K	264	GLY	2.0
2	H	83	VAL	2.0
3	O	79	VAL	2.0
1	G	148	PHE	2.0
2	B	136	LEU	2.0
2	H	187	GLU	2.0
1	G	195	SER	2.0
1	C	19	ARG	2.0
1	A	174	PHE	2.0
2	B	78	LEU	2.0
1	C	199	GLY	2.0
1	C	120	SER	2.0
3	K	141	VAL	2.0
3	I	260	ILE	2.0
3	M	98	ASN	2.0
3	O	216	THR	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	J	701	14/15	0.82	0.29	1.74	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	L	701	14/15	0.77	0.31	1.02	98,98,98,98	0
7	NAG	K	351	14/15	0.51	0.50	0.01	156,156,156,156	0
5	NAG	I	351	14/15	0.79	0.38	-0.09	115,115,115,115	0
5	NAG	M	351	14/15	0.78	0.31	-0.43	117,117,117,117	0
5	NAG	O	351	14/15	0.72	0.35	-0.51	140,140,140,140	0
8	NAG	P	701	14/15	0.80	0.28	-0.60	97,97,97,97	0
6	NAG	N	701	14/15	0.85	0.23	-1.25	96,96,96,96	0
5	NAG	I	352	14/15	0.77	0.30	-	175,175,175,175	0
6	MAN	J	704	11/12	0.78	0.21	-	148,148,148,148	0
5	BMA	I	353	11/12	0.54	0.36	-	172,172,172,172	0
7	NAG	K	352	14/15	0.54	0.50	-	167,167,167,167	0
6	NAG	J	702	14/15	0.88	0.29	-	105,105,105,105	0
5	NAG	O	352	14/15	0.69	0.45	-	177,177,177,177	0
8	NAG	L	702	14/15	0.85	0.24	-	126,126,126,126	0
5	NAG	M	352	14/15	0.62	0.41	-	162,162,162,162	0
8	MAN	L	705	11/12	0.54	0.47	-	162,162,162,162	0
8	MAN	P	704	11/12	0.80	0.21	-	144,144,144,144	0
8	MAN	L	704	11/12	0.76	0.25	-	160,160,160,160	0
6	MAN	N	704	11/12	0.71	0.54	-	132,132,132,132	0
6	MAN	J	705	11/12	0.74	0.31	-	171,171,171,171	0
6	NAG	N	702	14/15	0.83	0.29	-	115,115,115,115	0
8	NAG	P	702	14/15	0.88	0.20	-	116,116,116,116	0
8	MAN	P	705	11/12	0.46	0.45	-	174,174,174,174	0
8	NAG	P	706	14/15	0.76	0.45	-	177,177,177,177	0
8	BMA	L	703	11/12	0.78	0.22	-	118,118,118,118	0
5	BMA	M	353	11/12	0.40	0.49	-	168,168,168,168	0
8	NAG	L	706	14/15	0.62	0.44	-	173,173,173,173	0
6	MAN	N	705	11/12	0.79	0.23	-	148,148,148,148	0
6	BMA	J	703	11/12	0.66	0.32	-	135,135,135,135	0
5	BMA	O	353	11/12	0.11	0.61	-	190,190,190,190	0
8	BMA	P	703	11/12	0.75	0.21	-	154,154,154,154	0
6	BMA	N	703	11/12	0.79	0.32	-	140,140,140,140	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.