



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:28 am BST

PDB ID : 3Q6F
Title : Crystal structure of Fab of human mAb 2909 specific for quaternary neutralizing epitope of HIV-1 gp120
Authors : Spurrier, B.; Sampson, J.; Totrov, M.; Li, H.; O'Neal, T.; William, C.; Robinson, J.; Gorny, M.K.; Zolla-Pazner, S.; Kong, X.P.
Deposited on : 2010-12-31
Resolution : 3.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

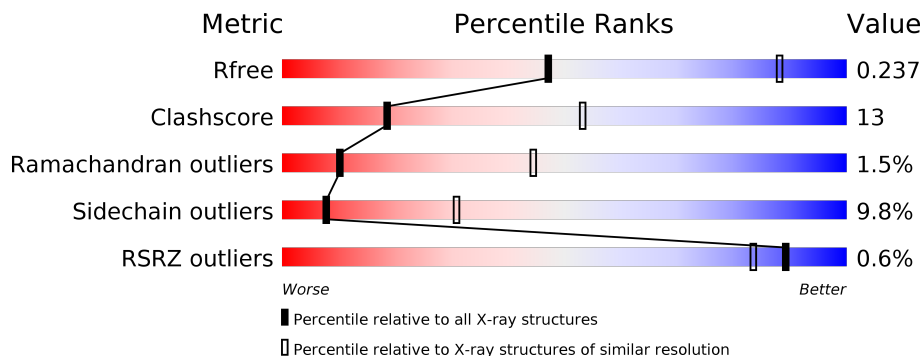
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">69% 25% 5%</p>
1	C	213	<div style="display: flex; align-items: center;"> <div style="width: 74%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">74% 23% .</p>
1	E	213	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">2% 66% 28% 5% .</p>
1	G	213	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">69% 27% .</p>
1	I	213	<div style="display: flex; align-items: center;"> <div style="width: 73%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">73% 24% .</p>
1	K	213	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">69% 27% .</p>

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Mol	Chain	Length	Quality of chain
2	B	233	
2	D	233	
2	F	233	
2	H	233	
2	J	233	
2	L	233	

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
2	TYS	D	100(A)	-	-	X	-
2	TYS	D	100(C)	-	-	X	-
2	TYS	J	100(C)	-	-	-	X
2	TYS	L	100(C)	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20084 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 Light chain of Fab of human mAb 2909.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1599	1000	272	322	5	0	0	0
1	C	212	1599	1000	272	322	5	0	0	0
1	E	212	1599	1000	272	322	5	0	0	0
1	G	212	1599	1000	272	322	5	0	0	0
1	I	212	1599	1000	272	322	5	0	0	0
1	K	212	1599	1000	272	322	5	0	0	0

- Molecule 2 is a protein called Heavy chain of Fab of human mAb 2909.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	228	1739	1094	285	350	10	0	0	0
2	D	228	1739	1094	285	350	10	0	0	0
2	F	228	1739	1094	285	350	10	0	0	0
2	H	228	1739	1094	285	350	10	0	0	0
2	J	230	1749	1099	287	353	10	0	0	0
2	L	229	1743	1096	286	351	10	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

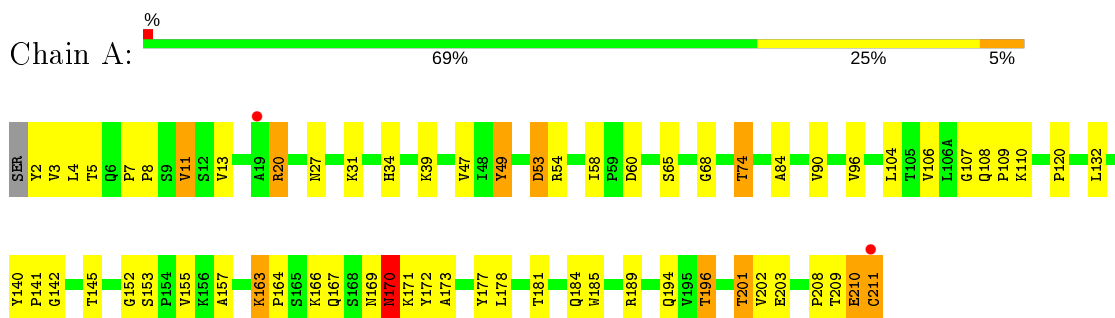


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0

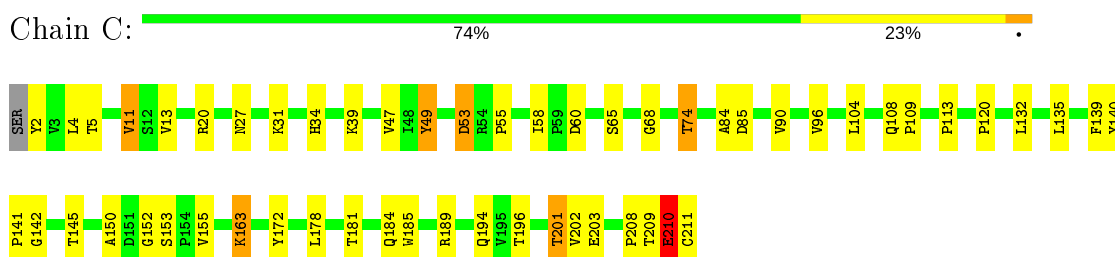
3 Residue-property plots [i](#)

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

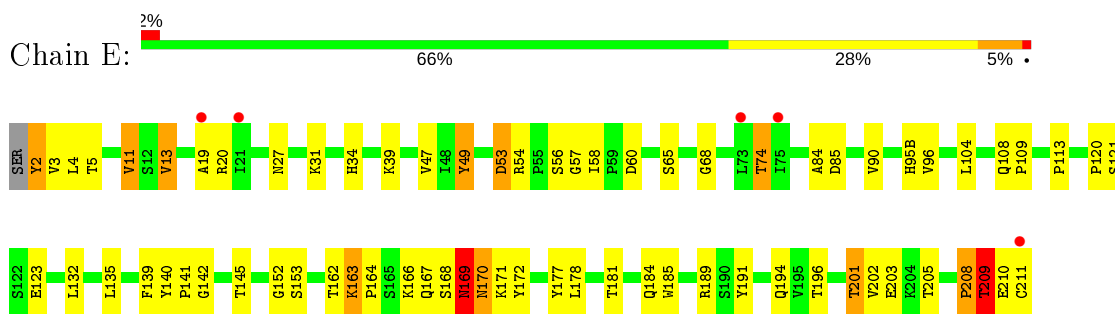
- Molecule 1: Light chain of Fab of human mAb 2909



- Molecule 1: Light chain of Fab of human mAb 2909

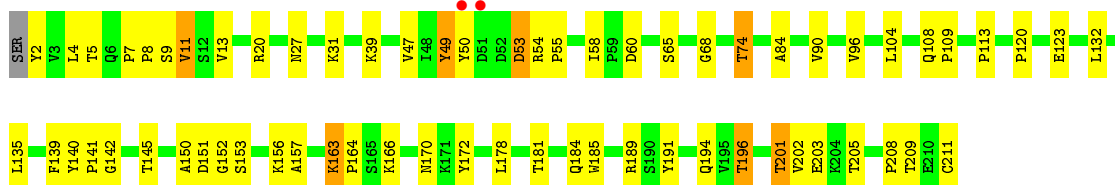


- Molecule 1: Light chain of Fab of human mAb 2909



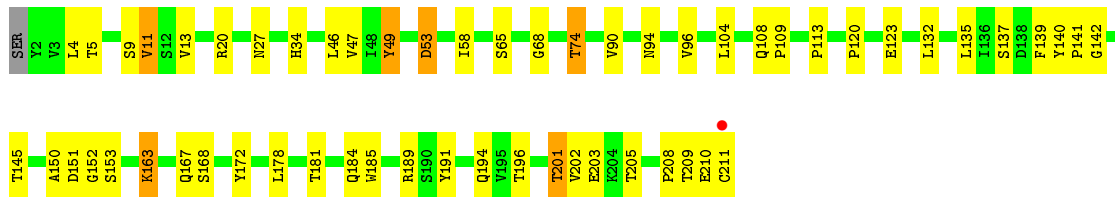
- Molecule 1: Light chain of Fab of human mAb 2909





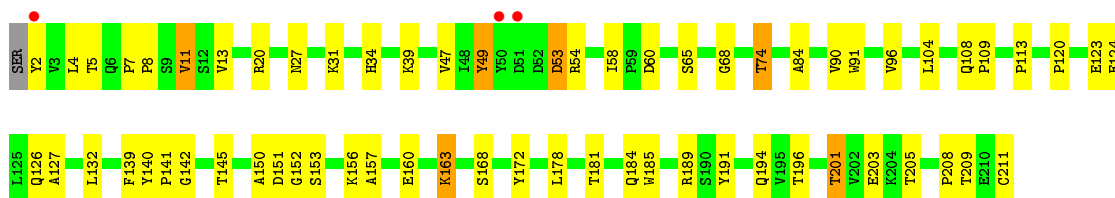
- Molecule 1: Light chain of Fab of human mAb 2909

Chain I: 73% 24%



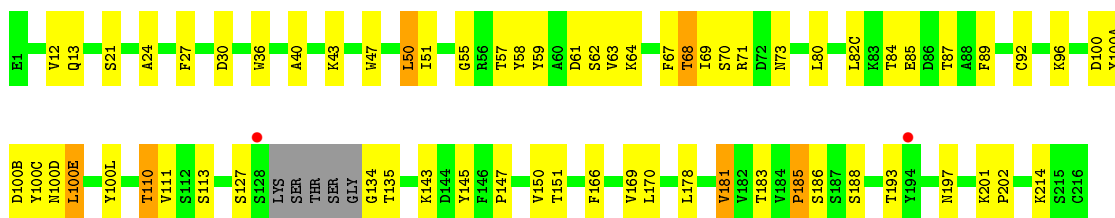
- Molecule 1: Light chain of Fab of human mAb 2909

Chain K: 69% 27%



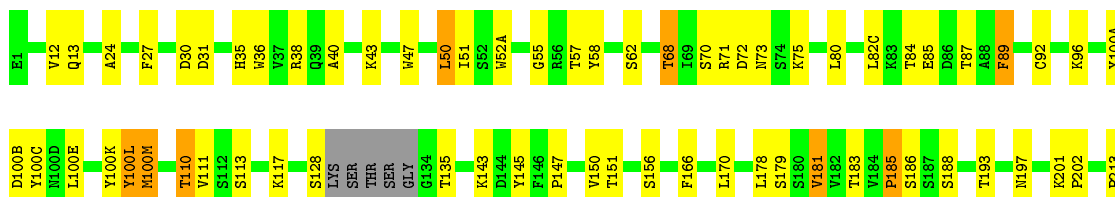
- Molecule 2: Heavy chain of Fab of human mAb 2909

Chain B: 70% 26%



- Molecule 2: Heavy chain of Fab of human mAb 2909

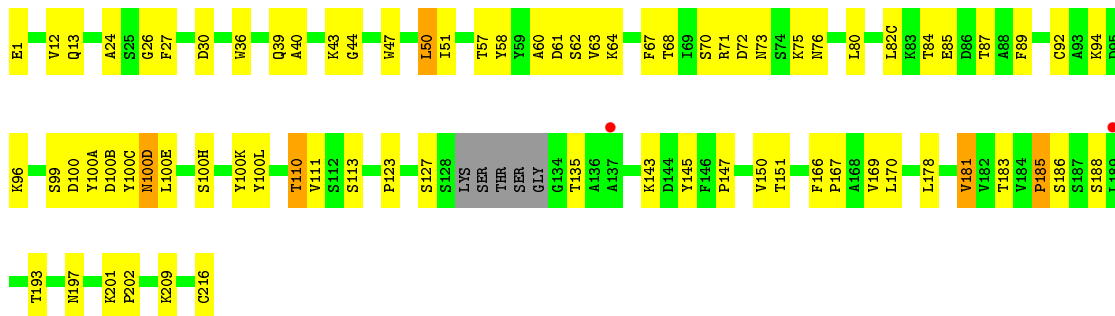
Chain D: 69% 25%



K214
S215
C216

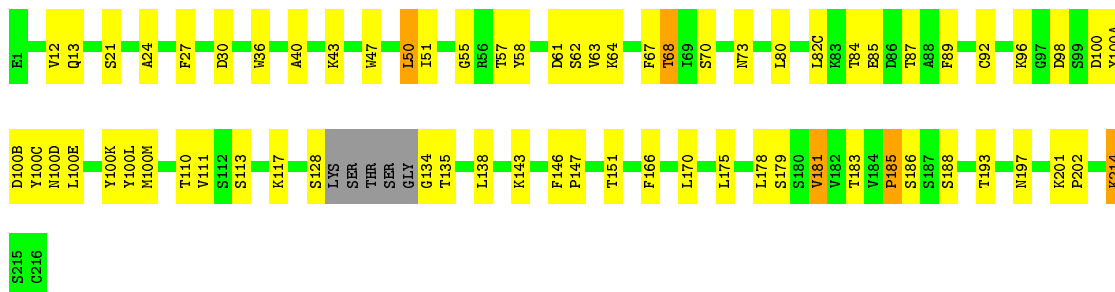
• Molecule 2: Heavy chain of Fab of human mAb 2909

Chain F: 65% 30%



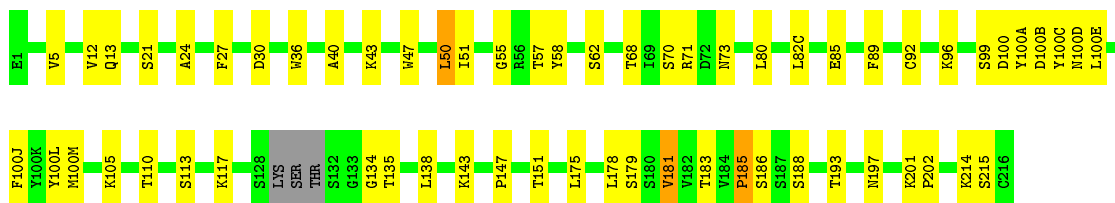
• Molecule 2: Heavy chain of Fab of human mAb 2909

Chain H: 69% 27%



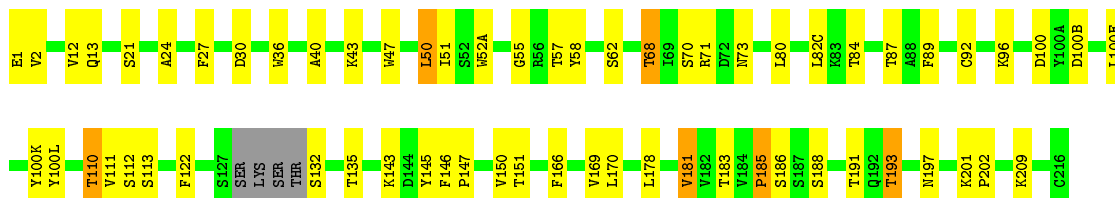
• Molecule 2: Heavy chain of Fab of human mAb 2909

Chain J: 73% 25%



• Molecule 2: Heavy chain of Fab of human mAb 2909

Chain L: 71% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.50Å 178.50Å 218.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.65 – 3.19 46.65 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.65-3.19) 99.3 (46.65-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.199 , 0.243 0.195 , 0.237	Depositor DCC
R_{free} test set	3393 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20084	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, TYS

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	0.44	0/1640	0.64	2/2244 (0.1%)
1	C	0.48	0/1640	0.65	2/2244 (0.1%)
1	E	0.41	0/1640	0.63	2/2244 (0.1%)
1	G	0.54	0/1640	0.77	3/2244 (0.1%)
1	I	0.55	0/1640	0.66	2/2244 (0.1%)
1	K	0.43	0/1640	0.75	3/2244 (0.1%)
2	B	0.47	0/1747	0.61	0/2371
2	D	0.51	0/1747	0.65	0/2371
2	F	0.50	0/1747	0.63	0/2371
2	H	0.59	0/1747	0.67	0/2371
2	J	0.62	0/1757	0.69	0/2384
2	L	0.47	0/1751	0.62	0/2376
All	All	0.51	0/20336	0.67	14/27708 (0.1%)

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	G	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	ARG	NE-CZ-NH1	-14.82	112.89	120.30
1	K	189	ARG	NE-CZ-NH2	14.76	127.68	120.30
1	K	189	ARG	NE-CZ-NH1	-14.63	112.99	120.30
1	G	189	ARG	NE-CZ-NH2	14.42	127.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	E	189	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	E	189	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	G	189	ARG	CD-NE-CZ	7.60	134.24	123.60
1	A	189	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	189	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	K	189	ARG	CD-NE-CZ	7.55	134.17	123.60
1	I	189	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	189	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	I	189	ARG	NE-CZ-NH1	6.90	123.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	157	ALA	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	1599	0	1534	46	0
1	C	1599	0	1534	42	0
1	E	1599	0	1534	65	0
1	G	1599	0	1534	42	0
1	I	1599	0	1534	41	0
1	K	1599	0	1534	43	0
2	B	1739	0	1660	39	0
2	D	1739	0	1659	69	0
2	F	1739	0	1660	62	0
2	H	1739	0	1659	48	0
2	J	1749	0	1668	40	0
2	L	1743	0	1663	46	0
3	A	7	0	10	0	0
3	C	7	0	10	1	0
3	E	7	0	10	1	0
3	G	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	7	0	10	0	0
3	K	7	0	10	0	0
All	All	20084	0	19233	520	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 13.

All (520) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100(A):TYS:HD1	2:D:100(B):ASP:N	1.38	1.37
2:J:96:LYS:HD2	2:J:100(L):TYR:OH	1.56	1.04
1:E:177:TYR:CE2	2:F:169:VAL:HG11	2.00	0.95
2:D:100(A):TYS:HD1	2:D:100(B):ASP:H	0.90	0.93
2:D:100(A):TYS:CD1	2:D:100(B):ASP:N	2.32	0.90
1:A:185:TRP:CZ2	1:A:208:PRO:HA	2.11	0.85
2:D:100(A):TYS:CD1	2:D:100(B):ASP:H	1.85	0.83
2:D:156:SER:HB3	1:E:56:SER:HB2	1.61	0.82
2:J:100(A):TYS:CD1	2:J:100(B):ASP:H	1.91	0.82
2:D:213:PRO:O	2:D:214:LYS:HB2	1.80	0.82
1:E:177:TYR:HE2	2:F:169:VAL:HG11	1.42	0.82
2:L:96:LYS:HD2	2:L:100(L):TYR:OH	1.82	0.78
1:E:209:THR:O	1:E:210:GLU:HG3	1.84	0.78
1:G:181:THR:OG1	1:G:184:GLN:HG3	1.85	0.76
2:D:100(A):TYS:HD1	2:D:100(A):TYS:C	2.14	0.74
2:L:50:LEU:HD21	2:L:58:TYR:HD2	1.53	0.74
1:A:167:GLN:OE1	1:A:173:ALA:HB2	1.88	0.73
1:A:20:ARG:HG3	1:A:74:THR:HG23	1.69	0.73
2:F:50:LEU:HD21	2:F:58:TYR:HD2	1.54	0.72
1:C:20:ARG:HG3	1:C:74:THR:HG23	1.73	0.71
1:E:2:TYR:CD2	1:E:31:LYS:HE3	2.25	0.71
1:I:181:THR:OG1	1:I:184:GLN:HG3	1.90	0.71
2:F:76:ASN:HD21	2:L:191:THR:HB	1.56	0.70
2:B:96:LYS:HD2	2:B:100(L):TYR:OH	1.91	0.70
1:G:20:ARG:HG3	1:G:74:THR:HG23	1.74	0.70
2:H:50:LEU:HD23	2:H:50:LEU:C	2.12	0.70
1:K:96:VAL:HB	2:L:47:TRP:CG	2.26	0.70
2:H:96:LYS:HD2	2:H:100(L):TYR:OH	1.92	0.69
2:F:100(C):TYS:HE1	2:F:100(C):TYS:O1	1.91	0.69
1:E:210:GLU:HB3	1:E:211:CYS:HA	1.74	0.69
2:F:50:LEU:HD21	2:F:58:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ARG:HG3	1:E:74:THR:HG23	1.75	0.69
2:B:100(A):TYS:CD1	2:B:100(B):ASP:H	2.05	0.69
2:D:214:LYS:CB	2:D:215:SER:HA	2.22	0.69
2:D:213:PRO:O	2:D:214:LYS:CB	2.41	0.69
1:E:2:TYR:CE2	1:E:31:LYS:HE3	2.26	0.68
2:L:50:LEU:HD21	2:L:58:TYR:CD2	2.29	0.68
2:B:50:LEU:HD21	2:B:58:TYR:HD2	1.59	0.68
1:E:181:THR:OG1	1:E:184:GLN:HG3	1.94	0.68
1:I:108:GLN:HB2	1:I:109:PRO:HD2	1.75	0.68
2:H:100(C):TYS:HD2	2:H:100(C):TYS:C	2.23	0.67
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.76	0.67
1:K:20:ARG:HG3	1:K:74:THR:HG23	1.76	0.67
1:A:109:PRO:HA	2:D:31:ASP:OD2	1.94	0.67
2:H:117:LYS:HA	1:I:123:GLU:HG3	1.77	0.67
1:C:181:THR:OG1	1:C:184:GLN:HG3	1.95	0.67
2:D:100(A):TYS:HE1	2:D:100(C):TYS:HA	1.77	0.67
2:D:50:LEU:HD21	2:D:58:TYR:HD2	1.59	0.66
1:I:163:LYS:CE	1:I:163:LYS:HA	2.25	0.66
1:A:142:GLY:HA3	1:A:172:TYR:CD1	2.30	0.66
2:J:100(A):TYS:HD1	2:J:100(B):ASP:H	1.59	0.66
2:J:100(A):TYS:CD1	2:J:100(B):ASP:N	2.59	0.66
2:L:1:GLU:HG2	2:L:2:VAL:H	1.60	0.66
1:A:108:GLN:HB2	1:A:109:PRO:HD2	1.76	0.66
1:I:4:LEU:HD11	1:I:90:VAL:HG22	1.77	0.66
2:F:76:ASN:ND2	2:L:191:THR:HB	2.10	0.66
1:E:142:GLY:HA3	1:E:172:TYR:CD1	2.31	0.66
1:G:108:GLN:HB2	1:G:109:PRO:HD2	1.76	0.66
1:A:181:THR:OG1	1:A:184:GLN:HG3	1.94	0.66
2:F:96:LYS:HD2	2:F:100(L):TYR:OH	1.96	0.66
2:J:50:LEU:HD21	2:J:58:TYR:HD2	1.59	0.66
2:D:100(C):TYS:OH	1:G:156:LYS:HG2	1.96	0.66
1:K:181:THR:OG1	1:K:184:GLN:HG3	1.96	0.66
1:C:108:GLN:HB2	1:C:109:PRO:HD2	1.78	0.65
2:B:50:LEU:HD21	2:B:58:TYR:CD2	2.31	0.65
1:C:142:GLY:HA3	1:C:172:TYR:CD1	2.32	0.65
1:E:121:SER:HB3	2:F:123:PRO:O	1.97	0.65
1:I:137:SER:HB2	1:I:167:GLN:HE22	1.61	0.65
1:E:108:GLN:HB2	1:E:109:PRO:HD2	1.77	0.65
1:K:156:LYS:HG3	1:K:157:ALA:H	1.61	0.65
2:D:50:LEU:HD21	2:D:58:TYR:CD2	2.32	0.64
1:G:196:THR:HG23	1:G:201:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:LEU:O	2:H:50:LEU:HD23	1.96	0.64
1:I:20:ARG:HG3	1:I:74:THR:HG23	1.77	0.64
1:E:177:TYR:CE2	2:F:169:VAL:CG1	2.76	0.64
2:B:50:LEU:HD23	2:B:50:LEU:C	2.18	0.64
2:D:156:SER:CB	1:E:56:SER:HB2	2.27	0.64
2:D:50:LEU:C	2:D:50:LEU:HD23	2.18	0.64
1:G:163:LYS:CE	1:G:163:LYS:HA	2.26	0.64
2:D:214:LYS:HB3	2:D:215:SER:HA	1.80	0.64
2:F:100(A):TYS:CD1	2:F:100(B):ASP:H	2.11	0.64
2:J:50:LEU:HD21	2:J:58:TYR:CD2	2.32	0.64
1:C:4:LEU:HD11	1:C:90:VAL:HG22	1.79	0.63
2:D:117:LYS:HE2	1:K:127:ALA:HB2	1.80	0.63
2:D:50:LEU:O	2:D:50:LEU:HD23	1.98	0.63
1:A:132:LEU:HD12	1:A:178:LEU:HD23	1.80	0.63
1:K:108:GLN:HB2	1:K:109:PRO:HD2	1.81	0.63
1:E:132:LEU:HD12	1:E:178:LEU:HD23	1.81	0.62
1:K:4:LEU:HD11	1:K:90:VAL:HG22	1.79	0.62
2:F:76:ASN:HD21	2:L:191:THR:CB	2.12	0.62
1:A:155:VAL:HG22	1:A:157:ALA:H	1.65	0.62
1:E:163:LYS:HA	1:E:163:LYS:CE	2.30	0.62
2:H:50:LEU:HD21	2:H:58:TYR:HD2	1.65	0.62
2:D:156:SER:O	1:E:57:GLY:N	2.33	0.62
2:J:178:LEU:HD12	2:J:178:LEU:C	2.20	0.62
1:A:163:LYS:HA	1:A:163:LYS:CE	2.30	0.61
2:B:100(A):TYS:HD1	2:B:100(B):ASP:H	1.64	0.61
2:D:178:LEU:C	2:D:178:LEU:HD12	2.20	0.61
1:I:120:PRO:HD3	1:I:132:LEU:CD2	2.30	0.61
1:I:163:LYS:HE3	1:I:163:LYS:HA	1.82	0.61
2:D:96:LYS:HD2	2:D:100(L):TYR:OH	2.00	0.61
1:K:142:GLY:HA3	1:K:172:TYR:CD1	2.36	0.61
2:B:50:LEU:HD23	2:B:50:LEU:O	2.00	0.61
1:E:4:LEU:HD11	1:E:90:VAL:HG22	1.83	0.61
1:E:96:VAL:HB	2:F:47:TRP:CG	2.36	0.61
1:E:2:TYR:HD1	1:E:3:VAL:N	1.99	0.60
1:K:163:LYS:HA	1:K:163:LYS:CE	2.30	0.60
1:C:163:LYS:HA	1:C:163:LYS:CE	2.30	0.60
1:E:120:PRO:HD3	1:E:132:LEU:HD23	1.83	0.60
2:H:50:LEU:HD21	2:H:58:TYR:CD2	2.37	0.60
1:G:142:GLY:HA3	1:G:172:TYR:CD1	2.36	0.60
1:G:47:VAL:O	1:G:58:ILE:HD11	2.02	0.60
2:J:135:THR:HA	2:J:186:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ASN:HD21	2:L:191:THR:CA	2.15	0.60
1:C:2:TYR:CD1	1:C:31:LYS:HE3	2.37	0.60
2:H:100(C):TYS:HD2	2:H:100(C):TYS:O	2.01	0.60
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.84	0.60
1:A:96:VAL:HB	2:B:47:TRP:CG	2.37	0.59
1:A:4:LEU:HD11	1:A:90:VAL:HG22	1.84	0.59
2:L:178:LEU:C	2:L:178:LEU:HD12	2.23	0.59
1:C:49:TYR:HD1	2:D:100(L):TYR:HH	1.50	0.59
2:D:185:PRO:HB2	2:D:188:SER:OG	2.03	0.59
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.85	0.59
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.84	0.59
1:G:166:LYS:HE3	1:G:170:ASN:O	2.02	0.59
1:I:120:PRO:HD3	1:I:132:LEU:HD23	1.84	0.59
2:J:50:LEU:HD23	2:J:50:LEU:C	2.22	0.59
2:F:50:LEU:C	2:F:50:LEU:HD23	2.24	0.58
2:H:178:LEU:C	2:H:178:LEU:HD12	2.23	0.58
1:C:208:PRO:O	1:C:210:GLU:N	2.33	0.58
1:C:47:VAL:O	1:C:58:ILE:HD11	2.02	0.58
1:E:120:PRO:HD3	1:E:132:LEU:CD2	2.34	0.58
1:I:96:VAL:HB	2:J:47:TRP:CG	2.39	0.58
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.86	0.58
1:A:2:TYR:CE1	1:A:31:LYS:HE3	2.39	0.58
1:K:47:VAL:O	1:K:58:ILE:HD11	2.04	0.58
1:G:163:LYS:HA	1:G:163:LYS:HE3	1.84	0.57
1:A:209:THR:O	1:A:210:GLU:CB	2.52	0.57
1:G:120:PRO:HD3	1:G:132:LEU:CD2	2.34	0.57
1:G:49:TYR:HD1	2:H:100(L):TYR:HH	1.50	0.57
1:E:166:LYS:HG2	1:E:172:TYR:CE2	2.38	0.57
1:G:96:VAL:HB	2:H:47:TRP:CG	2.39	0.57
1:C:150:ALA:HB3	1:I:94:ASN:ND2	2.19	0.57
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.86	0.57
2:J:68:THR:HG22	2:J:68:THR:O	2.04	0.57
2:B:178:LEU:C	2:B:178:LEU:HD12	2.25	0.57
2:H:134:GLY:O	2:H:186:SER:HB2	2.04	0.57
2:B:24:ALA:HB1	2:B:27:PHE:CE2	2.40	0.57
1:I:142:GLY:HA3	1:I:172:TYR:CD1	2.40	0.56
1:G:123:GLU:HG3	2:J:117:LYS:HA	1.88	0.56
1:I:132:LEU:HD12	1:I:178:LEU:HD23	1.87	0.56
1:E:2:TYR:CD1	1:E:3:VAL:N	2.73	0.56
2:J:185:PRO:HB2	2:J:188:SER:OG	2.06	0.56
2:D:24:ALA:HB1	2:D:27:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:LEU:HD12	1:K:178:LEU:HD23	1.88	0.56
1:E:196:THR:HG23	1:E:201:THR:OG1	2.05	0.56
2:B:84:THR:HG22	2:B:111:VAL:O	2.06	0.56
1:G:4:LEU:HD11	1:G:90:VAL:HG22	1.88	0.56
1:K:34:HIS:CD2	2:L:100(L):TYR:HB3	2.40	0.56
2:L:132:SER:HA	2:L:186:SER:OG	2.06	0.56
2:L:50:LEU:HD23	2:L:50:LEU:C	2.26	0.56
1:C:96:VAL:HB	2:D:47:TRP:CG	2.41	0.56
1:E:49:TYR:HD1	2:F:100(L):TYR:HH	1.53	0.56
2:B:135:THR:HA	2:B:186:SER:HB2	1.88	0.55
1:E:163:LYS:HA	1:E:163:LYS:HE3	1.88	0.55
1:A:166:LYS:HG3	1:A:170:ASN:HA	1.87	0.55
1:E:123:GLU:OE1	2:F:209:LYS:HE2	2.05	0.55
1:E:47:VAL:O	1:E:58:ILE:HD11	2.06	0.55
2:J:100(A):TYS:CZ	2:J:100(C):TYS:HA	2.37	0.55
2:F:185:PRO:HB2	2:F:188:SER:OG	2.06	0.55
2:H:24:ALA:HB1	2:H:27:PHE:CE2	2.42	0.55
2:J:50:LEU:HD23	2:J:50:LEU:O	2.07	0.55
1:C:132:LEU:HD12	1:C:178:LEU:HD23	1.88	0.55
1:G:132:LEU:HD12	1:G:178:LEU:HD23	1.88	0.55
1:K:120:PRO:HD3	1:K:132:LEU:CD2	2.37	0.55
2:L:24:ALA:HB1	2:L:27:PHE:CE2	2.42	0.55
2:D:36:TRP:NE1	2:D:80:LEU:HB2	2.21	0.55
2:F:24:ALA:HB1	2:F:27:PHE:CE2	2.42	0.55
2:D:100(A):TYS:HE1	2:D:100(C):TYS:CA	2.37	0.54
2:F:84:THR:HG22	2:F:111:VAL:O	2.07	0.54
1:C:2:TYR:CE1	1:C:31:LYS:HE3	2.42	0.54
1:E:11:VAL:HG12	1:E:104:LEU:HD12	1.89	0.54
2:H:100(C):TYS:C	2:H:100(C):TYS:CD2	2.80	0.54
1:I:196:THR:HG23	1:I:201:THR:OG1	2.07	0.54
1:K:163:LYS:HE3	1:K:163:LYS:HA	1.88	0.54
1:A:163:LYS:HE3	1:A:163:LYS:HA	1.87	0.54
2:D:84:THR:HG22	2:D:111:VAL:O	2.07	0.54
1:C:11:VAL:HG12	1:C:104:LEU:HD12	1.90	0.54
1:E:177:TYR:HE2	2:F:169:VAL:CG1	2.15	0.54
1:I:49:TYR:HD2	1:I:49:TYR:H	1.56	0.54
1:K:11:VAL:HG12	1:K:104:LEU:HD12	1.88	0.54
1:C:163:LYS:HA	1:C:163:LYS:HE3	1.88	0.54
1:G:49:TYR:HD2	1:G:49:TYR:H	1.56	0.54
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.22	0.54
2:B:185:PRO:HB2	2:B:188:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ASP:OD1	3:E:212:PEG:H12	2.08	0.54
1:E:123:GLU:OE1	2:F:209:LYS:CE	2.56	0.53
2:B:100(A):TYS:CD1	2:B:100(B):ASP:N	2.71	0.53
1:K:49:TYR:HD2	1:K:49:TYR:H	1.56	0.53
2:J:30:ASP:HA	2:J:73:ASN:ND2	2.22	0.53
1:A:47:VAL:O	1:A:58:ILE:HD11	2.08	0.53
1:G:120:PRO:HD3	1:G:132:LEU:HD23	1.89	0.53
2:L:185:PRO:HB2	2:L:188:SER:OG	2.08	0.53
1:K:120:PRO:HD3	1:K:132:LEU:HD23	1.91	0.53
2:F:76:ASN:ND2	2:L:191:THR:CB	2.71	0.53
1:A:49:TYR:H	1:A:49:TYR:HD2	1.57	0.53
2:J:134:GLY:O	2:J:186:SER:HB2	2.09	0.53
2:L:68:THR:HG22	2:L:68:THR:O	2.08	0.53
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.44	0.53
2:L:50:LEU:HD23	2:L:50:LEU:O	2.09	0.53
1:C:120:PRO:HD3	1:C:132:LEU:CD2	2.38	0.53
1:A:209:THR:O	1:A:210:GLU:HB2	2.09	0.52
1:C:185:TRP:CZ2	1:C:208:PRO:HA	2.43	0.52
1:C:120:PRO:HD3	1:C:132:LEU:HD23	1.91	0.52
2:F:50:LEU:O	2:F:50:LEU:HD23	2.08	0.52
1:I:11:VAL:HG12	1:I:104:LEU:HD12	1.92	0.52
1:I:47:VAL:O	1:I:58:ILE:HD11	2.08	0.52
2:D:117:LYS:HA	1:K:123:GLU:HG3	1.92	0.52
2:H:100(M):MET:N	2:H:100(M):MET:SD	2.83	0.52
2:J:24:ALA:HB1	2:J:27:PHE:CE2	2.44	0.52
1:C:49:TYR:HD2	1:C:49:TYR:H	1.57	0.52
2:L:84:THR:HG22	2:L:111:VAL:O	2.10	0.52
1:A:11:VAL:HG12	1:A:104:LEU:HD12	1.91	0.52
2:F:135:THR:HA	2:F:186:SER:HB2	1.91	0.52
2:H:100(A):TYS:CD2	2:H:100(B):ASP:H	2.23	0.52
2:F:51:ILE:HD13	2:F:71:ARG:HD2	1.92	0.52
1:G:11:VAL:HG12	1:G:104:LEU:HD12	1.92	0.52
1:I:34:HIS:CD2	2:J:100(L):TYR:HB3	2.45	0.52
2:L:100(B):ASP:OD1	2:L:100(E):LEU:HD12	2.10	0.52
2:F:147:PRO:HD2	2:F:202:PRO:CB	2.41	0.51
2:F:50:LEU:CD2	2:F:58:TYR:HD2	2.23	0.51
2:D:100(A):TYS:HE1	2:D:100(C):TYS:N	2.26	0.51
2:D:214:LYS:HG2	2:D:215:SER:HA	1.92	0.51
2:H:185:PRO:HB2	2:H:188:SER:OG	2.10	0.51
1:K:2:TYR:HE2	1:K:31:LYS:HD2	1.75	0.51
2:F:178:LEU:HD12	2:F:178:LEU:C	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HG23	2:H:51:ILE:O	2.10	0.51
1:A:196:THR:HG23	1:A:201:THR:OG1	2.10	0.51
1:C:34:HIS:NE2	2:D:100(L):TYR:HD2	2.09	0.51
2:D:135:THR:HA	2:D:186:SER:HB2	1.92	0.51
2:J:30:ASP:HA	2:J:73:ASN:HD22	1.76	0.51
2:H:100(A):TYS:O1	2:H:100(A):TYS:CE2	2.57	0.50
2:H:100(B):ASP:OD1	2:H:100(E):LEU:HD12	2.10	0.50
1:K:140:TYR:CD2	1:K:141:PRO:HA	2.45	0.50
2:B:51:ILE:O	2:B:51:ILE:HG23	2.12	0.50
1:C:34:HIS:CE1	2:D:100(L):TYR:CD2	3.00	0.50
1:K:196:THR:HG23	1:K:201:THR:OG1	2.12	0.50
1:A:110:LYS:HD3	2:D:52(A):TRP:NE1	2.26	0.50
1:G:47:VAL:O	1:G:55:PRO:HD2	2.11	0.50
1:I:49:TYR:HD1	2:J:100(L):TYR:CZ	2.30	0.50
1:K:156:LYS:HG3	1:K:157:ALA:N	2.27	0.49
2:H:135:THR:HA	2:H:186:SER:HB2	1.94	0.49
1:C:34:HIS:CE1	2:D:100(L):TYR:HD2	2.30	0.49
2:F:12:VAL:HG21	2:F:82(C):LEU:HD13	1.94	0.49
1:I:47:VAL:HA	1:I:58:ILE:CD1	2.43	0.49
2:B:100(C):TYS:O3	2:B:100(C):TYS:HE2	2.11	0.49
1:C:135:LEU:HD13	2:D:181:VAL:CG2	2.42	0.49
2:F:100(K):TYR:O	2:F:100(L):TYR:HB3	2.13	0.49
1:I:210:GLU:O	1:I:211:CYS:HB3	2.13	0.49
2:D:30:ASP:HA	2:D:73:ASN:ND2	2.28	0.48
2:H:201:LYS:N	2:H:202:PRO:CD	2.76	0.48
1:I:202:VAL:HG12	1:I:203:GLU:N	2.28	0.48
1:E:2:TYR:CE2	1:E:31:LYS:CE	2.95	0.48
2:L:135:THR:HA	2:L:186:SER:HB2	1.94	0.48
2:L:147:PRO:HD2	2:L:202:PRO:CB	2.42	0.48
2:F:51:ILE:HG23	2:F:51:ILE:O	2.13	0.48
2:J:147:PRO:HD2	2:J:202:PRO:CB	2.43	0.48
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.29	0.48
1:A:7:PRO:HA	2:D:100(C):TYS:O1	2.13	0.48
2:D:30:ASP:HA	2:D:73:ASN:HD22	1.79	0.48
2:D:43:LYS:N	2:D:43:LYS:HD2	2.28	0.48
2:D:12:VAL:HG21	2:D:82(C):LEU:HD13	1.96	0.48
1:A:209:THR:OG1	1:A:209:THR:O	2.28	0.48
2:F:87:THR:HG23	2:F:110:THR:HA	1.96	0.48
1:G:191:TYR:O	1:G:205:THR:HG23	2.14	0.48
2:J:201:LYS:N	2:J:202:PRO:CD	2.77	0.48
2:L:51:ILE:HG23	2:L:51:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:50:LEU:CD2	2:L:58:TYR:HD2	2.24	0.48
2:B:87:THR:HG23	2:B:110:THR:HA	1.96	0.48
1:G:49:TYR:HD1	2:H:100(L):TYR:OH	1.95	0.48
1:A:120:PRO:HD3	1:A:132:LEU:CD2	2.43	0.47
1:C:194:GLN:CG	1:C:203:GLU:HG3	2.44	0.47
2:H:147:PRO:HD2	2:H:202:PRO:CB	2.44	0.47
2:B:50:LEU:CD2	2:B:58:TYR:HD2	2.26	0.47
1:E:166:LYS:HE2	1:E:172:TYR:OH	2.14	0.47
1:E:169:ASN:H	1:E:169:ASN:ND2	2.10	0.47
2:L:30:ASP:HA	2:L:73:ASN:ND2	2.29	0.47
2:D:166:PHE:HE2	2:D:181:VAL:CG2	2.27	0.47
2:D:51:ILE:HG23	2:D:51:ILE:O	2.15	0.47
1:E:208:PRO:O	1:E:209:THR:C	2.53	0.47
1:I:191:TYR:O	1:I:205:THR:HG23	2.14	0.47
1:A:34:HIS:CD2	2:B:100(L):TYR:HB3	2.50	0.47
2:B:147:PRO:HD2	2:B:202:PRO:CB	2.44	0.47
2:B:68:THR:O	2:B:68:THR:HG22	2.13	0.47
1:C:135:LEU:HD13	2:D:181:VAL:HG22	1.95	0.47
1:E:140:TYR:CD2	1:E:141:PRO:HA	2.49	0.47
1:G:39:LYS:HG2	1:G:84:ALA:HB2	1.97	0.47
1:C:196:THR:HG23	1:C:201:THR:OG1	2.14	0.47
2:D:51:ILE:HD13	2:D:71:ARG:HD2	1.96	0.47
2:B:134:GLY:O	2:B:186:SER:HB2	2.15	0.47
2:D:100(A):TYS:C	2:D:100(A):TYS:CD1	2.86	0.47
2:D:68:THR:O	2:D:68:THR:HG22	2.15	0.47
1:C:140:TYR:CD2	1:C:141:PRO:HA	2.50	0.47
2:H:43:LYS:N	2:H:43:LYS:HD2	2.30	0.47
1:K:47:VAL:HA	1:K:58:ILE:CD1	2.44	0.47
2:D:100(L):TYR:C	2:D:100(L):TYR:CD1	2.89	0.47
1:E:191:TYR:O	1:E:205:THR:HG23	2.15	0.47
1:I:163:LYS:N	1:I:163:LYS:HD2	2.30	0.47
2:J:36:TRP:NE1	2:J:80:LEU:HB2	2.30	0.47
1:C:47:VAL:O	1:C:55:PRO:HD2	2.15	0.46
2:B:166:PHE:HE2	2:B:181:VAL:CG2	2.28	0.46
2:F:50:LEU:HD11	2:F:100(K):TYR:CE1	2.50	0.46
1:G:47:VAL:HA	1:G:58:ILE:CD1	2.46	0.46
2:L:201:LYS:N	2:L:202:PRO:CD	2.78	0.46
2:F:63:VAL:HG11	2:F:67:PHE:CD2	2.51	0.46
2:F:27:PHE:CD1	2:F:94:LYS:HD2	2.50	0.46
1:E:49:TYR:HD2	1:E:49:TYR:H	1.62	0.46
1:G:20:ARG:CG	1:G:74:THR:HG23	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:HG23	2:H:110:THR:HA	1.98	0.46
2:J:138:LEU:HD12	2:J:138:LEU:C	2.36	0.46
1:C:85:ASP:OD1	3:C:212:PEG:H11	2.16	0.46
1:A:120:PRO:HD3	1:A:132:LEU:HD23	1.98	0.46
2:B:30:ASP:HA	2:B:73:ASN:ND2	2.31	0.46
2:D:214:LYS:CG	2:D:215:SER:HA	2.45	0.46
2:D:147:PRO:HD2	2:D:202:PRO:CB	2.46	0.46
1:I:150:ALA:O	1:I:151:ASP:HB2	2.15	0.46
1:E:194:GLN:CG	1:E:203:GLU:HG3	2.46	0.46
1:C:150:ALA:HB3	1:I:94:ASN:HD21	1.80	0.46
1:K:91:TRP:CZ2	2:L:100(K):TYR:HE2	2.33	0.46
2:B:100(E):LEU:N	2:B:100(E):LEU:HD23	2.31	0.46
1:E:202:VAL:HG12	1:E:203:GLU:N	2.31	0.46
1:E:210:GLU:CB	1:E:211:CYS:HA	2.41	0.46
1:I:20:ARG:CG	1:I:74:THR:HG23	2.43	0.46
2:F:50:LEU:HD12	2:F:100(K):TYR:CD1	2.50	0.46
2:D:147:PRO:HD2	2:D:202:PRO:HB2	1.98	0.45
1:I:201:THR:O	1:I:201:THR:HG22	2.14	0.45
1:K:2:TYR:CE2	1:K:31:LYS:HD2	2.50	0.45
1:A:167:GLN:HG2	1:A:171:LYS:O	2.16	0.45
1:A:47:VAL:HA	1:A:58:ILE:CD1	2.46	0.45
1:E:47:VAL:HA	1:E:58:ILE:CD1	2.46	0.45
1:G:2:TYR:CE1	1:G:31:LYS:HE3	2.51	0.45
2:F:61:ASP:HA	2:F:64:LYS:HD2	1.99	0.45
2:J:5:VAL:HG13	2:J:105:LYS:HE2	1.99	0.45
2:B:12:VAL:HG21	2:B:82(C):LEU:HD13	1.98	0.45
2:B:51:ILE:HD13	2:B:71:ARG:HD2	1.98	0.45
2:D:201:LYS:N	2:D:202:PRO:CD	2.80	0.45
2:L:1:GLU:CG	2:L:2:VAL:H	2.28	0.45
1:I:185:TRP:CZ2	1:I:208:PRO:HA	2.51	0.45
1:K:194:GLN:HG3	1:K:203:GLU:HG3	1.97	0.45
1:K:191:TYR:O	1:K:205:THR:HG23	2.15	0.45
2:D:50:LEU:CD2	2:D:58:TYR:HD2	2.28	0.45
1:G:113:PRO:HA	1:G:139:PHE:HB3	1.99	0.45
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.99	0.45
1:A:106:VAL:O	1:A:107:GLY:N	2.50	0.45
2:D:100(M):MET:N	2:D:100(M):MET:SD	2.89	0.45
2:D:178:LEU:HD12	2:D:179:SER:N	2.31	0.45
1:A:110:LYS:HD3	2:D:52(A):TRP:CE2	2.52	0.45
2:D:87:THR:HG23	2:D:110:THR:HA	1.99	0.45
2:F:166:PHE:HE2	2:F:181:VAL:CG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG12	1:A:203:GLU:N	2.32	0.45
1:C:210:GLU:HA	1:C:211:CYS:HA	1.70	0.45
1:E:185:TRP:CZ2	1:E:208:PRO:HA	2.52	0.45
2:F:36:TRP:NE1	2:F:80:LEU:HB2	2.32	0.45
1:K:194:GLN:CG	1:K:203:GLU:HG3	2.47	0.45
2:L:51:ILE:HD13	2:L:71:ARG:HD2	1.99	0.45
2:H:84:THR:HG22	2:H:111:VAL:O	2.16	0.44
2:L:145:TYR:CE1	2:L:150:VAL:HG23	2.51	0.44
2:L:43:LYS:N	2:L:43:LYS:HD2	2.31	0.44
1:C:20:ARG:CG	1:C:74:THR:HG23	2.46	0.44
2:D:100(K):TYR:O	2:D:100(L):TYR:HB3	2.18	0.44
1:E:194:GLN:HG3	1:E:203:GLU:HG3	1.99	0.44
2:F:147:PRO:HD2	2:F:202:PRO:HB2	1.99	0.44
2:F:27:PHE:CE1	2:F:94:LYS:HD2	2.52	0.44
2:F:43:LYS:N	2:F:43:LYS:HD2	2.32	0.44
1:G:50:TYR:OH	2:H:98:ASP:CB	2.65	0.44
1:I:49:TYR:CD1	2:J:100(L):TYR:OH	2.70	0.44
2:H:30:ASP:HA	2:H:73:ASN:ND2	2.33	0.44
2:H:63:VAL:HG11	2:H:67:PHE:CD2	2.52	0.44
2:J:85:GLU:CD	2:J:85:GLU:H	2.21	0.44
1:C:163:LYS:HD2	1:C:163:LYS:N	2.31	0.44
1:E:39:LYS:HG2	1:E:84:ALA:HB2	2.00	0.44
1:G:163:LYS:HD2	1:G:163:LYS:N	2.31	0.44
1:G:166:LYS:HG3	1:G:170:ASN:HA	1.98	0.44
2:H:68:THR:O	2:H:68:THR:HG22	2.17	0.44
1:C:39:LYS:HG2	1:C:84:ALA:HB2	2.00	0.44
1:E:135:LEU:HD13	2:F:166:PHE:CE2	2.53	0.44
2:J:12:VAL:HG21	2:J:82(C):LEU:HD13	1.99	0.44
1:E:168:SER:C	1:E:170:ASN:H	2.21	0.44
2:F:72:ASP:OD2	2:F:75:LYS:HD2	2.18	0.44
1:G:202:VAL:HG12	1:G:203:GLU:N	2.32	0.44
1:I:113:PRO:HA	1:I:139:PHE:HB3	1.99	0.44
2:J:51:ILE:HG23	2:J:51:ILE:O	2.16	0.44
2:L:30:ASP:HA	2:L:73:ASN:HD22	1.81	0.44
2:H:166:PHE:HE2	2:H:181:VAL:CG2	2.31	0.44
2:H:85:GLU:H	2:H:85:GLU:CD	2.21	0.44
1:E:167:GLN:HG3	1:E:171:LYS:O	2.18	0.44
1:E:166:LYS:HG3	1:E:172:TYR:CZ	2.52	0.44
2:F:12:VAL:HG21	2:F:82(C):LEU:CD1	2.48	0.44
1:K:201:THR:HG22	1:K:201:THR:O	2.18	0.44
2:B:43:LYS:N	2:B:43:LYS:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:TYR:CE1	2:F:150:VAL:HG23	2.53	0.44
2:F:85:GLU:H	2:F:85:GLU:CD	2.22	0.44
1:I:49:TYR:CE2	1:I:53:ASP:HB3	2.53	0.44
1:G:135:LEU:HD13	2:H:181:VAL:CG2	2.48	0.43
1:C:47:VAL:HA	1:C:58:ILE:CD1	2.48	0.43
2:D:117:LYS:HB2	1:K:126:GLN:HG2	2.00	0.43
1:I:194:GLN:CG	1:I:203:GLU:HG3	2.49	0.43
2:J:178:LEU:HD12	2:J:179:SER:N	2.33	0.43
1:K:39:LYS:HG2	1:K:84:ALA:HB2	2.00	0.43
1:G:140:TYR:CD2	1:G:141:PRO:HA	2.54	0.43
2:B:145:TYR:CE1	2:B:150:VAL:HG23	2.53	0.43
2:F:100(A):TYS:CD1	2:F:100(B):ASP:N	2.79	0.43
2:L:36:TRP:NE1	2:L:80:LEU:HB2	2.32	0.43
1:A:20:ARG:CG	1:A:74:THR:HG23	2.45	0.43
1:E:20:ARG:CG	1:E:74:THR:HG23	2.48	0.43
1:G:150:ALA:O	1:G:151:ASP:HB2	2.18	0.43
1:K:124:GLU:HA	2:L:122:PHE:CE1	2.53	0.43
2:B:201:LYS:N	2:B:202:PRO:CD	2.82	0.43
2:H:138:LEU:HD12	2:H:138:LEU:C	2.38	0.43
1:I:194:GLN:HG3	1:I:203:GLU:HG3	2.00	0.43
1:I:49:TYR:HD1	2:J:100(L):TYR:OH	2.01	0.43
1:A:210:GLU:HB3	1:A:211:CYS:H	1.45	0.43
2:J:175:LEU:HD23	2:J:175:LEU:HA	1.70	0.43
1:A:163:LYS:HD2	1:A:163:LYS:N	2.33	0.43
1:K:49:TYR:CE2	1:K:53:ASP:HB3	2.54	0.43
1:K:123:GLU:OE1	2:L:209:LYS:HE2	2.19	0.43
1:C:194:GLN:HG3	1:C:203:GLU:HG3	2.00	0.43
1:G:194:GLN:CG	1:G:203:GLU:HG3	2.49	0.43
1:G:9:SER:O	1:G:11:VAL:HG23	2.18	0.43
2:L:12:VAL:HG21	2:L:82(C):LEU:HD13	2.00	0.43
1:I:9:SER:O	1:I:11:VAL:HG23	2.19	0.42
2:J:100(J):PHE:N	2:J:100(J):PHE:CD1	2.85	0.42
1:E:181:THR:HG23	1:E:184:GLN:OE1	2.19	0.42
1:E:201:THR:HG22	1:E:201:THR:O	2.18	0.42
1:E:54:ARG:HG3	1:E:58:ILE:HD11	2.01	0.42
1:G:185:TRP:CZ2	1:G:208:PRO:HA	2.54	0.42
2:H:100(A):TYS:O1	2:H:100(A):TYS:HE2	2.19	0.42
2:H:100(B):ASP:HB3	2:H:100(E):LEU:HB2	2.00	0.42
2:H:146:PHE:CE2	2:H:147:PRO:HB3	2.55	0.42
2:L:166:PHE:HE2	2:L:181:VAL:CG2	2.32	0.42
1:A:2:TYR:CD2	1:A:3:VAL:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:TYR:CZ	2:B:69:ILE:HG22	2.55	0.42
1:E:177:TYR:CD2	1:E:177:TYR:N	2.87	0.42
2:H:100(K):TYR:O	2:H:100(L):TYR:HB3	2.19	0.42
1:A:39:LYS:HG2	1:A:84:ALA:HB2	2.02	0.42
1:A:49:TYR:CE2	1:A:53:ASP:HB3	2.54	0.42
1:A:54:ARG:HG3	1:A:58:ILE:HD11	2.02	0.42
2:D:72:ASP:OD2	2:D:75:LYS:HD2	2.20	0.42
2:D:85:GLU:H	2:D:85:GLU:CD	2.23	0.42
2:J:51:ILE:HD13	2:J:71:ARG:HD2	2.02	0.42
1:A:194:GLN:CG	1:A:203:GLU:HG3	2.49	0.42
1:C:49:TYR:CE2	1:C:53:ASP:HB3	2.54	0.42
2:F:100(D):ASN:HD22	2:F:100(E):LEU:CD2	2.32	0.42
1:K:150:ALA:O	1:K:151:ASP:HB2	2.20	0.42
2:B:147:PRO:HD2	2:B:202:PRO:HB2	2.02	0.42
1:I:135:LEU:HD13	2:J:181:VAL:CG2	2.49	0.42
2:L:87:THR:HG23	2:L:110:THR:HA	2.01	0.42
1:C:113:PRO:HA	1:C:139:PHE:HB3	2.02	0.41
1:I:140:TYR:CD2	1:I:141:PRO:HA	2.55	0.41
1:A:209:THR:O	1:A:210:GLU:CG	2.68	0.41
2:B:63:VAL:HG11	2:B:67:PHE:CD2	2.55	0.41
2:B:85:GLU:CD	2:B:85:GLU:H	2.22	0.41
2:D:214:LYS:CB	2:D:215:SER:CA	2.95	0.41
1:E:163:LYS:HD2	1:E:163:LYS:N	2.35	0.41
1:E:166:LYS:CG	1:E:172:TYR:CZ	3.03	0.41
1:G:49:TYR:CE2	1:G:53:ASP:HB3	2.54	0.41
1:I:137:SER:HB2	1:I:167:GLN:NE2	2.30	0.41
2:J:43:LYS:N	2:J:43:LYS:HD2	2.34	0.41
2:J:50:LEU:CD2	2:J:58:TYR:HD2	2.30	0.41
1:K:160:GLU:CB	2:L:169:VAL:HG21	2.49	0.41
1:A:7:PRO:HA	1:A:8:PRO:HD3	1.92	0.41
1:C:210:GLU:HB3	1:C:211:CYS:HB2	2.02	0.41
1:E:113:PRO:HA	1:E:139:PHE:HB3	2.02	0.41
1:E:95(B):HIS:NE2	2:F:60:ALA:HA	2.35	0.41
2:F:30:ASP:HA	2:F:73:ASN:ND2	2.35	0.41
1:E:163:LYS:HA	1:E:164:PRO:HD3	1.95	0.41
1:E:162:THR:CG2	2:F:169:VAL:HG12	2.50	0.41
2:F:201:LYS:N	2:F:202:PRO:CD	2.83	0.41
2:H:61:ASP:HA	2:H:64:LYS:HD2	2.02	0.41
2:F:100(A):TYS:HD1	2:F:100(B):ASP:H	1.85	0.41
2:J:100(B):ASP:OD1	2:J:100(E):LEU:HD12	2.21	0.41
1:K:54:ARG:HG3	1:K:58:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:112:SER:HB3	2:L:146:PHE:CZ	2.56	0.41
1:C:202:VAL:HG12	1:C:203:GLU:N	2.34	0.41
1:K:163:LYS:N	1:K:163:LYS:HD2	2.36	0.41
1:A:163:LYS:HE3	1:A:164:PRO:CD	2.51	0.41
1:E:34:HIS:CD2	2:F:100(L):TYR:HB3	2.56	0.41
2:H:175:LEU:HD23	2:H:175:LEU:HA	1.79	0.41
1:K:7:PRO:HA	1:K:8:PRO:HD3	1.96	0.41
2:H:100(B):ASP:CG	2:H:100(E):LEU:HD12	2.41	0.41
2:L:100(K):TYR:O	2:L:100(L):TYR:HB3	2.21	0.41
2:L:30:ASP:O	2:L:52(A):TRP:HB2	2.20	0.41
1:A:177:TYR:CE2	2:B:169:VAL:HG11	2.55	0.41
2:B:100(B):ASP:CG	2:B:100(E):LEU:HG	2.41	0.41
2:D:145:TYR:CE1	2:D:150:VAL:HG23	2.55	0.41
1:K:91:TRP:CD2	2:L:100(K):TYR:HD2	2.39	0.41
1:E:49:TYR:CE2	1:E:53:ASP:HB3	2.56	0.41
2:F:166:PHE:HB3	2:F:167:PRO:CD	2.51	0.41
1:K:113:PRO:HA	1:K:139:PHE:HB3	2.02	0.41
1:K:34:HIS:CD2	2:L:100(L):TYR:CB	3.04	0.41
1:G:54:ARG:HG3	1:G:58:ILE:HD11	2.03	0.41
2:F:26:GLY:CA	2:L:193:THR:HG21	2.51	0.41
1:C:194:GLN:HG2	1:C:203:GLU:HG3	2.04	0.40
1:E:13:VAL:HG21	1:E:19:ALA:HB2	2.04	0.40
1:K:185:TRP:CZ2	1:K:208:PRO:HA	2.56	0.40
2:D:35:HIS:CG	2:D:100(M):MET:HE2	2.57	0.40
1:I:46:LEU:HD12	1:I:46:LEU:HA	1.89	0.40
2:F:50:LEU:CD1	2:F:100(K):TYR:CE1	3.03	0.40
2:F:39:GLN:HG3	2:F:44:GLY:O	2.22	0.40
2:F:63:VAL:HG11	2:F:67:PHE:CE2	2.56	0.40
1:G:163:LYS:HA	1:G:164:PRO:HD3	1.95	0.40
1:G:166:LYS:HD2	1:G:172:TYR:CE2	2.56	0.40
2:H:178:LEU:HD12	2:H:179:SER:N	2.37	0.40
2:B:61:ASP:HA	2:B:64:LYS:HD2	2.04	0.40
2:D:38:ARG:HA	2:D:89:PHE:O	2.21	0.40
1:G:7:PRO:HA	1:G:8:PRO:HD3	1.94	0.40
2:H:146:PHE:CD2	2:H:147:PRO:N	2.89	0.40
2:H:147:PRO:HD2	2:H:202:PRO:HB2	2.02	0.40
1:A:177:TYR:CD2	1:A:177:TYR:N	2.89	0.40
2:D:100(C):TYS:O3	2:D:100(C):TYS:HE1	2.22	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	210/213 (99%)	192 (91%)	13 (6%)	5 (2%)	6	34
1	C	210/213 (99%)	194 (92%)	12 (6%)	4 (2%)	8	39
1	E	210/213 (99%)	192 (91%)	13 (6%)	5 (2%)	6	34
1	G	210/213 (99%)	194 (92%)	14 (7%)	2 (1%)	15	54
1	I	210/213 (99%)	198 (94%)	10 (5%)	2 (1%)	15	54
1	K	210/213 (99%)	194 (92%)	14 (7%)	2 (1%)	15	54
2	B	222/233 (95%)	205 (92%)	13 (6%)	4 (2%)	8	41
2	D	222/233 (95%)	204 (92%)	15 (7%)	3 (1%)	11	46
2	F	222/233 (95%)	206 (93%)	13 (6%)	3 (1%)	11	46
2	H	222/233 (95%)	206 (93%)	12 (5%)	4 (2%)	8	41
2	J	224/233 (96%)	206 (92%)	15 (7%)	3 (1%)	12	47
2	L	223/233 (96%)	203 (91%)	17 (8%)	3 (1%)	12	47
All	All	2595/2676 (97%)	2394 (92%)	161 (6%)	40 (2%)	10	44

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLU
1	C	209	THR
2	D	214	LYS
1	E	208	PRO
1	A	68	GLY
1	A	170	ASN
1	C	68	GLY
1	E	68	GLY
1	E	169	ASN
1	E	209	THR
1	I	68	GLY
1	K	68	GLY

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Mol	Chain	Res	Type
1	A	152	GLY
1	A	169	ASN
2	B	214	LYS
1	C	152	GLY
1	E	152	GLY
2	F	127	SER
1	G	68	GLY
1	G	152	GLY
1	I	152	GLY
1	K	152	GLY
2	B	100	ASP
1	C	210	GLU
2	D	185	PRO
2	H	55	GLY
2	H	100	ASP
2	H	214	LYS
2	J	55	GLY
2	J	100	ASP
2	L	100	ASP
2	F	100	ASP
2	F	185	PRO
2	L	55	GLY
2	L	185	PRO
2	B	185	PRO
2	H	185	PRO
2	J	185	PRO
2	B	55	GLY
2	D	55	GLY

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	178/179 (99%)	161 (90%)	17 (10%)	8 32
1	C	178/179 (99%)	163 (92%)	15 (8%)	11 39
1	E	178/179 (99%)	161 (90%)	17 (10%)	8 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	178/179 (99%)	162 (91%)	16 (9%)	9	34
1	I	178/179 (99%)	164 (92%)	14 (8%)	12	43
1	K	178/179 (99%)	162 (91%)	16 (9%)	9	34
2	B	193/197 (98%)	172 (89%)	21 (11%)	6	26
2	D	193/197 (98%)	172 (89%)	21 (11%)	6	26
2	F	193/197 (98%)	171 (89%)	22 (11%)	5	24
2	H	193/197 (98%)	173 (90%)	20 (10%)	7	28
2	J	194/197 (98%)	173 (89%)	21 (11%)	6	27
2	L	193/197 (98%)	175 (91%)	18 (9%)	9	33
All	All	2227/2256 (99%)	2009 (90%)	218 (10%)	8	31

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	11	VAL
1	A	13	VAL
1	A	20	ARG
1	A	27	ASN
1	A	49	TYR
1	A	53	ASP
1	A	60	ASP
1	A	65	SER
1	A	74	THR
1	A	145	THR
1	A	153	SER
1	A	163	LYS
1	A	170	ASN
1	A	196	THR
1	A	201	THR
1	A	211	CYS
2	B	13	GLN
2	B	21	SER
2	B	50	LEU
2	B	57	THR
2	B	62	SER
2	B	68	THR
2	B	70	SER
2	B	89	PHE

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Mol	Chain	Res	Type
2	B	92	CYS
2	B	100(D)	ASN
2	B	100(E)	LEU
2	B	110	THR
2	B	113	SER
2	B	127	SER
2	B	143	LYS
2	B	151	THR
2	B	170	LEU
2	B	181	VAL
2	B	183	THR
2	B	193	THR
2	B	197	ASN
1	C	5	THR
1	C	11	VAL
1	C	13	VAL
1	C	27	ASN
1	C	49	TYR
1	C	53	ASP
1	C	60	ASP
1	C	65	SER
1	C	74	THR
1	C	145	THR
1	C	153	SER
1	C	155	VAL
1	C	163	LYS
1	C	201	THR
1	C	210	GLU
2	D	13	GLN
2	D	50	LEU
2	D	57	THR
2	D	62	SER
2	D	68	THR
2	D	70	SER
2	D	89	PHE
2	D	92	CYS
2	D	100(E)	LEU
2	D	100(L)	TYR
2	D	100(M)	MET
2	D	110	THR
2	D	113	SER
2	D	128	SER

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Mol	Chain	Res	Type
2	D	143	LYS
2	D	151	THR
2	D	170	LEU
2	D	181	VAL
2	D	183	THR
2	D	193	THR
2	D	197	ASN
1	E	2	TYR
1	E	5	THR
1	E	11	VAL
1	E	13	VAL
1	E	27	ASN
1	E	49	TYR
1	E	53	ASP
1	E	60	ASP
1	E	65	SER
1	E	74	THR
1	E	145	THR
1	E	153	SER
1	E	163	LYS
1	E	169	ASN
1	E	170	ASN
1	E	201	THR
1	E	209	THR
2	F	1	GLU
2	F	13	GLN
2	F	50	LEU
2	F	57	THR
2	F	62	SER
2	F	68	THR
2	F	70	SER
2	F	89	PHE
2	F	92	CYS
2	F	99	SER
2	F	100(D)	ASN
2	F	100(H)	SER
2	F	110	THR
2	F	113	SER
2	F	143	LYS
2	F	151	THR
2	F	170	LEU
2	F	181	VAL

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Mol	Chain	Res	Type
2	F	183	THR
2	F	193	THR
2	F	197	ASN
2	F	216	CYS
1	G	5	THR
1	G	11	VAL
1	G	13	VAL
1	G	27	ASN
1	G	49	TYR
1	G	53	ASP
1	G	60	ASP
1	G	65	SER
1	G	74	THR
1	G	145	THR
1	G	153	SER
1	G	163	LYS
1	G	196	THR
1	G	201	THR
1	G	209	THR
1	G	211	CYS
2	H	13	GLN
2	H	21	SER
2	H	50	LEU
2	H	57	THR
2	H	62	SER
2	H	68	THR
2	H	70	SER
2	H	89	PHE
2	H	92	CYS
2	H	100(D)	ASN
2	H	113	SER
2	H	128	SER
2	H	143	LYS
2	H	151	THR
2	H	170	LEU
2	H	181	VAL
2	H	183	THR
2	H	193	THR
2	H	197	ASN
2	H	214	LYS
1	I	5	THR
1	I	11	VAL

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Mol	Chain	Res	Type
1	I	13	VAL
1	I	27	ASN
1	I	49	TYR
1	I	53	ASP
1	I	65	SER
1	I	74	THR
1	I	145	THR
1	I	153	SER
1	I	163	LYS
1	I	168	SER
1	I	201	THR
1	I	209	THR
2	J	13	GLN
2	J	21	SER
2	J	50	LEU
2	J	57	THR
2	J	62	SER
2	J	70	SER
2	J	89	PHE
2	J	92	CYS
2	J	99	SER
2	J	100(D)	ASN
2	J	100(M)	MET
2	J	110	THR
2	J	113	SER
2	J	143	LYS
2	J	151	THR
2	J	181	VAL
2	J	183	THR
2	J	193	THR
2	J	197	ASN
2	J	214	LYS
2	J	215	SER
1	K	5	THR
1	K	11	VAL
1	K	13	VAL
1	K	27	ASN
1	K	49	TYR
1	K	53	ASP
1	K	60	ASP
1	K	65	SER
1	K	74	THR

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Mol	Chain	Res	Type
1	K	145	THR
1	K	153	SER
1	K	163	LYS
1	K	168	SER
1	K	201	THR
1	K	209	THR
1	K	211	CYS
2	L	13	GLN
2	L	21	SER
2	L	50	LEU
2	L	57	THR
2	L	62	SER
2	L	68	THR
2	L	70	SER
2	L	89	PHE
2	L	92	CYS
2	L	110	THR
2	L	113	SER
2	L	143	LYS
2	L	151	THR
2	L	170	LEU
2	L	181	VAL
2	L	183	THR
2	L	193	THR
2	L	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	32	ASN
1	A	170	ASN
2	B	100(D)	ASN
1	C	30	ASN
2	D	171	GLN
1	E	30	ASN
1	E	32	ASN
1	E	169	ASN
2	F	76	ASN
2	F	100(D)	ASN
2	F	171	GLN
1	G	30	ASN

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Mol	Chain	Res	Type
2	H	171	GLN
1	I	30	ASN
1	I	32	ASN
1	I	94	ASN
1	I	167	GLN
2	J	100(D)	ASN
1	K	30	ASN
1	K	32	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TYS	J	100(A)	2	15,16,17	1.28	1 (6%)	18,22,24	0.69	0
2	TYS	H	100(C)	2	15,16,17	1.43	2 (13%)	18,22,24	0.74	0
2	TYS	H	100(A)	2	15,16,17	1.22	2 (13%)	18,22,24	0.70	0
2	TYS	L	100(C)	2	15,16,17	1.20	1 (6%)	18,22,24	0.89	1 (5%)
2	TYS	L	100(A)	2	15,16,17	1.12	2 (13%)	18,22,24	0.56	0
2	TYS	D	100(C)	2	15,16,17	1.33	2 (13%)	18,22,24	1.21	3 (16%)
2	TYS	B	100(A)	2	15,16,17	1.20	2 (13%)	18,22,24	1.04	2 (11%)
2	TYS	B	100(C)	2	15,16,17	1.36	3 (20%)	18,22,24	0.87	1 (5%)
2	TYS	J	100(C)	2	15,16,17	1.27	1 (6%)	18,22,24	0.76	1 (5%)
2	TYS	F	100(A)	2	15,16,17	1.23	1 (6%)	18,22,24	0.81	0
2	TYS	F	100(C)	2	15,16,17	1.36	1 (6%)	18,22,24	1.04	2 (11%)
2	TYS	D	100(A)	2	15,16,17	1.17	1 (6%)	18,22,24	1.26	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	J	100(A)	2	-	7/10/11/13	0/1/1/1
2	TYS	H	100(C)	2	-	2/10/11/13	0/1/1/1
2	TYS	H	100(A)	2	-	7/10/11/13	0/1/1/1
2	TYS	L	100(C)	2	-	4/10/11/13	0/1/1/1
2	TYS	L	100(A)	2	-	0/10/11/13	0/1/1/1
2	TYS	D	100(C)	2	-	4/10/11/13	0/1/1/1
2	TYS	B	100(A)	2	-	4/10/11/13	0/1/1/1
2	TYS	B	100(C)	2	-	3/10/11/13	0/1/1/1
2	TYS	J	100(C)	2	-	1/10/11/13	0/1/1/1
2	TYS	F	100(A)	2	-	7/10/11/13	0/1/1/1
2	TYS	F	100(C)	2	-	3/10/11/13	0/1/1/1
2	TYS	D	100(A)	2	-	3/10/11/13	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	100(C)	TYS	OH-S	3.87	1.64	1.58
2	B	100(C)	TYS	OH-S	3.86	1.64	1.58
2	H	100(C)	TYS	OH-CZ	-3.82	1.36	1.42
2	J	100(A)	TYS	OH-S	3.67	1.63	1.58
2	J	100(C)	TYS	OH-S	3.60	1.63	1.58
2	F	100(A)	TYS	OH-S	3.50	1.63	1.58
2	H	100(A)	TYS	OH-S	2.99	1.62	1.58
2	B	100(A)	TYS	OH-S	2.97	1.62	1.58
2	L	100(C)	TYS	OH-S	2.93	1.62	1.58
2	D	100(C)	TYS	OH-CZ	-2.68	1.38	1.42
2	L	100(A)	TYS	OH-S	2.58	1.62	1.58
2	H	100(A)	TYS	OH-CZ	-2.29	1.38	1.42
2	D	100(A)	TYS	OH-S	2.18	1.61	1.58
2	D	100(C)	TYS	OH-S	2.18	1.61	1.58
2	H	100(C)	TYS	OH-S	2.14	1.61	1.58
2	L	100(A)	TYS	OH-CZ	-2.12	1.39	1.42
2	B	100(C)	TYS	O1-S	2.06	1.54	1.45
2	B	100(A)	TYS	OH-CZ	-2.02	1.39	1.42
2	B	100(C)	TYS	O2-S	2.01	1.53	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100(A)	TYS	OH-CZ-CE2	3.36	125.24	118.64
2	D	100(C)	TYS	CB-CA-C	-3.09	105.68	111.47
2	B	100(C)	TYS	O3-S-OH	2.60	112.08	105.83
2	B	100(A)	TYS	OH-CZ-CE2	2.46	123.47	118.64
2	D	100(A)	TYS	CB-CA-C	2.45	116.06	111.47
2	F	100(C)	TYS	CB-CA-C	2.31	115.80	111.47
2	D	100(C)	TYS	CG-CB-CA	-2.23	109.58	114.10
2	B	100(A)	TYS	O2-S-O1	-2.14	103.62	112.22
2	F	100(C)	TYS	O3-S-OH	2.13	110.96	105.83
2	L	100(C)	TYS	O3-S-OH	2.13	110.95	105.83
2	D	100(C)	TYS	OH-CZ-CE1	2.03	122.64	118.64
2	J	100(C)	TYS	O3-S-OH	2.00	110.66	105.83

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	100(A)	TYS	CZ-OH-S-O3
2	H	100(A)	TYS	CE1-CZ-OH-S
2	H	100(A)	TYS	CE2-CZ-OH-S
2	H	100(A)	TYS	CZ-OH-S-O2
2	H	100(A)	TYS	CZ-OH-S-O3
2	D	100(C)	TYS	CE1-CZ-OH-S
2	B	100(A)	TYS	CE1-CZ-OH-S
2	B	100(A)	TYS	CE2-CZ-OH-S
2	F	100(A)	TYS	CE2-CZ-OH-S
2	F	100(A)	TYS	CZ-OH-S-O3
2	H	100(C)	TYS	CA-CB-CG-CD2
2	D	100(A)	TYS	CA-CB-CG-CD1
2	H	100(C)	TYS	CA-CB-CG-CD1
2	D	100(A)	TYS	CA-CB-CG-CD2
2	B	100(C)	TYS	N-CA-CB-CG
2	L	100(C)	TYS	CA-CB-CG-CD1
2	L	100(C)	TYS	CA-CB-CG-CD2
2	B	100(A)	TYS	CA-CB-CG-CD2
2	B	100(A)	TYS	CA-CB-CG-CD1
2	J	100(A)	TYS	CA-CB-CG-CD2
2	J	100(A)	TYS	CA-CB-CG-CD1
2	F	100(A)	TYS	CA-CB-CG-CD1
2	F	100(A)	TYS	CA-CB-CG-CD2
2	L	100(C)	TYS	CE1-CZ-OH-S

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Mol	Chain	Res	Type	Atoms
2	L	100(C)	TYS	CE2-CZ-OH-S
2	B	100(C)	TYS	CE1-CZ-OH-S
2	B	100(C)	TYS	CE2-CZ-OH-S
2	F	100(A)	TYS	CE1-CZ-OH-S
2	F	100(C)	TYS	CE1-CZ-OH-S
2	F	100(C)	TYS	CE2-CZ-OH-S
2	D	100(A)	TYS	CZ-OH-S-O3
2	H	100(A)	TYS	CA-CB-CG-CD1
2	J	100(A)	TYS	CZ-OH-S-O1
2	J	100(A)	TYS	CZ-OH-S-O2
2	H	100(A)	TYS	CZ-OH-S-O1
2	F	100(A)	TYS	CZ-OH-S-O1
2	F	100(A)	TYS	CZ-OH-S-O2
2	H	100(A)	TYS	CA-CB-CG-CD2
2	D	100(C)	TYS	CA-CB-CG-CD2
2	J	100(C)	TYS	N-CA-CB-CG
2	F	100(C)	TYS	N-CA-CB-CG
2	D	100(C)	TYS	CA-CB-CG-CD1
2	J	100(A)	TYS	CE1-CZ-OH-S
2	J	100(A)	TYS	CE2-CZ-OH-S
2	D	100(C)	TYS	CE2-CZ-OH-S

There are no ring outliers.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	100(A)	TYS	4	0
2	H	100(C)	TYS	3	0
2	H	100(A)	TYS	3	0
2	D	100(C)	TYS	6	0
2	B	100(A)	TYS	3	0
2	B	100(C)	TYS	1	0
2	J	100(C)	TYS	1	0
2	F	100(A)	TYS	3	0
2	F	100(C)	TYS	1	0
2	D	100(A)	TYS	9	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	PEG	A	212	-	6,6,6	0.70	0	5,5,5	0.29	0
3	PEG	G	212	-	6,6,6	0.77	0	5,5,5	0.40	0
3	PEG	K	212	-	6,6,6	0.64	0	5,5,5	0.42	0
3	PEG	C	212	-	6,6,6	0.87	0	5,5,5	0.63	0
3	PEG	I	212	-	6,6,6	0.81	0	5,5,5	0.65	0
3	PEG	E	212	-	6,6,6	0.57	0	5,5,5	0.50	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	PEG	A	212	-	-	1/4/4/4	-
3	PEG	G	212	-	-	0/4/4/4	-
3	PEG	K	212	-	-	2/4/4/4	-
3	PEG	C	212	-	-	1/4/4/4	-
3	PEG	I	212	-	-	2/4/4/4	-
3	PEG	E	212	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	212	PEG	O1-C1-C2-O2
3	K	212	PEG	O2-C3-C4-O4
3	I	212	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	K	212	PEG	O1-C1-C2-O2
3	E	212	PEG	O1-C1-C2-O2
3	I	212	PEG	C1-C2-O2-C3
3	C	212	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	212	PEG	1	0
3	E	212	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	212/213 (99%)	-0.14	2 (0%) 84 75	66, 112, 153, 189	0
1	C	212/213 (99%)	-0.38	0 100 100	43, 83, 141, 172	0
1	E	212/213 (99%)	-0.03	5 (2%) 59 44	69, 122, 166, 193	0
1	G	212/213 (99%)	-0.34	2 (0%) 84 75	42, 72, 128, 163	0
1	I	212/213 (99%)	-0.40	1 (0%) 91 86	46, 69, 100, 174	0
1	K	212/213 (99%)	-0.14	3 (1%) 75 63	64, 106, 160, 200	0
2	B	226/233 (96%)	-0.27	2 (0%) 84 75	55, 103, 162, 211	0
2	D	226/233 (96%)	-0.25	0 100 100	52, 92, 133, 180	0
2	F	226/233 (96%)	-0.09	2 (0%) 84 75	58, 108, 160, 202	0
2	H	226/233 (96%)	-0.38	0 100 100	37, 67, 116, 181	0
2	J	228/233 (97%)	-0.38	0 100 100	35, 63, 118, 192	0
2	L	227/233 (97%)	-0.30	0 100 100	55, 98, 150, 201	0
All	All	2631/2676 (98%)	-0.26	17 (0%) 89 83	35, 91, 151, 211	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	194	TYR	2.8
1	A	211	CYS	2.8
1	E	211	CYS	2.6
1	E	19	ALA	2.6
2	F	137	ALA	2.6
1	G	51	ASP	2.5
1	K	51	ASP	2.5
2	B	128	SER	2.4
2	F	189	LEU	2.4
1	E	75	ILE	2.2
1	E	21	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	73	LEU	2.2
1	K	2	TYR	2.1
1	A	19	ALA	2.1
1	G	50	TYR	2.1
1	I	211	CYS	2.0
1	K	50	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TYS	L	100(C)	16/17	0.62	0.55	224,229,248,251	0
2	TYS	J	100(C)	16/17	0.66	0.50	164,175,193,197	0
2	TYS	F	100(C)	16/17	0.71	0.29	153,172,197,204	0
2	TYS	H	100(C)	16/17	0.74	0.34	180,223,231,232	0
2	TYS	D	100(C)	16/17	0.79	0.26	126,137,156,171	0
2	TYS	H	100(A)	16/17	0.80	0.22	157,169,186,190	0
2	TYS	L	100(A)	16/17	0.83	0.24	186,196,201,202	0
2	TYS	B	100(C)	16/17	0.83	0.25	128,134,156,170	0
2	TYS	F	100(A)	16/17	0.87	0.19	138,162,171,176	0
2	TYS	J	100(A)	16/17	0.90	0.23	125,151,182,192	0
2	TYS	D	100(A)	16/17	0.91	0.14	119,130,154,155	0
2	TYS	B	100(A)	16/17	0.95	0.16	103,115,130,137	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	K	212	7/7	0.76	0.21	84,91,102,107	0
3	PEG	C	212	7/7	0.76	0.23	67,87,98,102	0
3	PEG	I	212	7/7	0.80	0.25	73,79,95,97	0
3	PEG	G	212	7/7	0.90	0.28	76,85,93,96	0
3	PEG	E	212	7/7	0.90	0.13	84,91,95,96	0
3	PEG	A	212	7/7	0.91	0.12	67,84,95,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.