Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:20 AM GMT

PDB ID	:	3LQA
Title	:	Crystal structure of clade C gp120 in complex with sCD4 and 21c Fab
Authors	:	Diskin, R.; Marcovecchio, P.M.; Bjorkman, P.J.
Deposited on	:	2010-02-08
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

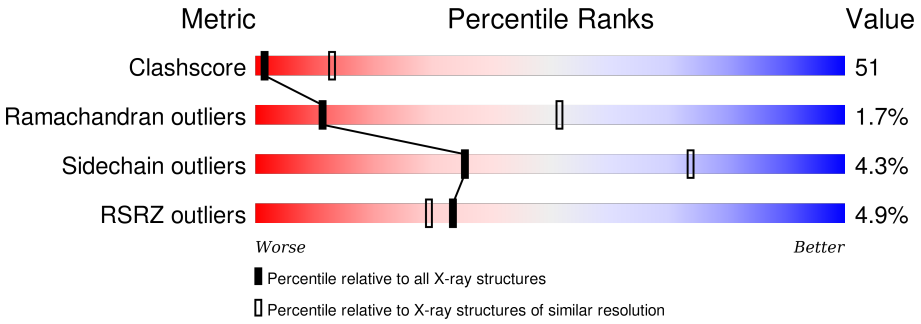
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	C	192	3% 30% 55% 6% • 9%
2	G	332	10% 28% 48% 10% 13%
3	H	231	2% 35% 51% 10% • •
4	L	217	% 47% 42% 7% • •

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
5	NAG	G	2500	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6945 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 T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	175	Total	C	N	O	S	0	0	0
			1361	850	238	269	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	183	ILE	-	EXPRESSION TAG	UNP P01730
C	184	ASP	-	EXPRESSION TAG	UNP P01730
C	185	GLY	-	EXPRESSION TAG	UNP P01730
C	186	ARG	-	EXPRESSION TAG	UNP P01730
C	187	HIS	-	EXPRESSION TAG	UNP P01730
C	188	HIS	-	EXPRESSION TAG	UNP P01730
C	189	HIS	-	EXPRESSION TAG	UNP P01730
C	190	HIS	-	EXPRESSION TAG	UNP P01730
C	191	HIS	-	EXPRESSION TAG	UNP P01730
C	192	HIS	-	EXPRESSION TAG	UNP P01730

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	290	Total	C	N	O	S	0	0	0
			2271	1434	386	433	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	294	GLY	-	LINKER	UNP Q1PHM6
G	323	ALA	-	LINKER	UNP Q1PHM6
G	324	GLY	-	LINKER	UNP Q1PHM6
G	89	ILE	THR	ENGINEERED	UNP Q1PHM6
G	226	ASP	ASN	ENGINEERED	UNP Q1PHM6
G	232	ILE	THR	ENGINEERED	UNP Q1PHM6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	285	THR	ASN	ENGINEERED	UNP Q1PHM6
G	329	ASN	SER	ENGINEERED	UNP Q1PHM6
G	388	ILE	THR	ENGINEERED	UNP Q1PHM6
G	447	ASP	ASN	ENGINEERED	UNP Q1PHM6
G	495	SER	-	EXPRESSION TAG	UNP Q1PHM6
G	496	GLY	-	EXPRESSION TAG	UNP Q1PHM6
G	497	HIS	-	EXPRESSION TAG	UNP Q1PHM6
G	498	HIS	-	EXPRESSION TAG	UNP Q1PHM6
G	499	HIS	-	EXPRESSION TAG	UNP Q1PHM6
G	500	HIS	-	EXPRESSION TAG	UNP Q1PHM6
G	501	HIS	-	EXPRESSION TAG	UNP Q1PHM6
G	502	HIS	-	EXPRESSION TAG	UNP Q1PHM6

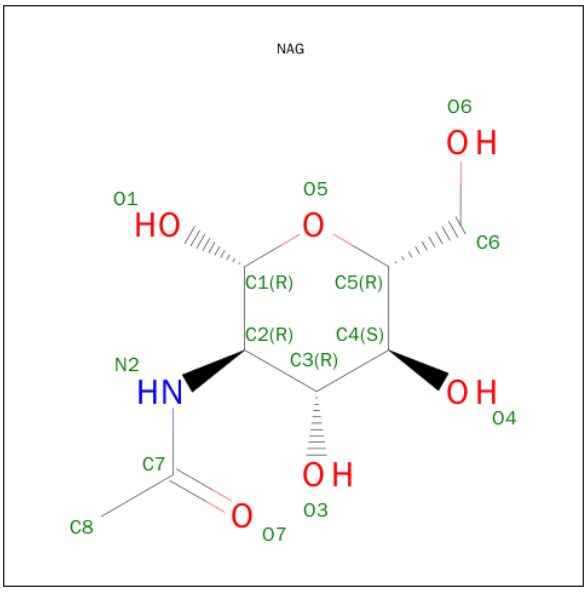
- Molecule 3 is a protein called Heavy chain of anti HIV Fab from human 21c antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	225	Total	C	N	O	S	0	0	0
			1685	1068	277	333	7			

- Molecule 4 is a protein called Light chain of anti HIV Fab from human 21c antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1572	984	262	321	5			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



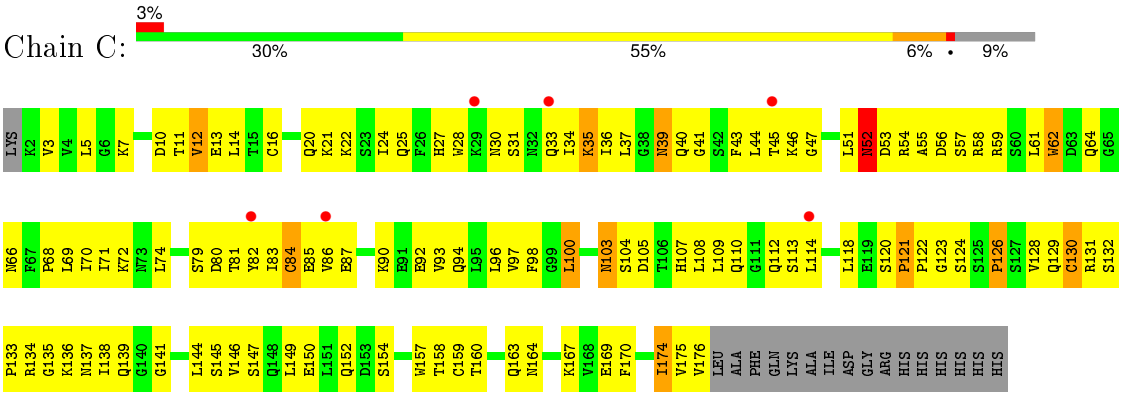
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0

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

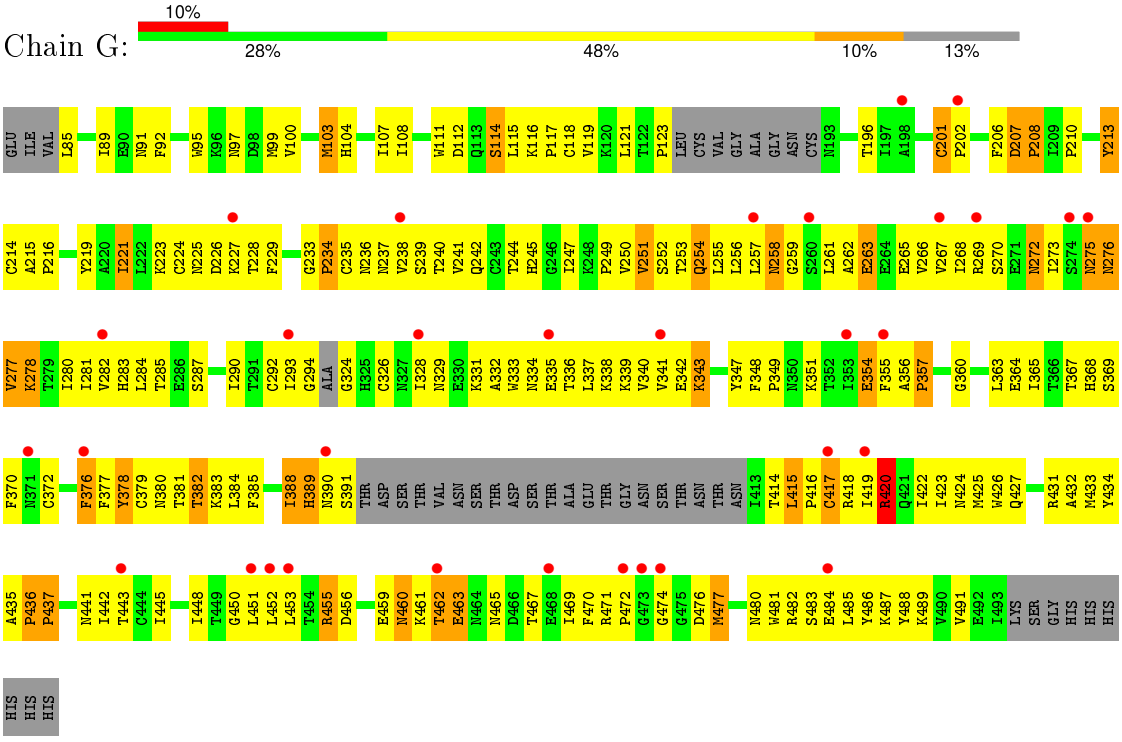
- Molecule 1: T-cell surface glycoprotein CD4

Chain C:



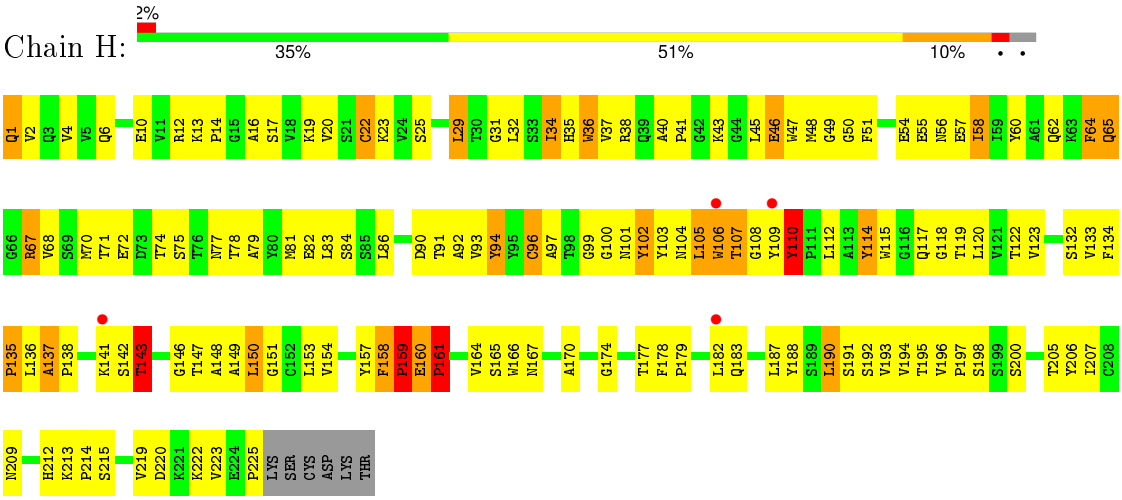
- Molecule 2: Envelope glycoprotein gp160

Chain G:



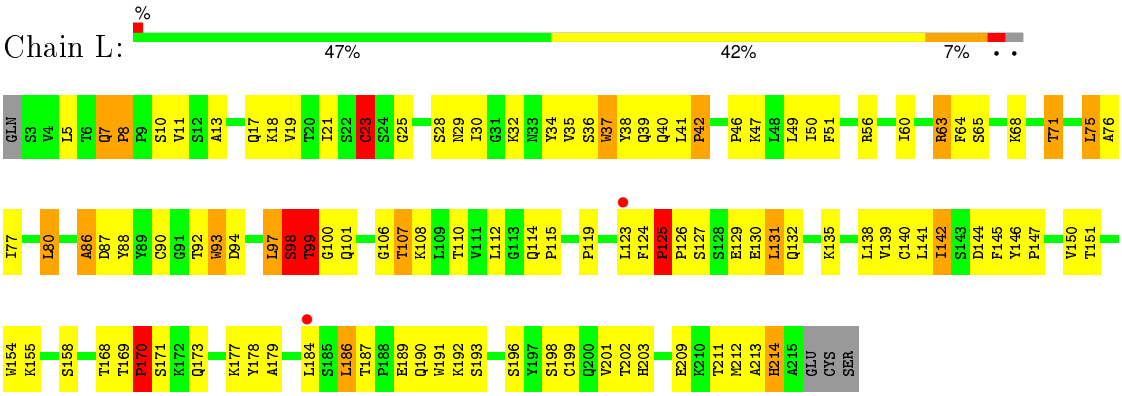
- Molecule 3: Heavy chain of anti HIV Fab from human 21c antibody

Chain H:



• Molecule 4: Light chain of anti HIV Fab from human 21c antibody

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.73Å 187.93Å 151.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.00 – 3.40 83.88 – 3.39	Depositor EDS
% Data completeness (in resolution range)	79.6 (84.00-3.40) 78.9 (83.88-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.322 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	90.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 83.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	1 of 14987 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6945	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.89	1/1380 (0.1%)	1.48	15/1862 (0.8%)
2	G	1.04	7/2316 (0.3%)	1.57	41/3142 (1.3%)
3	H	1.18	4/1728 (0.2%)	1.66	33/2358 (1.4%)
4	L	1.08	2/1610 (0.1%)	1.46	16/2197 (0.7%)
All	All	1.06	14/7034 (0.2%)	1.55	105/9559 (1.1%)

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
3	H	0	4
4	L	0	3
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	258	ASN	CB-CG	12.20	1.79	1.51
2	G	272	ASN	CB-CG	7.98	1.69	1.51
4	L	37	TRP	CB-CG	-7.20	1.37	1.50
2	G	441	ASN	CB-CG	6.95	1.67	1.51
2	G	258	ASN	CA-CB	6.68	1.70	1.53
3	H	115	TRP	CB-CG	-6.32	1.38	1.50
3	H	4	VAL	CB-CG2	-6.10	1.40	1.52
1	C	62	TRP	CB-CG	5.94	1.60	1.50
2	G	380	ASN	CB-CG	5.82	1.64	1.51
3	H	64	PHE	CB-CG	-5.64	1.41	1.51
3	H	46	GLU	CG-CD	5.55	1.60	1.51
4	L	110	THR	CA-CB	5.19	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	272	ASN	CA-CB	5.14	1.66	1.53
2	G	103	MET	CG-SD	5.02	1.94	1.81

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	160	GLU	C-N-CD	-19.55	77.58	120.60
3	H	58	ILE	N-CA-C	-14.99	70.53	111.00
3	H	158	PHE	C-N-CD	-14.53	88.63	120.60
2	G	276	ASN	N-CA-CB	-10.18	92.27	110.60
3	H	105	LEU	CA-CB-CG	9.28	136.64	115.30
4	L	63	ARG	NE-CZ-NH1	-9.04	115.78	120.30
3	H	105	LEU	CB-CA-C	-8.96	93.17	110.20
4	L	97	LEU	CA-CB-CG	8.82	135.59	115.30
2	G	389	HIS	N-CA-C	8.66	134.38	111.00
2	G	467	THR	N-CA-C	8.49	133.92	111.00
3	H	29	LEU	CA-CB-CG	8.19	134.14	115.30
3	H	160	GLU	C-N-CA	8.05	155.79	122.00
2	G	251	VAL	N-CA-C	-8.03	89.31	111.00
2	G	380	ASN	N-CA-C	-7.99	89.44	111.00
3	H	105	LEU	CB-CG-CD1	7.69	124.08	111.00
2	G	390	ASN	N-CA-C	7.63	131.60	111.00
3	H	105	LEU	CB-CG-CD2	-7.51	98.23	111.00
4	L	75	LEU	CB-CG-CD1	-7.26	98.66	111.00
3	H	67	ARG	N-CA-C	7.26	130.59	111.00
4	L	98	SER	CB-CA-C	-7.17	96.48	110.10
1	C	174	ILE	N-CA-C	7.04	130.01	111.00
2	G	114	SER	N-CA-C	6.93	129.72	111.00
3	H	29	LEU	CB-CG-CD1	-6.87	99.33	111.00
2	G	476	ASP	N-CA-C	-6.78	92.70	111.00
2	G	207	ASP	C-N-CD	-6.64	105.99	120.60
3	H	159	PRO	CA-N-CD	-6.51	102.38	111.50
3	H	109	TYR	N-CA-C	6.51	128.58	111.00
3	H	75	SER	N-CA-C	6.50	128.55	111.00
2	G	277	VAL	N-CA-C	6.49	128.53	111.00
2	G	343	LYS	N-CA-C	6.49	128.53	111.00
2	G	275	ASN	CA-C-N	-6.47	102.97	117.20
2	G	213	TYR	N-CA-C	-6.44	93.60	111.00
4	L	99	THR	N-CA-C	6.44	128.39	111.00
4	L	17	GLN	N-CA-C	6.43	128.35	111.00
1	C	110	GLN	N-CA-C	6.38	128.22	111.00
1	C	35	LYS	N-CA-CB	-6.35	99.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	278	LYS	N-CA-C	6.34	128.12	111.00
3	H	65	GLN	CA-CB-CG	6.32	127.29	113.40
2	G	201	CYS	CA-CB-SG	6.26	125.27	114.00
3	H	65	GLN	CB-CA-C	-6.24	97.92	110.40
4	L	142	ILE	N-CA-C	-6.19	94.30	111.00
2	G	437	PRO	N-CA-C	6.18	128.17	112.10
4	L	193	SER	N-CA-C	6.18	127.68	111.00
2	G	441	ASN	CB-CA-C	6.13	122.67	110.40
1	C	146	VAL	N-CA-C	-6.13	94.45	111.00
1	C	59	ARG	CA-CB-CG	-6.08	100.03	113.40
2	G	284	LEU	N-CA-C	6.04	127.30	111.00
2	G	263	GLU	N-CA-C	6.02	127.25	111.00
3	H	34	ILE	N-CA-C	5.93	127.01	111.00
1	C	100	LEU	CA-CB-CG	5.93	128.93	115.30
2	G	450	GLY	N-CA-C	5.90	127.85	113.10
3	H	133	VAL	CG1-CB-CG2	5.89	120.32	110.90
2	G	221	ILE	N-CA-C	-5.82	95.28	111.00
2	G	455	ARG	NE-CZ-NH2	-5.82	117.39	120.30
3	H	106	TRP	N-CA-C	-5.81	95.32	111.00
2	G	420	ARG	CB-CG-CD	5.80	126.69	111.60
3	H	190	LEU	N-CA-C	5.75	126.52	111.00
4	L	7	GLN	C-N-CD	5.72	140.41	128.40
4	L	93	TRP	N-CA-C	-5.72	95.57	111.00
2	G	234	PRO	N-CA-C	-5.71	97.26	112.10
4	L	23	CYS	CA-CB-SG	5.70	124.27	114.00
1	C	12	VAL	CB-CA-C	-5.70	100.57	111.40
1	C	105	ASP	CB-CA-C	-5.66	99.08	110.40
2	G	376	PHE	N-CA-C	-5.66	95.73	111.00
3	H	143	THR	N-CA-C	5.66	126.27	111.00
1	C	59	ARG	NE-CZ-NH1	-5.61	117.49	120.30
3	H	1	GLN	C-N-CA	5.53	135.53	121.70
3	H	219	VAL	CG1-CB-CG2	-5.53	102.05	110.90
3	H	83	LEU	N-CA-C	-5.52	96.11	111.00
2	G	259	GLY	N-CA-C	5.50	126.86	113.10
2	G	420	ARG	NE-CZ-NH2	-5.49	117.55	120.30
2	G	343	LYS	CB-CA-C	-5.49	99.43	110.40
3	H	161	PRO	CA-N-CD	-5.48	103.83	111.50
1	C	139	GLN	N-CA-CB	-5.43	100.82	110.60
3	H	132	SER	N-CA-C	-5.40	96.42	111.00
4	L	98	SER	CA-C-N	-5.40	105.33	117.20
3	H	164	VAL	N-CA-C	5.38	125.53	111.00
2	G	477	MET	CA-CB-CG	-5.38	104.15	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	22	CYS	CA-CB-SG	-5.38	104.31	114.00
3	H	1	GLN	CB-CA-C	-5.37	99.65	110.40
1	C	81	THR	N-CA-C	-5.37	96.51	111.00
3	H	105	LEU	N-CA-C	-5.36	96.54	111.00
2	G	456	ASP	N-CA-C	5.33	125.40	111.00
4	L	209	GLU	N-CA-C	5.31	125.34	111.00
1	C	105	ASP	N-CA-C	5.31	125.33	111.00
4	L	80	LEU	CA-CB-CG	5.30	127.50	115.30
4	L	147	PRO	N-CA-C	-5.29	98.33	112.10
3	H	4	VAL	CG1-CB-CG2	-5.29	102.43	110.90
3	H	137	ALA	C-N-CD	5.26	139.44	128.40
2	G	354	GLU	CA-CB-CG	5.25	124.94	113.40
3	H	159	PRO	N-CA-C	-5.25	98.46	112.10
2	G	463	GLU	N-CA-C	-5.23	96.87	111.00
1	C	174	ILE	CG1-CB-CG2	5.20	122.83	111.40
4	L	125	PRO	CA-N-CD	-5.19	104.23	111.50
1	C	136	LYS	N-CA-C	-5.17	97.03	111.00
2	G	420	ARG	N-CA-CB	-5.17	101.30	110.60
2	G	378	TYR	N-CA-CB	-5.16	101.31	110.60
2	G	257	LEU	N-CA-C	5.15	124.90	111.00
2	G	442	ILE	N-CA-C	5.11	124.79	111.00
1	C	123	GLY	N-CA-C	5.10	125.84	113.10
2	G	258	ASN	N-CA-CB	5.09	119.76	110.60
2	G	292	CYS	CA-CB-SG	5.08	123.14	114.00
2	G	382	THR	N-CA-C	-5.07	97.31	111.00
2	G	420	ARG	CA-CB-CG	-5.07	102.25	113.40
2	G	347	TYR	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	102	TYR	Sidechain
3	H	110	TYR	Sidechain
3	H	114	TYR	Sidechain
3	H	94	TYR	Sidechain
4	L	34	TYR	Sidechain
4	L	98	SER	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1361	0	1382	159	0
2	G	2271	0	2232	278	0
3	H	1685	0	1645	202	0
4	L	1572	0	1530	126	0
5	G	56	0	51	11	0
All	All	6945	0	6840	700	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 51.

All (700) 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)
5:G:2500:NAG:C1	5:G:2500:NAG:C2	1.75	1.56
2:G:258:ASN:CB	2:G:258:ASN:CG	1.79	1.51
3:H:158:PHE:HB3	3:H:159:PRO:HD2	1.22	1.20
2:G:420:ARG:HH12	3:H:55:GLU:HB2	1.06	1.13
2:G:355:PHE:HB3	2:G:385:PHE:HB3	1.23	1.12
4:L:7:GLN:HE21	4:L:107:THR:HG22	1.06	1.10
1:C:37:LEU:HD11	1:C:44:LEU:HD11	1.30	1.09
1:C:3:VAL:HG22	1:C:94:GLN:HB3	1.32	1.08
3:H:91:THR:HG22	3:H:123:VAL:H	1.05	1.08
2:G:420:ARG:HG2	3:H:56:ASN:HB3	1.34	1.08
2:G:354:GLU:HG3	2:G:469:ILE:HG12	1.29	1.08
2:G:420:ARG:HH22	3:H:55:GLU:N	1.54	1.05
2:G:420:ARG:NE	3:H:56:ASN:HD22	1.55	1.04
4:L:29:ASN:ND2	4:L:30:ILE:HG12	1.73	1.03
3:H:16:ALA:O	3:H:86:LEU:HD13	1.60	1.02
1:C:157:TRP:HE1	1:C:174:ILE:HD12	1.19	1.02
2:G:123:PRO:HD3	3:H:105:LEU:HD13	1.40	1.02
3:H:158:PHE:CB	3:H:159:PRO:HD2	1.86	1.01
2:G:223:LYS:HE3	2:G:241:VAL:HG11	1.44	0.99
2:G:329:ASN:HD21	2:G:331:LYS:HB2	1.26	0.98
4:L:7:GLN:NE2	4:L:107:THR:HG22	1.79	0.98
4:L:5:LEU:HD21	4:L:29:ASN:ND2	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:29:LEU:H	3:H:77:ASN:ND2	1.62	0.96
2:G:337:LEU:O	2:G:341:VAL:HG13	1.66	0.96
3:H:86:LEU:HD23	3:H:123:VAL:HG22	1.48	0.95
3:H:56:ASN:OD1	3:H:57:GLU:HG3	1.66	0.95
2:G:100:VAL:HG11	2:G:482:ARG:HG2	1.48	0.95
1:C:21:LYS:HA	1:C:64:GLN:O	1.66	0.94
3:H:149:ALA:HB2	3:H:195:THR:HG22	1.49	0.94
1:C:3:VAL:HG11	1:C:164:ASN:HD22	1.33	0.94
2:G:420:ARG:HH12	3:H:55:GLU:CB	1.81	0.93
4:L:155:LYS:HG2	4:L:158:SER:HA	1.50	0.93
2:G:275:ASN:HD21	2:G:277:VAL:HB	1.32	0.93
2:G:247:ILE:HG23	2:G:484:GLU:OE1	1.68	0.92
3:H:29:LEU:H	3:H:77:ASN:HD21	1.12	0.92
3:H:48:MET:HG2	3:H:64:PHE:CZ	2.04	0.92
3:H:91:THR:HG22	3:H:123:VAL:N	1.83	0.91
2:G:420:ARG:NH1	3:H:55:GLU:HB2	1.85	0.91
1:C:103:ASN:HD22	1:C:104:SER:H	1.12	0.91
2:G:420:ARG:HE	3:H:56:ASN:HD22	1.15	0.91
2:G:420:ARG:CG	3:H:56:ASN:HB3	2.00	0.90
1:C:103:ASN:HD22	1:C:104:SER:N	1.70	0.90
2:G:354:GLU:HB2	2:G:469:ILE:HA	1.51	0.90
1:C:132:SER:HA	1:C:157:TRP:CE3	2.08	0.88
4:L:97:LEU:HD22	4:L:99:THR:HG23	1.53	0.88
3:H:35:HIS:CD2	3:H:50:GLY:HA3	2.09	0.88
3:H:158:PHE:HB3	3:H:159:PRO:CD	2.05	0.87
2:G:337:LEU:O	2:G:340:VAL:HG22	1.73	0.87
1:C:53:ASP:O	1:C:54:ARG:HG2	1.74	0.86
1:C:37:LEU:HD11	1:C:44:LEU:CD1	2.05	0.86
1:C:154:SER:HA	1:C:174:ILE:HG22	1.58	0.85
2:G:329:ASN:ND2	2:G:331:LYS:HB2	1.90	0.85
2:G:383:LYS:NZ	2:G:416:PRO:HG3	1.93	0.84
2:G:383:LYS:HZ3	2:G:416:PRO:HG3	1.41	0.84
2:G:253:THR:CG2	2:G:369:SER:H	1.90	0.84
3:H:91:THR:CG2	3:H:123:VAL:H	1.89	0.84
1:C:98:PHE:HE1	1:C:120:SER:HG	1.23	0.84
2:G:85:LEU:HD22	2:G:240:THR:H	1.43	0.84
2:G:262:ALA:HB2	2:G:283:HIS:CD2	2.12	0.84
2:G:223:LYS:HE2	2:G:488:TYR:HE2	1.43	0.84
2:G:420:ARG:CZ	3:H:56:ASN:H	1.91	0.84
2:G:420:ARG:NH2	3:H:56:ASN:H	1.76	0.83
2:G:272:ASN:HB3	2:G:275:ASN:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:333:TRP:CZ2	2:G:384:LEU:HD21	2.13	0.83
4:L:186:LEU:HD23	4:L:186:LEU:N	1.92	0.83
1:C:37:LEU:CD1	1:C:44:LEU:HD11	2.10	0.82
2:G:266:VAL:HB	2:G:343:LYS:HE2	1.62	0.81
3:H:32:LEU:HD13	3:H:107:THR:HG21	1.62	0.81
2:G:348:PHE:HB3	2:G:351:LYS:HD2	1.61	0.81
2:G:92:PHE:CE2	2:G:224:CYS:HB2	2.16	0.81
1:C:132:SER:OG	1:C:134:ARG:HB2	1.81	0.81
3:H:158:PHE:CB	3:H:159:PRO:CD	2.57	0.81
1:C:54:ARG:HA	1:C:72:LYS:HE2	1.63	0.80
2:G:95:TRP:HA	2:G:482:ARG:NH1	1.96	0.80
1:C:53:ASP:HB2	4:L:32:LYS:NZ	1.96	0.80
2:G:435:ALA:HB1	2:G:436:PRO:HD2	1.63	0.80
4:L:7:GLN:HE21	4:L:107:THR:CG2	1.92	0.79
2:G:270:SER:CB	2:G:273:ILE:HD13	2.13	0.79
2:G:223:LYS:CE	2:G:241:VAL:HG11	2.13	0.78
1:C:157:TRP:NE1	1:C:174:ILE:HD12	1.97	0.78
3:H:36:TRP:CD1	3:H:81:MET:HG3	2.19	0.78
2:G:422:ILE:HG12	2:G:433:MET:HG3	1.65	0.78
1:C:46:LYS:HB2	2:G:360:GLY:HA3	1.65	0.77
3:H:29:LEU:HD11	3:H:34:ILE:HD11	1.66	0.77
1:C:45:THR:HG22	2:G:365:ILE:HG21	1.66	0.77
3:H:86:LEU:HD23	3:H:123:VAL:CG2	2.15	0.77
2:G:420:ARG:HG2	3:H:56:ASN:CB	2.13	0.77
1:C:150:GLU:O	1:C:176:VAL:HG11	1.84	0.77
4:L:71:THR:HG23	4:L:71:THR:O	1.84	0.77
4:L:150:VAL:HG12	4:L:170:PRO:HG3	1.67	0.77
3:H:22:CYS:HB2	3:H:36:TRP:HH2	1.48	0.76
4:L:126:PRO:HB2	4:L:131:LEU:HD11	1.68	0.76
1:C:43:PHE:CB	2:G:365:ILE:HD11	2.16	0.75
3:H:29:LEU:N	3:H:77:ASN:HD21	1.85	0.75
2:G:382:THR:HG21	5:G:2000:NAG:H62	1.69	0.74
1:C:51:LEU:O	1:C:53:ASP:O	2.05	0.74
4:L:29:ASN:HD21	4:L:30:ILE:HG12	1.49	0.74
2:G:349:PRO:O	2:G:351:LYS:HG3	1.88	0.74
2:G:272:ASN:ND2	5:G:1500:NAG:H62	2.01	0.74
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.69	0.74
4:L:19:VAL:CG1	4:L:80:LEU:HD22	2.18	0.74
2:G:333:TRP:CH2	2:G:384:LEU:HD21	2.22	0.73
2:G:388:ILE:H	2:G:388:ILE:HD13	1.52	0.73
2:G:381:THR:HG22	2:G:415:LEU:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:294:GLY:HA2	2:G:324:GLY:N	2.03	0.73
4:L:123:LEU:HD22	4:L:212:MET:HB2	1.70	0.73
2:G:270:SER:HB2	2:G:273:ILE:HD13	1.71	0.73
4:L:97:LEU:HD23	4:L:98:SER:H	1.53	0.73
4:L:124:PHE:HB3	4:L:125:PRO:HD2	1.71	0.73
3:H:32:LEU:HD13	3:H:107:THR:CG2	2.18	0.73
2:G:100:VAL:HG11	2:G:482:ARG:CG	2.17	0.73
2:G:275:ASN:ND2	2:G:277:VAL:HB	2.04	0.73
3:H:182:LEU:HD12	3:H:188:TYR:CE1	2.24	0.73
1:C:109:LEU:O	1:C:112:GLN:HB2	1.90	0.72
2:G:459:GLU:O	2:G:460:ASN:HB2	1.88	0.72
2:G:123:PRO:CD	3:H:105:LEU:HD13	2.20	0.72
2:G:253:THR:O	2:G:255:LEU:N	2.21	0.72
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.72	0.72
2:G:418:ARG:HB3	2:G:420:ARG:HD2	1.71	0.72
4:L:7:GLN:NE2	4:L:107:THR:CG2	2.51	0.72
2:G:215:ALA:HB2	2:G:221:ILE:HG12	1.72	0.72
2:G:119:VAL:HB	2:G:433:MET:HB3	1.72	0.71
2:G:461:LYS:HE2	2:G:463:GLU:OE2	1.91	0.71
1:C:53:ASP:HB2	4:L:32:LYS:HZ3	1.53	0.71
2:G:275:ASN:HD22	2:G:278:LYS:HG2	1.53	0.71
1:C:43:PHE:HB3	2:G:365:ILE:HD11	1.71	0.71
1:C:27:HIS:CE1	1:C:35:LYS:HE3	2.24	0.71
1:C:45:THR:CG2	2:G:365:ILE:HG21	2.21	0.71
3:H:142:SER:HB3	3:H:148:ALA:HB1	1.73	0.71
2:G:111:TRP:CZ2	2:G:251:VAL:HG21	2.26	0.71
4:L:186:LEU:HD12	4:L:190:GLN:CB	2.21	0.71
1:C:35:LYS:O	1:C:47:GLY:HA3	1.92	0.70
1:C:40:GLN:HG3	2:G:474:GLY:O	1.91	0.70
3:H:190:LEU:HD12	3:H:191:SER:N	2.06	0.70
2:G:422:ILE:O	3:H:55:GLU:HB3	1.92	0.70
2:G:206:PHE:CE2	2:G:208:PRO:HA	2.26	0.70
1:C:31:SER:HB2	1:C:80:ASP:OD1	1.92	0.70
2:G:91:ASN:ND2	2:G:234:PRO:HA	2.06	0.70
1:C:129:GLN:CG	1:C:137:ASN:HD21	2.03	0.70
2:G:459:GLU:O	2:G:460:ASN:CB	2.40	0.70
3:H:19:LYS:HB2	3:H:82:GLU:HG2	1.74	0.69
3:H:193:VAL:HG11	4:L:141:LEU:HD13	1.74	0.69
3:H:159:PRO:HB2	3:H:214:PRO:CB	2.22	0.69
4:L:29:ASN:CG	4:L:30:ILE:H	1.95	0.69
4:L:87:ASP:OD1	4:L:108:LYS:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:97:ASN:HD21	2:G:99:MET:HE2	1.56	0.69
2:G:290:ILE:HG12	2:G:328:ILE:HG12	1.74	0.69
2:G:455:ARG:HB3	2:G:470:PHE:CD1	2.27	0.69
2:G:111:TRP:CZ3	2:G:115:LEU:HD12	2.28	0.69
3:H:158:PHE:HD1	3:H:159:PRO:HD3	1.58	0.69
2:G:270:SER:OG	2:G:273:ILE:HD13	1.93	0.68
1:C:138:ILE:CG2	1:C:144:LEU:HD21	2.23	0.68
2:G:337:LEU:HD22	2:G:389:HIS:CE1	2.28	0.68
3:H:17:SER:HA	3:H:84:SER:HA	1.74	0.68
2:G:97:ASN:HD21	2:G:99:MET:CE	2.06	0.68
4:L:186:LEU:HD12	4:L:190:GLN:HB2	1.73	0.68
2:G:385:PHE:CE1	2:G:472:PRO:HG3	2.29	0.68
1:C:7:LYS:HE3	1:C:169:GLU:O	1.94	0.68
4:L:127:SER:O	4:L:131:LEU:HD13	1.94	0.67
4:L:49:LEU:HD11	4:L:64:PHE:CD1	2.29	0.67
1:C:108:LEU:O	1:C:176:VAL:HA	1.93	0.67
4:L:30:ILE:HD13	4:L:92:THR:OG1	1.94	0.67
1:C:71:ILE:HG22	1:C:74:LEU:HD23	1.76	0.67
3:H:174:GLY:O	3:H:194:VAL:HG23	1.94	0.67
2:G:206:PHE:HE2	2:G:208:PRO:HA	1.60	0.67
3:H:97:ALA:HB1	3:H:112:LEU:HD22	1.76	0.67
3:H:167:ASN:HB3	3:H:170:ALA:HB3	1.77	0.67
4:L:41:LEU:HD23	4:L:86:ALA:HB2	1.76	0.67
3:H:62:GLN:HA	3:H:65:GLN:HG2	1.75	0.67
1:C:129:GLN:CD	1:C:137:ASN:HD21	1.98	0.67
2:G:91:ASN:HD22	2:G:234:PRO:HA	1.61	0.66
4:L:155:LYS:CG	4:L:158:SER:HA	2.24	0.66
2:G:455:ARG:HB3	2:G:470:PHE:CE1	2.30	0.66
1:C:33:GLN:HB2	2:G:459:GLU:CG	2.25	0.66
4:L:112:LEU:HA	4:L:146:TYR:OH	1.95	0.66
2:G:418:ARG:CB	2:G:420:ARG:HD2	2.24	0.66
2:G:253:THR:HG22	2:G:369:SER:N	2.12	0.65
2:G:354:GLU:CG	2:G:469:ILE:HG12	2.17	0.65
3:H:29:LEU:HD11	3:H:34:ILE:CD1	2.26	0.65
3:H:104:ASN:O	3:H:107:THR:OG1	2.07	0.65
4:L:36:SER:CB	4:L:51:PHE:HA	2.27	0.65
2:G:363:LEU:HD21	2:G:420:ARG:CZ	2.27	0.65
2:G:338:LYS:HA	2:G:341:VAL:HG22	1.78	0.65
4:L:18:LYS:HG3	4:L:77:ILE:O	1.96	0.65
2:G:336:THR:O	2:G:340:VAL:HG13	1.97	0.65
2:G:419:ILE:C	2:G:420:ARG:HG3	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:PRO:HD3	3:H:105:LEU:CD1	2.22	0.64
2:G:254:GLN:NE2	2:G:368:HIS:HB2	2.12	0.64
4:L:138:LEU:HD22	4:L:184:LEU:HD23	1.79	0.64
2:G:481:TRP:HA	2:G:481:TRP:CE3	2.31	0.64
3:H:158:PHE:CD1	3:H:159:PRO:CD	2.80	0.64
1:C:138:ILE:HG22	1:C:144:LEU:HD21	1.79	0.64
2:G:424:ASN:OD1	2:G:431:ARG:HG2	1.97	0.64
2:G:223:LYS:HE2	2:G:488:TYR:CE2	2.30	0.64
1:C:20:GLN:HE21	1:C:22:LYS:HD2	1.62	0.64
2:G:261:LEU:HD21	2:G:287:SER:HB3	1.78	0.64
3:H:158:PHE:CD1	3:H:159:PRO:HD3	2.32	0.64
2:G:100:VAL:HG21	2:G:482:ARG:HD3	1.80	0.64
2:G:420:ARG:HH21	3:H:54:GLU:HG2	1.61	0.64
4:L:192:LYS:O	4:L:214:HIS:NE2	2.32	0.63
3:H:212:HIS:ND1	3:H:214:PRO:HD2	2.14	0.63
3:H:64:PHE:O	3:H:68:VAL:HG12	1.99	0.63
4:L:130:GLU:HG2	4:L:135:LYS:O	1.98	0.63
3:H:158:PHE:O	3:H:159:PRO:HG2	1.97	0.63
3:H:36:TRP:HB2	3:H:70:MET:CE	2.28	0.63
3:H:117:GLN:HG3	3:H:118:GLY:O	1.98	0.63
4:L:36:SER:HB2	4:L:51:PHE:HA	1.80	0.63
2:G:338:LYS:O	2:G:341:VAL:HG22	1.99	0.63
4:L:129:GLU:O	4:L:132:GLN:HB3	1.99	0.63
3:H:99:GLY:HA3	3:H:110:TYR:HD1	1.63	0.62
4:L:114:GLN:NE2	4:L:177:LYS:HG2	2.14	0.62
2:G:261:LEU:HD21	2:G:287:SER:CB	2.29	0.62
4:L:119:PRO:HA	4:L:145:PHE:HB3	1.81	0.62
2:G:420:ARG:HE	3:H:56:ASN:ND2	1.93	0.62
2:G:253:THR:C	2:G:255:LEU:H	2.02	0.62
2:G:253:THR:HG22	2:G:369:SER:H	1.64	0.62
2:G:107:ILE:HG22	2:G:426:TRP:HH2	1.64	0.62
4:L:154:TRP:CZ3	4:L:199:CYS:HB2	2.34	0.62
3:H:177:THR:HG22	3:H:190:LEU:HD11	1.82	0.62
1:C:113:SER:HB3	1:C:147:SER:O	2.00	0.62
2:G:227:LYS:HD2	2:G:263:GLU:OE1	2.00	0.61
2:G:381:THR:HG22	2:G:415:LEU:CD1	2.30	0.61
1:C:103:ASN:ND2	1:C:104:SER:N	2.45	0.61
2:G:253:THR:CG2	2:G:369:SER:N	2.61	0.61
2:G:256:LEU:HD23	2:G:480:ASN:ND2	2.14	0.61
4:L:123:LEU:HD12	4:L:199:CYS:HB3	1.83	0.61
3:H:37:VAL:HG13	3:H:46:GLU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:254:GLN:HE21	2:G:368:HIS:HB2	1.63	0.61
4:L:19:VAL:HG11	4:L:80:LEU:HD22	1.82	0.61
3:H:146:GLY:O	3:H:198:SER:N	2.25	0.61
2:G:103:MET:HG2	2:G:485:LEU:HD11	1.82	0.61
2:G:332:ALA:O	2:G:336:THR:HG23	2.01	0.61
1:C:28:TRP:CE2	1:C:69:LEU:HB2	2.36	0.61
1:C:36:ILE:HD11	1:C:51:LEU:HD12	1.82	0.60
4:L:5:LEU:HD21	4:L:29:ASN:HD21	1.65	0.60
3:H:94:TYR:O	3:H:119:THR:HG22	2.00	0.60
3:H:141:LYS:NZ	4:L:212:MET:HG3	2.16	0.60
4:L:173:GLN:HB3	4:L:177:LYS:O	2.01	0.60
1:C:103:ASN:ND2	1:C:104:SER:H	1.92	0.60
2:G:461:LYS:HB3	2:G:461:LYS:NZ	2.17	0.60
1:C:20:GLN:HE21	1:C:22:LYS:CD	2.15	0.60
3:H:159:PRO:HB2	3:H:214:PRO:HB3	1.84	0.60
3:H:177:THR:HG23	3:H:192:SER:HB2	1.82	0.60
3:H:142:SER:O	3:H:148:ALA:HA	2.01	0.60
2:G:95:TRP:HA	2:G:482:ARG:HH11	1.65	0.60
2:G:254:GLN:NE2	2:G:381:THR:OG1	2.33	0.60
2:G:104:HIS:HE1	2:G:477:MET:HB2	1.67	0.60
2:G:253:THR:HG21	2:G:369:SER:H	1.67	0.60
3:H:47:TRP:CD2	4:L:101:GLN:HB3	2.37	0.60
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.37	0.59
3:H:206:TYR:O	3:H:222:LYS:HG3	2.02	0.59
2:G:266:VAL:HB	2:G:343:LYS:CE	2.31	0.59
4:L:19:VAL:HG12	4:L:80:LEU:HD22	1.83	0.59
1:C:43:PHE:HB2	2:G:365:ILE:HD11	1.82	0.59
3:H:23:LYS:HA	3:H:78:THR:HG22	1.84	0.59
3:H:207:ILE:HG12	3:H:222:LYS:HB2	1.85	0.59
2:G:290:ILE:HD11	2:G:448:ILE:HD11	1.83	0.59
5:G:2500:NAG:C2	5:G:2500:NAG:O5	2.42	0.59
3:H:36:TRP:HB2	3:H:70:MET:HE3	1.85	0.59
4:L:71:THR:O	4:L:71:THR:CG2	2.51	0.59
3:H:138:PRO:HG2	3:H:225:PRO:HB3	1.84	0.59
2:G:280:ILE:HG22	2:G:282:VAL:HG23	1.83	0.59
2:G:384:LEU:C	2:G:384:LEU:HD23	2.23	0.59
2:G:420:ARG:HH22	3:H:55:GLU:H	1.44	0.58
1:C:43:PHE:HB3	2:G:365:ILE:CD1	2.33	0.58
2:G:420:ARG:CZ	3:H:56:ASN:N	2.66	0.58
2:G:420:ARG:NE	3:H:56:ASN:ND2	2.39	0.58
4:L:30:ILE:CG2	4:L:68:LYS:HE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.85	0.58
2:G:111:TRP:CE3	2:G:115:LEU:HD12	2.38	0.58
4:L:186:LEU:HD23	4:L:186:LEU:H	1.67	0.58
3:H:193:VAL:HG11	4:L:141:LEU:CD1	2.33	0.58
4:L:41:LEU:HB3	4:L:42:PRO:HD2	1.85	0.58
2:G:356:ALA:HB1	2:G:357:PRO:HD2	1.86	0.58
2:G:383:LYS:HE2	5:G:2000:NAG:O7	2.03	0.58
1:C:58:ARG:HB3	1:C:61:LEU:HD23	1.84	0.58
3:H:178:PHE:HB3	3:H:179:PRO:HD2	1.86	0.58
2:G:253:THR:HG23	2:G:368:HIS:HA	1.84	0.57
3:H:110:TYR:N	3:H:110:TYR:HD2	2.02	0.57
2:G:333:TRP:O	2:G:337:LEU:HG	2.03	0.57
3:H:48:MET:HG2	3:H:64:PHE:CE2	2.38	0.57
2:G:388:ILE:N	2:G:388:ILE:HD13	2.19	0.57
4:L:186:LEU:N	4:L:186:LEU:CD2	2.65	0.57
3:H:20:VAL:HG11	3:H:119:THR:HG21	1.87	0.57
3:H:143:THR:HA	3:H:147:THR:O	2.04	0.57
3:H:154:VAL:HB	3:H:190:LEU:O	2.04	0.57
3:H:150:LEU:H	3:H:150:LEU:HD23	1.69	0.57
1:C:61:LEU:HD22	1:C:61:LEU:N	2.20	0.57
2:G:225:ASN:HB2	2:G:237:ASN:O	2.05	0.57
1:C:37:LEU:HD11	1:C:44:LEU:CG	2.34	0.57
4:L:142:ILE:HD12	4:L:201:VAL:CG2	2.35	0.56
2:G:266:VAL:HG22	2:G:285:THR:H	1.70	0.56
3:H:165:SER:OG	3:H:209:ASN:HB2	2.04	0.56
4:L:7:GLN:NE2	4:L:106:GLY:HA2	2.20	0.56
2:G:290:ILE:CD1	2:G:448:ILE:HD11	2.35	0.56
2:G:253:THR:HG21	2:G:364:GLU:O	2.04	0.56
1:C:33:GLN:HB2	2:G:459:GLU:HG3	1.85	0.56
2:G:268:ILE:HG23	2:G:280:ILE:HG23	1.87	0.56
1:C:44:LEU:HD13	1:C:62:TRP:HH2	1.69	0.56
2:G:436:PRO:HB2	2:G:437:PRO:HD2	1.87	0.56
1:C:14:LEU:HD22	1:C:93:VAL:HG11	1.87	0.56
2:G:461:LYS:O	2:G:461:LYS:HG2	2.04	0.56
3:H:110:TYR:CD2	3:H:110:TYR:N	2.74	0.56
1:C:53:ASP:HB2	4:L:32:LYS:HZ1	1.70	0.56
1:C:3:VAL:HG22	1:C:94:GLN:CB	2.22	0.56
3:H:212:HIS:CE1	3:H:215:SER:OG	2.59	0.56
2:G:261:LEU:HD21	2:G:287:SER:OG	2.06	0.56
2:G:455:ARG:HA	2:G:469:ILE:O	2.05	0.56
1:C:107:HIS:HD2	1:C:175:VAL:HG11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:60:TYR:HE1	3:H:70:MET:HG3	1.70	0.56
4:L:8:PRO:O	4:L:107:THR:HB	2.06	0.55
3:H:160:GLU:N	3:H:161:PRO:HD3	2.16	0.55
4:L:21:ILE:HG21	4:L:107:THR:HG21	1.88	0.55
3:H:103:TYR:CD1	3:H:103:TYR:O	2.58	0.55
2:G:85:LEU:HD23	2:G:240:THR:HG22	1.87	0.55
1:C:52:ASN:N	1:C:52:ASN:HD22	2.02	0.55
4:L:140:CYS:HB2	4:L:154:TRP:CZ2	2.41	0.55
3:H:135:PRO:HB2	3:H:223:VAL:HG13	1.89	0.55
4:L:5:LEU:HD11	4:L:92:THR:CG2	2.37	0.55
1:C:5:LEU:CD2	1:C:96:LEU:HB2	2.36	0.55
3:H:150:LEU:O	3:H:150:LEU:HD23	2.06	0.55
4:L:93:TRP:CZ3	4:L:100:GLY:HA2	2.42	0.55
2:G:462:THR:O	2:G:462:THR:HG22	2.07	0.55
1:C:40:GLN:O	1:C:41:GLY:C	2.44	0.55
4:L:138:LEU:N	4:L:138:LEU:HD12	2.22	0.54
2:G:425:MET:SD	2:G:432:ALA:HB2	2.47	0.54
2:G:245:HIS:N	2:G:488:TYR:OH	2.40	0.54
2:G:117:PRO:HD3	2:G:434:TYR:OH	2.07	0.54
2:G:268:ILE:HG22	2:G:273:ILE:HD12	1.89	0.54
2:G:335:GLU:O	2:G:338:LYS:HB2	2.08	0.54
2:G:97:ASN:O	2:G:100:VAL:HG22	2.08	0.54
4:L:30:ILE:HD12	4:L:35:VAL:HG22	1.89	0.54
3:H:99:GLY:HA3	3:H:110:TYR:CD1	2.43	0.54
4:L:29:ASN:CG	4:L:30:ILE:N	2.61	0.54
4:L:171:SER:O	4:L:178:TYR:HA	2.08	0.54
2:G:461:LYS:HB3	2:G:461:LYS:HZ3	1.73	0.54
1:C:12:VAL:HG22	1:C:13:GLU:N	2.23	0.54
3:H:167:ASN:CB	3:H:170:ALA:HB3	2.38	0.54
2:G:228:THR:HG21	2:G:265:GLU:HB2	1.90	0.54
3:H:36:TRP:H	3:H:70:MET:HE1	1.73	0.53
2:G:214:CYS:SG	2:G:242:GLN:O	2.66	0.53
4:L:191:TRP:CH2	4:L:214:HIS:HB2	2.42	0.53
2:G:481:TRP:HE3	2:G:481:TRP:HA	1.71	0.53
2:G:89:ILE:HG12	2:G:236:ASN:HA	1.89	0.53
2:G:383:LYS:HZ1	5:G:2000:NAG:H81	1.72	0.53
3:H:193:VAL:HG21	4:L:141:LEU:HD11	1.90	0.53
3:H:2:VAL:HG11	3:H:114:TYR:CE1	2.43	0.53
2:G:272:ASN:ND2	5:G:1500:NAG:C6	2.65	0.53
4:L:125:PRO:HB3	4:L:212:MET:SD	2.48	0.53
1:C:20:GLN:NE2	1:C:22:LYS:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:103:TYR:N	3:H:103:TYR:CD2	2.76	0.53
3:H:142:SER:HB3	3:H:149:ALA:H	1.73	0.53
4:L:37:TRP:CD2	4:L:75:LEU:HD13	2.44	0.53
4:L:186:LEU:HD12	4:L:190:GLN:HB3	1.91	0.53
2:G:471:ARG:HG2	2:G:471:ARG:HH11	1.73	0.53
2:G:282:VAL:HB	2:G:451:LEU:HB2	1.91	0.53
1:C:36:ILE:O	1:C:47:GLY:N	2.31	0.53
1:C:37:LEU:HD12	1:C:45:THR:O	2.08	0.53
4:L:29:ASN:ND2	4:L:30:ILE:H	2.07	0.53
2:G:275:ASN:ND2	2:G:278:LYS:HG2	2.23	0.53
3:H:182:LEU:C	3:H:182:LEU:HD23	2.30	0.52
2:G:215:ALA:HB2	2:G:221:ILE:CD1	2.40	0.52
3:H:102:TYR:CE2	3:H:110:TYR:HA	2.43	0.52
2:G:367:THR:HB	2:G:379:CYS:O	2.09	0.52
2:G:426:TRP:CE3	2:G:477:MET:HG3	2.43	0.52
1:C:21:LYS:O	1:C:21:LYS:HG3	2.09	0.52
4:L:155:LYS:HG2	4:L:158:SER:CA	2.31	0.52
4:L:40:GLN:O	4:L:86:ALA:HB1	2.09	0.52
3:H:197:PRO:HG2	3:H:200:SER:HB2	1.89	0.52
1:C:46:LYS:HE3	2:G:360:GLY:HA3	1.92	0.52
1:C:53:ASP:O	1:C:54:ARG:CG	2.54	0.52
1:C:138:ILE:HG21	1:C:144:LEU:HD21	1.91	0.52
1:C:144:LEU:HD22	1:C:145:SER:N	2.25	0.52
3:H:209:ASN:OD1	3:H:220:ASP:HB3	2.10	0.52
3:H:31:GLY:HA2	3:H:72:GLU:OE1	2.08	0.52
2:G:348:PHE:HB3	2:G:351:LYS:CD	2.34	0.52
1:C:133:PRO:HG3	1:C:157:TRP:HB3	1.92	0.52
1:C:144:LEU:C	1:C:144:LEU:HD13	2.29	0.52
3:H:35:HIS:CD2	3:H:47:TRP:HE1	2.28	0.52
1:C:33:GLN:HG3	2:G:459:GLU:HG3	1.92	0.52
2:G:281:ILE:O	2:G:451:LEU:O	2.28	0.52
3:H:137:ALA:O	3:H:138:PRO:C	2.46	0.52
1:C:45:THR:CG2	2:G:365:ILE:HD13	2.40	0.51
4:L:29:ASN:HD22	4:L:92:THR:HG21	1.75	0.51
3:H:104:ASN:C	3:H:107:THR:H	2.13	0.51
2:G:103:MET:CE	2:G:213:TYR:HB2	2.39	0.51
4:L:87:ASP:CG	4:L:108:LYS:HG3	2.31	0.51
2:G:328:ILE:HG21	2:G:333:TRP:HE1	1.74	0.51
3:H:34:ILE:HD12	3:H:72:GLU:HG2	1.93	0.51
2:G:339:LYS:O	2:G:343:LYS:HG2	2.10	0.51
1:C:36:ILE:HD11	1:C:82:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:O	1:C:52:ASN:C	2.48	0.51
2:G:338:LYS:HB3	2:G:338:LYS:NZ	2.26	0.51
4:L:151:THR:HG23	4:L:202:THR:HB	1.92	0.51
2:G:270:SER:OG	2:G:280:ILE:HG12	2.10	0.51
2:G:253:THR:OG1	2:G:254:GLN:N	2.44	0.51
2:G:256:LEU:HD23	2:G:480:ASN:HD22	1.74	0.51
2:G:85:LEU:HD22	2:G:239:SER:OG	2.10	0.51
4:L:41:LEU:HB3	4:L:42:PRO:CD	2.40	0.51
2:G:483:SER:O	2:G:486:TYR:HD2	1.92	0.51
2:G:229:PHE:CE2	2:G:235:CYS:HB2	2.45	0.51
1:C:154:SER:HB3	1:C:176:VAL:HB	1.92	0.51
2:G:340:VAL:CG2	2:G:341:VAL:N	2.73	0.51
3:H:60:TYR:HE1	3:H:70:MET:CG	2.23	0.51
1:C:58:ARG:CB	1:C:61:LEU:HD23	2.41	0.51
3:H:97:ALA:CB	3:H:112:LEU:HD22	2.41	0.51
4:L:5:LEU:HD11	4:L:92:THR:HG22	1.91	0.51
3:H:38:ARG:O	3:H:38:ARG:HG3	2.11	0.51
1:C:24:ILE:HD13	1:C:87:GLU:HB3	1.92	0.51
2:G:282:VAL:HG11	2:G:451:LEU:HD12	1.92	0.50
2:G:254:GLN:O	2:G:255:LEU:HD23	2.11	0.50
3:H:110:TYR:HD2	3:H:110:TYR:H	1.58	0.50
2:G:272:ASN:ND2	5:G:1500:NAG:H4	2.26	0.50
3:H:60:TYR:OH	3:H:70:MET:N	2.42	0.50
2:G:435:ALA:HB1	2:G:436:PRO:CD	2.37	0.50
1:C:36:ILE:HG23	1:C:55:ALA:HB1	1.94	0.50
3:H:36:TRP:CH2	3:H:96:CYS:HB2	2.46	0.50
1:C:120:SER:OG	1:C:121:PRO:HD2	2.12	0.50
3:H:71:THR:O	3:H:79:ALA:HB1	2.11	0.50
2:G:453:LEU:HD23	2:G:472:PRO:HA	1.94	0.50
2:G:272:ASN:CB	2:G:275:ASN:HB2	2.36	0.50
1:C:138:ILE:HG22	1:C:144:LEU:CD2	2.41	0.50
2:G:378:TYR:CD1	2:G:420:ARG:HD3	2.46	0.50
2:G:376:PHE:CD2	2:G:423:ILE:HD13	2.47	0.50
3:H:38:ARG:HA	3:H:93:VAL:O	2.12	0.50
4:L:65:SER:OG	4:L:76:ALA:HB3	2.12	0.50
1:C:83:ILE:HG12	1:C:92:GLU:CB	2.42	0.50
4:L:198:SER:OG	4:L:211:THR:HA	2.12	0.50
2:G:268:ILE:HG23	2:G:280:ILE:CG2	2.42	0.50
2:G:326:CYS:O	2:G:414:THR:HG23	2.12	0.50
2:G:420:ARG:CB	3:H:56:ASN:HB3	2.41	0.49
2:G:334:ASN:HA	2:G:337:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:267:VAL:HG11	2:G:269:ARG:NH2	2.26	0.49
1:C:71:ILE:CG2	1:C:74:LEU:HD23	2.41	0.49
2:G:420:ARG:CB	2:G:420:ARG:HH11	2.24	0.49
2:G:419:ILE:C	2:G:420:ARG:CG	2.81	0.49
4:L:151:THR:CG2	4:L:202:THR:HB	2.42	0.49
3:H:150:LEU:HD23	3:H:194:VAL:O	2.11	0.49
3:H:158:PHE:O	3:H:159:PRO:O	2.30	0.49
3:H:138:PRO:HD3	3:H:150:LEU:CB	2.43	0.49
1:C:33:GLN:CG	2:G:459:GLU:HG3	2.43	0.49
2:G:215:ALA:HB2	2:G:221:ILE:CG1	2.40	0.49
4:L:142:ILE:HD12	4:L:201:VAL:HG21	1.94	0.49
2:G:269:ARG:HH12	2:G:283:HIS:CD2	2.30	0.49
2:G:253:THR:C	2:G:255:LEU:N	2.66	0.49
2:G:463:GLU:CB	2:G:465:ASN:HD22	2.26	0.49
1:C:79:SER:OG	1:C:97:VAL:N	2.44	0.49
1:C:28:TRP:CD2	1:C:84:CYS:HB2	2.48	0.48
3:H:158:PHE:CG	3:H:159:PRO:CD	2.97	0.48
3:H:22:CYS:HB2	3:H:36:TRP:CH2	2.39	0.48
1:C:144:LEU:HD22	1:C:145:SER:H	1.79	0.48
4:L:28:SER:O	4:L:94:ASP:OD2	2.30	0.48
2:G:420:ARG:NH1	2:G:420:ARG:HB3	2.28	0.48
1:C:27:HIS:NE2	1:C:35:LYS:HE3	2.28	0.48
3:H:23:LYS:HG3	3:H:78:THR:CG2	2.43	0.48
2:G:103:MET:O	2:G:107:ILE:HG12	2.14	0.48
3:H:31:GLY:CA	3:H:72:GLU:OE1	2.61	0.48
2:G:208:PRO:HG3	5:G:1000:NAG:O7	2.13	0.48
3:H:100:GLY:O	3:H:101:ASN:C	2.51	0.48
3:H:182:LEU:HD12	3:H:188:TYR:CZ	2.49	0.48
3:H:151:GLY:HA2	3:H:166:TRP:HH2	1.77	0.48
3:H:142:SER:CB	3:H:148:ALA:HB1	2.44	0.48
3:H:150:LEU:N	3:H:150:LEU:HD23	2.28	0.48
1:C:44:LEU:HD13	1:C:62:TRP:CH2	2.49	0.48
4:L:19:VAL:HG11	4:L:80:LEU:CD2	2.43	0.48
2:G:250:VAL:HG23	2:G:250:VAL:O	2.14	0.48
1:C:85:GLU:HG2	1:C:90:LYS:HD3	1.96	0.48
1:C:37:LEU:HD23	1:C:57:SER:HB3	1.96	0.48
2:G:461:LYS:O	2:G:463:GLU:N	2.46	0.48
4:L:173:GLN:OE1	4:L:179:ALA:HB2	2.14	0.48
4:L:37:TRP:CG	4:L:75:LEU:HD13	2.49	0.48
2:G:420:ARG:HH11	2:G:420:ARG:HB3	1.78	0.48
4:L:7:GLN:HB3	4:L:23:CYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:272:ASN:HB3	2:G:275:ASN:CB	2.40	0.47
3:H:179:PRO:HG2	4:L:168:THR:CG2	2.44	0.47
3:H:141:LYS:HZ3	4:L:212:MET:HG3	1.78	0.47
1:C:61:LEU:H	1:C:61:LEU:HD22	1.79	0.47
3:H:19:LYS:CB	3:H:82:GLU:HG2	2.44	0.47
1:C:129:GLN:HG2	1:C:137:ASN:HD21	1.76	0.47
2:G:223:LYS:O	2:G:238:VAL:HG13	2.13	0.47
3:H:150:LEU:CD2	3:H:150:LEU:N	2.77	0.47
4:L:25:GLY:O	4:L:71:THR:HG23	2.15	0.47
3:H:159:PRO:CB	3:H:214:PRO:HB3	2.44	0.47
2:G:420:ARG:NH2	3:H:55:GLU:N	2.40	0.47
1:C:11:THR:HG23	1:C:72:LYS:HB3	1.95	0.47
3:H:47:TRP:CG	4:L:101:GLN:HB3	2.50	0.47
1:C:33:GLN:HB2	2:G:459:GLU:HG2	1.96	0.47
1:C:12:VAL:CG2	1:C:13:GLU:N	2.78	0.47
3:H:205:THR:HB	3:H:222:LYS:HD2	1.95	0.47
3:H:1:GLN:NE2	3:H:25:SER:HB3	2.30	0.47
4:L:29:ASN:HD22	4:L:30:ILE:HG12	1.74	0.47
4:L:13:ALA:HB3	4:L:80:LEU:HD23	1.97	0.47
1:C:109:LEU:HD23	1:C:176:VAL:C	2.35	0.47
2:G:333:TRP:HA	2:G:336:THR:OG1	2.15	0.46
3:H:64:PHE:HB3	3:H:68:VAL:CG1	2.45	0.46
3:H:183:GLN:HB3	3:H:187:LEU:O	2.16	0.46
1:C:128:VAL:HG23	1:C:141:GLY:O	2.15	0.46
3:H:212:HIS:HE1	3:H:214:PRO:HB2	1.79	0.46
3:H:6:GLN:OE1	3:H:118:GLY:N	2.47	0.46
3:H:190:LEU:HD12	3:H:191:SER:H	1.78	0.46
3:H:91:THR:HG22	3:H:122:THR:HA	1.97	0.46
1:C:132:SER:O	1:C:135:GLY:N	2.49	0.46
2:G:436:PRO:CB	2:G:437:PRO:HD2	2.45	0.46
1:C:61:LEU:CD2	1:C:61:LEU:H	2.29	0.46
3:H:106:TRP:C	3:H:108:GLY:H	2.17	0.46
3:H:10:GLU:OE2	3:H:12:ARG:CZ	2.64	0.46
1:C:100:LEU:HD12	1:C:170:PHE:HB2	1.98	0.46
2:G:420:ARG:HH22	3:H:55:GLU:CA	2.28	0.46
3:H:64:PHE:HB3	3:H:68:VAL:HG11	1.97	0.46
1:C:131:ARG:HG2	1:C:137:ASN:HD22	1.80	0.46
2:G:121:LEU:HD23	2:G:196:THR:OG1	2.15	0.46
1:C:57:SER:HB2	1:C:68:PRO:O	2.14	0.46
1:C:36:ILE:CG2	1:C:55:ALA:HB1	2.45	0.46
1:C:43:PHE:CE1	2:G:426:TRP:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:340:VAL:HG23	2:G:341:VAL:N	2.31	0.46
3:H:134:PHE:CD2	4:L:130:GLU:HB2	2.50	0.46
1:C:56:ASP:O	1:C:70:ILE:HB	2.15	0.46
2:G:370:PHE:CE2	2:G:377:PHE:HB2	2.51	0.46
4:L:191:TRP:CZ3	4:L:214:HIS:HB2	2.51	0.46
3:H:138:PRO:HD3	3:H:150:LEU:HB3	1.98	0.45
4:L:114:GLN:HB3	4:L:115:PRO:HD2	1.98	0.45
3:H:51:PHE:HA	3:H:58:ILE:HA	1.98	0.45
1:C:158:THR:HG23	1:C:169:GLU:HG3	1.97	0.45
2:G:261:LEU:N	2:G:261:LEU:HD12	2.30	0.45
4:L:38:TYR:HA	4:L:47:LYS:O	2.17	0.45
1:C:28:TRP:CE2	1:C:84:CYS:HB2	2.51	0.45
2:G:252:SER:OG	2:G:255:LEU:O	2.22	0.45
4:L:63:ARG:HD2	4:L:63:ARG:HH11	1.49	0.45
1:C:174:ILE:HG23	1:C:175:VAL:N	2.31	0.45
1:C:20:GLN:O	1:C:22:LYS:N	2.49	0.45
4:L:39:GLN:HG3	4:L:88:TYR:CE1	2.52	0.45
2:G:378:TYR:O	2:G:417:CYS:SG	2.74	0.45
1:C:133:PRO:HD3	1:C:157:TRP:CD2	2.51	0.45
2:G:331:LYS:O	2:G:335:GLU:OE2	2.35	0.45
1:C:12:VAL:O	1:C:12:VAL:HG13	2.17	0.45
3:H:35:HIS:HD2	3:H:47:TRP:HE1	1.64	0.45
2:G:378:TYR:OH	2:G:423:ILE:HG13	2.16	0.45
4:L:97:LEU:CD2	4:L:99:THR:HG23	2.36	0.45
4:L:126:PRO:HG2	4:L:191:TRP:CD1	2.52	0.45
4:L:30:ILE:HG22	4:L:68:LYS:HE2	1.99	0.45
2:G:262:ALA:O	2:G:285:THR:HA	2.17	0.45
3:H:32:LEU:HD22	3:H:51:PHE:CE2	2.51	0.45
1:C:58:ARG:HA	3:H:106:TRP:HH2	1.80	0.45
1:C:100:LEU:HD11	1:C:159:CYS:HB2	1.98	0.45
3:H:136:LEU:HB3	4:L:124:PHE:CD2	2.52	0.45
3:H:45:LEU:HD21	4:L:46:PRO:HG2	1.99	0.45
2:G:112:ASP:O	2:G:116:LYS:HG2	2.17	0.45
3:H:13:LYS:O	3:H:14:PRO:C	2.54	0.45
2:G:420:ARG:HH21	3:H:54:GLU:CG	2.29	0.44
2:G:210:PRO:HA	2:G:247:ILE:O	2.17	0.44
2:G:266:VAL:O	2:G:343:LYS:HE2	2.17	0.44
4:L:37:TRP:CE3	4:L:75:LEU:HD22	2.52	0.44
4:L:114:GLN:HE22	4:L:177:LYS:HG2	1.81	0.44
1:C:61:LEU:HB3	1:C:66:ASN:HB3	1.98	0.44
2:G:354:GLU:OE2	2:G:388:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:TRP:CE2	2:G:251:VAL:HG21	2.52	0.44
4:L:37:TRP:CD1	4:L:50:ILE:HB	2.52	0.44
1:C:36:ILE:CD1	1:C:51:LEU:HD12	2.47	0.44
1:C:132:SER:O	1:C:133:PRO:C	2.54	0.44
2:G:337:LEU:HD22	2:G:389:HIS:NE2	2.33	0.44
3:H:68:VAL:HG23	3:H:82:GLU:O	2.17	0.44
3:H:47:TRP:CH2	3:H:49:GLY:HA2	2.53	0.44
4:L:56:ARG:HD2	4:L:60:ILE:CG2	2.47	0.44
1:C:46:LYS:HD2	1:C:52:ASN:O	2.17	0.44
4:L:144:ASP:OD2	4:L:173:GLN:NE2	2.51	0.44
2:G:420:ARG:NH1	3:H:56:ASN:N	2.65	0.44
1:C:134:ARG:HD3	1:C:152:GLN:HB3	2.00	0.44
3:H:148:ALA:O	3:H:196:VAL:N	2.42	0.44
4:L:154:TRP:CH2	4:L:199:CYS:HB2	2.52	0.44
2:G:461:LYS:NZ	2:G:461:LYS:CB	2.80	0.44
3:H:158:PHE:CD1	3:H:159:PRO:N	2.86	0.44
4:L:169:THR:O	4:L:170:PRO:O	2.36	0.44
2:G:276:ASN:OD1	2:G:277:VAL:HG23	2.18	0.44
3:H:141:LYS:HZ1	4:L:212:MET:HG3	1.82	0.44
2:G:118:CYS:N	2:G:201:CYS:SG	2.91	0.44
1:C:121:PRO:O	1:C:122:PRO:C	2.57	0.43
2:G:463:GLU:HB3	2:G:465:ASN:HD22	1.83	0.43
2:G:207:ASP:HA	2:G:208:PRO:HD2	1.47	0.43
2:G:452:LEU:O	2:G:453:LEU:HD23	2.17	0.43
1:C:46:LYS:HE3	2:G:360:GLY:CA	2.48	0.43
1:C:51:LEU:O	1:C:53:ASP:N	2.51	0.43
1:C:30:ASN:OD1	1:C:34:ILE:O	2.36	0.43
1:C:12:VAL:CG1	1:C:74:LEU:HD21	2.48	0.43
3:H:38:ARG:O	3:H:38:ARG:CG	2.64	0.43
1:C:39:ASN:HD22	1:C:39:ASN:H	1.65	0.43
4:L:187:THR:OG1	4:L:189:GLU:HB3	2.18	0.43
2:G:272:ASN:ND2	5:G:1500:NAG:C4	2.76	0.43
3:H:36:TRP:CG	3:H:81:MET:HG3	2.53	0.43
2:G:267:VAL:HG11	2:G:269:ARG:HH21	1.82	0.43
2:G:426:TRP:HE3	2:G:477:MET:HG3	1.82	0.43
1:C:130:CYS:HA	1:C:158:THR:O	2.18	0.43
1:C:86:VAL:O	1:C:87:GLU:C	2.57	0.43
1:C:132:SER:HA	1:C:157:TRP:HE3	1.71	0.43
3:H:6:GLN:OE1	3:H:118:GLY:CA	2.67	0.43
2:G:338:LYS:CA	2:G:341:VAL:HG22	2.48	0.43
2:G:357:PRO:HB2	2:G:382:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:215:ALA:HB1	2:G:219:TYR:O	2.18	0.43
3:H:67:ARG:HD2	3:H:84:SER:O	2.19	0.43
2:G:471:ARG:HG2	2:G:471:ARG:NH1	2.34	0.43
2:G:483:SER:O	2:G:486:TYR:CD2	2.70	0.43
2:G:103:MET:HE2	2:G:213:TYR:HB2	2.01	0.43
2:G:213:TYR:O	2:G:244:THR:HG23	2.19	0.43
1:C:160:THR:HG21	1:C:167:LYS:HD2	2.00	0.43
3:H:213:LYS:N	3:H:214:PRO:CD	2.82	0.43
2:G:108:ILE:HD12	2:G:427:GLN:HG2	2.01	0.43
3:H:149:ALA:CB	3:H:195:THR:HG22	2.34	0.43
2:G:267:VAL:HG11	2:G:269:ARG:NE	2.34	0.43
1:C:114:LEU:HB2	1:C:149:LEU:HD11	2.00	0.43
4:L:37:TRP:CZ2	4:L:75:LEU:HB2	2.54	0.43
1:C:85:GLU:OE2	1:C:90:LYS:HE2	2.19	0.43
1:C:132:SER:C	1:C:135:GLY:H	2.22	0.42
2:G:227:LYS:CD	2:G:263:GLU:OE1	2.66	0.42
2:G:418:ARG:HB2	2:G:420:ARG:HD2	1.98	0.42
1:C:3:VAL:HG21	1:C:164:ASN:ND2	2.35	0.42
4:L:124:PHE:CB	4:L:125:PRO:HD2	2.41	0.42
3:H:90:ASP:O	3:H:91:THR:C	2.58	0.42
1:C:132:SER:HG	1:C:134:ARG:HB2	1.80	0.42
1:C:96:LEU:HD22	1:C:121:PRO:HG3	2.00	0.42
2:G:225:ASN:O	2:G:226:ASP:C	2.56	0.42
2:G:116:LYS:HG3	2:G:202:PRO:HG3	2.02	0.42
2:G:97:ASN:C	2:G:97:ASN:OD1	2.57	0.42
3:H:136:LEU:HD21	4:L:139:VAL:HG21	2.00	0.42
1:C:24:ILE:HG22	1:C:25:GLN:O	2.20	0.42
2:G:338:LYS:C	2:G:341:VAL:HG22	2.39	0.42
3:H:153:LEU:HD12	3:H:191:SER:HB3	2.01	0.42
1:C:58:ARG:HA	3:H:106:TRP:CH2	2.55	0.42
4:L:10:SER:C	4:L:11:VAL:HG23	2.39	0.42
2:G:223:LYS:HE3	2:G:241:VAL:HG21	2.02	0.42
1:C:53:ASP:CB	4:L:32:LYS:HZ1	2.33	0.42
3:H:47:TRP:CZ2	3:H:49:GLY:CA	3.03	0.42
1:C:133:PRO:N	1:C:157:TRP:HB3	2.34	0.42
3:H:58:ILE:O	3:H:58:ILE:CG2	2.68	0.42
4:L:150:VAL:HG22	4:L:151:THR:N	2.35	0.42
3:H:193:VAL:HG21	4:L:141:LEU:HD21	2.02	0.42
3:H:146:GLY:O	3:H:197:PRO:HA	2.20	0.42
4:L:196:SER:HB3	4:L:213:ALA:HB2	2.01	0.42
2:G:368:HIS:CG	2:G:368:HIS:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:489:LYS:HE2	2:G:491:VAL:HG13	2.02	0.41
2:G:420:ARG:NH2	3:H:54:GLU:HG2	2.30	0.41
2:G:103:MET:HE1	2:G:213:TYR:HB2	2.01	0.41
1:C:114:LEU:O	1:C:145:SER:HA	2.20	0.41
1:C:12:VAL:HG12	1:C:74:LEU:HD21	2.02	0.41
2:G:280:ILE:O	2:G:453:LEU:N	2.48	0.41
1:C:133:PRO:HD3	1:C:157:TRP:CG	2.54	0.41
3:H:36:TRP:HB2	3:H:70:MET:HE1	2.02	0.41
2:G:348:PHE:CB	2:G:351:LYS:HD2	2.42	0.41
3:H:153:LEU:HD12	3:H:153:LEU:HA	1.70	0.41
1:C:85:GLU:HG2	1:C:90:LYS:CD	2.51	0.41
3:H:41:PRO:HD3	3:H:92:ALA:HA	2.02	0.41
2:G:420:ARG:NH2	3:H:56:ASN:N	2.58	0.41
1:C:133:PRO:CD	1:C:157:TRP:HB3	2.50	0.41
1:C:58:ARG:HG2	3:H:106:TRP:CH2	2.55	0.41
3:H:1:GLN:HE22	3:H:25:SER:HB3	1.85	0.41
3:H:32:LEU:HD13	3:H:107:THR:HG23	2.01	0.41
1:C:133:PRO:CG	1:C:157:TRP:HB3	2.50	0.41
2:G:92:PHE:CD1	2:G:489:LYS:HB2	2.56	0.41
1:C:33:GLN:CB	2:G:459:GLU:HG3	2.49	0.41
1:C:36:ILE:HG22	1:C:37:LEU:N	2.34	0.41
1:C:52:ASN:ND2	1:C:53:ASP:H	2.18	0.41
1:C:57:SER:CB	1:C:68:PRO:O	2.69	0.41
1:C:174:ILE:CG2	1:C:176:VAL:HG23	2.50	0.41
3:H:31:GLY:C	3:H:72:GLU:OE1	2.59	0.41
2:G:253:THR:HG23	2:G:254:GLN:HG2	2.02	0.41
5:G:1000:NAG:H83	5:G:1000:NAG:O3	2.21	0.41
1:C:118:LEU:HD23	1:C:126:PRO:HB2	2.03	0.41
2:G:244:THR:HA	2:G:488:TYR:CZ	2.55	0.41
1:C:132:SER:C	1:C:134:ARG:N	2.69	0.41
3:H:149:ALA:HA	3:H:195:THR:HA	2.02	0.41
2:G:436:PRO:HA	2:G:437:PRO:HD3	1.90	0.41
3:H:157:TYR:CE2	3:H:188:TYR:O	2.73	0.41
3:H:93:VAL:HG22	3:H:120:LEU:HD13	2.02	0.41
1:C:124:SER:HB3	1:C:163:GLN:HE21	1.86	0.41
3:H:158:PHE:CG	3:H:159:PRO:N	2.89	0.41
2:G:223:LYS:HE3	2:G:241:VAL:CG1	2.31	0.41
1:C:45:THR:HG21	2:G:365:ILE:HG21	2.00	0.41
1:C:7:LYS:HD2	1:C:10:ASP:OD2	2.20	0.41
3:H:197:PRO:HG2	3:H:200:SER:CB	2.51	0.41
4:L:37:TRP:CZ3	4:L:90:CYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:37:TRP:N	4:L:50:ILE:O	2.43	0.41
1:C:36:ILE:HG21	1:C:69:LEU:HD11	2.03	0.41
2:G:104:HIS:O	2:G:108:ILE:HG12	2.21	0.41
1:C:61:LEU:CD2	1:C:61:LEU:N	2.84	0.41
1:C:58:ARG:HG2	3:H:106:TRP:HH2	1.85	0.41
2:G:341:VAL:HG23	2:G:342:GLU:N	2.36	0.40
2:G:233:GLY:HA2	2:G:234:PRO:HD3	1.85	0.40
4:L:119:PRO:HD3	4:L:203:HIS:CD2	2.56	0.40
2:G:245:HIS:CE1	2:G:487:LYS:NZ	2.89	0.40
4:L:123:LEU:HD22	4:L:212:MET:CB	2.45	0.40
2:G:114:SER:OG	2:G:206:PHE:HB2	2.21	0.40
2:G:100:VAL:HG12	2:G:485:LEU:HD12	2.03	0.40
2:G:455:ARG:CA	2:G:469:ILE:O	2.70	0.40
2:G:338:LYS:HZ3	2:G:338:LYS:HB3	1.86	0.40
2:G:276:ASN:OD1	2:G:277:VAL:N	2.52	0.40
2:G:111:TRP:CZ2	2:G:251:VAL:CG2	2.98	0.40
3:H:158:PHE:O	3:H:159:PRO:CG	2.60	0.40
2:G:388:ILE:N	2:G:388:ILE:CD1	2.85	0.40
4:L:56:ARG:HD2	4:L:60:ILE:HG22	2.03	0.40
1:C:37:LEU:HD21	1:C:57:SER:OG	2.21	0.40
3:H:36:TRP:O	3:H:48:MET:HB2	2.21	0.40
3:H:138:PRO:HD3	3:H:150:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	173/192 (90%)	168 (97%)	3 (2%)	2 (1%)	16 59
2	G	282/332 (85%)	273 (97%)	3 (1%)	6 (2%)	9 47
3	H	223/231 (96%)	216 (97%)	4 (2%)	3 (1%)	15 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	L	211/217 (97%)	204 (97%)	3 (1%)	4 (2%)	10 49
All	All	889/972 (92%)	861 (97%)	13 (2%)	15 (2%)	11 51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	ASN
1	C	126	PRO
2	G	208	PRO
2	G	216	PRO
2	G	254	GLN
2	G	460	ASN
2	G	462	THR
3	H	159	PRO
3	H	161	PRO
4	L	99	THR
3	H	107	THR
4	L	42	PRO
4	L	86	ALA
4	L	170	PRO
2	G	249	PRO

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	C	159/173 (92%)	152 (96%)	7 (4%)	35 73
2	G	261/296 (88%)	250 (96%)	11 (4%)	36 74
3	H	188/194 (97%)	181 (96%)	7 (4%)	41 77
4	L	176/180 (98%)	167 (95%)	9 (5%)	29 69
All	All	784/843 (93%)	750 (96%)	34 (4%)	35 74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	CYS
1	C	39	ASN
1	C	52	ASN
1	C	84	CYS
1	C	103	ASN
1	C	121	PRO
1	C	130	CYS
2	G	293	ILE
2	G	357	PRO
2	G	372	CYS
2	G	388	ILE
2	G	391	SER
2	G	415	LEU
2	G	417	CYS
2	G	420	ARG
2	G	436	PRO
2	G	443	THR
2	G	445	ILE
3	H	36	TRP
3	H	74	THR
3	H	96	CYS
3	H	110	TYR
3	H	135	PRO
3	H	143	THR
3	H	150	LEU
4	L	8	PRO
4	L	23	CYS
4	L	71	THR
4	L	107	THR
4	L	125	PRO
4	L	131	LEU
4	L	170	PRO
4	L	186	LEU
4	L	214	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	C	33	GLN
1	C	39	ASN
1	C	52	ASN
1	C	73	ASN

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Mol	Chain	Res	Type
1	C	103	ASN
1	C	107	HIS
1	C	110	GLN
1	C	129	GLN
1	C	137	ASN
1	C	139	GLN
1	C	163	GLN
1	C	164	ASN
2	G	91	ASN
2	G	102	GLN
2	G	105	GLN
2	G	236	ASN
2	G	254	GLN
2	G	275	ASN
2	G	283	HIS
2	G	329	ASN
2	G	389	HIS
2	G	390	ASN
2	G	464	ASN
2	G	465	ASN
2	G	480	ASN
3	H	1	GLN
3	H	35	HIS
3	H	56	ASN
3	H	77	ASN
4	L	7	GLN
4	L	81	GLN
4	L	194	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	G	1000	2	14,14,15	2.36	3 (21%)	15,19,21	1.81	2 (13%)
5	NAG	G	1500	2	14,14,15	2.89	3 (21%)	15,19,21	1.41	3 (20%)
5	NAG	G	2000	2	14,14,15	2.46	4 (28%)	15,19,21	1.43	2 (13%)
5	NAG	G	2500	2	14,14,15	4.61	3 (21%)	15,19,21	1.07	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	G	1000	2	-	0/6/23/26	0/1/1/1
5	NAG	G	1500	2	-	2/6/23/26	0/1/1/1
5	NAG	G	2000	2	-	0/6/23/26	0/1/1/1
5	NAG	G	2500	2	1/1/5/7	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2500	NAG	C8-C7	2.08	1.54	1.50
5	G	2000	NAG	C3-C2	2.08	1.57	1.52
5	G	1000	NAG	C3-C2	2.13	1.57	1.52
5	G	1500	NAG	C2-N2	2.13	1.50	1.46
5	G	2000	NAG	O5-C5	2.22	1.48	1.43
5	G	2000	NAG	C4-C5	2.39	1.58	1.53
5	G	1500	NAG	C8-C7	2.57	1.55	1.50
5	G	2500	NAG	C3-C2	3.81	1.61	1.52
5	G	1000	NAG	O5-C5	4.99	1.54	1.43
5	G	1000	NAG	O5-C1	6.32	1.54	1.43
5	G	2000	NAG	C1-C2	8.16	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1500	NAG	C1-C2	10.00	1.66	1.52
5	G	2500	NAG	C1-C2	16.31	1.75	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	1000	NAG	C2-N2-C7	-4.01	117.89	123.04
5	G	1500	NAG	O7-C7-C8	-2.90	116.74	122.06
5	G	2000	NAG	C3-C2-N2	-2.45	104.69	110.56
5	G	2500	NAG	O7-C7-C8	-2.44	117.59	122.06
5	G	1500	NAG	C3-C2-N2	-2.39	104.84	110.56
5	G	1500	NAG	C8-C7-N2	3.34	122.50	116.11
5	G	2000	NAG	C1-O5-C5	3.48	116.66	112.25
5	G	1000	NAG	C1-O5-C5	3.60	116.82	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	2500	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1500	NAG	C8-C7-N2-C2
5	G	1500	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1000	NAG	2	0
5	G	1500	NAG	4	0
5	G	2000	NAG	3	0
5	G	2500	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	175/192 (91%)	0.35	6 (3%) 49 44	51, 103, 139, 185	0
2	G	290/332 (87%)	0.69	32 (11%) 7 7	52, 118, 174, 225	0
3	H	225/231 (97%)	0.36	4 (1%) 71 65	36, 84, 136, 185	0
4	L	213/217 (98%)	0.26	2 (0%) 85 81	39, 83, 133, 162	0
All	All	903/972 (92%)	0.44	44 (4%) 33 29	36, 97, 162, 225	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	390	ASN	5.5
3	H	109	TYR	4.8
2	G	443	THR	4.3
2	G	257	LEU	4.2
2	G	353	ILE	3.8
2	G	484	GLU	3.7
3	H	141	LYS	3.6
3	H	106	TRP	3.3
2	G	282	VAL	3.2
1	C	82	TYR	3.2
2	G	451	LEU	3.1
2	G	452	LEU	3.1
2	G	267	VAL	3.0
2	G	202	PRO	2.9
2	G	328	ILE	2.9
3	H	182	LEU	2.9
2	G	468	GLU	2.8
2	G	293	ILE	2.7
2	G	269	ARG	2.7
4	L	184	LEU	2.6
2	G	227	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	114	LEU	2.6
1	C	86	VAL	2.5
1	C	33	GLN	2.5
2	G	376	PHE	2.5
2	G	355	PHE	2.5
2	G	335	GLU	2.5
2	G	238	VAL	2.4
2	G	417	CYS	2.4
4	L	123	LEU	2.4
2	G	474	GLY	2.4
2	G	274	SER	2.4
2	G	371	ASN	2.4
2	G	473	GLY	2.3
2	G	198	ALA	2.2
2	G	453	LEU	2.2
2	G	419	ILE	2.2
2	G	472	PRO	2.2
2	G	462	THR	2.1
2	G	260	SER	2.1
1	C	45	THR	2.1
2	G	275	ASN	2.1
1	C	29	LYS	2.0
2	G	341	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	G	2000	14/15	0.74	0.31	-0.28	125,125,125,125	0
5	NAG	G	1000	14/15	0.87	0.17	-1.21	105,105,105,105	0
5	NAG	G	2500	14/15	0.82	0.17	-	136,136,136,136	0
5	NAG	G	1500	14/15	0.90	0.29	-	122,122,122,122	0

6.5 Other polymers (i)

There are no such residues in this entry.