Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:24 AM BST

PDB ID	:	3TZV
Title	:	Crystal structure of an iNKT TCR in complex with CD1d-lysophosphatidylcholine
Authors	:	Lopez-Sagaseta, J.; Adams, E.J.
Deposited on	:	2011-09-27
Resolution	:	3.06 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:

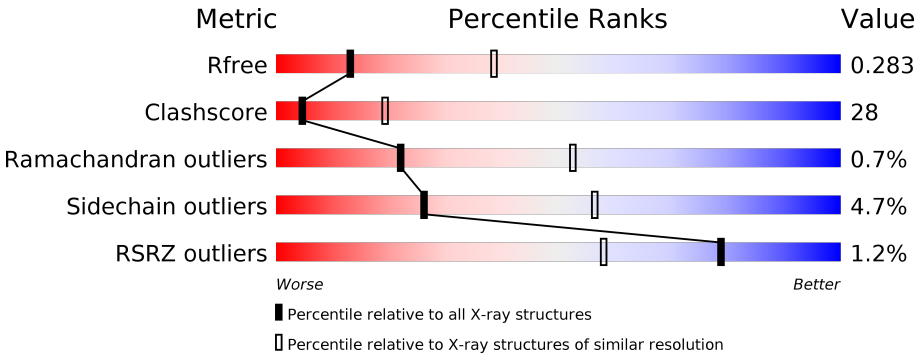
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 <=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	68% 21% • 8%
1	G	213	% 69% 23% • 6%
2	B	259	3% 55% 34% • 9%
2	H	259	% 59% 33% • 6%
3	C	276	42% 50% • 5%
4	D	99	59% 34% • •

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Mol	Chain	Length	Quality of chain
5	E	2	100%

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
6	LSC	C	303	-	-	-	X
9	GOL	C	306	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9519 atoms, of which 10 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 Invariant Natural Killer T Cell Receptor chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	4	0	0
			1419	886	233	291	9			
1	G	201	Total	C	N	O	S	2	0	0
			1516	947	250	310	9			

- Molecule 2 is a protein called Invariant Natural Killer T Cell Receptor chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1819	1153	321	338	7			
2	H	244	Total	C	N	O	S	0	0	0
			1865	1181	325	352	7			

- Molecule 3 is a protein called Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	8	0	0
			2045	1315	348	375	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	PRO	-	expression tag	UNP P15813
C	42	GLN	ASN	engineered mutation	UNP P15813
C	108	GLN	ASN	engineered mutation	UNP P15813
C	163	GLN	ASN	engineered mutation	UNP P15813

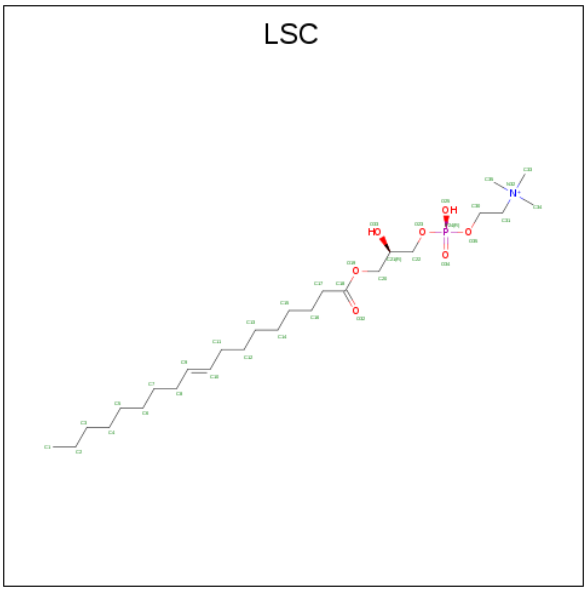
- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	4	0	0
			757	481	131	143	2			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

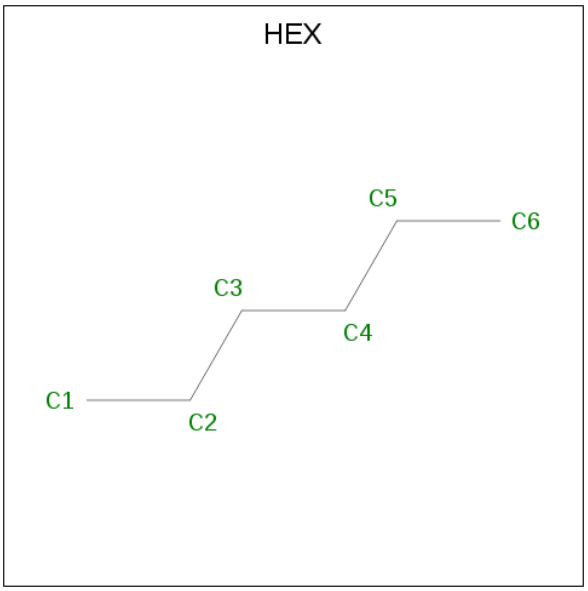
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is (4R,7R,18E)-4,7-dihydroxy-N,N,N-trimethyl-10-oxo-3,5,9-trioxa-4-phosphahexacos-18-en-1-aminium 4-oxide (three-letter code: LSC) (formula: $C_{26}H_{53}NO_7P$).



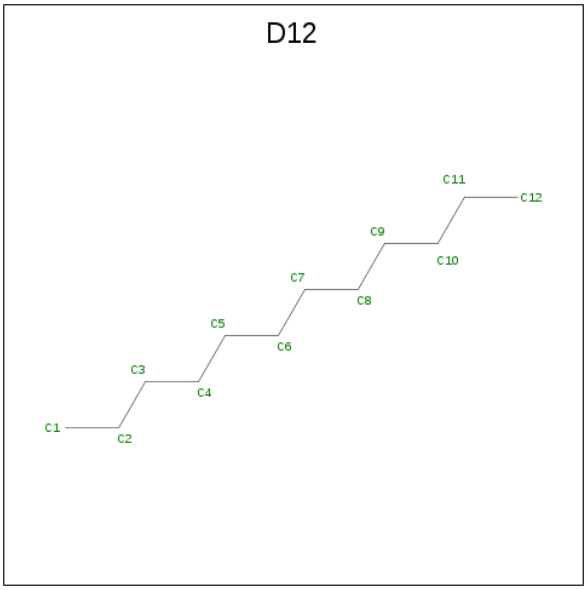
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



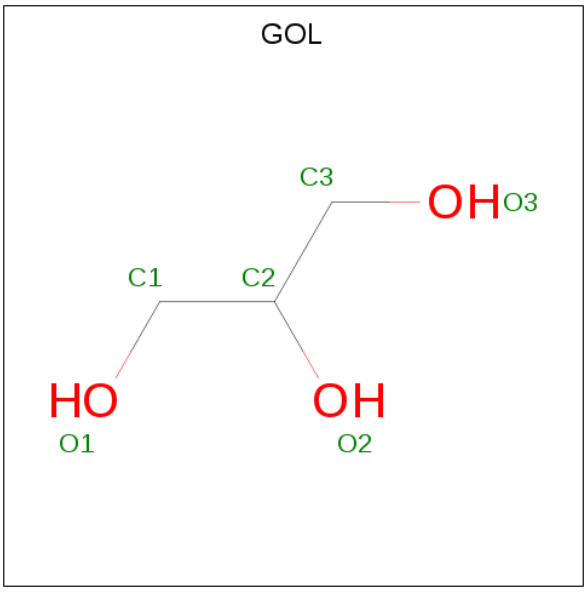
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C 6 6	0	0

- Molecule 8 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C 12 12	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		

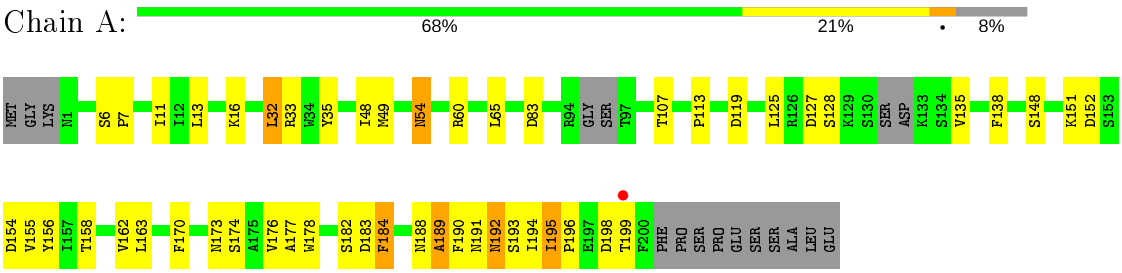
- Molecule 10 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	H	O	0	0
			3	2	1		
10	G	4	Total	H	O	0	0
			12	8	4		

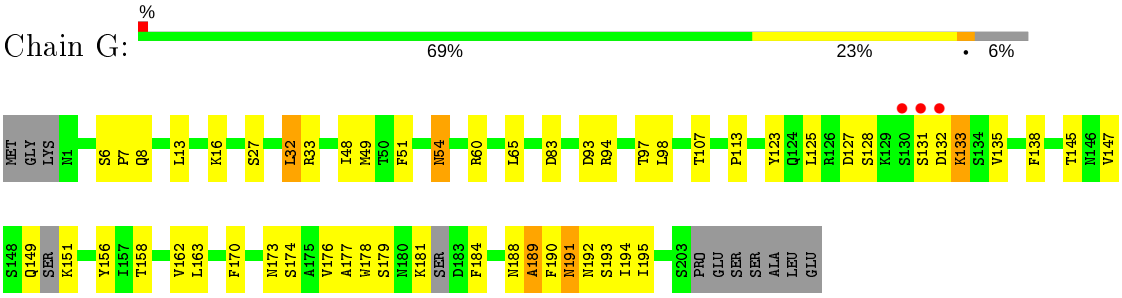
3 Residue-property plots

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

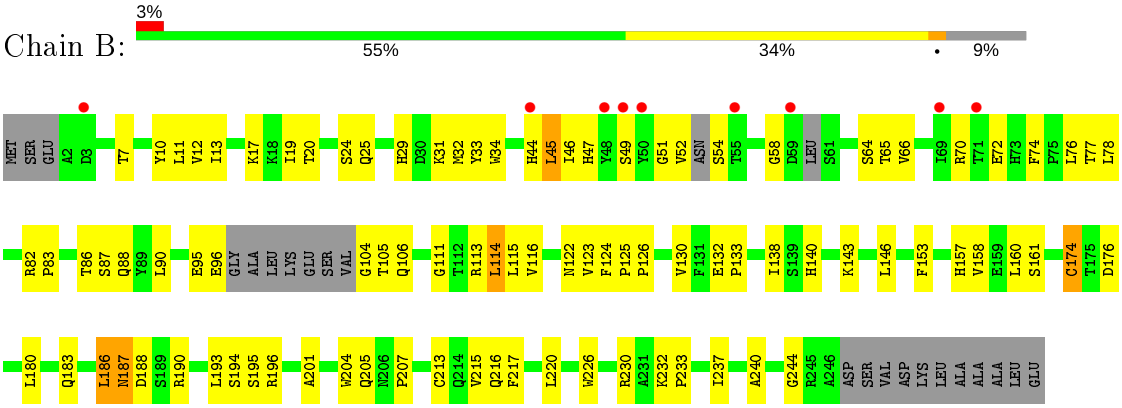
- Molecule 1: Invariant Natural Killer T Cell Receptor chain A



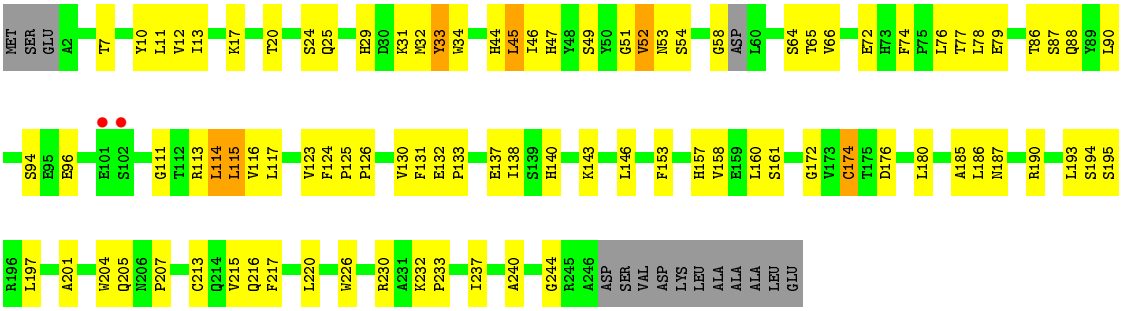
- Molecule 1: Invariant Natural Killer T Cell Receptor chain A



- Molecule 2: Invariant Natural Killer T Cell Receptor chain B

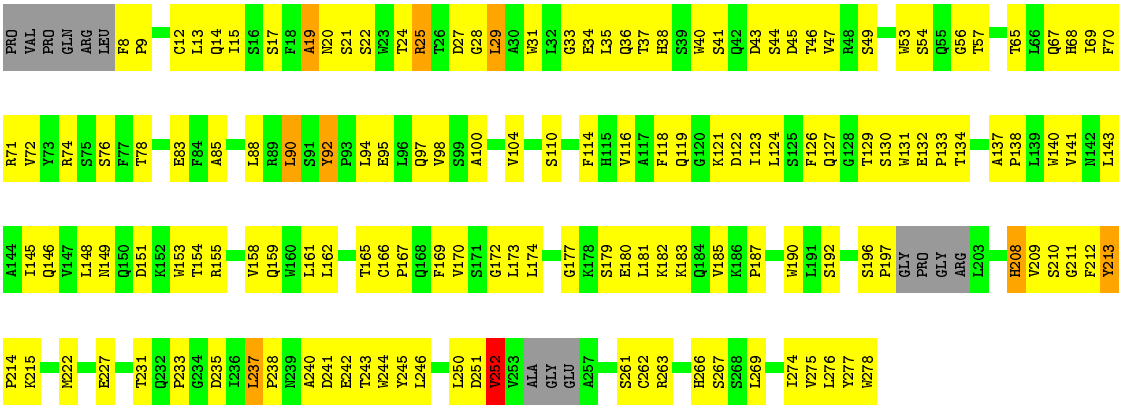


- Molecule 2: Invariant Natural Killer T Cell Receptor chain B



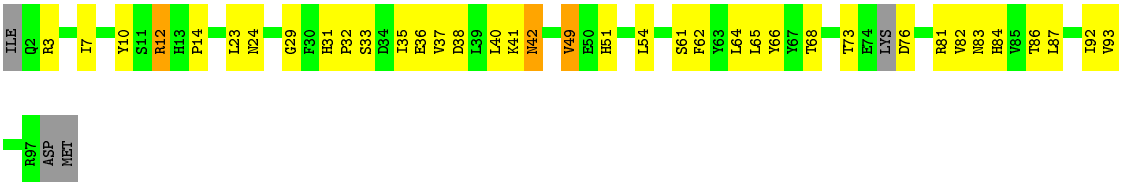
• Molecule 3: Antigen-presenting glycoprotein CD1d

Chain C:



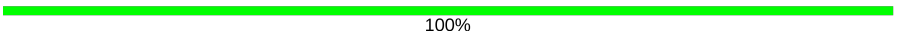
• Molecule 4: Beta-2-microglobulin

Chain D:



• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.59Å 117.61Å 190.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.02 – 3.06 20.02 – 3.06	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.02-3.06) 93.6 (20.02-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.04Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.236 , 0.288 0.230 , 0.283	Depositor DCC
R_{free} test set	1362 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9519	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, D12, HEX, FUC, LSC

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	0.24	0/1445	0.44	0/1976
1	G	0.25	0/1544	0.44	0/2100
2	B	0.23	0/1869	0.42	0/2552
2	H	0.23	0/1917	0.41	0/2618
3	C	0.22	0/2107	0.39	0/2880
4	D	0.22	0/778	0.38	0/1061
All	All	0.23	0/9660	0.42	0/13187

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	191	ASN	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	1419	0	1254	81	0
1	G	1516	0	1409	69	0
2	B	1819	0	1679	99	0
2	H	1865	0	1723	93	0
3	C	2045	0	1904	180	0
4	D	757	0	686	46	0
5	E	24	0	22	0	0
6	C	35	0	52	7	0
7	C	6	0	14	0	0
8	C	12	0	26	4	0
9	C	6	0	8	5	0
10	C	1	2	0	0	0
10	G	4	8	0	0	0
All	All	9509	10	8777	514	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 28.

All (514) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:CB	1:A:196:PRO:HD2	1.84	1.05
1:A:151:LYS:HA	1:A:155:VAL:O	1.59	1.03
1:A:158:THR:HG22	1:A:176:VAL:H	1.25	1.01
1:G:158:THR:HG22	1:G:176:VAL:H	1.25	0.99
1:G:135:VAL:HG23	1:G:178:TRP:HB3	1.44	0.97
1:A:135:VAL:HG23	1:A:178:TRP:HB3	1.45	0.96
3:C:269:LEU:HD13	3:C:274:ILE:HG13	1.50	0.92
3:C:46:THR:HA	3:C:67:GLN:HE21	1.33	0.92
3:C:40:TRP:CE3	8:C:305:D12:H12	2.06	0.90
2:H:13:ILE:HD11	2:H:17:LYS:CB	2.02	0.90
3:C:133:PRO:HB3	3:C:145:ILE:HD11	1.52	0.89
1:A:182:SER:CB	1:A:183:ASP:CB	2.51	0.89
1:G:145:THR:HA	1:G:194:ILE:HD11	1.54	0.88
2:H:13:ILE:HD11	2:H:17:LYS:HB2	1.53	0.88
3:C:131:TRP:H	3:C:149:ASN:HD21	1.16	0.88
2:B:13:ILE:HD11	2:B:17:LYS:CB	2.03	0.87
2:B:13:ILE:HD11	2:B:17:LYS:HB2	1.55	0.87
1:A:158:THR:CG2	1:A:176:VAL:H	1.91	0.84
1:G:158:THR:CG2	1:G:176:VAL:H	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CZ	1:A:189:ALA:HB2	2.12	0.83
1:A:6:SER:HB2	1:G:16:LYS:HE3	1.60	0.83
3:C:241:ASP:OD1	9:C:306:GOL:H11	1.79	0.83
1:A:152:ASP:O	1:A:155:VAL:N	2.12	0.82
1:G:184:PHE:CZ	1:G:189:ALA:HB2	2.13	0.81
1:A:195:ILE:CB	1:A:196:PRO:CD	2.57	0.81
1:G:179:SER:OG	1:G:181:LYS:HG2	1.81	0.79
3:C:13:LEU:HB2	3:C:29:LEU:HD13	1.65	0.79
3:C:94:LEU:HD22	3:C:118:PHE:CE1	2.17	0.79
1:A:194:ILE:HD12	1:A:195:ILE:H	1.48	0.79
4:D:40:LEU:HD21	4:D:81:ARG:NH1	1.98	0.78
3:C:240:ALA:HB3	9:C:306:GOL:H12	1.66	0.78
3:C:34:GLU:OE2	3:C:215:LYS:HB2	1.84	0.78
1:A:13:LEU:HB2	1:A:16:LYS:HD3	1.65	0.78
2:B:114:LEU:O	2:B:114:LEU:HD12	1.85	0.77
3:C:148:LEU:HD11	6:C:303:LSC:H6A	1.65	0.77
3:C:250:LEU:HD23	3:C:251:ASP:H	1.49	0.77
1:G:125:LEU:HD23	2:H:133:PRO:HA	1.67	0.77
2:H:114:LEU:O	2:H:114:LEU:HD12	1.85	0.76
1:G:13:LEU:HB2	1:G:16:LYS:HD3	1.68	0.76
3:C:13:LEU:HB2	3:C:29:LEU:CD1	2.16	0.75
2:B:130:VAL:HG23	2:B:240:ALA:HB3	1.69	0.75
3:C:277:TYR:O	3:C:278:TRP:HB2	1.84	0.75
1:A:182:SER:CB	1:A:184:PHE:H	2.00	0.74
4:D:92:ILE:O	4:D:92:ILE:HD12	1.87	0.74
4:D:33:SER:HB3	4:D:62:PHE:CZ	2.23	0.74
2:B:95:GLU:HG2	2:B:96:GLU:H	1.52	0.74
2:H:130:VAL:HG23	2:H:240:ALA:HB3	1.69	0.74
4:D:10:TYR:CE1	4:D:24:ASN:HB2	2.21	0.74
1:A:182:SER:CB	1:A:184:PHE:N	2.51	0.73
3:C:46:THR:HA	3:C:67:GLN:NE2	2.03	0.73
1:A:184:PHE:HZ	1:A:189:ALA:HB2	1.53	0.73
3:C:240:ALA:HB3	9:C:306:GOL:H32	1.71	0.73
3:C:31:TRP:CZ3	3:C:36:GLN:HB2	2.23	0.73
2:B:76:LEU:HD23	2:B:77:THR:N	2.04	0.73
1:A:16:LYS:HE3	1:G:6:SER:HB2	1.71	0.73
2:B:186:LEU:N	2:B:186:LEU:HD23	2.04	0.72
1:G:191:ASN:OD1	1:G:192:ASN:CA	2.37	0.72
2:H:76:LEU:HD23	2:H:77:THR:N	2.04	0.72
3:C:133:PRO:HB3	3:C:145:ILE:CD1	2.19	0.72
3:C:94:LEU:HD22	3:C:118:PHE:CZ	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:ILE:CD1	2:H:17:LYS:HB2	2.20	0.71
2:B:13:ILE:CD1	2:B:17:LYS:HB2	2.21	0.71
2:B:158:VAL:HG13	2:B:215:VAL:HG13	1.71	0.71
2:H:158:VAL:HG13	2:H:215:VAL:HG13	1.71	0.71
3:C:241:ASP:HB2	3:C:243:THR:HG23	1.73	0.71
3:C:238:PRO:HG2	4:D:65:LEU:HD22	1.74	0.70
1:G:147:VAL:HG22	1:G:193:SER:OG	1.91	0.70
3:C:235:ASP:O	3:C:237:LEU:HD13	1.91	0.70
3:C:88:LEU:CB	3:C:90:LEU:HD21	2.21	0.70
4:D:49:VAL:HG12	4:D:68:THR:HG21	1.71	0.70
2:B:20:THR:HG22	2:B:77:THR:HG23	1.74	0.70
3:C:67:GLN:HG2	3:C:71:ARG:NH2	2.06	0.70
2:H:220:LEU:HD13	2:H:233:PRO:HG2	1.74	0.70
1:G:184:PHE:HZ	1:G:189:ALA:HB2	1.55	0.69
1:G:93:ASP:OD2	1:G:94:ARG:HG2	1.92	0.69
2:H:130:VAL:HG23	2:H:240:ALA:CB	2.23	0.69
1:G:149:GLN:O	1:G:151:LYS:N	2.26	0.69
6:C:303:LSC:O25	1:G:27:SER:OG	2.09	0.69
2:B:130:VAL:HG23	2:B:240:ALA:CB	2.23	0.69
3:C:29:LEU:HD12	3:C:29:LEU:N	2.08	0.69
2:B:160:LEU:HD23	2:B:161:SER:N	2.07	0.69
1:G:194:ILE:O	1:G:194:ILE:HD12	1.93	0.69
3:C:131:TRP:O	3:C:132:GLU:HG3	1.92	0.68
2:B:29:HIS:CE1	2:B:95:GLU:HG3	2.29	0.68
2:B:220:LEU:HD13	2:B:233:PRO:HG2	1.74	0.68
2:H:160:LEU:HD23	2:H:161:SER:N	2.09	0.68
1:G:32:LEU:HD13	1:G:33:ARG:N	2.09	0.68
3:C:166:CYS:N	3:C:167:PRO:HD2	2.09	0.67
1:A:32:LEU:HD13	1:A:33:ARG:N	2.08	0.67
1:A:198:ASP:OD2	2:B:140:HIS:ND1	2.26	0.67
1:A:188:ASN:O	1:A:190:PHE:N	2.28	0.67
3:C:250:LEU:HD23	3:C:251:ASP:N	2.08	0.67
3:C:118:PHE:HB3	3:C:123:ILE:HG21	1.77	0.67
4:D:49:VAL:HA	4:D:68:THR:HG22	1.76	0.67
2:H:20:THR:HG22	2:H:77:THR:HG23	1.76	0.67
1:G:158:THR:HG22	1:G:176:VAL:N	2.05	0.66
1:A:158:THR:HG22	1:A:176:VAL:N	2.05	0.66
3:C:40:TRP:HE3	8:C:305:D12:H12	1.55	0.66
2:H:66:VAL:HG11	2:H:74:PHE:CZ	2.30	0.66
1:G:33:ARG:HG2	1:G:48:ILE:CD1	2.26	0.66
2:B:13:ILE:HD11	2:B:17:LYS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:VAL:H	3:C:67:GLN:NE2	1.94	0.65
3:C:118:PHE:HB2	3:C:123:ILE:HD13	1.79	0.65
2:H:13:ILE:HD11	2:H:17:LYS:HB3	1.77	0.65
1:A:33:ARG:HG2	1:A:48:ILE:CD1	2.26	0.65
1:G:191:ASN:OD1	1:G:192:ASN:N	2.29	0.65
1:A:6:SER:CB	1:G:16:LYS:HE3	2.26	0.65
1:G:162:VAL:HG22	1:G:173:ASN:OD1	1.97	0.64
2:B:66:VAL:HG11	2:B:74:PHE:CZ	2.31	0.64
3:C:88:LEU:HB2	3:C:90:LEU:HD21	1.78	0.64
1:A:135:VAL:HG23	1:A:178:TRP:CB	2.26	0.64
1:A:182:SER:CB	1:A:183:ASP:CA	2.75	0.64
3:C:54:SER:O	3:C:173:LEU:HD21	1.96	0.64
2:B:183:GLN:HB3	2:B:186:LEU:HD21	1.79	0.64
1:A:191:ASN:ND2	2:H:185:ALA:C	2.51	0.64
3:C:187:PRO:HB3	3:C:212:PHE:HB3	1.78	0.64
3:C:166:CYS:O	3:C:170:VAL:HG23	1.98	0.64
1:G:54:ASN:N	1:G:54:ASN:OD1	2.31	0.64
1:G:188:ASN:O	1:G:190:PHE:N	2.31	0.63
3:C:153:TRP:CZ2	6:C:303:LSC:H35	2.34	0.63
3:C:211:GLY:HA3	4:D:12:ARG:NH2	2.14	0.63
1:G:135:VAL:HG23	1:G:178:TRP:CB	2.25	0.63
1:A:54:ASN:N	1:A:54:ASN:OD1	2.31	0.63
1:G:163:LEU:HB3	2:H:174:CYS:CB	2.28	0.63
1:G:163:LEU:HB3	2:H:174:CYS:HB2	1.80	0.62
1:G:191:ASN:OD1	1:G:192:ASN:HB2	1.99	0.62
1:A:170:PHE:CE2	2:B:143:LYS:HE3	2.33	0.62
3:C:127:GLN:HB2	3:C:132:GLU:OE1	1.99	0.62
1:A:194:ILE:CD1	1:A:195:ILE:H	2.12	0.62
3:C:213:TYR:C	3:C:213:TYR:CD2	2.73	0.62
3:C:151:ASP:OD1	3:C:154:THR:HG22	2.00	0.62
1:A:191:ASN:HD21	2:H:185:ALA:C	2.04	0.61
1:A:48:ILE:HD11	2:B:105:THR:OG1	2.01	0.61
3:C:241:ASP:CB	3:C:243:THR:HG23	2.30	0.61
2:H:123:VAL:O	2:H:230:ARG:NH2	2.34	0.61
3:C:211:GLY:HA3	4:D:12:ARG:HH21	1.65	0.60
1:G:188:ASN:O	1:G:191:ASN:N	2.34	0.60
1:A:194:ILE:HG13	1:A:195:ILE:N	2.16	0.60
3:C:208:HIS:N	3:C:208:HIS:CD2	2.69	0.60
2:B:77:THR:C	2:B:78:LEU:HD12	2.22	0.60
1:A:192:ASN:O	1:A:194:ILE:N	2.35	0.60
1:A:125:LEU:HD23	2:B:133:PRO:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:THR:O	3:C:69:ILE:HD13	2.02	0.60
3:C:34:GLU:O	3:C:35:LEU:HD23	2.02	0.59
3:C:213:TYR:CD2	3:C:214:PRO:N	2.70	0.59
1:A:49:MET:CE	1:A:65:LEU:HB2	2.31	0.59
2:B:123:VAL:O	2:B:230:ARG:NH2	2.35	0.59
3:C:133:PRO:HD3	3:C:145:ILE:HD13	1.82	0.59
1:G:49:MET:CE	1:G:65:LEU:HB2	2.32	0.59
3:C:88:LEU:HB3	3:C:90:LEU:HD21	1.84	0.59
1:A:162:VAL:HG22	1:A:173:ASN:OD1	2.02	0.59
3:C:177:GLY:O	3:C:181:LEU:HD13	2.03	0.59
1:G:135:VAL:CG2	1:G:178:TRP:HB3	2.26	0.58
2:H:77:THR:C	2:H:78:LEU:HD12	2.23	0.58
1:G:60:ARG:NH2	1:G:83:ASP:OD1	2.35	0.58
2:H:66:VAL:HG11	2:H:74:PHE:CE2	2.37	0.58
2:B:95:GLU:HG2	2:B:96:GLU:N	2.17	0.58
1:A:170:PHE:CZ	2:B:143:LYS:HE3	2.39	0.58
3:C:213:TYR:C	3:C:213:TYR:HD2	2.07	0.58
3:C:240:ALA:CB	9:C:306:GOL:H12	2.32	0.58
3:C:237:LEU:HD23	4:D:10:TYR:CE2	2.38	0.58
4:D:37:VAL:HG11	4:D:66:TYR:CD1	2.38	0.57
4:D:38:ASP:OD2	4:D:81:ARG:NH2	2.36	0.57
1:G:49:MET:HE3	1:G:65:LEU:HB2	1.85	0.57
1:A:125:LEU:HD23	2:B:132:GLU:O	2.04	0.57
2:B:66:VAL:HG11	2:B:74:PHE:CE2	2.38	0.57
1:A:135:VAL:CG2	1:A:178:TRP:HB3	2.27	0.57
4:D:10:TYR:CD1	4:D:24:ASN:HB2	2.40	0.57
1:A:60:ARG:NH2	1:A:83:ASP:OD1	2.38	0.57
4:D:3:ARG:O	4:D:86:THR:HG21	2.05	0.57
1:A:119:ASP:OD1	2:B:140:HIS:NE2	2.37	0.56
3:C:35:LEU:HD21	3:C:213:TYR:HE1	1.69	0.56
2:B:133:PRO:HG3	2:B:146:LEU:HD12	1.86	0.56
2:B:133:PRO:HD2	2:B:204:TRP:CZ2	2.40	0.56
2:H:226:TRP:HB2	2:H:232:LYS:HE2	1.87	0.56
4:D:7:ILE:HB	4:D:93:VAL:HG21	1.86	0.56
2:H:133:PRO:HG3	2:H:146:LEU:HD12	1.88	0.56
3:C:231:THR:O	3:C:233:PRO:HD3	2.06	0.56
3:C:46:THR:CA	3:C:67:GLN:NE2	2.68	0.56
3:C:40:TRP:CZ3	3:C:70:PHE:HB3	2.41	0.56
2:H:133:PRO:HD2	2:H:204:TRP:CZ2	2.41	0.56
3:C:68:HIS:HA	3:C:71:ARG:NH1	2.21	0.56
1:A:188:ASN:O	1:A:191:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:TRP:CZ3	8:C:305:D12:H12	2.41	0.55
1:A:182:SER:CA	1:A:183:ASP:CB	2.84	0.55
3:C:29:LEU:HD12	3:C:29:LEU:H	1.72	0.55
2:H:216:GLN:OE1	2:H:237:ILE:HD11	2.06	0.55
3:C:72:VAL:HG11	6:C:303:LSC:H21	1.87	0.55
3:C:67:GLN:HG2	3:C:71:ARG:HH21	1.71	0.55
2:B:25:GLN:HG2	2:B:32:MET:HE3	1.88	0.55
3:C:238:PRO:HB3	3:C:244:TRP:CZ3	2.41	0.55
1:A:194:ILE:CG1	1:A:195:ILE:N	2.69	0.55
3:C:9:PRO:HD2	3:C:33:GLY:HA2	1.88	0.55
1:A:191:ASN:HB2	2:H:187:ASN:CA	2.37	0.55
1:A:35:TYR:OH	2:B:106:GLN:HB2	2.07	0.55
1:A:148:SER:OG	1:G:151:LYS:HE3	2.07	0.55
2:B:216:GLN:HA	2:B:237:ILE:HD13	1.89	0.55
1:G:113:PRO:HD3	1:G:162:VAL:HG21	1.89	0.54
2:H:24:SER:HA	2:H:72:GLU:O	2.07	0.54
3:C:121:LYS:O	3:C:123:ILE:HG23	2.08	0.54
1:G:7:PRO:O	1:G:107:THR:HG23	2.08	0.54
2:B:207:PRO:HA	2:B:244:GLY:O	2.06	0.54
2:B:31:LYS:HA	2:B:49:SER:O	2.07	0.54
2:B:24:SER:HA	2:B:72:GLU:O	2.08	0.54
3:C:129:THR:HA	3:C:159:GLN:OE1	2.08	0.54
2:H:34:TRP:O	2:H:46:ILE:HG12	2.08	0.54
1:A:184:PHE:CE2	1:A:189:ALA:HB2	2.42	0.54
1:G:156:TYR:O	1:G:177:ALA:HA	2.08	0.54
1:G:191:ASN:OD1	1:G:192:ASN:CB	2.56	0.54
2:B:47:HIS:CB	2:B:66:VAL:HG21	2.37	0.54
4:D:41:LYS:HG2	4:D:42:ASN:ND2	2.22	0.54
2:H:114:LEU:C	2:H:114:LEU:HD12	2.28	0.54
2:H:31:LYS:HA	2:H:49:SER:O	2.08	0.54
1:A:7:PRO:O	1:A:107:THR:HG23	2.08	0.54
2:H:216:GLN:HA	2:H:237:ILE:HD13	1.89	0.54
2:B:226:TRP:HB2	2:B:232:LYS:HE2	1.90	0.54
2:B:76:LEU:C	2:B:76:LEU:HD23	2.29	0.54
3:C:100:ALA:HB2	3:C:114:PHE:HA	1.90	0.54
3:C:222:MET:CB	3:C:227:GLU:HA	2.38	0.54
1:A:188:ASN:O	1:A:189:ALA:C	2.45	0.53
3:C:154:THR:HG23	3:C:155:ARG:N	2.23	0.53
3:C:25:ARG:C	3:C:25:ARG:HD2	2.28	0.53
2:H:207:PRO:HA	2:H:244:GLY:O	2.08	0.53
2:H:25:GLN:CG	2:H:32:MET:HE3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:ASP:OD1	3:C:71:ARG:NE	2.39	0.53
1:A:113:PRO:HD3	1:A:162:VAL:HG21	1.89	0.53
2:B:216:GLN:OE1	2:B:237:ILE:HD11	2.07	0.53
3:C:170:VAL:O	3:C:174:LEU:HG	2.09	0.53
1:G:184:PHE:CE2	1:G:189:ALA:HB2	2.44	0.53
2:H:47:HIS:CB	2:H:66:VAL:HG21	2.37	0.53
4:D:10:TYR:CE1	4:D:24:ASN:CB	2.90	0.53
3:C:241:ASP:O	3:C:242:GLU:HB2	2.08	0.53
2:H:76:LEU:C	2:H:76:LEU:HD23	2.29	0.53
3:C:190:TRP:CZ2	4:D:14:PRO:HG3	2.43	0.53
3:C:185:VAL:HG12	3:C:211:GLY:O	2.09	0.53
3:C:25:ARG:O	3:C:25:ARG:HD2	2.09	0.53
2:B:160:LEU:HD23	2:B:160:LEU:C	2.29	0.53
2:B:34:TRP:CD1	2:B:74:PHE:CE1	2.97	0.53
2:B:90:LEU:HD23	2:B:111:GLY:CA	2.38	0.53
3:C:14:GLN:HB3	3:C:98:VAL:HB	1.91	0.53
3:C:116:VAL:HG12	3:C:124:LEU:HD12	1.90	0.52
2:B:114:LEU:C	2:B:114:LEU:HD12	2.30	0.52
3:C:76:SER:HB3	6:C:303:LSC:H14	1.89	0.52
3:C:34:GLU:C	3:C:35:LEU:HD23	2.29	0.52
3:C:250:LEU:CD2	3:C:251:ASP:N	2.72	0.52
2:B:34:TRP:O	2:B:46:ILE:HG12	2.10	0.52
3:C:41:SER:OG	3:C:44:SER:HB3	2.09	0.52
2:H:66:VAL:CG1	2:H:74:PHE:CE2	2.92	0.52
2:H:34:TRP:CD1	2:H:74:PHE:CE1	2.97	0.52
2:H:90:LEU:HD23	2:H:111:GLY:CA	2.40	0.52
3:C:140:TRP:CZ3	3:C:141:VAL:HG22	2.43	0.52
3:C:76:SER:HA	1:G:94:ARG:HH12	1.75	0.52
2:H:90:LEU:HD23	2:H:111:GLY:HA2	1.92	0.52
1:A:138:PHE:CZ	1:A:194:ILE:HG21	2.45	0.52
2:B:187:ASN:N	2:B:187:ASN:OD1	2.31	0.52
2:B:176:ASP:HB2	2:B:193:LEU:HD12	1.92	0.52
3:C:116:VAL:CG1	3:C:124:LEU:HD12	2.40	0.52
3:C:8:PHE:CE2	3:C:181:LEU:HD23	2.45	0.52
3:C:74:ARG:O	3:C:78:THR:OG1	2.28	0.52
1:A:156:TYR:O	1:A:177:ALA:HA	2.10	0.52
1:A:49:MET:HE3	1:A:65:LEU:HB2	1.92	0.52
3:C:161:LEU:HA	3:C:165:THR:HB	1.92	0.52
3:C:57:THR:HG23	3:C:172:GLY:HA2	1.92	0.52
1:G:188:ASN:O	1:G:189:ALA:C	2.47	0.52
2:B:10:TYR:CD2	2:B:157:HIS:HB3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:PHE:O	1:G:195:ILE:HD11	2.10	0.51
3:C:151:ASP:CG	3:C:154:THR:HG22	2.31	0.51
2:H:10:TYR:CD2	2:H:157:HIS:HB3	2.44	0.51
2:H:176:ASP:HB2	2:H:193:LEU:HD12	1.92	0.51
2:B:25:GLN:OE1	2:B:29:HIS:HB2	2.11	0.51
2:B:95:GLU:CG	2:B:96:GLU:H	2.10	0.51
3:C:179:SER:O	3:C:182:LYS:HG2	2.09	0.51
3:C:187:PRO:HB3	3:C:212:PHE:HD1	1.75	0.51
3:C:8:PHE:CD2	3:C:181:LEU:HD23	2.45	0.51
3:C:122:ASP:HB3	3:C:134:THR:HG21	1.92	0.51
3:C:261:SER:HB2	3:C:276:LEU:O	2.10	0.51
2:B:47:HIS:CD2	2:B:66:VAL:HG23	2.46	0.51
2:H:160:LEU:C	2:H:160:LEU:HD23	2.31	0.51
2:B:220:LEU:HD12	2:B:220:LEU:N	2.25	0.51
2:B:90:LEU:HD23	2:B:111:GLY:HA2	1.91	0.51
1:A:11:ILE:O	1:G:8:GLN:HB2	2.11	0.51
2:B:66:VAL:CG1	2:B:74:PHE:CE2	2.94	0.51
1:A:191:ASN:HB2	2:H:187:ASN:CB	2.41	0.51
2:H:25:GLN:HG2	2:H:32:MET:HE3	1.91	0.51
1:G:191:ASN:OD1	1:G:192:ASN:HA	2.09	0.51
2:H:88:GLN:HG3	2:H:113:ARG:HG2	1.93	0.51
3:C:143:LEU:HA	3:C:146:GLN:OE1	2.11	0.50
3:C:210:SER:HB3	3:C:245:TYR:CD1	2.46	0.50
3:C:90:LEU:HD23	3:C:90:LEU:N	2.26	0.50
3:C:92:TYR:N	3:C:92:TYR:CD2	2.78	0.50
4:D:54:LEU:HA	4:D:64:LEU:HD13	1.92	0.50
4:D:54:LEU:HD12	4:D:64:LEU:HD13	1.93	0.50
4:D:49:VAL:HB	4:D:68:THR:HG22	1.94	0.50
3:C:15:ILE:HD13	4:D:62:PHE:HE1	1.76	0.50
4:D:10:TYR:O	4:D:23:LEU:HD12	2.11	0.50
4:D:49:VAL:HB	4:D:68:THR:CG2	2.41	0.50
3:C:237:LEU:N	3:C:237:LEU:CD1	2.74	0.50
4:D:33:SER:HB3	4:D:62:PHE:CE2	2.46	0.50
2:H:47:HIS:CD2	2:H:66:VAL:HG23	2.46	0.50
2:B:88:GLN:HG3	2:B:113:ARG:HG2	1.93	0.50
3:C:130:SER:HB2	3:C:149:ASN:ND2	2.26	0.50
3:C:35:LEU:HD21	3:C:213:TYR:CE1	2.46	0.50
2:H:25:GLN:OE1	2:H:29:HIS:HB2	2.11	0.50
1:G:163:LEU:C	1:G:163:LEU:HD12	2.31	0.50
2:B:158:VAL:HG13	2:B:215:VAL:CG1	2.40	0.50
2:B:45:LEU:HD13	2:B:58:GLY:HA3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:SER:HB2	2:B:76:LEU:HD21	1.94	0.50
3:C:262:CYS:O	3:C:275:VAL:HA	2.11	0.50
2:B:25:GLN:CG	2:B:32:MET:HE3	2.42	0.49
2:H:52:VAL:O	2:H:53:ASN:HB2	2.12	0.49
3:C:213:TYR:HD2	3:C:214:PRO:N	2.10	0.49
1:A:127:ASP:OD1	1:A:128:SER:N	2.45	0.49
1:A:16:LYS:HE3	1:G:6:SER:CB	2.40	0.49
2:H:114:LEU:C	2:H:114:LEU:CD1	2.81	0.49
2:H:45:LEU:HD13	2:H:58:GLY:HA3	1.94	0.49
1:G:127:ASP:OD1	1:G:128:SER:N	2.46	0.49
1:G:33:ARG:HG2	1:G:48:ILE:HD13	1.94	0.49
2:H:158:VAL:HG13	2:H:215:VAL:CG1	2.39	0.49
2:H:79:GLU:OE1	2:H:79:GLU:HA	2.12	0.49
2:H:64:SER:HB2	2:H:76:LEU:HD21	1.94	0.49
1:A:33:ARG:HG2	1:A:48:ILE:HD13	1.95	0.49
3:C:212:PHE:CE2	3:C:244:TRP:HB2	2.48	0.49
4:D:40:LEU:HD21	4:D:81:ARG:HH12	1.73	0.49
1:A:163:LEU:C	1:A:163:LEU:HD12	2.33	0.49
3:C:126:PHE:CD1	3:C:158:VAL:HG11	2.48	0.49
2:B:186:LEU:H	2:B:186:LEU:HD23	1.75	0.49
3:C:266:HIS:CG	3:C:267:SER:H	2.31	0.49
3:C:92:TYR:H	3:C:92:TYR:HD2	1.59	0.49
3:C:180:GLU:O	3:C:183:LYS:HG2	2.13	0.48
4:D:49:VAL:CB	4:D:68:THR:HG22	2.43	0.48
1:A:191:ASN:ND2	2:H:186:LEU:N	2.62	0.48
1:A:32:LEU:C	1:A:32:LEU:CD1	2.81	0.48
1:A:152:ASP:OD2	2:H:185:ALA:CB	2.61	0.48
1:A:163:LEU:HB3	2:B:174:CYS:CB	2.44	0.48
3:C:20:ASN:C	3:C:22:SER:H	2.15	0.48
3:C:222:MET:HB3	3:C:227:GLU:CB	2.43	0.48
3:C:31:TRP:CH2	3:C:36:GLN:HB2	2.49	0.48
2:H:94:SER:OG	2:H:96:GLU:HB2	2.13	0.48
1:A:163:LEU:HB3	2:B:174:CYS:HB3	1.95	0.48
1:A:182:SER:CB	1:A:183:ASP:C	2.82	0.48
3:C:123:ILE:HG13	3:C:124:LEU:N	2.28	0.48
3:C:46:THR:HG22	3:C:67:GLN:NE2	2.28	0.48
1:G:132:ASP:O	1:G:133:LYS:C	2.51	0.48
1:G:32:LEU:CD1	1:G:32:LEU:C	2.82	0.48
2:H:160:LEU:HD13	2:H:195:SER:HB2	1.95	0.48
2:H:220:LEU:N	2:H:220:LEU:HD12	2.27	0.48
1:A:138:PHE:O	1:A:174:SER:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LEU:HD13	2:B:195:SER:HB2	1.95	0.48
3:C:153:TRP:CZ2	6:C:303:LSC:C35	2.96	0.48
3:C:222:MET:HB2	3:C:227:GLU:HA	1.95	0.48
4:D:37:VAL:HB	4:D:66:TYR:CE1	2.48	0.48
1:G:60:ARG:NH2	1:G:83:ASP:OD2	2.46	0.48
2:B:125:PRO:HD3	2:B:233:PRO:HB3	1.96	0.48
4:D:84:HIS:H	4:D:87:LEU:HB2	1.78	0.48
2:H:125:PRO:HD3	2:H:233:PRO:HB3	1.96	0.48
2:B:122:ASN:ND2	2:B:188:ASP:OD2	2.47	0.47
2:H:47:HIS:CG	2:H:66:VAL:CG2	2.98	0.47
1:G:163:LEU:HB3	2:H:174:CYS:HB3	1.96	0.47
1:A:191:ASN:ND2	2:H:186:LEU:CA	2.77	0.47
1:G:32:LEU:HD13	1:G:32:LEU:C	2.35	0.47
2:H:25:GLN:CD	2:H:32:MET:HE3	2.34	0.47
4:D:7:ILE:HD11	4:D:82:VAL:HB	1.96	0.47
2:B:114:LEU:C	2:B:114:LEU:CD1	2.82	0.47
1:A:198:ASP:OD2	2:B:140:HIS:CE1	2.68	0.47
4:D:65:LEU:HD12	4:D:66:TYR:N	2.29	0.47
2:B:47:HIS:CG	2:B:66:VAL:CG2	2.97	0.47
1:G:138:PHE:O	1:G:174:SER:HA	2.14	0.47
2:B:86:THR:HA	2:B:114:LEU:CD1	2.45	0.47
3:C:116:VAL:O	3:C:123:ILE:HG12	2.15	0.47
1:A:32:LEU:HD13	1:A:32:LEU:C	2.34	0.47
3:C:12:CYS:C	3:C:13:LEU:HD12	2.36	0.47
2:H:86:THR:O	2:H:87:SER:HB2	2.13	0.47
3:C:187:PRO:HB2	3:C:209:VAL:HG12	1.97	0.47
1:G:125:LEU:HB3	2:H:132:GLU:O	2.14	0.47
2:B:51:GLY:O	2:B:54:SER:HB3	2.15	0.46
2:B:86:THR:O	2:B:87:SER:HB2	2.15	0.46
1:G:133:LYS:O	2:H:131:PHE:HE2	1.97	0.46
3:C:37:THR:OG1	3:C:38:HIS:ND1	2.35	0.46
2:H:11:LEU:HD12	2:H:12:VAL:N	2.30	0.46
1:A:60:ARG:NH2	1:A:83:ASP:OD2	2.47	0.46
3:C:95:GLU:HG3	4:D:32:PRO:HB3	1.97	0.46
1:G:179:SER:HG	1:G:181:LYS:HG2	1.81	0.46
3:C:181:LEU:N	3:C:181:LEU:HD12	2.29	0.46
3:C:187:PRO:HB3	3:C:212:PHE:CD1	2.50	0.46
3:C:53:TRP:CH2	3:C:181:LEU:HD11	2.50	0.46
3:C:21:SER:HA	3:C:92:TYR:CE1	2.51	0.46
3:C:269:LEU:CD1	3:C:274:ILE:HG13	2.35	0.46
3:C:213:TYR:CD2	3:C:214:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:VAL:HG22	3:C:116:VAL:HG23	1.98	0.46
2:H:51:GLY:O	2:H:54:SER:HB3	2.15	0.46
2:H:47:HIS:CG	2:H:66:VAL:HG21	2.51	0.46
3:C:137:ALA:HA	3:C:138:PRO:HD3	1.81	0.46
3:C:213:TYR:CD2	3:C:214:PRO:CA	2.99	0.46
4:D:29:GLY:HA2	4:D:61:SER:HB2	1.97	0.46
2:B:47:HIS:CG	2:B:66:VAL:HG21	2.51	0.45
2:B:82:ARG:HG3	2:B:83:PRO:HD2	1.99	0.45
3:C:116:VAL:CG1	3:C:124:LEU:CD1	2.94	0.45
1:A:152:ASP:OD2	2:H:185:ALA:HB3	2.17	0.45
1:A:174:SER:OG	2:B:196:ARG:HD2	2.17	0.45
2:H:86:THR:HA	2:H:114:LEU:CD1	2.47	0.45
2:B:11:LEU:HD12	2:B:12:VAL:N	2.32	0.45
3:C:140:TRP:CE3	3:C:140:TRP:C	2.90	0.45
4:D:49:VAL:CA	4:D:68:THR:HG22	2.44	0.45
1:A:191:ASN:ND2	2:H:185:ALA:O	2.50	0.45
1:G:125:LEU:CD2	2:H:133:PRO:HA	2.41	0.45
2:B:186:LEU:CD2	2:B:186:LEU:N	2.76	0.45
3:C:240:ALA:HB3	9:C:306:GOL:C3	2.43	0.45
3:C:28:GLY:HA3	8:C:305:D12:H31	1.99	0.45
1:A:151:LYS:CA	1:A:155:VAL:O	2.49	0.44
3:C:237:LEU:HD13	3:C:237:LEU:N	2.31	0.44
4:D:33:SER:HB3	4:D:62:PHE:CE1	2.53	0.44
3:C:20:ASN:C	3:C:22:SER:N	2.71	0.44
2:H:31:LYS:HE2	2:H:33:TYR:CE2	2.52	0.44
2:B:124:PHE:CB	2:B:190:ARG:HD3	2.47	0.44
3:C:119:GLN:HA	3:C:119:GLN:OE1	2.18	0.44
3:C:17:SER:OG	3:C:25:ARG:NE	2.48	0.44
2:B:176:ASP:OD2	2:B:194:SER:HB3	2.17	0.44
2:B:201:ALA:O	2:B:205:GLN:HG3	2.18	0.44
3:C:166:CYS:N	3:C:167:PRO:CD	2.80	0.44
1:G:125:LEU:HD23	2:H:133:PRO:CA	2.41	0.44
2:H:126:PRO:CA	2:H:153:PHE:HB3	2.48	0.44
1:A:125:LEU:HD23	2:B:133:PRO:CA	2.48	0.44
2:B:70:ARG:HE	2:B:70:ARG:HB2	1.65	0.44
3:C:47:VAL:N	3:C:67:GLN:NE2	2.64	0.44
2:H:176:ASP:OD2	2:H:194:SER:HB3	2.18	0.43
2:B:95:GLU:O	2:B:96:GLU:CB	2.64	0.43
3:C:49:SER:HB3	3:C:54:SER:HB2	2.00	0.43
2:H:124:PHE:CB	2:H:190:ARG:HD3	2.48	0.43
1:A:125:LEU:CD2	2:B:133:PRO:HA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:PRO:CA	2:B:153:PHE:HB3	2.48	0.43
3:C:129:THR:HG22	3:C:159:GLN:OE1	2.18	0.43
3:C:251:ASP:C	3:C:252:VAL:HG22	2.38	0.43
3:C:266:HIS:CG	3:C:267:SER:N	2.87	0.43
2:B:95:GLU:HB3	2:B:104:GLY:HA3	2.00	0.43
1:G:123:TYR:CE2	2:H:137:GLU:HG3	2.53	0.43
2:H:34:TRP:HD1	2:H:74:PHE:CE1	2.37	0.43
3:C:114:PHE:HB3	3:C:126:PHE:HB3	2.01	0.43
3:C:208:HIS:HD2	3:C:208:HIS:N	2.17	0.43
1:A:191:ASN:HB2	2:H:187:ASN:HA	2.01	0.43
1:A:125:LEU:HB3	2:B:132:GLU:O	2.19	0.43
2:B:47:HIS:CD2	2:B:66:VAL:CG2	3.02	0.43
3:C:19:ALA:O	3:C:92:TYR:HB3	2.19	0.43
3:C:69:ILE:HD12	3:C:69:ILE:N	2.34	0.43
4:D:51:HIS:HB3	4:D:66:TYR:CD2	2.53	0.43
3:C:222:MET:HB3	3:C:227:GLU:HA	1.99	0.43
2:H:138:ILE:HG23	2:H:201:ALA:HB1	2.01	0.43
3:C:277:TYR:HB2	3:C:278:TRP:CE3	2.53	0.43
3:C:237:LEU:HD23	4:D:10:TYR:CD2	2.54	0.43
3:C:85:ALA:HA	3:C:90:LEU:HG	2.00	0.42
2:H:47:HIS:CD2	2:H:66:VAL:CG2	3.02	0.42
3:C:131:TRP:C	3:C:132:GLU:HG3	2.39	0.42
3:C:158:VAL:O	3:C:162:LEU:HG	2.19	0.42
6:C:303:LSC:H22A	6:C:303:LSC:H30	2.01	0.42
2:H:201:ALA:O	2:H:205:GLN:HG3	2.20	0.42
3:C:196:SER:HA	3:C:197:PRO:HD3	1.85	0.42
1:G:193:SER:O	1:G:195:ILE:HG13	2.19	0.42
3:C:37:THR:OG1	3:C:38:HIS:N	2.51	0.42
2:H:130:VAL:HG23	2:H:240:ALA:HB1	2.01	0.42
2:H:140:HIS:C	2:H:140:HIS:CD2	2.93	0.42
1:A:152:ASP:C	1:A:154:ASP:N	2.73	0.42
2:B:25:GLN:OE1	2:B:32:MET:HE2	2.20	0.42
3:C:83:GLU:HB3	1:G:98:LEU:HD11	2.00	0.42
4:D:35:ILE:HD13	4:D:84:HIS:HD2	1.84	0.42
4:D:49:VAL:CB	4:D:68:THR:CG2	2.98	0.42
2:H:126:PRO:HD3	2:H:217:PHE:CD1	2.54	0.42
3:C:131:TRP:H	3:C:149:ASN:ND2	1.98	0.42
4:D:37:VAL:HB	4:D:66:TYR:CZ	2.55	0.42
2:H:176:ASP:HB2	2:H:193:LEU:CD1	2.50	0.42
1:A:33:ARG:HG2	1:A:48:ILE:HD12	2.01	0.42
2:B:138:ILE:HG23	2:B:201:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:SER:HA	3:C:182:LYS:HE2	2.02	0.42
3:C:231:THR:O	3:C:231:THR:HG23	2.20	0.42
2:B:140:HIS:C	2:B:140:HIS:CD2	2.93	0.41
3:C:129:THR:O	3:C:155:ARG:NH1	2.51	0.41
3:C:192:SER:HB3	3:C:208:HIS:NE2	2.35	0.41
3:C:54:SER:C	3:C:56:GLY:H	2.24	0.41
2:B:76:LEU:C	2:B:76:LEU:CD2	2.88	0.41
2:B:77:THR:O	2:B:78:LEU:HD12	2.20	0.41
4:D:31:HIS:ND1	4:D:32:PRO:HA	2.35	0.41
2:H:114:LEU:HD13	2:H:116:VAL:HG23	2.02	0.41
3:C:211:GLY:CA	4:D:12:ARG:NH2	2.83	0.41
1:G:33:ARG:HG2	1:G:48:ILE:HD12	2.02	0.41
3:C:133:PRO:CB	3:C:145:ILE:CD1	2.96	0.41
2:H:76:LEU:C	2:H:76:LEU:CD2	2.89	0.41
2:B:114:LEU:HD13	2:B:116:VAL:HG23	2.02	0.41
3:C:153:TRP:HB2	1:G:51:PHE:CZ	2.56	0.41
3:C:49:SER:HB3	3:C:54:SER:CB	2.50	0.41
4:D:73:THR:CG2	4:D:76:ASP:OD2	2.68	0.41
2:B:176:ASP:HB2	2:B:193:LEU:CD1	2.51	0.41
2:B:13:ILE:HG21	2:B:19:ILE:HD11	2.03	0.41
3:C:13:LEU:O	3:C:29:LEU:HD12	2.21	0.41
1:G:60:ARG:NH2	1:G:83:ASP:CG	2.74	0.41
1:G:131:SER:HA	1:G:132:ASP:HA	1.47	0.41
2:B:12:VAL:HG13	2:B:12:VAL:O	2.21	0.41
3:C:173:LEU:O	3:C:177:GLY:N	2.51	0.41
3:C:95:GLU:HG3	4:D:32:PRO:CB	2.51	0.41
2:B:86:THR:HA	2:B:114:LEU:HD12	2.03	0.40
3:C:263:ARG:HA	3:C:274:ILE:O	2.21	0.40
3:C:190:TRP:CH2	4:D:14:PRO:HG3	2.57	0.40
1:A:33:ARG:CG	1:A:48:ILE:HD13	2.51	0.40
2:B:126:PRO:HD3	2:B:217:PHE:CD1	2.56	0.40
2:B:34:TRP:HD1	2:B:74:PHE:CE1	2.37	0.40
1:G:33:ARG:CG	1:G:48:ILE:HD13	2.51	0.40
3:C:97:GLN:O	3:C:116:VAL:HG23	2.21	0.40
3:C:169:PHE:CE2	3:C:173:LEU:HD11	2.57	0.40
3:C:250:LEU:HD22	3:C:252:VAL:HG22	2.03	0.40
3:C:29:LEU:N	3:C:29:LEU:CD1	2.79	0.40
1:G:170:PHE:CZ	2:H:143:LYS:HE3	2.56	0.40
3:C:104:VAL:HA	3:C:110:SER:HB3	2.02	0.40
3:C:245:TYR:CD2	3:C:246:LEU:N	2.90	0.40
3:C:116:VAL:HG11	3:C:124:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ARG:HA	4:D:12:ARG:HD2	1.90	0.40
2:H:115:LEU:HD22	2:H:117:LEU:HD21	2.04	0.40
2:H:172:GLY:O	2:H:197:LEU:HA	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	190/213 (89%)	173 (91%)	12 (6%)	5 (3%)	5 22
1	G	195/213 (92%)	184 (94%)	9 (5%)	2 (1%)	15 45
2	B	228/259 (88%)	223 (98%)	5 (2%)	0	100 100
2	H	240/259 (93%)	232 (97%)	8 (3%)	0	100 100
3	C	257/276 (93%)	233 (91%)	22 (9%)	2 (1%)	19 50
4	D	91/99 (92%)	90 (99%)	1 (1%)	0	100 100
All	All	1201/1319 (91%)	1135 (94%)	57 (5%)	9 (1%)	22 52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ALA
1	A	192	ASN
1	A	195	ILE
1	G	189	ALA
1	G	133	LYS
1	A	184	PHE
1	A	193	SER
3	C	19	ALA
3	C	252	VAL

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	147/193 (76%)	144 (98%)	3 (2%)	55	78
1	G	169/193 (88%)	166 (98%)	3 (2%)	59	80
2	B	187/226 (83%)	174 (93%)	13 (7%)	15	41
2	H	192/226 (85%)	181 (94%)	11 (6%)	20	49
3	C	213/242 (88%)	202 (95%)	11 (5%)	23	52
4	D	81/94 (86%)	76 (94%)	5 (6%)	18	46
All	All	989/1174 (84%)	943 (95%)	46 (5%)	26	56

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	54	ASN
1	A	199	THR
2	B	7	THR
2	B	33	TYR
2	B	44	HIS
2	B	45	LEU
2	B	52	VAL
2	B	65	THR
2	B	114	LEU
2	B	115	LEU
2	B	174	CYS
2	B	180	LEU
2	B	186	LEU
2	B	187	ASN
2	B	213	CYS
3	C	24	THR
3	C	25	ARG
3	C	27	ASP
3	C	29	LEU
3	C	43	ASP
3	C	90	LEU

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Mol	Chain	Res	Type
3	C	92	TYR
3	C	208	HIS
3	C	213	TYR
3	C	237	LEU
3	C	252	VAL
4	D	12	ARG
4	D	36	GLU
4	D	42	ASN
4	D	49	VAL
4	D	83	ASN
1	G	32	LEU
1	G	54	ASN
1	G	97	THR
2	H	7	THR
2	H	33	TYR
2	H	44	HIS
2	H	45	LEU
2	H	52	VAL
2	H	65	THR
2	H	114	LEU
2	H	115	LEU
2	H	174	CYS
2	H	180	LEU
2	H	213	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	ASN
2	B	29	HIS
3	C	67	GLN
3	C	97	GLN
3	C	149	ASN
3	C	239	ASN
4	D	13	HIS
4	D	42	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides 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	E	1	3,5	14,14,15	0.54	0	17,19,21	1.16	0
5	FUC	E	2	5	10,10,11	0.75	0	14,14,16	0.76	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
5	NAG	E	1	3,5	-	3/6/23/26	0/1/1/1
5	FUC	E	2	5	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	$\#\|Z\| > 2$
7	HEX	C	304	-	5,5,5	0.22	0	4,4,4	0.38	0
9	GOL	C	306	-	5,5,5	0.36	0	5,5,5	0.30	0
8	D12	C	305	-	11,11,11	0.23	0	10,10,10	0.59	0
6	LSC	C	303	-	34,34,34	0.89	1 (2%)	39,41,41	0.85	2 (5%)

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
7	HEX	C	304	-	-	0/3/3/3	-
9	GOL	C	306	-	-	2/4/4/4	-
8	D12	C	305	-	-	2/9/9/9	-
6	LSC	C	303	-	-	13/36/36/36	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	303	LSC	O19-C18	4.31	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	303	LSC	O19-C18-C17	2.79	120.67	111.91
6	C	303	LSC	C30-C31-N32	-2.15	108.59	115.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	306	GOL	O1-C1-C2-C3
6	C	303	LSC	O35-C30-C31-N32
6	C	303	LSC	O33-C21-C22-O23
6	C	303	LSC	C5-C6-C7-C8
6	C	303	LSC	C10-C11-C12-C13
6	C	303	LSC	C4-C5-C6-C7
6	C	303	LSC	C12-C13-C14-C15
8	C	305	D12	C3-C4-C5-C6
8	C	305	D12	C9-C10-C11-C12
6	C	303	LSC	C20-C21-C22-O23
9	C	306	GOL	O1-C1-C2-O2
6	C	303	LSC	C11-C12-C13-C14
6	C	303	LSC	O19-C20-C21-C22
6	C	303	LSC	C30-C31-N32-C34
6	C	303	LSC	O19-C20-C21-O33
6	C	303	LSC	C16-C17-C18-O19
6	C	303	LSC	C16-C17-C18-O32

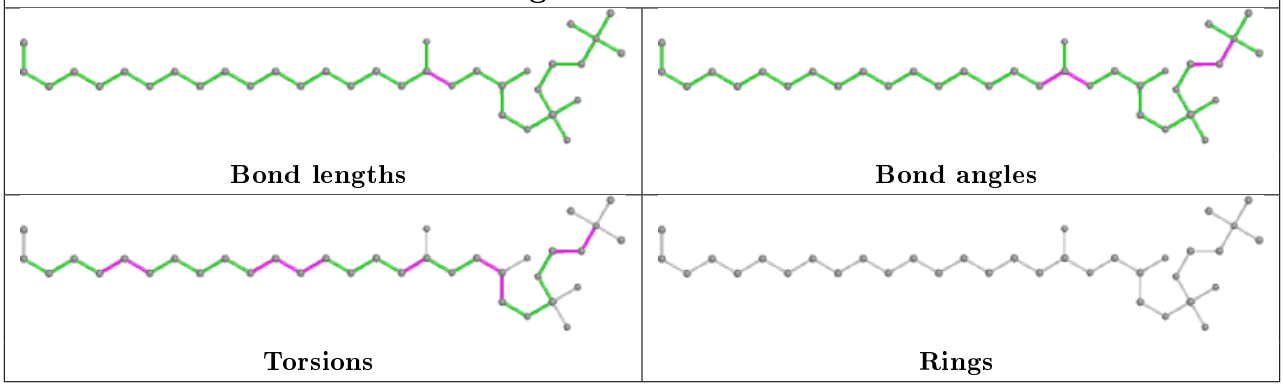
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	306	GOL	5	0
8	C	305	D12	4	0
6	C	303	LSC	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LSC C 303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	196/213 (92%)	-0.11	1 (0%) 91 79	28, 60, 122, 148	1 (0%)
1	G	201/213 (94%)	-0.17	3 (1%) 73 51	28, 60, 110, 146	1 (0%)
2	B	236/259 (91%)	-0.04	9 (3%) 40 20	26, 65, 107, 157	0
2	H	244/259 (94%)	-0.13	2 (0%) 86 70	24, 62, 110, 193	0
3	C	263/276 (95%)	-0.38	0 100 100	41, 73, 106, 130	2 (0%)
4	D	95/99 (95%)	-0.32	0 100 100	45, 73, 113, 128	1 (1%)
All	All	1235/1319 (93%)	-0.18	15 (1%) 79 58	24, 66, 112, 193	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	ASP	5.7
2	H	101	GLU	5.3
2	B	71	THR	4.5
2	B	48	TYR	3.0
1	G	131	SER	2.9
2	H	102	SER	2.9
2	B	69	ILE	2.8
2	B	49	SER	2.6
1	A	199	THR	2.6
2	B	50	TYR	2.5
2	B	44	HIS	2.4
1	G	132	ASP	2.3
1	G	130	SER	2.2
2	B	59	ASP	2.2
2	B	55	THR	2.1

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
5	FUC	E	2	10/11	0.81	0.35	79,88,95,100	0
5	NAG	E	1	14/15	0.85	0.27	81,92,109,111	0

6.4 Ligands (i)

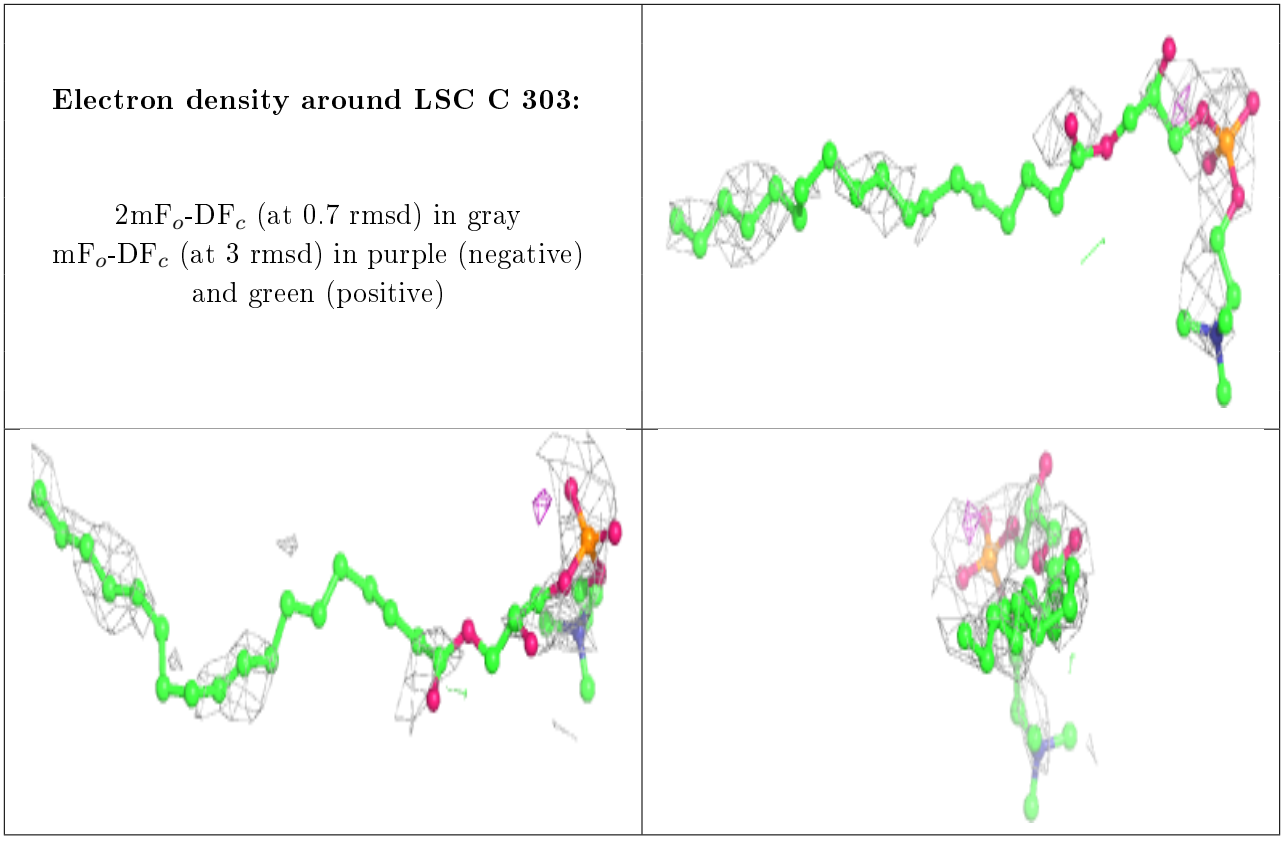
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LSC	C	303	35/35	0.66	0.49	52,136,192,193	0
9	GOL	C	306	6/6	0.84	0.32	38,57,62,67	0
8	D12	C	305	12/12	0.89	0.33	46,58,65,66	0
7	HEX	C	304	6/6	0.93	0.19	29,47,54,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LSC C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.