



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:44 pm BST

PDB ID : 1XY3
Title : Urate oxidase from aspergillus flavus complexed with guanine
Authors : Retailleau, P.; Colloc'h, N.; Vivares, D.; Bonnete, F.; Castro, B.; El Hajji, M.; Prange, T.
Deposited on : 2004-11-09
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

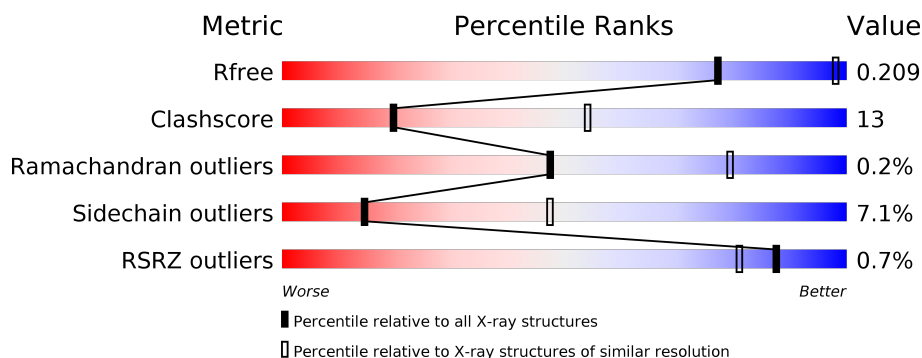
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	B	301	<div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	C	301	<div> <div>70%</div> <div>27%</div> <div>• •</div> </div>
1	D	301	<div> <div>%</div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	E	301	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	F	301	<div> <div>%</div> <div>70%</div> <div>25%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	301	 2% 70% 26% . .
1	H	301	 % 71% 23% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GUN	F	905	-	-	-	X
2	GUN	H	907	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18945 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.

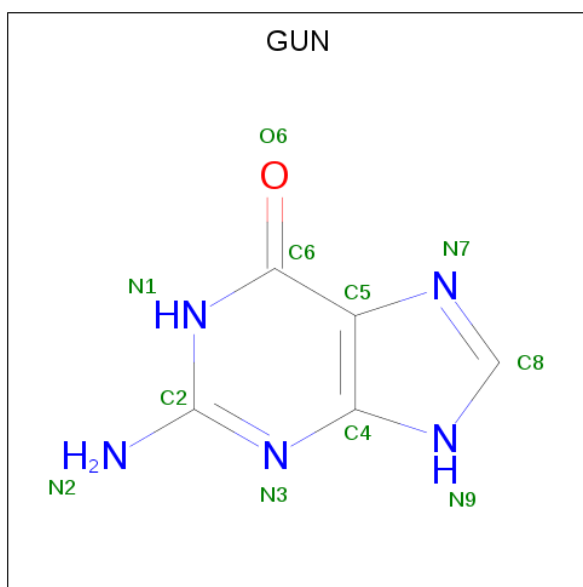
- Molecule 1 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			
1	B	295	Total	C	N	O	S	0	0	0
			2357	1490	409	451	7			
1	C	299	Total	C	N	O	S	0	0	1
			2374	1500	413	454	7			
1	D	295	Total	C	N	O	S	0	0	0
			2352	1486	408	451	7			
1	E	295	Total	C	N	O	S	0	0	0
			2348	1485	407	449	7			
1	F	295	Total	C	N	O	S	0	0	0
			2349	1484	408	450	7			
1	G	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			
1	H	295	Total	C	N	O	S	0	0	0
			2359	1491	409	452	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
B	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
C	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
D	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
E	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
F	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
G	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511
H	1	SAC	SER	MODIFIED RESIDUE	UNP Q00511

- Molecule 2 is GUANINE (three-letter code: GUN) (formula: C₅H₅N₅O).

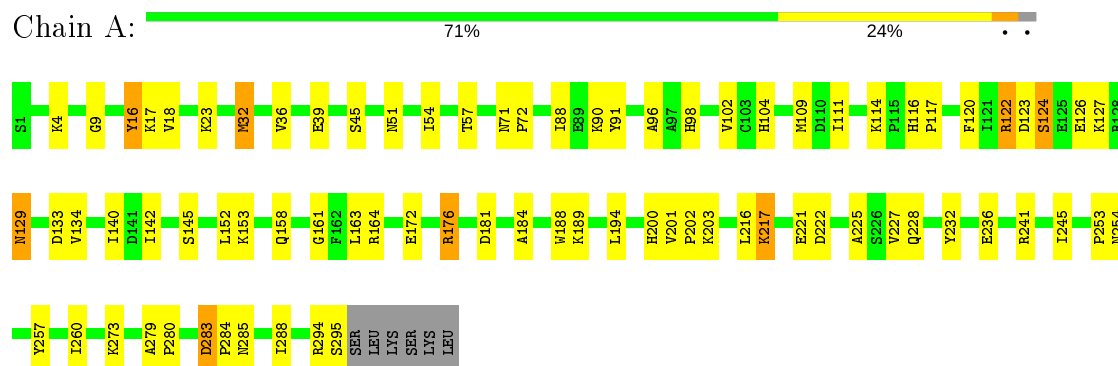


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	5	5	1		
2	B	1	Total	C	N	O	0	0
			11	5	5	1		
2	C	1	Total	C	N	O	0	0
			11	5	5	1		
2	D	1	Total	C	N	O	0	0
			11	5	5	1		
2	E	1	Total	C	N	O	0	0
			11	5	5	1		
2	F	1	Total	C	N	O	0	0
			11	5	5	1		
2	G	1	Total	C	N	O	0	0
			11	5	5	1		
2	H	1	Total	C	N	O	0	0
			11	5	5	1		

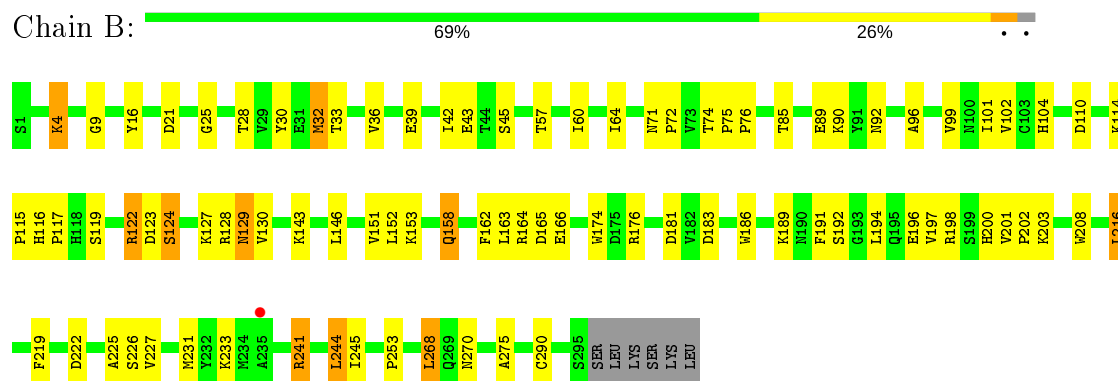
3 Residue-property plots [i](#)

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

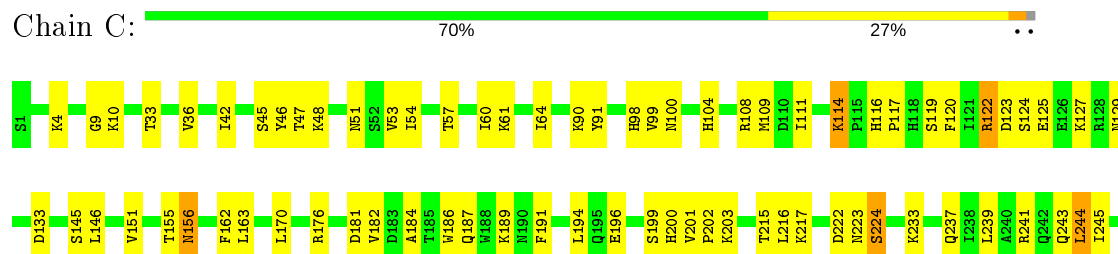
• Molecule 1: Uricase



• Molecule 1: Uricase

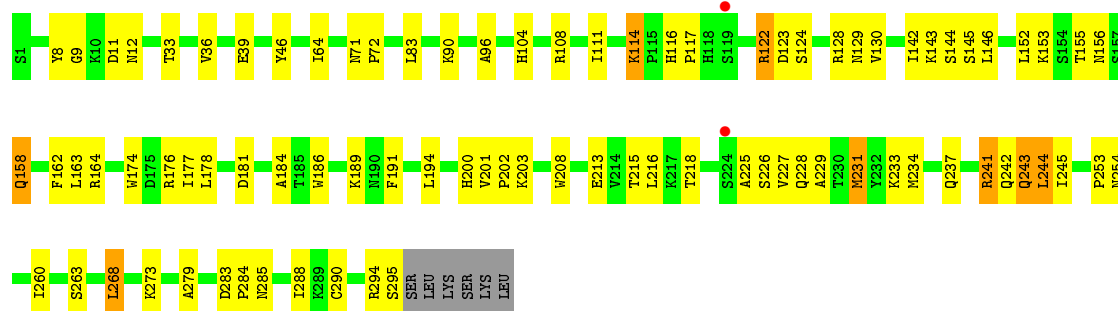


• Molecule 1: Uricase

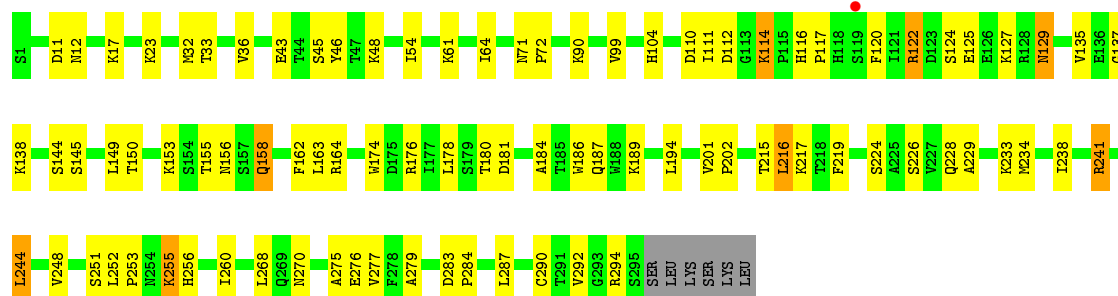




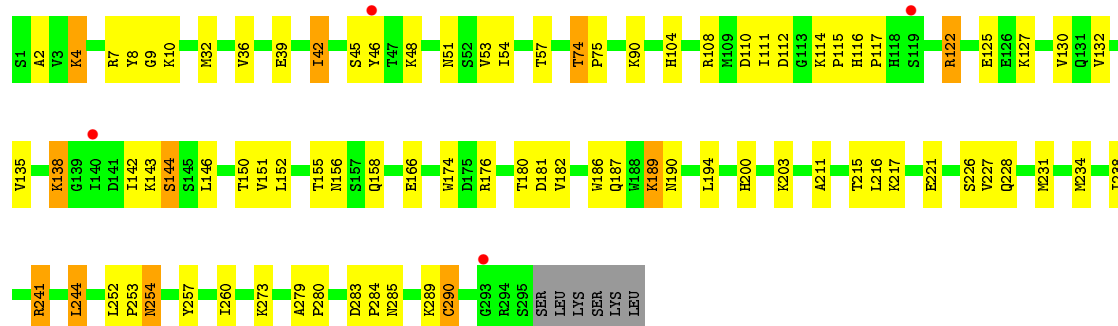
- Molecule 1: Uricase



- Molecule 1: Uricase

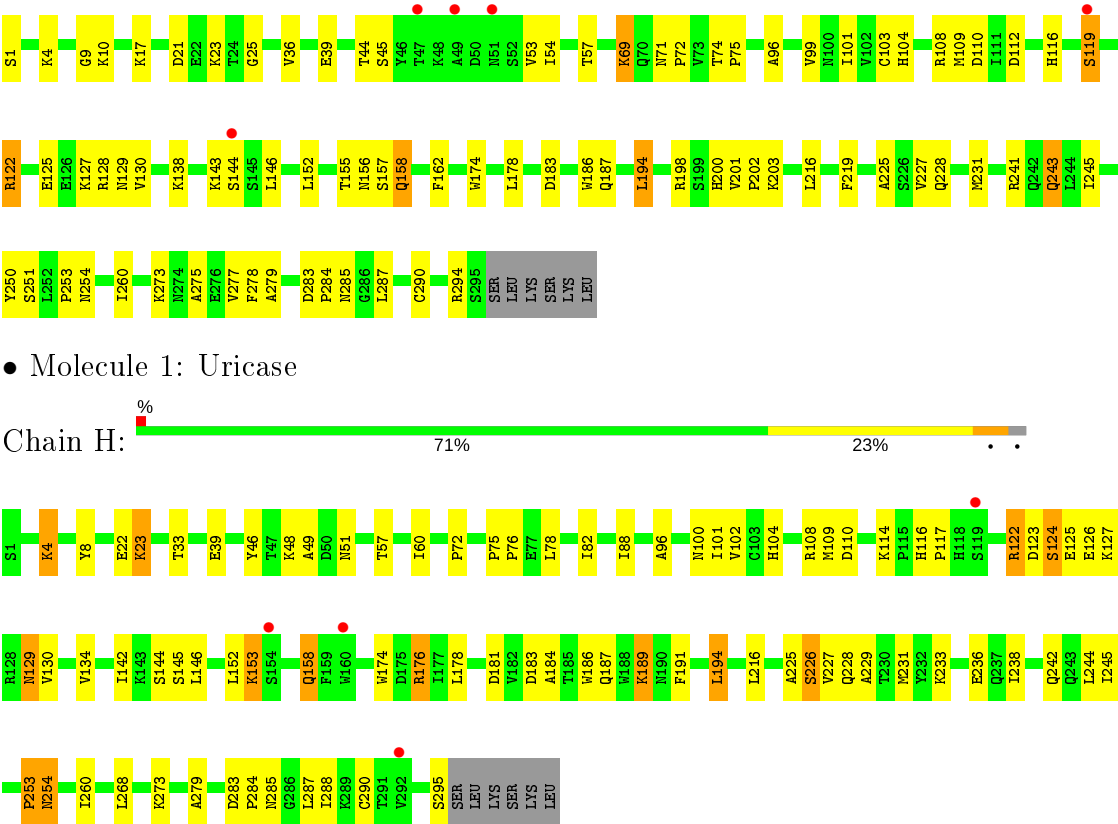


- Molecule 1: Uricase



- Molecule 1: Uricase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 141.94Å 135.08Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 134.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.20) 93.7 (134.94-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 3.19Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.172 , 0.208 0.174 , 0.209	Depositor DCC
R_{free} test set	4804 reflections (9.33%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18945	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/2406	0.53	0/3265
1	B	0.42	0/2401	0.51	0/3258
1	C	0.42	0/2421	0.52	0/3286
1	D	0.43	0/2396	0.51	0/3252
1	E	0.40	0/2395	0.50	0/3252
1	F	0.42	0/2396	0.50	0/3252
1	G	0.38	0/2406	0.49	0/3265
1	H	0.41	0/2406	0.50	0/3265
All	All	0.42	0/19227	0.51	0/26095

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2359	0	2320	61	0
1	B	2357	0	2319	65	0
1	C	2374	0	2333	55	0
1	D	2352	0	2307	70	0
1	E	2348	0	2301	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2349	0	2303	61	0
1	G	2359	0	2320	67	0
1	H	2359	0	2320	62	0
2	A	11	0	5	3	0
2	B	11	0	5	3	0
2	C	11	0	5	1	0
2	D	11	0	5	3	0
2	E	11	0	5	1	0
2	F	11	0	5	2	0
2	G	11	0	5	0	0
2	H	11	0	5	3	0
All	All	18945	0	18563	475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (475) 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:G:36:VAL:HG22	1:G:99:VAL:HG22	1.31	1.08
1:H:176:ARG:HH22	2:H:907:GUN:HN22	1.15	0.91
1:A:88:ILE:HD13	1:A:134:VAL:HG12	1.53	0.89
1:H:102:VAL:HG22	1:H:129:ASN:HD22	1.36	0.89
1:E:180:THR:HG21	1:E:252:LEU:HD12	1.58	0.84
1:F:45:SER:HB3	1:F:54:ILE:HD11	1.60	0.82
1:D:231:MET:HE3	1:D:290:CYS:HB2	1.62	0.81
1:D:215:THR:HA	1:D:234:MET:HE2	1.62	0.81
1:D:71:ASN:HB3	1:D:72:PRO:HD2	1.64	0.81
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.48	0.79
1:G:53:VAL:HG23	1:G:54:ILE:HD12	1.66	0.78
1:D:231:MET:CE	1:D:290:CYS:HB2	2.14	0.78
1:B:158:GLN:HB3	1:B:174:TRP:HA	1.67	0.77
1:A:200:HIS:HD2	1:A:203:LYS:HE2	1.50	0.76
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.51	0.76
1:D:39:GLU:HB2	1:D:96:ALA:HB3	1.67	0.75
1:B:186:TRP:HB2	1:B:245:ILE:HD12	1.69	0.75
1:G:227:VAL:O	1:G:231:MET:HG2	1.87	0.74
1:A:200:HIS:CD2	1:A:203:LYS:HE2	2.23	0.74
1:F:260:ILE:HD11	1:F:279:ALA:HB2	1.68	0.73
1:D:116:HIS:ND1	1:D:117:PRO:HD2	2.03	0.73
1:F:181:ASP:HB2	1:F:253:PRO:HG2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:HIS:HD2	1:E:127:LYS:NZ	1.88	0.72
1:G:178:LEU:HD23	1:G:219:PHE:CE1	2.24	0.72
1:G:231:MET:CE	1:G:290:CYS:HB2	2.19	0.71
1:B:104:HIS:HD2	1:B:127:LYS:NZ	1.88	0.71
1:H:226:SER:HB3	1:H:229:ALA:HB3	1.73	0.71
1:F:45:SER:CB	1:F:54:ILE:HD11	2.19	0.71
1:A:39:GLU:HB2	1:A:96:ALA:HB3	1.73	0.71
1:E:162:PHE:HA	1:F:51:ASN:O	1.92	0.70
1:G:294:ARG:HH11	1:G:294:ARG:HG2	1.56	0.69
1:F:257:TYR:HE2	1:F:280:PRO:HG3	1.58	0.68
1:G:231:MET:HE2	1:G:290:CYS:HB2	1.74	0.68
1:B:158:GLN:O	1:B:225:ALA:HA	1.93	0.68
1:H:260:ILE:HD11	1:H:279:ALA:HB2	1.75	0.68
1:C:200:HIS:HD2	1:C:203:LYS:NZ	1.91	0.68
1:A:104:HIS:HD2	1:A:127:LYS:NZ	1.92	0.68
1:A:134:VAL:HG22	1:A:140:ILE:HG23	1.76	0.68
1:E:181:ASP:O	1:E:253:PRO:HD2	1.94	0.68
1:F:45:SER:HB3	1:F:54:ILE:CD1	2.24	0.68
1:D:176:ARG:HH22	2:D:903:GUN:HN22	1.40	0.67
1:E:229:ALA:O	1:E:233:LYS:HG3	1.95	0.67
1:E:180:THR:CG2	1:E:252:LEU:HD12	2.24	0.67
1:H:102:VAL:HG22	1:H:129:ASN:ND2	2.10	0.67
1:A:200:HIS:HD2	1:A:203:LYS:CE	2.09	0.66
1:D:116:HIS:CG	1:D:117:PRO:HD2	2.31	0.66
1:D:294:ARG:HG2	1:D:294:ARG:NH1	2.11	0.66
1:H:254:ASN:O	1:H:285:ASN:HB2	1.95	0.66
1:C:57:THR:HA	1:C:60:ILE:HD12	1.75	0.66
1:E:163:LEU:HD23	1:E:164:ARG:N	2.11	0.65
1:C:176:ARG:HH22	2:C:902:GUN:HN22	1.44	0.65
1:E:178:LEU:HD23	1:E:219:PHE:CE1	2.31	0.65
1:G:200:HIS:HD2	1:G:203:LYS:NZ	1.95	0.65
1:G:45:SER:CB	1:G:54:ILE:HD11	2.26	0.65
1:H:288:ILE:N	1:H:288:ILE:HD12	2.11	0.65
1:H:181:ASP:O	1:H:253:PRO:HD2	1.95	0.65
1:G:155:THR:OG1	1:G:156:ASN:N	2.29	0.65
1:D:254:ASN:O	1:D:285:ASN:HB2	1.96	0.64
1:A:254:ASN:O	1:A:285:ASN:HB2	1.97	0.64
1:C:90:LYS:HG2	1:C:91:TYR:CE2	2.33	0.64
1:G:45:SER:HB3	1:G:54:ILE:HD11	1.80	0.64
1:H:287:LEU:C	1:H:288:ILE:HD12	2.18	0.64
1:A:260:ILE:HD11	1:A:279:ALA:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:SER:HB3	1:G:54:ILE:CD1	2.29	0.63
1:F:257:TYR:CE2	1:F:280:PRO:HG3	2.33	0.63
1:D:254:ASN:ND2	1:D:288:ILE:HD12	2.14	0.63
1:E:158:GLN:HB3	1:E:174:TRP:HA	1.80	0.62
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.13	0.62
1:G:186:TRP:HB2	1:G:245:ILE:HD12	1.80	0.62
1:B:28:THR:HG22	1:B:30:TYR:CE2	2.34	0.62
1:D:231:MET:HE3	1:D:290:CYS:CB	2.28	0.62
1:A:176:ARG:HH22	2:A:900:GUN:HN22	1.48	0.61
1:H:176:ARG:NH2	2:H:907:GUN:HN22	1.93	0.61
1:B:186:TRP:HD1	1:B:245:ILE:HD11	1.63	0.61
1:E:260:ILE:HD11	1:E:279:ALA:HB2	1.81	0.61
1:B:85:THR:O	1:B:89:GLU:HG3	2.00	0.61
1:E:217:LYS:NZ	1:G:112:ASP:OD2	2.33	0.61
1:F:116:HIS:CG	1:F:117:PRO:HD2	2.35	0.61
1:B:200:HIS:HD2	1:B:203:LYS:NZ	1.99	0.61
1:D:200:HIS:HD2	1:D:203:LYS:NZ	1.99	0.61
1:D:215:THR:CA	1:D:234:MET:HE2	2.31	0.61
1:F:104:HIS:HD2	1:F:127:LYS:NZ	1.98	0.60
1:H:194:LEU:O	1:H:194:LEU:HD22	2.01	0.60
1:E:215:THR:HA	1:E:234:MET:HE2	1.83	0.60
1:G:243:GLN:HE21	1:G:243:GLN:HA	1.66	0.59
1:B:36:VAL:HG22	1:B:99:VAL:HG22	1.85	0.59
1:D:108:ARG:HD3	1:D:116:HIS:O	2.03	0.59
1:E:241:ARG:HG2	1:E:241:ARG:HH11	1.68	0.59
1:B:104:HIS:HD2	1:B:127:LYS:HZ1	1.48	0.59
1:G:283:ASP:HB2	1:G:284:PRO:HA	1.83	0.59
1:H:101:ILE:HB	1:H:130:VAL:HG22	1.83	0.59
1:C:181:ASP:O	1:C:253:PRO:HD2	2.03	0.59
1:B:222:ASP:OD1	1:B:233:LYS:NZ	2.35	0.59
1:G:101:ILE:HB	1:G:130:VAL:HG22	1.85	0.59
1:G:158:GLN:O	1:G:225:ALA:HA	2.03	0.58
1:E:176:ARG:HH22	2:E:904:GUN:HN22	1.50	0.58
1:D:254:ASN:HD21	1:D:288:ILE:HD12	1.69	0.58
1:E:241:ARG:CG	1:E:241:ARG:HH11	2.17	0.57
1:B:123:ASP:O	1:B:124:SER:HB2	2.04	0.57
1:H:227:VAL:O	1:H:231:MET:HG2	2.04	0.57
1:D:242:GLN:HG3	1:D:245:ILE:HG12	1.86	0.57
1:H:145:SER:HB2	1:H:184:ALA:O	2.05	0.57
1:D:163:LEU:HD23	1:D:164:ARG:N	2.19	0.57
1:D:144:SER:HB2	1:D:186:TRP:NE1	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:THR:HA	1:H:60:ILE:HD12	1.87	0.57
1:C:61:LYS:HA	1:C:64:ILE:HD12	1.87	0.57
1:E:270:ASN:O	1:E:275:ALA:HA	2.05	0.57
1:C:51:ASN:O	1:D:162:PHE:HA	2.04	0.56
1:D:241:ARG:HG2	1:D:241:ARG:HH11	1.71	0.56
1:A:122:ARG:HG3	1:A:122:ARG:O	2.05	0.56
1:F:176:ARG:HH22	2:F:905:GUN:HN22	1.54	0.56
1:B:16:TYR:CE1	1:D:177:ILE:HD11	2.40	0.56
1:H:189:LYS:HD3	1:H:244:LEU:CD1	2.35	0.56
1:B:101:ILE:HB	1:B:130:VAL:HG22	1.86	0.56
1:E:178:LEU:HD23	1:E:219:PHE:HE1	1.69	0.56
1:A:57:THR:HG23	2:B:901:GUN:N7	2.19	0.56
1:C:33:THR:OG1	1:C:104:HIS:HE1	1.89	0.56
1:B:201:VAL:HG12	1:B:202:PRO:HD3	1.88	0.55
1:D:11:ASP:OD1	1:D:12:ASN:N	2.37	0.55
1:D:158:GLN:O	1:D:225:ALA:HA	2.06	0.55
1:D:260:ILE:HD11	1:D:279:ALA:HB2	1.89	0.55
1:H:75:PRO:HB2	1:H:76:PRO:HD2	1.89	0.55
1:D:181:ASP:O	1:D:253:PRO:HD2	2.06	0.55
1:H:124:SER:OG	1:H:126:GLU:HB3	2.07	0.55
1:D:215:THR:HG23	1:D:234:MET:CE	2.37	0.55
1:D:215:THR:HG23	1:D:234:MET:HE2	1.88	0.55
1:E:90:LYS:NZ	1:F:166:GLU:OE2	2.40	0.55
1:B:151:VAL:HG23	1:B:219:PHE:CZ	2.42	0.54
1:C:116:HIS:ND1	1:C:117:PRO:HD2	2.22	0.54
1:E:228:GLN:OE1	1:E:228:GLN:N	2.32	0.54
1:F:283:ASP:HB2	1:F:284:PRO:HA	1.90	0.54
1:G:231:MET:HE1	1:G:290:CYS:HB2	1.90	0.54
1:A:116:HIS:CG	1:A:117:PRO:HD2	2.42	0.54
1:D:254:ASN:HD21	1:D:288:ILE:CD1	2.20	0.54
1:A:181:ASP:HB2	1:A:253:PRO:HG2	1.90	0.54
1:D:227:VAL:HG23	2:D:903:GUN:N2	2.23	0.54
1:G:254:ASN:O	1:G:285:ASN:HB2	2.07	0.54
1:A:88:ILE:CD1	1:A:134:VAL:HG12	2.31	0.54
1:E:116:HIS:CG	1:E:117:PRO:HD2	2.42	0.54
1:B:176:ARG:HH22	2:B:901:GUN:HN22	1.55	0.54
1:C:53:VAL:HG23	1:C:54:ILE:HD13	1.89	0.54
1:E:256:HIS:NE2	1:F:10:LYS:NZ	2.56	0.54
1:F:227:VAL:HG23	2:F:905:GUN:N2	2.23	0.54
1:E:145:SER:HB2	1:E:184:ALA:O	2.08	0.54
1:A:90:LYS:HG3	1:A:90:LYS:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HH11	1:B:241:ARG:CG	2.20	0.54
1:A:90:LYS:HG2	1:A:91:TYR:CE2	2.43	0.54
1:B:39:GLU:HB2	1:B:96:ALA:HB3	1.90	0.54
1:C:36:VAL:HG22	1:C:99:VAL:HG22	1.90	0.54
1:A:9:GLY:HA3	1:A:36:VAL:O	2.08	0.54
1:C:260:ILE:HD11	1:C:279:ALA:HB2	1.90	0.53
1:H:229:ALA:O	1:H:233:LYS:HG3	2.08	0.53
1:C:116:HIS:CG	1:C:117:PRO:HD2	2.43	0.53
1:C:191:PHE:HD1	1:C:196:GLU:HG2	1.74	0.53
1:G:231:MET:HE2	1:G:290:CYS:CB	2.39	0.53
1:B:122:ARG:O	1:B:122:ARG:HG3	2.09	0.53
1:A:111:ILE:HD12	1:C:217:LYS:HA	1.91	0.53
1:E:287:LEU:O	1:F:8:TYR:HA	2.09	0.53
1:F:144:SER:HB2	1:F:186:TRP:NE1	2.23	0.53
1:C:163:LEU:C	1:C:163:LEU:HD23	2.29	0.53
1:H:39:GLU:HB2	1:H:96:ALA:HB3	1.91	0.53
1:A:227:VAL:HG23	2:A:900:GUN:N2	2.23	0.53
1:D:241:ARG:HH11	1:D:241:ARG:CG	2.21	0.53
1:E:180:THR:HG21	1:E:252:LEU:CD1	2.36	0.53
1:G:39:GLU:HB2	1:G:96:ALA:HB3	1.90	0.53
1:C:108:ARG:HD3	1:C:116:HIS:O	2.09	0.52
1:G:36:VAL:CG2	1:G:99:VAL:HG22	2.22	0.52
1:H:33:THR:OG1	1:H:104:HIS:HE1	1.92	0.52
1:E:43:GLU:H	1:E:43:GLU:CD	2.11	0.52
1:G:144:SER:HB2	1:G:186:TRP:NE1	2.24	0.52
1:H:142:ILE:HD12	1:H:191:PHE:CE2	2.44	0.52
1:D:146:LEU:HD12	1:D:146:LEU:O	2.09	0.52
1:B:152:LEU:HD23	1:B:153:LYS:N	2.24	0.52
1:D:158:GLN:HB3	1:D:174:TRP:HA	1.91	0.52
1:E:104:HIS:HD2	1:E:127:LYS:HZ2	1.58	0.52
1:E:150:THR:CG2	1:E:255:LYS:HE2	2.40	0.52
1:F:211:ALA:HA	1:F:238:ILE:HD11	1.92	0.52
1:A:45:SER:HB2	1:A:54:ILE:CD1	2.40	0.52
1:C:122:ARG:O	1:C:122:ARG:HG3	2.08	0.52
1:H:104:HIS:HD2	1:H:127:LYS:NZ	2.07	0.52
1:G:17:LYS:NZ	1:G:71:ASN:O	2.43	0.52
1:G:9:GLY:HA3	1:G:36:VAL:O	2.10	0.52
1:G:109:MET:HE2	1:G:119:SER:HB3	1.90	0.52
1:D:237:GLN:O	1:D:241:ARG:HG3	2.10	0.52
1:F:9:GLY:HA3	1:F:36:VAL:O	2.10	0.52
1:A:145:SER:HB2	1:A:184:ALA:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:VAL:HG23	1:F:54:ILE:CD1	2.40	0.52
1:F:152:LEU:HD23	1:F:152:LEU:C	2.30	0.51
1:C:9:GLY:HA3	1:C:36:VAL:O	2.11	0.51
1:F:111:ILE:O	1:F:112:ASP:HB2	2.10	0.51
1:F:7:ARG:HG2	1:F:39:GLU:HG3	1.93	0.51
1:H:122:ARG:HG3	1:H:122:ARG:O	2.10	0.51
1:H:158:GLN:HG2	1:H:174:TRP:O	2.11	0.51
1:H:231:MET:HE2	1:H:290:CYS:HB2	1.92	0.51
1:A:161:GLY:N	1:A:172:GLU:OE2	2.32	0.51
1:D:229:ALA:O	1:D:233:LYS:HG3	2.10	0.51
1:D:243:GLN:HE21	1:D:243:GLN:HA	1.75	0.51
1:D:111:ILE:O	1:D:114:LYS:HG2	2.10	0.51
1:G:104:HIS:HD2	1:G:127:LYS:CE	2.24	0.51
1:G:10:LYS:HD2	1:G:57:THR:HB	1.93	0.51
1:A:217:LYS:HE2	1:A:221:GLU:OE2	2.11	0.51
1:G:260:ILE:HD11	1:G:279:ALA:HB2	1.92	0.51
1:B:152:LEU:HD23	1:B:152:LEU:C	2.31	0.51
1:F:144:SER:HB2	1:F:186:TRP:CE2	2.46	0.51
1:F:241:ARG:HH11	1:F:241:ARG:HG2	1.76	0.51
1:D:33:THR:OG1	1:D:104:HIS:HE1	1.94	0.50
1:E:276:GLU:OE1	1:G:69:LYS:NZ	2.30	0.50
1:G:178:LEU:HD23	1:G:219:PHE:HE1	1.76	0.50
1:A:158:GLN:O	1:A:225:ALA:HA	2.11	0.50
1:H:283:ASP:HB2	1:H:284:PRO:HA	1.93	0.50
1:D:227:VAL:O	1:D:231:MET:HG2	2.12	0.50
1:D:215:THR:CG2	1:D:234:MET:HE2	2.41	0.50
1:F:254:ASN:O	1:F:285:ASN:HB2	2.12	0.50
1:A:181:ASP:O	1:A:253:PRO:HD2	2.12	0.49
1:C:283:ASP:HB2	1:C:284:PRO:HA	1.93	0.49
1:A:283:ASP:HB2	1:A:284:PRO:HA	1.92	0.49
1:A:90:LYS:CG	1:A:91:TYR:CE2	2.95	0.49
1:D:283:ASP:HB2	1:D:284:PRO:HA	1.94	0.49
1:E:33:THR:OG1	1:E:104:HIS:HE1	1.95	0.49
1:F:166:GLU:OE1	1:F:166:GLU:N	2.30	0.49
1:B:21:ASP:O	1:B:25:GLY:N	2.40	0.49
1:F:135:VAL:HB	1:F:138:LYS:HB2	1.94	0.49
1:B:33:THR:OG1	1:B:104:HIS:HE1	1.95	0.49
1:A:16:TYR:CD1	1:C:278:PHE:HB2	2.48	0.49
1:F:215:THR:HG23	1:F:234:MET:HE1	1.94	0.49
1:F:90:LYS:O	1:F:90:LYS:HG3	2.11	0.49
1:H:228:GLN:HG3	1:H:288:ILE:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:O	1:C:114:LYS:HG2	2.13	0.49
1:B:123:ASP:O	1:D:123:ASP:O	2.30	0.49
1:E:228:GLN:HB3	1:F:46:TYR:CD2	2.47	0.49
1:G:146:LEU:C	1:G:146:LEU:HD12	2.34	0.49
1:B:43:GLU:CD	1:B:43:GLU:H	2.15	0.49
1:C:123:ASP:O	1:C:124:SER:HB2	2.13	0.49
1:C:289:LYS:O	1:C:290:CYS:HB3	2.12	0.49
1:G:228:GLN:HB3	1:H:46:TYR:CD2	2.48	0.49
1:C:186:TRP:HB2	1:C:245:ILE:HD12	1.94	0.48
1:G:152:LEU:C	1:G:152:LEU:HD23	2.34	0.48
1:C:98:HIS:ND1	1:C:133:ASP:OD1	2.32	0.48
1:C:90:LYS:O	1:C:90:LYS:HG3	2.14	0.48
1:B:90:LYS:O	1:B:90:LYS:HG3	2.13	0.48
1:B:163:LEU:HD23	1:B:164:ARG:N	2.29	0.48
1:D:158:GLN:HG2	1:D:174:TRP:O	2.13	0.48
1:A:91:TYR:CD2	1:A:91:TYR:N	2.81	0.48
1:C:42:ILE:O	1:C:45:SER:OG	2.31	0.48
1:H:116:HIS:ND1	1:H:117:PRO:HD2	2.29	0.48
1:B:231:MET:HE1	1:B:290:CYS:HB2	1.94	0.48
1:G:36:VAL:HG22	1:G:99:VAL:CG2	2.22	0.48
1:A:116:HIS:ND1	1:A:117:PRO:HD2	2.29	0.48
1:A:17:LYS:NZ	1:A:71:ASN:O	2.47	0.48
1:E:45:SER:HB2	1:E:54:ILE:HD11	1.96	0.48
1:E:17:LYS:HG3	1:G:277:VAL:HG22	1.95	0.48
1:H:123:ASP:OD1	1:H:123:ASP:N	2.45	0.48
1:H:226:SER:HB3	1:H:229:ALA:CB	2.43	0.48
1:H:116:HIS:CG	1:H:117:PRO:HD2	2.48	0.48
1:H:158:GLN:O	1:H:225:ALA:HA	2.14	0.48
1:F:289:LYS:O	1:F:290:CYS:HB3	2.14	0.48
2:A:900:GUN:N7	1:B:57:THR:HG23	2.29	0.47
1:C:222:ASP:OD2	1:C:224:SER:HB2	2.14	0.47
1:F:150:THR:HB	1:H:122:ARG:HB3	1.96	0.47
1:F:180:THR:HG21	1:F:252:LEU:HD13	1.96	0.47
1:A:124:SER:HB3	1:A:126:GLU:H	1.79	0.47
1:G:231:MET:HE3	1:G:250:TYR:HB3	1.95	0.47
1:G:74:THR:HA	1:G:75:PRO:C	2.34	0.47
1:H:146:LEU:C	1:H:146:LEU:HD12	2.34	0.47
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.50	0.47
1:F:241:ARG:CG	1:F:241:ARG:HH11	2.28	0.47
1:B:268:LEU:HA	1:B:268:LEU:HD12	1.73	0.47
1:E:135:VAL:HG11	1:E:138:LYS:HD3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:294:ARG:HG2	1:G:294:ARG:NH1	2.27	0.47
1:B:9:GLY:HA3	1:B:36:VAL:O	2.15	0.47
1:D:71:ASN:HB3	1:D:72:PRO:CD	2.39	0.47
1:G:200:HIS:HD2	1:G:203:LYS:HZ2	1.59	0.47
1:H:146:LEU:O	1:H:146:LEU:HD12	2.15	0.47
1:C:265:HIS:O	1:C:266:LYS:HB2	2.14	0.47
1:E:11:ASP:O	1:E:12:ASN:HB2	2.14	0.47
1:F:53:VAL:HG23	1:F:54:ILE:HD12	1.96	0.47
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.79	0.47
1:C:146:LEU:HD12	1:C:146:LEU:C	2.35	0.47
1:C:233:LYS:O	1:C:237:GLN:HG3	2.13	0.47
1:D:142:ILE:HD12	1:D:191:PHE:CE2	2.50	0.47
1:F:155:THR:HG23	1:F:156:ASN:N	2.29	0.47
1:F:4:LYS:HE2	1:F:4:LYS:HB3	1.62	0.47
1:H:242:GLN:HG3	1:H:245:ILE:HG12	1.95	0.47
1:A:45:SER:HB2	1:A:54:ILE:HD11	1.96	0.47
1:D:128:ARG:HD2	1:D:208:TRP:CD1	2.50	0.47
1:E:201:VAL:N	1:E:202:PRO:CD	2.78	0.47
1:F:42:ILE:O	1:F:45:SER:OG	2.32	0.47
1:G:178:LEU:CD2	1:G:219:PHE:CE1	2.97	0.47
1:B:166:GLU:N	1:B:166:GLU:OE1	2.31	0.47
1:D:155:THR:O	1:D:156:ASN:HB2	2.14	0.47
1:F:108:ARG:HD3	1:F:116:HIS:O	2.15	0.47
1:H:189:LYS:HE2	1:H:244:LEU:CD1	2.45	0.46
1:E:122:ARG:O	1:E:122:ARG:HG3	2.14	0.46
1:E:127:LYS:HB2	1:E:129:ASN:HD21	1.80	0.46
1:F:74:THR:HA	1:F:75:PRO:C	2.33	0.46
1:B:244:LEU:HD12	1:B:244:LEU:HA	1.71	0.46
1:E:155:THR:O	1:E:156:ASN:HB2	2.16	0.46
1:E:292:VAL:HG13	1:F:2:ALA:O	2.15	0.46
1:D:189:LYS:HE3	1:D:244:LEU:CD1	2.45	0.46
1:G:103:CYS:HB2	1:G:128:ARG:O	2.15	0.46
1:A:163:LEU:HD23	1:A:164:ARG:N	2.30	0.46
1:E:111:ILE:O	1:E:114:LYS:HG3	2.16	0.46
1:G:251:SER:O	1:G:253:PRO:HD3	2.15	0.46
1:B:186:TRP:CD1	1:B:245:ILE:HD11	2.47	0.46
1:E:61:LYS:HA	1:E:64:ILE:HD12	1.97	0.46
1:B:227:VAL:O	1:B:231:MET:HG2	2.15	0.46
1:F:257:TYR:CE2	1:F:280:PRO:HB3	2.50	0.46
1:B:146:LEU:HD12	1:B:146:LEU:C	2.36	0.46
1:B:227:VAL:HG23	2:B:901:GUN:N2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PHE:CD1	1:C:120:PHE:N	2.83	0.46
1:H:48:LYS:O	1:H:49:ALA:HB3	2.15	0.46
1:G:109:MET:CE	1:G:119:SER:HB3	2.46	0.46
1:G:1:SAC:OG	1:H:236:GLU:HG2	2.16	0.46
1:D:189:LYS:HE3	1:D:244:LEU:HD12	1.98	0.45
1:A:18:VAL:O	1:A:18:VAL:HG13	2.16	0.45
1:A:54:ILE:O	1:A:54:ILE:HG22	2.15	0.45
1:C:200:HIS:HD2	1:C:203:LYS:HZ3	1.59	0.45
1:E:104:HIS:HD2	1:E:127:LYS:HZ1	1.65	0.45
1:F:158:GLN:HG2	1:F:174:TRP:O	2.17	0.45
1:H:181:ASP:HB2	1:H:253:PRO:HG2	1.98	0.45
1:H:288:ILE:N	1:H:288:ILE:CD1	2.79	0.45
1:B:165:ASP:HB2	1:B:166:GLU:OE1	2.16	0.45
1:E:251:SER:O	1:E:253:PRO:HD3	2.16	0.45
1:B:201:VAL:CB	1:B:202:PRO:HD3	2.46	0.45
1:C:155:THR:OG1	1:C:156:ASN:N	2.50	0.45
1:F:151:VAL:CG1	1:H:109:MET:HE3	2.47	0.45
1:H:78:LEU:HG	1:H:82:ILE:HD12	1.98	0.45
1:B:114:LYS:HA	1:B:115:PRO:HD3	1.86	0.45
1:F:135:VAL:HG12	1:F:138:LYS:HG3	1.99	0.45
1:G:157:SER:C	1:G:158:GLN:HG3	2.37	0.45
1:D:152:LEU:C	1:D:152:LEU:HD23	2.37	0.45
1:D:254:ASN:ND2	1:D:288:ILE:CD1	2.80	0.45
1:D:64:ILE:HG12	1:D:83:LEU:HD21	1.99	0.45
1:H:152:LEU:HD23	1:H:152:LEU:C	2.36	0.45
1:B:201:VAL:HG12	1:B:202:PRO:CD	2.47	0.45
1:C:10:LYS:HD3	1:C:57:THR:HB	1.98	0.45
1:D:116:HIS:CE1	1:D:117:PRO:HD2	2.52	0.45
1:G:122:ARG:HG3	1:G:122:ARG:O	2.17	0.45
1:C:4:LYS:HE2	1:C:4:LYS:HB3	1.66	0.45
1:A:45:SER:CB	1:A:54:ILE:HD11	2.47	0.44
1:C:182:VAL:HG11	1:C:215:THR:HG21	1.98	0.44
1:F:151:VAL:HG12	1:H:109:MET:HE3	1.99	0.44
1:H:153:LYS:HG2	1:H:178:LEU:HB3	1.99	0.44
1:A:104:HIS:HD2	1:A:127:LYS:HZ1	1.66	0.44
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.79	0.44
1:B:241:ARG:CG	1:B:241:ARG:NH1	2.78	0.44
1:C:201:VAL:N	1:C:202:PRO:CD	2.80	0.44
1:D:123:ASP:O	1:D:124:SER:HB2	2.16	0.44
1:B:191:PHE:CD2	1:B:197:VAL:HG22	2.52	0.44
1:E:283:ASP:HB2	1:E:284:PRO:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:MET:CE	1:C:151:VAL:HG12	2.47	0.44
1:E:215:THR:CA	1:E:234:MET:HE2	2.47	0.44
1:B:200:HIS:HD2	1:B:203:LYS:HZ3	1.63	0.44
1:E:46:TYR:CD2	1:F:228:GLN:HB3	2.53	0.44
1:H:158:GLN:HB3	1:H:174:TRP:HA	1.99	0.44
1:C:162:PHE:CZ	1:C:170:LEU:HD23	2.53	0.44
1:E:241:ARG:CG	1:E:241:ARG:NH1	2.78	0.44
1:H:125:GLU:O	1:H:127:LYS:HE2	2.18	0.44
1:G:178:LEU:CD2	1:G:219:PHE:HE1	2.31	0.44
1:A:120:PHE:N	1:A:120:PHE:CD1	2.86	0.43
1:E:120:PHE:CD1	1:E:120:PHE:N	2.86	0.43
1:E:149:LEU:HD21	1:E:216:LEU:CD1	2.47	0.43
1:H:144:SER:HB2	1:H:186:TRP:NE1	2.33	0.43
1:B:128:ARG:HD2	1:B:208:TRP:CD1	2.52	0.43
1:D:145:SER:HB2	1:D:184:ALA:O	2.18	0.43
1:G:144:SER:HB2	1:G:186:TRP:CD1	2.52	0.43
1:D:241:ARG:CG	1:D:241:ARG:NH1	2.80	0.43
1:E:144:SER:HB2	1:E:186:TRP:NE1	2.33	0.43
1:F:132:VAL:HG22	1:F:142:ILE:HG12	2.01	0.43
1:H:189:LYS:HE2	1:H:244:LEU:HD12	1.99	0.43
1:B:181:ASP:O	1:B:253:PRO:HD2	2.19	0.43
1:B:30:TYR:N	1:B:30:TYR:CD2	2.86	0.43
1:C:290:CYS:HB3	1:D:46:TYR:CE2	2.53	0.43
1:G:71:ASN:HB3	1:G:72:PRO:CD	2.49	0.43
1:C:287:LEU:O	1:D:8:TYR:HA	2.18	0.43
1:D:176:ARG:NH2	2:D:903:GUN:HN22	2.12	0.43
1:H:268:LEU:HD12	1:H:268:LEU:HA	1.85	0.43
1:A:232:TYR:HE2	1:A:236:GLU:OE2	2.01	0.43
1:A:88:ILE:HD13	1:A:134:VAL:CG1	2.36	0.43
1:B:231:MET:HE2	1:B:290:CYS:HB3	2.01	0.43
1:C:109:MET:CE	1:C:119:SER:HB3	2.48	0.43
1:D:218:THR:HG21	1:D:234:MET:HG3	1.99	0.43
1:E:189:LYS:HE2	1:E:244:LEU:CD1	2.48	0.43
1:C:239:LEU:HD23	1:C:245:ILE:HG22	1.99	0.43
1:C:237:GLN:O	1:C:241:ARG:HG3	2.17	0.43
1:C:156:ASN:ND2	1:C:223:ASN:ND2	2.66	0.43
1:C:47:THR:C	1:C:48:LYS:HD3	2.39	0.43
1:E:277:VAL:HG22	1:G:17:LYS:HG3	2.01	0.43
1:G:158:GLN:HB3	1:G:174:TRP:HA	2.00	0.43
1:G:162:PHE:HA	1:H:51:ASN:O	2.18	0.43
1:F:244:LEU:HA	1:F:244:LEU:HD13	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HA	1:C:53:VAL:HG21	2.00	0.42
1:E:215:THR:HG23	1:E:234:MET:HE2	2.01	0.42
1:A:153:LYS:NZ	1:A:222:ASP:O	2.53	0.42
1:A:228:GLN:HG3	1:A:288:ILE:HG21	2.01	0.42
1:A:51:ASN:O	1:B:162:PHE:HA	2.19	0.42
1:F:122:ARG:O	1:F:122:ARG:HG3	2.18	0.42
1:G:201:VAL:N	1:G:202:PRO:CD	2.82	0.42
1:H:4:LYS:HE2	1:H:4:LYS:HB3	1.33	0.42
1:A:142:ILE:HG22	1:A:188:TRP:HD1	1.83	0.42
1:A:201:VAL:N	1:A:202:PRO:CD	2.82	0.42
1:B:76:PRO:HB2	1:B:130:VAL:HG11	2.00	0.42
1:F:10:LYS:HD3	1:F:57:THR:HB	2.02	0.42
1:G:104:HIS:HD2	1:G:127:LYS:HE3	1.84	0.42
1:A:32:MET:HB2	1:A:102:VAL:O	2.20	0.42
1:C:200:HIS:HD2	1:C:203:LYS:HZ1	1.65	0.42
1:F:217:LYS:NZ	1:F:221:GLU:OE2	2.51	0.42
1:G:21:ASP:O	1:G:25:GLY:N	2.45	0.42
1:B:201:VAL:CG1	1:B:202:PRO:HD3	2.48	0.42
1:B:42:ILE:O	1:B:45:SER:OG	2.36	0.42
1:E:149:LEU:HD12	1:E:149:LEU:C	2.40	0.42
1:H:108:ARG:HD3	1:H:116:HIS:O	2.19	0.42
1:E:149:LEU:HD21	1:E:216:LEU:HD11	2.01	0.42
1:A:123:ASP:N	1:A:123:ASP:OD1	2.48	0.42
1:C:46:TYR:CD2	1:D:228:GLN:HB3	2.55	0.42
1:D:268:LEU:HD13	1:G:174:TRP:CG	2.55	0.42
1:G:200:HIS:HD2	1:G:203:LYS:HZ3	1.67	0.42
1:H:231:MET:HE3	1:H:290:CYS:HB3	2.01	0.42
1:C:145:SER:HB2	1:C:184:ALA:O	2.19	0.42
1:D:244:LEU:HA	1:D:244:LEU:HD13	1.85	0.42
1:E:228:GLN:HG3	1:F:46:TYR:CE2	2.55	0.42
1:F:146:LEU:HD12	1:F:146:LEU:O	2.20	0.42
1:F:182:VAL:HG11	1:F:215:THR:HG21	2.02	0.42
1:A:283:ASP:CB	1:A:284:PRO:HA	2.50	0.41
1:B:151:VAL:CG2	1:B:219:PHE:CE2	3.03	0.41
1:C:104:HIS:HD2	1:C:127:LYS:NZ	2.18	0.41
1:E:71:ASN:HB3	1:E:72:PRO:CD	2.50	0.41
1:F:257:TYR:HE2	1:F:280:PRO:CG	2.29	0.41
1:H:88:ILE:HD13	1:H:134:VAL:HG12	2.02	0.41
1:G:287:LEU:O	1:H:8:TYR:HA	2.20	0.41
1:E:124:SER:OG	1:E:125:GLU:N	2.53	0.41
1:F:130:VAL:HG23	1:F:130:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:228:GLN:HG3	1:H:288:ILE:CG2	2.50	0.41
1:B:270:ASN:O	1:B:275:ALA:HA	2.20	0.41
1:D:201:VAL:N	1:D:202:PRO:CD	2.83	0.41
1:E:238:ILE:CG2	1:E:248:VAL:HG21	2.49	0.41
1:A:102:VAL:HA	1:A:129:ASN:HD22	1.85	0.41
1:A:152:LEU:HD23	1:A:152:LEU:C	2.40	0.41
1:E:268:LEU:HA	1:E:268:LEU:HD12	1.88	0.41
1:E:36:VAL:HG22	1:E:99:VAL:HG22	2.03	0.41
1:E:153:LYS:HE3	1:E:153:LYS:HB2	1.83	0.41
1:G:275:ALA:HB1	1:G:278:PHE:CZ	2.55	0.41
1:G:194:LEU:O	1:G:198:ARG:HG3	2.21	0.41
1:G:228:GLN:HG2	1:H:46:TYR:CZ	2.55	0.41
1:A:257:TYR:CE2	1:A:280:PRO:HG3	2.56	0.41
1:B:71:ASN:HB3	1:B:72:PRO:CD	2.50	0.41
1:B:74:THR:HA	1:B:75:PRO:C	2.41	0.41
1:C:244:LEU:HA	1:C:244:LEU:HD13	1.92	0.41
1:D:153:LYS:HG2	1:D:178:LEU:HB3	2.02	0.41
1:F:114:LYS:HA	1:F:115:PRO:HD3	1.88	0.41
1:G:4:LYS:HE2	1:G:4:LYS:HB3	1.88	0.41
1:G:57:THR:HG1	2:H:907:GUN:C8	2.33	0.41
1:A:188:TRP:CE3	1:A:245:ILE:HD13	2.56	0.41
1:B:102:VAL:HG22	1:B:129:ASN:HD22	1.85	0.41
1:B:60:ILE:O	1:B:64:ILE:HG13	2.21	0.41
1:D:263:SER:OG	1:G:273:LYS:HD2	2.20	0.41
1:D:9:GLY:HA3	1:D:36:VAL:O	2.21	0.41
1:A:4:LYS:HB3	1:A:4:LYS:HE2	1.79	0.41
1:B:32:MET:HB2	1:B:102:VAL:O	2.21	0.41
1:A:98:HIS:ND1	1:A:133:ASP:OD1	2.52	0.41
1:A:71:ASN:HB3	1:A:72:PRO:HD2	2.02	0.41
1:G:108:ARG:HD3	1:G:116:HIS:O	2.21	0.41
1:B:192:SER:OG	1:B:196:GLU:OE1	2.32	0.40
1:D:122:ARG:O	1:D:122:ARG:HG3	2.21	0.40
1:E:111:ILE:O	1:E:112:ASP:HB2	2.21	0.40
1:F:200:HIS:HD2	1:F:203:LYS:NZ	2.19	0.40
1:H:194:LEU:HD22	1:H:194:LEU:C	2.41	0.40
1:C:243:GLN:HG3	1:C:243:GLN:O	2.22	0.40
1:F:189:LYS:NZ	1:F:190:ASN:O	2.48	0.40
1:A:45:SER:CB	1:A:54:ILE:CD1	2.99	0.40
1:B:4:LYS:HB3	1:B:4:LYS:HE2	1.29	0.40
1:E:137:GLY:C	1:E:138:LYS:HG3	2.41	0.40
1:B:151:VAL:HG23	1:B:219:PHE:CE2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ARG:NH1	1:D:294:ARG:CG	2.82	0.40
1:E:144:SER:HB2	1:E:186:TRP:CE2	2.56	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	293/301 (97%)	284 (97%)	9 (3%)	0	100	100
1	B	293/301 (97%)	280 (96%)	12 (4%)	1 (0%)	41	74
1	C	297/301 (99%)	283 (95%)	14 (5%)	0	100	100
1	D	293/301 (97%)	280 (96%)	13 (4%)	0	100	100
1	E	293/301 (97%)	279 (95%)	13 (4%)	1 (0%)	41	74
1	F	293/301 (97%)	280 (96%)	13 (4%)	0	100	100
1	G	293/301 (97%)	282 (96%)	11 (4%)	0	100	100
1	H	293/301 (97%)	282 (96%)	9 (3%)	2 (1%)	22	61
All	All	2348/2408 (98%)	2250 (96%)	94 (4%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	23	LYS
1	E	23	LYS
1	H	253	PRO
1	B	124	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/266 (98%)	244 (94%)	16 (6%)	18	53
1	B	259/266 (97%)	241 (93%)	18 (7%)	15	49
1	C	261/266 (98%)	244 (94%)	17 (6%)	17	51
1	D	258/266 (97%)	240 (93%)	18 (7%)	15	48
1	E	257/266 (97%)	241 (94%)	16 (6%)	18	53
1	F	258/266 (97%)	236 (92%)	22 (8%)	10	38
1	G	260/266 (98%)	243 (94%)	17 (6%)	17	51
1	H	260/266 (98%)	237 (91%)	23 (9%)	10	36
All	All	2073/2128 (97%)	1926 (93%)	147 (7%)	14	47

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	23	LYS
1	A	32	MET
1	A	114	LYS
1	A	122	ARG
1	A	124	SER
1	A	129	ASN
1	A	176	ARG
1	A	189	LYS
1	A	194	LEU
1	A	216	LEU
1	A	217	LYS
1	A	241	ARG
1	A	273	LYS
1	A	283	ASP
1	A	295	SER
1	B	4	LYS
1	B	32	MET
1	B	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	110	ASP
1	B	119	SER
1	B	122	ARG
1	B	129	ASN
1	B	143	LYS
1	B	158	GLN
1	B	183	ASP
1	B	189	LYS
1	B	194	LEU
1	B	198	ARG
1	B	216	LEU
1	B	226	SER
1	B	241	ARG
1	B	244	LEU
1	B	268	LEU
1	C	100	ASN
1	C	114	LYS
1	C	122	ARG
1	C	125	GLU
1	C	129	ASN
1	C	156	ASN
1	C	187	GLN
1	C	189	LYS
1	C	194	LEU
1	C	199	SER
1	C	216	LEU
1	C	224	SER
1	C	244	LEU
1	C	273	LYS
1	C	290	CYS
1	C	297	LEU
1	C	298	LYS
1	D	90	LYS
1	D	114	LYS
1	D	122	ARG
1	D	129	ASN
1	D	130	VAL
1	D	143	LYS
1	D	158	GLN
1	D	194	LEU
1	D	213	GLU
1	D	216	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	226	SER
1	D	231	MET
1	D	241	ARG
1	D	243	GLN
1	D	244	LEU
1	D	268	LEU
1	D	273	LYS
1	D	295	SER
1	E	32	MET
1	E	48	LYS
1	E	110	ASP
1	E	114	LYS
1	E	122	ARG
1	E	129	ASN
1	E	158	GLN
1	E	187	GLN
1	E	194	LEU
1	E	216	LEU
1	E	224	SER
1	E	226	SER
1	E	241	ARG
1	E	244	LEU
1	E	255	LYS
1	E	290	CYS
1	F	4	LYS
1	F	32	MET
1	F	42	ILE
1	F	48	LYS
1	F	74	THR
1	F	110	ASP
1	F	122	ARG
1	F	125	GLU
1	F	138	LYS
1	F	143	LYS
1	F	144	SER
1	F	187	GLN
1	F	189	LYS
1	F	194	LEU
1	F	216	LEU
1	F	226	SER
1	F	231	MET
1	F	241	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	244	LEU
1	F	254	ASN
1	F	273	LYS
1	F	290	CYS
1	G	23	LYS
1	G	44	THR
1	G	69	LYS
1	G	110	ASP
1	G	119	SER
1	G	122	ARG
1	G	125	GLU
1	G	129	ASN
1	G	138	LYS
1	G	143	LYS
1	G	158	GLN
1	G	183	ASP
1	G	187	GLN
1	G	194	LEU
1	G	216	LEU
1	G	241	ARG
1	G	243	GLN
1	H	4	LYS
1	H	22	GLU
1	H	23	LYS
1	H	72	PRO
1	H	100	ASN
1	H	110	ASP
1	H	114	LYS
1	H	122	ARG
1	H	124	SER
1	H	129	ASN
1	H	153	LYS
1	H	158	GLN
1	H	176	ARG
1	H	183	ASP
1	H	187	GLN
1	H	189	LYS
1	H	194	LEU
1	H	216	LEU
1	H	226	SER
1	H	238	ILE
1	H	254	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	273	LYS
1	H	295	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	129	ASN
1	A	200	HIS
1	B	86	HIS
1	B	104	HIS
1	B	118	HIS
1	B	129	ASN
1	B	131	GLN
1	B	187	GLN
1	B	200	HIS
1	C	12	ASN
1	C	104	HIS
1	C	129	ASN
1	C	156	ASN
1	C	200	HIS
1	D	86	HIS
1	D	104	HIS
1	D	129	ASN
1	D	200	HIS
1	D	243	GLN
1	D	254	ASN
1	D	285	ASN
1	E	86	HIS
1	E	104	HIS
1	E	129	ASN
1	E	200	HIS
1	F	86	HIS
1	F	104	HIS
1	F	129	ASN
1	F	158	GLN
1	F	200	HIS
1	G	86	HIS
1	G	104	HIS
1	G	200	HIS
1	G	243	GLN
1	H	104	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	129	ASN
1	H	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SAC	H	1	1	4,5,9	0.67	0	0,5,11	0.00	-
1	SAC	C	1	1	4,5,9	0.57	0	0,5,11	0.00	-
1	SAC	B	1	1	7,8,9	0.95	0	8,9,11	1.58	3 (37%)
1	SAC	A	1	1	4,5,9	0.78	0	0,5,11	0.00	-
1	SAC	G	1	1	4,5,9	0.43	0	0,5,11	0.00	-
1	SAC	F	1	1	4,5,9	0.55	0	0,5,11	0.00	-
1	SAC	E	1	1	4,5,9	0.80	0	0,5,11	0.00	-
1	SAC	D	1	1	7,8,9	0.97	0	8,9,11	1.50	2 (25%)

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
1	SAC	H	1	1	-	2/2/4/10	-
1	SAC	C	1	1	-	0/2/4/10	-
1	SAC	B	1	1	-	0/7/8/10	-
1	SAC	A	1	1	-	2/2/4/10	-
1	SAC	G	1	1	-	1/2/4/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SAC	F	1	1	-	0/2/4/10	-
1	SAC	E	1	1	-	0/2/4/10	-
1	SAC	D	1	1	-	2/7/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	SAC	O-C-CA	-2.35	118.61	124.78
1	D	1	SAC	O-C-CA	-2.32	118.70	124.78
1	D	1	SAC	OAC-C1A-N	-2.22	117.86	121.95
1	B	1	SAC	OAC-C1A-N	-2.15	118.00	121.95
1	B	1	SAC	C-CA-N	2.02	113.37	109.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	1	SAC	C-CA-CB-OG
1	A	1	SAC	C-CA-CB-OG
1	G	1	SAC	C-CA-CB-OG
1	H	1	SAC	N-CA-CB-OG
1	A	1	SAC	N-CA-CB-OG
1	D	1	SAC	C-CA-CB-OG
1	D	1	SAC	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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
2	GUN	C	902	-	9,12,12	2.65	3 (33%)	8,17,17	3.89	4 (50%)
2	GUN	E	904	-	9,12,12	2.53	4 (44%)	8,17,17	3.87	3 (37%)
2	GUN	B	901	-	9,12,12	2.77	4 (44%)	8,17,17	3.75	3 (37%)
2	GUN	F	905	-	9,12,12	2.69	4 (44%)	8,17,17	3.86	4 (50%)
2	GUN	A	900	-	9,12,12	2.58	4 (44%)	8,17,17	3.69	4 (50%)
2	GUN	H	907	-	9,12,12	2.71	4 (44%)	8,17,17	3.85	4 (50%)
2	GUN	G	906	-	9,12,12	2.63	4 (44%)	8,17,17	3.87	4 (50%)
2	GUN	D	903	-	9,12,12	2.39	3 (33%)	8,17,17	3.89	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GUN	C	902	-	-	-	0/2/2/2
2	GUN	E	904	-	-	-	0/2/2/2
2	GUN	B	901	-	-	-	0/2/2/2
2	GUN	F	905	-	-	-	0/2/2/2
2	GUN	A	900	-	-	-	0/2/2/2
2	GUN	H	907	-	-	-	0/2/2/2
2	GUN	G	906	-	-	-	0/2/2/2
2	GUN	D	903	-	-	-	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	905	GUN	C6-N1	5.79	1.43	1.33
2	B	901	GUN	C6-N1	5.76	1.43	1.33
2	A	900	GUN	C6-N1	5.54	1.42	1.33
2	H	907	GUN	C6-N1	5.51	1.42	1.33
2	G	906	GUN	C6-N1	5.48	1.42	1.33
2	E	904	GUN	C6-N1	5.43	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	GUN	C6-N1	5.25	1.42	1.33
2	D	903	GUN	C6-N1	5.22	1.42	1.33
2	H	907	GUN	C6-C5	4.91	1.49	1.41
2	C	902	GUN	C6-C5	4.85	1.49	1.41
2	B	901	GUN	C6-C5	4.67	1.49	1.41
2	G	906	GUN	C6-C5	4.48	1.49	1.41
2	F	905	GUN	C6-C5	4.18	1.48	1.41
2	A	900	GUN	C6-C5	4.04	1.48	1.41
2	E	904	GUN	C6-C5	3.78	1.47	1.41
2	D	903	GUN	C6-C5	3.64	1.47	1.41
2	F	905	GUN	C4-N9	2.68	1.39	1.34
2	A	900	GUN	C4-N9	2.64	1.39	1.34
2	B	901	GUN	C2-N1	2.64	1.40	1.35
2	C	902	GUN	C4-N9	2.60	1.39	1.34
2	E	904	GUN	C2-N1	2.54	1.39	1.35
2	F	905	GUN	C2-N1	2.47	1.39	1.35
2	H	907	GUN	C2-N1	2.44	1.39	1.35
2	G	906	GUN	C2-N1	2.38	1.39	1.35
2	A	900	GUN	C2-N1	2.34	1.39	1.35
2	E	904	GUN	C4-N9	2.32	1.39	1.34
2	B	901	GUN	C4-N9	2.31	1.39	1.34
2	D	903	GUN	C2-N1	2.26	1.39	1.35
2	H	907	GUN	C4-N9	2.10	1.38	1.34
2	G	906	GUN	C4-N9	2.02	1.38	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	GUN	C5-C6-N1	-8.83	111.36	123.43
2	D	903	GUN	C5-C6-N1	-8.69	111.55	123.43
2	E	904	GUN	C5-C6-N1	-8.63	111.63	123.43
2	B	901	GUN	C5-C6-N1	-8.59	111.68	123.43
2	F	905	GUN	C5-C6-N1	-8.57	111.71	123.43
2	G	906	GUN	C5-C6-N1	-8.56	111.72	123.43
2	H	907	GUN	C5-C6-N1	-8.40	111.94	123.43
2	A	900	GUN	C5-C6-N1	-8.38	111.97	123.43
2	H	907	GUN	C6-N1-C2	5.55	124.74	115.93
2	F	905	GUN	C6-N1-C2	5.49	124.66	115.93
2	C	902	GUN	C6-N1-C2	5.47	124.62	115.93
2	E	904	GUN	C6-N1-C2	5.46	124.61	115.93
2	D	903	GUN	C6-N1-C2	5.45	124.59	115.93
2	G	906	GUN	C6-N1-C2	5.40	124.51	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	GUN	C6-N1-C2	5.15	124.11	115.93
2	A	900	GUN	C6-N1-C2	5.10	124.03	115.93
2	D	903	GUN	N3-C2-N1	-3.16	123.01	127.22
2	G	906	GUN	N3-C2-N1	-3.09	123.11	127.22
2	E	904	GUN	N3-C2-N1	-3.06	123.14	127.22
2	H	907	GUN	N3-C2-N1	-2.99	123.24	127.22
2	A	900	GUN	N3-C2-N1	-2.71	123.61	127.22
2	F	905	GUN	N3-C2-N1	-2.64	123.70	127.22
2	B	901	GUN	N3-C2-N1	-2.55	123.82	127.22
2	H	907	GUN	C6-C5-C4	-2.39	118.52	120.80
2	G	906	GUN	C6-C5-C4	-2.38	118.53	120.80
2	C	902	GUN	N3-C2-N1	-2.28	124.18	127.22
2	F	905	GUN	C6-C5-C4	-2.10	118.80	120.80
2	C	902	GUN	C6-C5-C4	-2.07	118.82	120.80
2	D	903	GUN	C6-C5-C4	-2.06	118.83	120.80
2	A	900	GUN	C6-C5-C4	-2.01	118.88	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	902	GUN	1	0
2	E	904	GUN	1	0
2	B	901	GUN	3	0
2	F	905	GUN	2	0
2	A	900	GUN	3	0
2	H	907	GUN	3	0
2	D	903	GUN	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/301 (97%)	-0.10	0 100 100	16, 31, 47, 62	0
1	B	294/301 (97%)	-0.02	1 (0%) 94 92	21, 39, 51, 54	0
1	C	298/301 (99%)	-0.03	0 100 100	19, 32, 51, 65	0
1	D	294/301 (97%)	0.03	2 (0%) 87 81	20, 37, 55, 58	0
1	E	294/301 (97%)	0.06	1 (0%) 94 92	26, 44, 59, 62	0
1	F	294/301 (97%)	0.09	4 (1%) 75 63	24, 44, 59, 67	0
1	G	294/301 (97%)	0.16	5 (1%) 70 57	24, 47, 70, 75	0
1	H	294/301 (97%)	0.06	4 (1%) 75 63	19, 39, 66, 70	0
All	All	2356/2408 (97%)	0.03	17 (0%) 87 81	16, 39, 59, 75	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	49	ALA	3.2
1	H	154	SER	3.1
1	G	47	THR	2.6
1	D	224	SER	2.6
1	B	235	ALA	2.4
1	G	144	SER	2.4
1	H	119	SER	2.3
1	F	293	GLY	2.3
1	F	119	SER	2.2
1	H	160	TRP	2.2
1	H	292	VAL	2.1
1	G	119	SER	2.1
1	E	119	SER	2.1
1	G	51	ASN	2.1
1	F	46	TYR	2.1
1	F	140	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	119	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SAC	E	1	6/10	0.81	0.28	51,53,54,71	0
1	SAC	F	1	6/10	0.84	0.26	50,65,65,66	0
1	SAC	C	1	6/10	0.84	0.23	48,63,63,63	0
1	SAC	H	1	6/10	0.87	0.31	58,59,59,82	0
1	SAC	A	1	6/10	0.89	0.25	53,56,59,69	0
1	SAC	G	1	6/10	0.92	0.36	51,57,59,73	0
1	SAC	B	1	9/10	0.93	0.33	37,46,61,72	0
1	SAC	D	1	9/10	0.93	0.25	39,43,56,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GUN	F	905	11/11	0.71	0.52	35,35,35,35	11
2	GUN	H	907	11/11	0.77	0.44	61,61,61,61	11
2	GUN	B	901	11/11	0.80	0.47	50,50,50,50	11
2	GUN	G	906	11/11	0.81	0.53	43,43,43,43	11
2	GUN	D	903	11/11	0.81	0.49	53,53,53,53	11
2	GUN	A	900	11/11	0.89	0.42	39,39,39,39	11
2	GUN	E	904	11/11	0.89	0.35	31,51,51,51	11
2	GUN	C	902	11/11	0.92	0.31	36,36,36,36	11

6.5 Other polymers [i](#)

There are no such residues in this entry.