



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

PDB ID : 4DC9
Title : Hexameric ring of Methanococcus voltae RadA
Authors : Du, L.; Luo, Y.
Deposited on : 2012-01-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

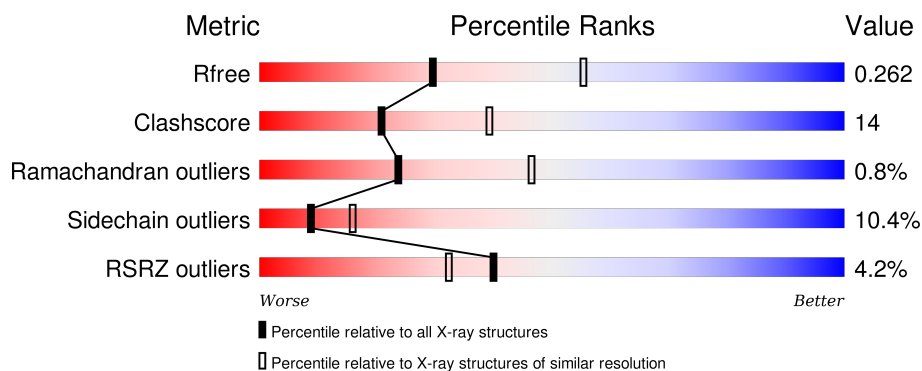
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	266	<div> <div>3%</div> <div>68% 25% . .</div> </div>
1	B	266	<div> <div>5%</div> <div>65% 27% . .</div> </div>
1	C	266	<div> <div>5%</div> <div>55% 36% 5% .</div> </div>
1	D	266	<div> <div>3%</div> <div>69% 24% . .</div> </div>
1	E	266	<div> <div>6%</div> <div>70% 23% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	266	

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	NO3	C	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12092 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 DNA repair and recombination protein radA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0
1	B	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0
1	C	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0
1	D	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0
1	E	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0
1	F	257	Total 1997	C 1252	N 349	O 387	S 9	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

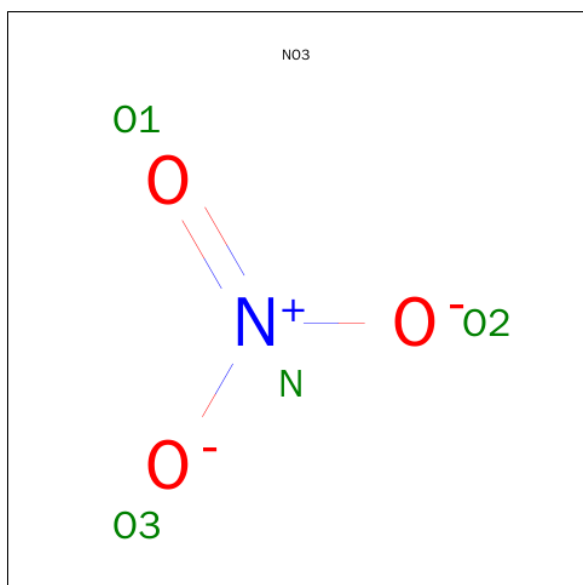
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	EXPRESSION TAG	UNP O73948
A	58	SER	-	EXPRESSION TAG	UNP O73948
A	59	HIS	-	EXPRESSION TAG	UNP O73948
A	60	MET	-	EXPRESSION TAG	UNP O73948
B	57	GLY	-	EXPRESSION TAG	UNP O73948
B	58	SER	-	EXPRESSION TAG	UNP O73948
B	59	HIS	-	EXPRESSION TAG	UNP O73948
B	60	MET	-	EXPRESSION TAG	UNP O73948
C	57	GLY	-	EXPRESSION TAG	UNP O73948
C	58	SER	-	EXPRESSION TAG	UNP O73948
C	59	HIS	-	EXPRESSION TAG	UNP O73948
C	60	MET	-	EXPRESSION TAG	UNP O73948
D	57	GLY	-	EXPRESSION TAG	UNP O73948
D	58	SER	-	EXPRESSION TAG	UNP O73948
D	59	HIS	-	EXPRESSION TAG	UNP O73948
D	60	MET	-	EXPRESSION TAG	UNP O73948
E	57	GLY	-	EXPRESSION TAG	UNP O73948

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	58	SER	-	EXPRESSION TAG	UNP O73948
E	59	HIS	-	EXPRESSION TAG	UNP O73948
E	60	MET	-	EXPRESSION TAG	UNP O73948
F	57	GLY	-	EXPRESSION TAG	UNP O73948
F	58	SER	-	EXPRESSION TAG	UNP O73948
F	59	HIS	-	EXPRESSION TAG	UNP O73948
F	60	MET	-	EXPRESSION TAG	UNP O73948

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		
2	D	1	Total	N	O	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	N	O	0	0
			4	1	3		
2	E	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		
2	F	1	Total	N	O	0	0
			4	1	3		

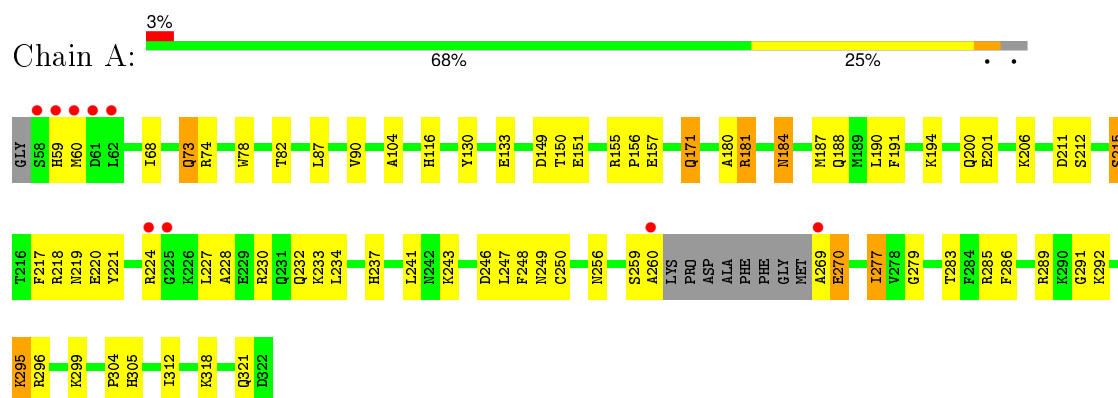
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	10	Total	O	0	0
			10	10		
3	C	5	Total	O	0	0
			5	5		
3	D	10	Total	O	0	0
			10	10		
3	E	11	Total	O	0	0
			11	11		
3	F	13	Total	O	0	0
			13	13		

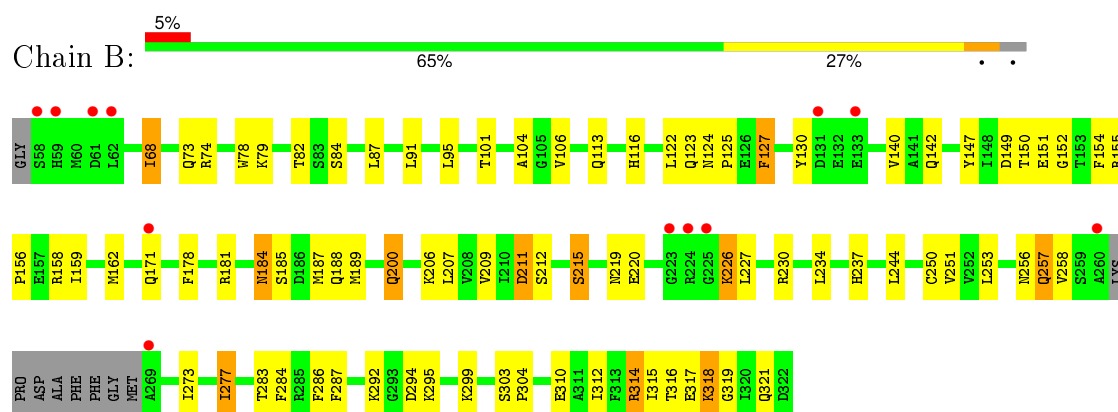
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

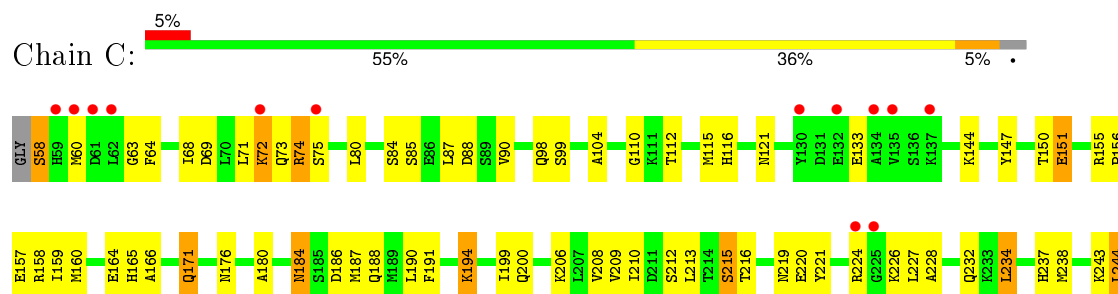
- Molecule 1: DNA repair and recombination protein radA

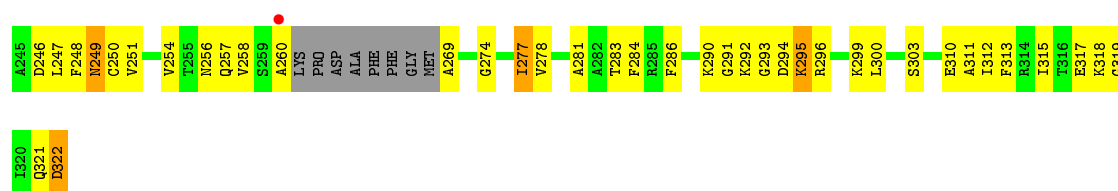


- Molecule 1: DNA repair and recombination protein radA

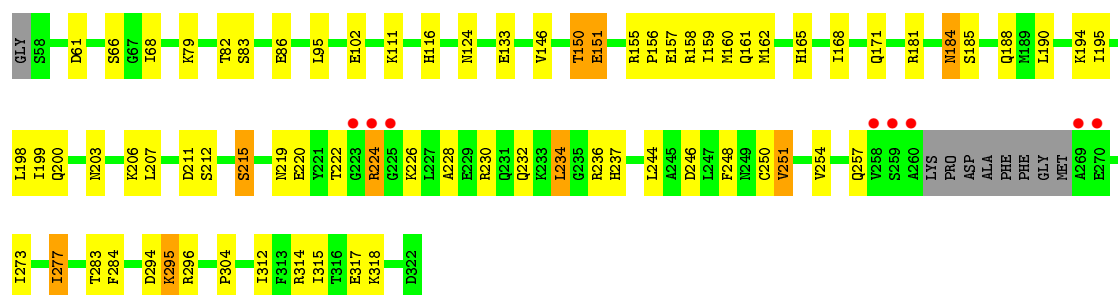


- Molecule 1: DNA repair and recombination protein radA

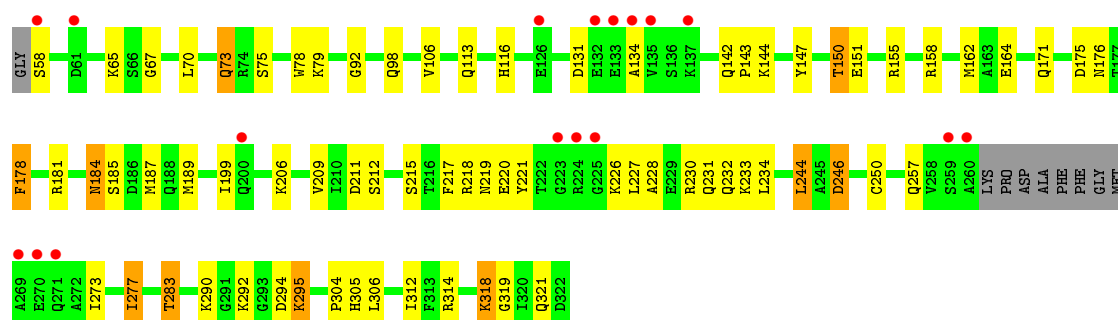




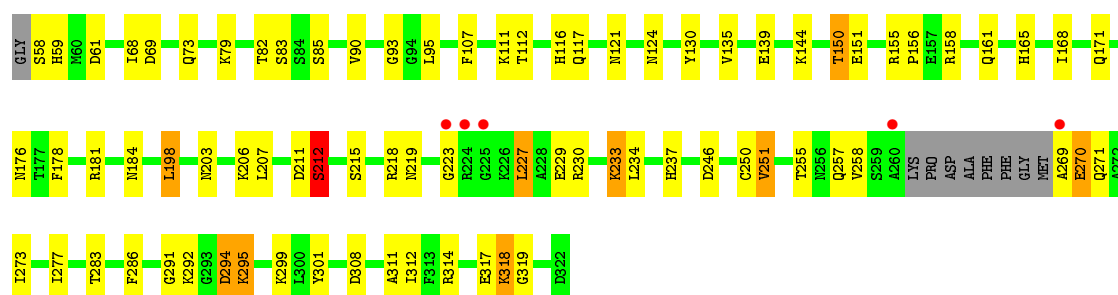
- Molecule 1: DNA repair and recombination protein rada



- Molecule 1: DNA repair and recombination protein rada



- Molecule 1: DNA repair and recombination protein rada



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.35Å 118.58Å 141.73Å 90.00° 138.05° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 39.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.60) 90.1 (39.19-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.266 0.203 , 0.262	Depositor DCC
R_{free} test set	2923 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.6	EDS
Estimated twinning fraction	0.000 for h+2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	3 of 57374 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12092	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NO3

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	0.74	0/2028	0.89	1/2727 (0.0%)
1	B	0.71	1/2028 (0.0%)	0.88	3/2727 (0.1%)
1	C	0.64	0/2028	0.79	1/2727 (0.0%)
1	D	0.69	0/2028	0.83	0/2727
1	E	0.69	1/2028 (0.0%)	0.84	1/2727 (0.0%)
1	F	0.71	0/2028	0.94	5/2727 (0.2%)
All	All	0.70	2/12168 (0.0%)	0.86	11/16362 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	TRP	CD2-CE2	5.84	1.48	1.41
1	E	78	TRP	CD2-CE2	5.25	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	61	ASP	CB-CG-OD2	17.63	134.17	118.30
1	F	61	ASP	OD1-CG-OD2	-7.77	108.54	123.30
1	E	244	LEU	CA-CB-CG	6.06	129.23	115.30
1	F	294	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	314	ARG	NE-CZ-NH2	5.86	123.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	233	LYS	CD-CE-NZ	5.41	124.13	111.70
1	B	211	ASP	CB-CG-OD1	5.33	123.10	118.30
1	F	181	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	B	314	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	F	212	SER	CB-CA-C	-5.13	100.35	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	221	TYR	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	1997	0	1976	54	1
1	B	1997	0	1976	62	0
1	C	1997	0	1976	79	0
1	D	1997	0	1976	52	0
1	E	1997	0	1976	56	1
1	F	1997	0	1976	59	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	2	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	1	0
3	A	13	0	0	2	0
3	B	10	0	0	0	0
3	C	5	0	0	2	0
3	D	10	0	0	1	0
3	E	11	0	0	0	0
3	F	13	0	0	1	0
All	All	12092	0	11856	345	1

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 14.

All (345) 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:E:292:LYS:H	1:E:295:LYS:HE3	1.03	1.16
1:C:292:LYS:H	1:C:295:LYS:HE2	0.97	1.09
1:C:292:LYS:H	1:C:295:LYS:CE	1.74	0.99
1:C:292:LYS:N	1:C:295:LYS:HE2	1.77	0.98
1:D:116:HIS:HE1	1:D:155:ARG:H	1.10	0.98
1:E:150:THR:HG22	1:E:212:SER:H	1.31	0.96
1:E:73:GLN:HG3	1:E:98:GLN:OE1	1.65	0.94
1:E:292:LYS:N	1:E:295:LYS:HE3	1.83	0.92
1:D:206:LYS:O	1:D:250:CYS:HB2	1.70	0.91
1:D:116:HIS:CE1	1:D:155:ARG:H	1.90	0.91
1:E:150:THR:CG2	1:E:212:SER:H	1.83	0.90
1:A:292:LYS:H	1:A:295:LYS:CE	1.84	0.90
1:D:257:GLN:HB3	1:D:273:ILE:HD12	1.52	0.90
1:D:188:GLN:HE21	1:D:237:HIS:CE1	1.88	0.90
1:C:116:HIS:HE1	1:C:155:ARG:H	1.20	0.87
1:D:124:ASN:HB2	1:D:168:ILE:HD11	1.56	0.87
1:B:318:LYS:HD3	1:B:321:GLN:NE2	1.90	0.87
1:F:292:LYS:H	1:F:295:LYS:HE2	1.38	0.86
1:E:116:HIS:HE1	1:E:155:ARG:H	1.24	0.86
1:B:95:LEU:HD13	1:B:253:LEU:HD11	1.58	0.84
1:F:116:HIS:HE1	1:F:155:ARG:H	1.26	0.83
1:F:144:LYS:HE3	1:F:176:ASN:HD22	1.41	0.83
1:C:188:GLN:HE21	1:C:237:HIS:CE1	1.97	0.83
1:A:116:HIS:HE1	1:A:155:ARG:H	1.25	0.82
1:C:110:GLY:HA2	2:C:401:NO3:O2	1.77	0.82
1:E:292:LYS:H	1:E:295:LYS:CE	1.89	0.82
1:A:150:THR:HG22	1:A:151:GLU:HG3	1.63	0.80
1:D:257:GLN:HB3	1:D:273:ILE:CD1	2.13	0.79
1:D:150:THR:HG22	1:D:151:GLU:HG2	1.63	0.78
1:A:292:LYS:H	1:A:295:LYS:HE2	1.49	0.77
1:C:228:ALA:O	1:C:232:GLN:HG3	1.83	0.77
1:C:116:HIS:CE1	1:C:155:ARG:H	2.01	0.77
1:C:269:ALA:HB2	3:C:501:HOH:O	1.83	0.77
1:F:144:LYS:HE3	1:F:176:ASN:ND2	1.99	0.77
1:F:124:ASN:HB2	1:F:168:ILE:HD11	1.66	0.77
1:B:318:LYS:CD	1:B:321:GLN:NE2	2.48	0.77
1:B:150:THR:HB	1:B:212:SER:H	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:H	1:A:295:LYS:HE3	1.52	0.75
1:F:116:HIS:CE1	1:F:155:ARG:H	2.04	0.75
1:E:131:ASP:HB3	1:E:134:ALA:HB3	1.68	0.74
1:B:292:LYS:H	1:B:295:LYS:HE3	1.52	0.73
1:E:67:GLY:HA2	1:E:70:LEU:HD12	1.70	0.72
1:B:147:TYR:CE1	1:B:209:VAL:HG11	2.24	0.72
1:C:150:THR:HB	1:C:212:SER:H	1.56	0.71
1:C:184:ASN:ND2	1:C:187:MET:H	1.89	0.70
1:C:71:LEU:CD2	1:C:74:ARG:HH21	2.04	0.70
1:A:237:HIS:HD2	3:A:701:HOH:O	1.75	0.70
1:B:257:GLN:HB3	1:B:273:ILE:HD12	1.73	0.70
1:E:116:HIS:CE1	1:E:155:ARG:H	2.09	0.70
1:C:110:GLY:CA	2:C:401:NO3:O2	2.40	0.70
1:E:158:ARG:HH11	1:E:319:GLY:HA2	1.56	0.69
1:F:150:THR:CG2	1:F:212:SER:H	2.03	0.69
1:A:291:GLY:HA3	1:A:295:LYS:HE3	1.73	0.69
1:F:207:LEU:HD12	1:F:251:VAL:HG22	1.75	0.69
1:F:292:LYS:N	1:F:295:LYS:HE2	2.07	0.68
1:B:188:GLN:HE21	1:B:237:HIS:CE1	2.11	0.67
1:C:58:SER:HB3	1:C:60:MET:H	1.59	0.67
1:A:188:GLN:HE21	1:A:237:HIS:CE1	2.12	0.66
1:F:198:LEU:O	1:F:203:ASN:HB2	1.95	0.66
1:B:200:GLN:HA	1:B:200:GLN:OE1	1.95	0.66
1:E:175:ASP:HB2	1:F:68:ILE:HD12	1.78	0.66
1:C:238:MET:HE2	1:C:281:ALA:HB3	1.78	0.65
1:A:219:ASN:HB3	1:B:277:ILE:HG12	1.78	0.65
1:C:188:GLN:HE21	1:C:237:HIS:HE1	1.43	0.65
1:D:219:ASN:HB3	1:E:277:ILE:HG12	1.79	0.64
1:D:222:THR:OG1	1:E:227:LEU:CD2	2.46	0.64
1:E:147:TYR:CE1	1:E:209:VAL:HG11	2.32	0.64
1:F:237:HIS:HD2	3:F:501:HOH:O	1.81	0.63
1:E:98:GLN:HG2	1:E:246:ASP:HA	1.77	0.63
1:A:270:GLU:HA	1:A:270:GLU:OE2	1.99	0.63
1:C:212:SER:HB2	1:C:215:SER:HB3	1.78	0.62
1:F:150:THR:HG22	1:F:212:SER:H	1.63	0.62
1:A:150:THR:HB	1:A:212:SER:H	1.64	0.62
1:D:116:HIS:HE1	1:D:155:ARG:N	1.91	0.62
1:B:101:THR:HB	1:B:253:LEU:CD2	2.30	0.61
1:F:144:LYS:CE	1:F:176:ASN:HD22	2.11	0.61
1:B:150:THR:HG22	1:B:151:GLU:HG3	1.81	0.61
1:C:150:THR:HG22	1:C:151:GLU:HG2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:PRO:O	1:C:159:ILE:HB	2.01	0.60
1:C:257:GLN:HG3	1:C:258:VAL:N	2.16	0.60
1:C:116:HIS:HE1	1:C:155:ARG:N	1.93	0.60
1:A:157:GLU:H	1:A:157:GLU:CD	2.04	0.60
1:E:257:GLN:HB3	1:E:273:ILE:HD12	1.83	0.60
1:D:228:ALA:O	1:D:232:GLN:HG3	2.01	0.60
1:F:124:ASN:HB2	1:F:168:ILE:CD1	2.30	0.60
1:B:188:GLN:HE21	1:B:237:HIS:HE1	1.50	0.59
1:E:295:LYS:HD2	1:E:312:ILE:HD11	1.84	0.59
1:C:71:LEU:CD2	1:C:74:ARG:NH2	2.65	0.59
1:C:90:VAL:HG21	1:C:311:ALA:HB2	1.83	0.59
1:B:116:HIS:HE1	1:B:155:ARG:H	1.51	0.59
1:A:292:LYS:O	1:A:295:LYS:HG3	2.03	0.59
1:F:90:VAL:HG21	1:F:311:ALA:HB2	1.84	0.59
1:B:294:ASP:OD1	1:B:314:ARG:HD2	2.02	0.59
1:F:111:LYS:HB2	2:F:402:NO3:O2	2.03	0.58
1:B:207:LEU:HD13	1:B:251:VAL:HG22	1.84	0.58
1:B:295:LYS:HD2	1:B:312:ILE:HD11	1.85	0.58
1:A:104:ALA:HA	1:A:256:ASN:O	2.04	0.58
1:F:257:GLN:HB3	1:F:273:ILE:CD1	2.33	0.58
1:F:212:SER:HA	1:F:255:THR:OG1	2.03	0.58
1:C:180:ALA:HB1	1:C:191:PHE:CD1	2.39	0.58
1:F:207:LEU:CD1	1:F:251:VAL:HG22	2.33	0.57
1:B:113:GLN:HG3	1:B:315:ILE:HG21	1.84	0.57
1:A:292:LYS:N	1:A:295:LYS:HE3	2.17	0.57
1:C:157:GLU:O	1:C:160:MET:HB2	2.05	0.57
1:A:228:ALA:O	1:A:232:GLN:HG3	2.04	0.57
1:A:184:ASN:ND2	1:A:187:MET:H	2.03	0.57
1:B:318:LYS:CD	1:B:321:GLN:HE22	2.16	0.57
1:C:199:ILE:HD12	1:C:248:PHE:CD2	2.40	0.57
1:B:184:ASN:C	1:B:184:ASN:HD22	2.06	0.57
1:E:184:ASN:HB2	1:E:220:GLU:OE1	2.04	0.56
1:C:84:SER:HA	1:C:322:ASP:OXT	2.05	0.56
1:D:111:LYS:HB2	2:D:402:NO3:O3	2.05	0.56
1:B:212:SER:HB2	1:B:215:SER:HB3	1.88	0.56
1:D:188:GLN:NE2	1:D:237:HIS:CE1	2.69	0.56
1:F:206:LYS:O	1:F:250:CYS:HB2	2.05	0.56
1:D:222:THR:OG1	1:E:227:LEU:HD21	2.05	0.56
1:A:171:GLN:HE21	1:A:171:GLN:CA	2.19	0.56
1:C:71:LEU:HD22	1:C:74:ARG:HH21	1.71	0.56
1:E:184:ASN:ND2	1:E:187:MET:H	2.03	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:GLY:HA3	1:C:295:LYS:HE3	1.88	0.56
1:A:171:GLN:HE21	1:A:171:GLN:HA	1.71	0.56
1:B:158:ARG:NH1	1:B:319:GLY:HA2	2.20	0.56
1:D:158:ARG:O	1:D:162:MET:HG3	2.07	0.55
1:D:124:ASN:CB	1:D:168:ILE:HD11	2.34	0.55
1:E:158:ARG:NH1	1:E:319:GLY:HA2	2.22	0.55
1:C:164:GLU:O	1:C:166:ALA:N	2.39	0.55
1:C:171:GLN:HE21	1:C:171:GLN:N	2.05	0.55
1:B:286:PHE:HA	1:B:299:LYS:O	2.07	0.55
1:E:150:THR:HG22	1:E:212:SER:N	2.13	0.54
1:A:150:THR:C	1:A:151:GLU:HG3	2.26	0.54
1:A:156:PRO:HD2	1:A:157:GLU:OE1	2.07	0.54
1:C:295:LYS:HD2	1:C:312:ILE:HD11	1.90	0.54
1:C:184:ASN:HD21	1:C:187:MET:H	1.56	0.53
1:F:107:PHE:H	1:F:257:GLN:HE22	1.56	0.53
1:B:219:ASN:HB3	1:C:277:ILE:HG12	1.90	0.53
1:A:260:ALA:HB1	1:A:269:ALA:HB1	1.90	0.53
1:C:269:ALA:CB	3:C:501:HOH:O	2.47	0.53
1:C:147:TYR:CE1	1:C:209:VAL:HG11	2.44	0.53
1:A:116:HIS:CE1	1:A:155:ARG:H	2.15	0.53
1:B:147:TYR:CD1	1:B:209:VAL:HG11	2.43	0.53
1:F:301:TYR:HA	1:F:308:ASP:OD1	2.08	0.53
1:F:158:ARG:NH1	1:F:319:GLY:HA2	2.23	0.53
1:C:286:PHE:HA	1:C:299:LYS:O	2.09	0.53
1:F:294:ASP:OD1	1:F:314:ARG:HD2	2.09	0.53
1:E:294:ASP:OD1	1:E:314:ARG:HD2	2.09	0.52
1:B:116:HIS:CE1	1:B:155:ARG:H	2.28	0.52
1:E:228:ALA:O	1:E:232:GLN:HG3	2.09	0.52
1:C:206:LYS:O	1:C:250:CYS:HB2	2.10	0.52
1:E:199:ILE:O	1:E:199:ILE:HG22	2.09	0.52
1:D:198:LEU:O	1:D:203:ASN:HB2	2.10	0.52
1:B:156:PRO:O	1:B:159:ILE:HB	2.10	0.52
1:A:295:LYS:HD2	1:A:312:ILE:HD11	1.91	0.51
1:C:248:PHE:O	1:C:249:ASN:C	2.47	0.51
1:C:73:GLN:HG3	1:C:98:GLN:OE1	2.11	0.51
1:D:207:LEU:CD1	1:D:251:VAL:HG22	2.41	0.51
1:B:79:LYS:HA	1:B:95:LEU:O	2.11	0.51
1:D:79:LYS:HA	1:D:95:LEU:O	2.10	0.51
1:D:212:SER:OG	1:D:215:SER:HB3	2.12	0.50
1:A:150:THR:HG21	1:A:215:SER:HB3	1.93	0.50
1:C:110:GLY:HA3	1:C:315:ILE:HD11	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:GLN:HB3	1:F:273:ILE:HD12	1.93	0.50
1:A:181:ARG:NH2	3:A:705:HOH:O	2.44	0.50
1:F:295:LYS:HD2	1:F:312:ILE:HD11	1.93	0.50
1:F:286:PHE:HA	1:F:299:LYS:O	2.11	0.50
1:B:185:SER:O	1:B:189:MET:HG3	2.12	0.50
1:C:300:LEU:HD11	1:C:303:SER:HB3	1.94	0.50
1:F:211:ASP:HA	1:F:255:THR:OG1	2.12	0.50
1:A:243:LYS:HE2	1:A:247:LEU:CD1	2.42	0.50
1:B:178:PHE:HB3	1:C:64:PHE:HB3	1.94	0.49
1:E:318:LYS:NZ	1:E:321:GLN:HE22	2.09	0.49
1:B:303:SER:HB2	1:B:304:PRO:HD2	1.94	0.49
1:D:237:HIS:HD2	3:D:503:HOH:O	1.95	0.49
1:F:317:GLU:OE1	1:F:318:LYS:HE3	2.13	0.49
1:F:292:LYS:O	1:F:295:LYS:HG2	2.11	0.49
1:B:101:THR:HB	1:B:253:LEU:HD23	1.94	0.49
1:F:139:GLU:O	1:F:206:LYS:HE2	2.13	0.49
1:B:124:ASN:O	1:B:125:PRO:C	2.50	0.49
1:C:150:THR:HG23	1:C:216:THR:HG23	1.95	0.49
1:B:299:LYS:HD2	1:B:310:GLU:HG2	1.94	0.49
1:B:185:SER:OG	1:B:220:GLU:OE2	2.30	0.49
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.59	0.49
1:C:238:MET:CE	1:C:281:ALA:HB3	2.42	0.49
1:F:107:PHE:N	1:F:257:GLN:HE22	2.10	0.49
1:B:316:THR:OG1	1:B:318:LYS:HD2	2.12	0.48
1:C:171:GLN:HE21	1:C:171:GLN:CA	2.24	0.48
1:B:130:TYR:CE2	1:B:140:VAL:HG21	2.48	0.48
1:A:180:ALA:HB1	1:A:191:PHE:CE1	2.48	0.48
1:C:219:ASN:HB3	1:D:277:ILE:HG12	1.95	0.48
1:E:206:LYS:HA	1:E:250:CYS:HB3	1.94	0.48
1:E:305:HIS:C	1:E:306:LEU:HD12	2.34	0.48
1:E:150:THR:CG2	1:E:151:GLU:HG3	2.43	0.48
1:C:164:GLU:C	1:C:166:ALA:H	2.17	0.48
1:C:98:GLN:HG2	1:C:246:ASP:HA	1.95	0.47
1:D:206:LYS:HA	1:D:206:LYS:HD3	1.74	0.47
1:E:158:ARG:HH11	1:E:162:MET:HE2	1.79	0.47
1:B:152:GLY:O	1:B:155:ARG:NH2	2.45	0.47
1:D:207:LEU:HD12	1:D:251:VAL:HG22	1.96	0.47
1:A:116:HIS:HE1	1:A:155:ARG:N	2.03	0.47
1:B:150:THR:HG21	1:B:215:SER:HB3	1.97	0.47
1:B:283:THR:HG22	1:B:304:PRO:HD3	1.95	0.47
1:B:154:PHE:O	1:B:155:ARG:NH1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:GLN:HG3	1:F:258:VAL:H	1.80	0.47
1:E:79:LYS:NZ	1:E:92:GLY:O	2.38	0.47
1:E:231:GLN:HA	1:E:231:GLN:OE1	2.14	0.47
1:E:211:ASP:HA	1:E:212:SER:HA	1.57	0.47
1:E:150:THR:HG21	1:E:212:SER:H	1.75	0.47
1:F:151:GLU:OE2	1:F:212:SER:OG	2.33	0.47
1:A:269:ALA:O	1:A:270:GLU:HB2	2.15	0.47
1:E:142:GLN:N	1:E:143:PRO:CD	2.78	0.47
1:A:304:PRO:HB2	1:A:305:HIS:CD2	2.50	0.47
1:A:291:GLY:CA	1:A:295:LYS:HE3	2.43	0.47
1:A:149:ASP:OD1	1:A:149:ASP:C	2.52	0.47
1:B:207:LEU:CD1	1:B:251:VAL:HG22	2.44	0.47
1:B:150:THR:HB	1:B:212:SER:N	2.25	0.46
1:F:150:THR:HG23	1:F:151:GLU:HG3	1.96	0.46
1:A:217:PHE:O	1:A:221:TYR:HD2	1.98	0.46
1:E:219:ASN:HB3	1:F:277:ILE:HG12	1.96	0.46
1:A:286:PHE:HA	1:A:299:LYS:O	2.15	0.46
1:A:206:LYS:C	1:A:250:CYS:HB2	2.35	0.46
1:B:106:VAL:HA	1:B:257:GLN:HE22	1.80	0.46
1:B:184:ASN:C	1:B:184:ASN:ND2	2.69	0.46
1:E:185:SER:OG	1:E:220:GLU:OE2	2.20	0.46
1:E:147:TYR:HA	1:E:209:VAL:HB	1.97	0.46
1:E:106:VAL:HA	1:E:257:GLN:HE22	1.79	0.46
1:D:165:HIS:ND1	1:D:318:LYS:HE3	2.31	0.46
1:F:82:THR:O	1:F:83:SER:HB2	2.15	0.46
1:C:80:LEU:HD11	1:C:121:ASN:HB3	1.97	0.46
1:F:206:LYS:C	1:F:250:CYS:HB2	2.36	0.46
1:C:158:ARG:HH11	1:C:319:GLY:HA2	1.81	0.46
1:E:178:PHE:N	1:E:178:PHE:CD1	2.84	0.46
1:C:208:VAL:HG21	1:C:244:LEU:HD11	1.98	0.46
1:B:318:LYS:HD2	1:B:321:GLN:NE2	2.30	0.45
1:E:283:THR:HG22	1:E:304:PRO:HD3	1.98	0.45
1:E:189:MET:SD	1:E:233:LYS:HG2	2.57	0.45
1:C:184:ASN:C	1:C:184:ASN:HD22	2.20	0.45
1:E:144:LYS:HE2	1:E:176:ASN:OD1	2.16	0.45
1:B:104:ALA:HA	1:B:256:ASN:O	2.17	0.45
1:B:113:GLN:HG3	1:B:315:ILE:CG2	2.45	0.45
1:B:158:ARG:O	1:B:162:MET:HG3	2.17	0.45
1:F:292:LYS:H	1:F:295:LYS:CE	2.20	0.45
1:A:78:TRP:HB3	1:A:130:TYR:HB3	1.99	0.45
1:F:59:HIS:HE1	1:F:69:ASP:OD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASP:OD1	1:D:314:ARG:HD2	2.16	0.44
1:F:291:GLY:HA3	1:F:295:LYS:HE2	1.98	0.44
1:F:144:LYS:CE	1:F:176:ASN:ND2	2.73	0.44
1:E:158:ARG:HD2	1:E:158:ARG:HA	1.82	0.44
1:F:144:LYS:HG2	1:F:176:ASN:HB3	1.99	0.44
1:C:180:ALA:HB1	1:C:191:PHE:CG	2.53	0.44
1:F:227:LEU:HA	1:F:227:LEU:HD23	1.84	0.44
1:C:190:LEU:O	1:C:194:LYS:HD3	2.18	0.44
1:B:277:ILE:HA	1:B:277:ILE:HD13	1.90	0.44
1:F:117:GLN:NE2	1:F:121:ASN:OD1	2.50	0.44
1:D:184:ASN:HB2	1:D:220:GLU:OE1	2.18	0.44
1:A:150:THR:HB	1:A:212:SER:N	2.30	0.44
1:D:155:ARG:HA	1:D:155:ARG:HD3	1.78	0.44
1:D:124:ASN:HB2	1:D:168:ILE:CD1	2.38	0.44
1:F:150:THR:HG21	1:F:212:SER:H	1.80	0.44
1:E:217:PHE:O	1:E:221:TYR:HD2	2.00	0.44
1:D:156:PRO:O	1:D:159:ILE:HB	2.18	0.44
1:B:206:LYS:C	1:B:250:CYS:HB2	2.39	0.44
1:D:102:GLU:HA	1:D:254:VAL:HG23	2.00	0.44
1:A:243:LYS:HE2	1:A:247:LEU:HD12	2.00	0.44
1:A:180:ALA:HB1	1:A:191:PHE:CD1	2.53	0.44
1:F:95:LEU:HG	1:F:95:LEU:H	1.71	0.44
1:B:226:LYS:HE3	1:C:228:ALA:HB3	2.00	0.43
1:D:161:GLN:NE2	1:D:317:GLU:HB2	2.33	0.43
1:D:295:LYS:HD2	1:D:312:ILE:HD11	1.99	0.43
1:C:213:LEU:HD13	1:C:254:VAL:HG11	2.00	0.43
1:A:171:GLN:HG3	1:B:68:ILE:HD11	1.99	0.43
1:C:69:ASP:O	1:C:73:GLN:HB2	2.18	0.43
1:C:274:GLY:HA3	1:C:278:VAL:HG21	2.00	0.43
1:D:211:ASP:HA	1:D:212:SER:HA	1.64	0.43
1:A:78:TRP:CB	1:A:130:TYR:HB3	2.48	0.43
1:C:290:LYS:HA	1:C:296:ARG:HD3	1.99	0.43
1:E:185:SER:O	1:E:189:MET:HG3	2.18	0.43
1:A:74:ARG:HH12	1:F:156:PRO:HG2	1.84	0.43
1:F:90:VAL:CG2	1:F:311:ALA:HB2	2.48	0.43
1:D:157:GLU:O	1:D:160:MET:HB2	2.19	0.43
1:E:150:THR:HG23	1:E:151:GLU:HG3	2.01	0.43
1:D:284:PHE:CE2	1:D:304:PRO:HD2	2.54	0.43
1:D:82:THR:O	1:D:83:SER:HB2	2.19	0.43
1:A:211:ASP:HA	1:A:212:SER:HA	1.79	0.43
1:D:222:THR:HG1	1:E:227:LEU:HD21	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASN:HB3	1:B:127:PHE:HB2	2.01	0.43
1:D:185:SER:OG	1:D:220:GLU:OE2	2.18	0.43
1:C:295:LYS:C	1:C:296:ARG:HG2	2.40	0.42
1:B:149:ASP:OD1	1:B:152:GLY:N	2.52	0.42
1:C:184:ASN:HB2	1:C:220:GLU:OE1	2.19	0.42
1:C:104:ALA:HA	1:C:256:ASN:O	2.19	0.42
1:A:237:HIS:O	1:A:241:LEU:HG	2.20	0.42
1:C:180:ALA:HB1	1:C:191:PHE:CE1	2.54	0.42
1:C:312:ILE:HG12	1:C:313:PHE:N	2.35	0.42
1:A:295:LYS:O	1:A:296:ARG:HD3	2.20	0.42
1:C:243:LYS:HG3	1:C:247:LEU:HD12	2.01	0.42
1:A:82:THR:CB	1:A:87:LEU:HD23	2.50	0.42
1:E:113:GLN:HG2	2:E:401:NO3:O2	2.20	0.42
1:E:175:ASP:HB2	1:F:68:ILE:CD1	2.48	0.42
1:A:248:PHE:O	1:A:249:ASN:C	2.57	0.42
1:C:322:ASP:N	1:C:322:ASP:OD2	2.52	0.42
1:C:144:LYS:HG3	1:C:176:ASN:HD22	1.84	0.42
1:D:188:GLN:HE21	1:D:237:HIS:HE1	1.53	0.42
1:F:116:HIS:HE1	1:F:155:ARG:N	2.06	0.42
1:C:260:ALA:HA	1:C:269:ALA:O	2.19	0.42
1:E:199:ILE:O	1:E:199:ILE:CG2	2.67	0.42
1:D:199:ILE:HD13	1:D:248:PHE:CD2	2.55	0.42
1:B:211:ASP:HA	1:B:212:SER:HA	1.89	0.42
1:E:318:LYS:HB2	1:E:321:GLN:HE21	1.85	0.42
1:A:279:GLY:HA2	1:A:285:ARG:CZ	2.50	0.42
1:A:59:HIS:CD2	1:F:178:PHE:HE2	2.38	0.42
1:A:184:ASN:HB2	1:A:220:GLU:OE1	2.20	0.41
1:F:269:ALA:O	1:F:270:GLU:CB	2.67	0.41
1:C:184:ASN:C	1:C:184:ASN:ND2	2.73	0.41
1:D:146:VAL:HG11	1:D:195:ILE:HD11	2.03	0.41
1:F:130:TYR:CD1	1:F:135:VAL:HB	2.54	0.41
1:D:190:LEU:HG	1:D:194:LYS:HE2	2.02	0.41
1:F:79:LYS:HD3	1:F:93:GLY:HA3	2.02	0.41
1:D:66:SER:C	1:D:68:ILE:N	2.73	0.41
1:C:234:LEU:O	1:C:238:MET:HG2	2.20	0.41
1:D:222:THR:OG1	1:E:227:LEU:HD22	2.21	0.41
1:B:124:ASN:O	1:B:127:PHE:N	2.50	0.41
1:C:210:ILE:HB	1:C:254:VAL:HG12	2.02	0.41
1:F:229:GLU:O	1:F:233:LYS:HB2	2.21	0.41
1:B:82:THR:C	1:B:84:SER:H	2.23	0.41
1:D:206:LYS:C	1:D:250:CYS:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLN:O	1:F:165:HIS:HD2	2.03	0.41
1:C:299:LYS:HD2	1:C:310:GLU:HG2	2.03	0.41
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.77	0.41
1:A:150:THR:HG22	1:A:151:GLU:CG	2.41	0.41
1:D:296:ARG:HG3	1:D:315:ILE:HD12	2.02	0.41
1:C:71:LEU:HD23	1:C:74:ARG:NH2	2.34	0.41
1:C:257:GLN:HG3	1:C:258:VAL:H	1.86	0.41
1:E:290:LYS:HB2	1:E:290:LYS:HE3	1.80	0.41
1:E:147:TYR:CD1	1:E:209:VAL:HG11	2.55	0.41
1:D:161:GLN:HE21	1:D:317:GLU:HB2	1.85	0.41
1:A:277:ILE:HG12	1:F:219:ASN:HB3	2.03	0.41
1:C:112:THR:O	1:C:115:MET:HB2	2.21	0.40
1:B:184:ASN:ND2	1:B:187:MET:H	2.19	0.40
1:D:111:LYS:HE3	1:D:111:LYS:HB2	1.96	0.40
1:C:68:ILE:HG23	1:C:72:LYS:HE3	2.04	0.40
1:D:158:ARG:HG3	1:D:158:ARG:O	2.19	0.40
1:C:206:LYS:C	1:C:250:CYS:HB2	2.41	0.40
1:B:284:PHE:CE2	1:B:304:PRO:HD2	2.56	0.40
1:D:230:ARG:O	1:D:234:LEU:HB2	2.21	0.40
1:B:258:VAL:HG12	1:B:287:PHE:HE1	1.87	0.40
1:C:99:SER:CB	1:C:284:PHE:HE1	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LYS:NZ	1:E:295:LYS:NZ[2_555]	1.72	0.48

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	253/266 (95%)	238 (94%)	12 (5%)	3 (1%)	16	33
1	B	253/266 (95%)	234 (92%)	18 (7%)	1 (0%)	39	65
1	C	253/266 (95%)	233 (92%)	16 (6%)	4 (2%)	12	24
1	D	253/266 (95%)	240 (95%)	12 (5%)	1 (0%)	39	65
1	E	253/266 (95%)	238 (94%)	14 (6%)	1 (0%)	39	65
1	F	253/266 (95%)	234 (92%)	17 (7%)	2 (1%)	24	46
All	All	1518/1596 (95%)	1417 (93%)	89 (6%)	12 (1%)	24	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	270	GLU
1	A	224	ARG
1	C	165	HIS
1	C	249	ASN
1	C	293	GLY
1	D	224	ARG
1	F	223	GLY
1	E	164	GLU
1	A	270	GLU
1	B	123	GLN
1	A	73	GLN
1	C	63	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/221 (97%)	191 (89%)	24 (11%)	7	13
1	B	215/221 (97%)	194 (90%)	21 (10%)	10	19
1	C	215/221 (97%)	187 (87%)	28 (13%)	5	9
1	D	215/221 (97%)	195 (91%)	20 (9%)	11	21
1	E	215/221 (97%)	195 (91%)	20 (9%)	11	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	215/221 (97%)	194 (90%)	21 (10%)	10	19
All	All	1290/1326 (97%)	1156 (90%)	134 (10%)	9	16

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	MET
1	A	68	ILE
1	A	73	GLN
1	A	90	VAL
1	A	133	GLU
1	A	171	GLN
1	A	181	ARG
1	A	184	ASN
1	A	190	LEU
1	A	194	LYS
1	A	200	GLN
1	A	201	GLU
1	A	215	SER
1	A	218	ARG
1	A	227	LEU
1	A	230	ARG
1	A	246	ASP
1	A	259	SER
1	A	277	ILE
1	A	283	THR
1	A	289	ARG
1	A	295	LYS
1	A	318	LYS
1	A	321	GLN
1	B	68	ILE
1	B	73	GLN
1	B	74	ARG
1	B	87	LEU
1	B	91	LEU
1	B	127	PHE
1	B	142	GLN
1	B	171	GLN
1	B	181	ARG
1	B	184	ASN
1	B	200	GLN
1	B	215	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	226	LYS
1	B	227	LEU
1	B	230	ARG
1	B	234	LEU
1	B	244	LEU
1	B	257	GLN
1	B	277	ILE
1	B	317	GLU
1	B	318	LYS
1	C	58	SER
1	C	72	LYS
1	C	74	ARG
1	C	75	SER
1	C	85	SER
1	C	87	LEU
1	C	88	ASP
1	C	133	GLU
1	C	151	GLU
1	C	171	GLN
1	C	184	ASN
1	C	194	LYS
1	C	200	GLN
1	C	215	SER
1	C	224	ARG
1	C	226	LYS
1	C	227	LEU
1	C	234	LEU
1	C	244	LEU
1	C	251	VAL
1	C	277	ILE
1	C	283	THR
1	C	294	ASP
1	C	295	LYS
1	C	317	GLU
1	C	318	LYS
1	C	321	GLN
1	C	322	ASP
1	D	61	ASP
1	D	86	GLU
1	D	133	GLU
1	D	150	THR
1	D	151	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	171	GLN
1	D	181	ARG
1	D	184	ASN
1	D	200	GLN
1	D	215	SER
1	D	224	ARG
1	D	226	LYS
1	D	234	LEU
1	D	236	ARG
1	D	244	LEU
1	D	246	ASP
1	D	251	VAL
1	D	277	ILE
1	D	283	THR
1	D	295	LYS
1	E	58	SER
1	E	65	LYS
1	E	73	GLN
1	E	75	SER
1	E	150	THR
1	E	171	GLN
1	E	178	PHE
1	E	181	ARG
1	E	184	ASN
1	E	215	SER
1	E	218	ARG
1	E	226	LYS
1	E	230	ARG
1	E	234	LEU
1	E	244	LEU
1	E	246	ASP
1	E	277	ILE
1	E	283	THR
1	E	295	LYS
1	E	318	LYS
1	F	58	SER
1	F	73	GLN
1	F	85	SER
1	F	112	THR
1	F	150	THR
1	F	171	GLN
1	F	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	198	LEU
1	F	212	SER
1	F	215	SER
1	F	218	ARG
1	F	227	LEU
1	F	230	ARG
1	F	233	LYS
1	F	234	LEU
1	F	246	ASP
1	F	251	VAL
1	F	271	GLN
1	F	283	THR
1	F	295	LYS
1	F	318	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	171	GLN
1	A	184	ASN
1	A	237	HIS
1	A	257	GLN
1	A	276	HIS
1	A	305	HIS
1	B	116	HIS
1	B	142	GLN
1	B	171	GLN
1	B	184	ASN
1	B	237	HIS
1	B	257	GLN
1	B	280	HIS
1	B	321	GLN
1	C	116	HIS
1	C	171	GLN
1	C	176	ASN
1	C	184	ASN
1	C	200	GLN
1	C	237	HIS
1	C	242	ASN
1	C	305	HIS
1	D	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	116	HIS
1	D	161	GLN
1	D	184	ASN
1	D	237	HIS
1	E	116	HIS
1	E	171	GLN
1	E	184	ASN
1	E	237	HIS
1	E	257	GLN
1	E	271	GLN
1	E	321	GLN
1	F	73	GLN
1	F	116	HIS
1	F	165	HIS
1	F	171	GLN
1	F	176	ASN
1	F	184	ASN
1	F	237	HIS
1	F	257	GLN
1	F	271	GLN

5.3.3 RNA [i](#)

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	NO3	A	401	-	3,3,3	2.38	2 (66%)	3,3,3	0.33	0
2	NO3	A	402	-	3,3,3	2.28	2 (66%)	3,3,3	0.30	0
2	NO3	B	401	-	3,3,3	2.45	2 (66%)	3,3,3	0.10	0
2	NO3	B	402	-	3,3,3	2.15	2 (66%)	3,3,3	0.25	0
2	NO3	C	401	-	3,3,3	2.26	2 (66%)	3,3,3	0.38	0
2	NO3	C	402	-	3,3,3	2.40	2 (66%)	3,3,3	0.20	0
2	NO3	D	401	-	3,3,3	2.59	2 (66%)	3,3,3	0.17	0
2	NO3	D	402	-	3,3,3	2.31	2 (66%)	3,3,3	0.31	0
2	NO3	E	401	-	3,3,3	2.39	2 (66%)	3,3,3	0.37	0
2	NO3	E	402	-	3,3,3	2.16	2 (66%)	3,3,3	0.17	0
2	NO3	F	401	-	3,3,3	2.73	2 (66%)	3,3,3	0.34	0
2	NO3	F	402	-	3,3,3	2.23	2 (66%)	3,3,3	0.38	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
2	NO3	A	401	-	-	0/0/0/0	0/0/0/0
2	NO3	A	402	-	-	0/0/0/0	0/0/0/0
2	NO3	B	401	-	-	0/0/0/0	0/0/0/0
2	NO3	B	402	-	-	0/0/0/0	0/0/0/0
2	NO3	C	401	-	-	0/0/0/0	0/0/0/0
2	NO3	C	402	-	-	0/0/0/0	0/0/0/0
2	NO3	D	401	-	-	0/0/0/0	0/0/0/0
2	NO3	D	402	-	-	0/0/0/0	0/0/0/0
2	NO3	E	401	-	-	0/0/0/0	0/0/0/0
2	NO3	E	402	-	-	0/0/0/0	0/0/0/0
2	NO3	F	401	-	-	0/0/0/0	0/0/0/0
2	NO3	F	402	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	402	NO3	O2-N	2.46	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	NO3	O3-N	2.51	1.38	1.25
2	A	402	NO3	O2-N	2.57	1.38	1.25
2	F	402	NO3	O2-N	2.59	1.38	1.25
2	C	401	NO3	O3-N	2.60	1.38	1.25
2	E	402	NO3	O3-N	2.65	1.39	1.25
2	D	402	NO3	O3-N	2.66	1.39	1.25
2	A	401	NO3	O3-N	2.70	1.39	1.25
2	B	402	NO3	O2-N	2.72	1.39	1.25
2	F	402	NO3	O3-N	2.79	1.39	1.25
2	A	402	NO3	O3-N	2.85	1.40	1.25
2	E	401	NO3	O3-N	2.87	1.40	1.25
2	C	402	NO3	O3-N	2.89	1.40	1.25
2	C	401	NO3	O2-N	2.90	1.40	1.25
2	D	402	NO3	O2-N	2.94	1.40	1.25
2	B	401	NO3	O3-N	2.94	1.40	1.25
2	E	401	NO3	O2-N	2.95	1.40	1.25
2	C	402	NO3	O2-N	2.96	1.40	1.25
2	B	401	NO3	O2-N	3.02	1.41	1.25
2	A	401	NO3	O2-N	3.09	1.41	1.25
2	D	401	NO3	O2-N	3.15	1.41	1.25
2	D	401	NO3	O3-N	3.18	1.41	1.25
2	F	401	NO3	O2-N	3.33	1.42	1.25
2	F	401	NO3	O3-N	3.37	1.42	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NO3	2	0
2	D	402	NO3	1	0
2	E	401	NO3	1	0
2	F	402	NO3	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	257/266 (96%)	-0.25	9 (3%)	48	40	22, 44, 79, 121	0
1	B	257/266 (96%)	-0.11	12 (4%)	35	28	26, 52, 99, 122	0
1	C	257/266 (96%)	0.10	14 (5%)	29	22	35, 65, 99, 144	0
1	D	257/266 (96%)	-0.23	8 (3%)	52	45	28, 52, 81, 109	0
1	E	257/266 (96%)	-0.12	17 (6%)	22	16	26, 51, 96, 131	0
1	F	257/266 (96%)	-0.30	5 (1%)	70	64	27, 48, 77, 117	0
All	All	1542/1596 (96%)	-0.15	65 (4%)	40	32	22, 52, 94, 144	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	224	ARG	6.8
1	A	269	ALA	5.7
1	B	224	ARG	5.2
1	C	59	HIS	5.1
1	E	260	ALA	4.7
1	E	269	ALA	4.6
1	F	269	ALA	4.5
1	C	134	ALA	4.4
1	A	224	ARG	4.4
1	B	61	ASP	4.0
1	F	224	ARG	4.0
1	B	269	ALA	4.0
1	C	60	MET	4.0
1	C	260	ALA	3.8
1	C	62	LEU	3.7
1	D	260	ALA	3.7
1	E	270	GLU	3.7
1	B	225	GLY	3.6
1	D	270	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	223	GLY	3.5
1	D	224	ARG	3.5
1	D	269	ALA	3.5
1	E	223	GLY	3.4
1	E	58	SER	3.4
1	C	137	LYS	3.3
1	A	58	SER	3.2
1	D	225	GLY	3.1
1	C	135	VAL	3.1
1	B	133	GLU	3.1
1	C	224	ARG	3.0
1	B	223	GLY	3.0
1	E	225	GLY	2.9
1	C	72	LYS	2.9
1	C	61	ASP	2.9
1	E	133	GLU	2.9
1	E	126	GLU	2.9
1	E	259	SER	2.8
1	C	225	GLY	2.8
1	F	225	GLY	2.8
1	B	58	SER	2.7
1	A	61	ASP	2.7
1	E	200	GLN	2.6
1	B	171	GLN	2.6
1	B	59	HIS	2.6
1	F	260	ALA	2.5
1	E	271	GLN	2.5
1	E	137	LYS	2.4
1	B	62	LEU	2.4
1	A	59	HIS	2.4
1	A	260	ALA	2.3
1	C	75	SER	2.3
1	D	259	SER	2.3
1	E	135	VAL	2.3
1	C	130	TYR	2.2
1	A	62	LEU	2.2
1	B	131	ASP	2.2
1	F	223	GLY	2.2
1	A	225	GLY	2.1
1	A	60	MET	2.1
1	B	260	ALA	2.1
1	E	61	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	132	GLU	2.1
1	E	132	GLU	2.1
1	E	134	ALA	2.1
1	D	258	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NO3	D	401	4/4	0.97	0.13	1.09	38,43,46,50	0
2	NO3	E	402	4/4	0.99	0.15	0.96	32,35,38,39	0
2	NO3	F	401	4/4	0.93	0.14	0.93	34,43,44,45	0
2	NO3	F	402	4/4	0.96	0.14	0.70	45,46,51,52	0
2	NO3	A	402	4/4	0.98	0.13	0.58	39,40,43,44	0
2	NO3	B	402	4/4	0.98	0.15	0.18	39,39,42,43	0
2	NO3	A	401	4/4	0.98	0.12	-0.20	37,37,39,39	0
2	NO3	D	402	4/4	0.97	0.12	-0.33	49,50,50,53	0
2	NO3	C	401	4/4	0.95	0.14	-0.34	47,51,56,57	0
2	NO3	E	401	4/4	0.98	0.09	-0.93	37,39,39,43	0
2	NO3	B	401	4/4	0.98	0.09	-1.73	34,38,39,39	0
2	NO3	C	402	4/4	0.97	0.07	-2.78	45,49,50,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.