



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:01 PM UTC

PDB ID : 4DC9 / pdb_00004dc9
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

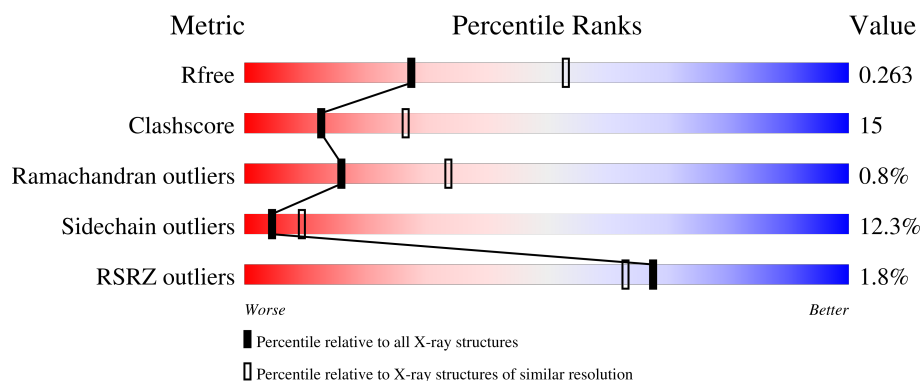
1 Overall quality at a glance ⓘ

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of 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	266	2% 67% 26% • • •
1	B	266	3% 61% 31% 5% •
1	C	266	3% 53% 37% 6% •
1	D	266	64% 27% 5% •
1	E	266	2% 66% 26% • •

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Mol	Chain	Length	Quality of chain
1	F	266	% 65% 28% ...

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:

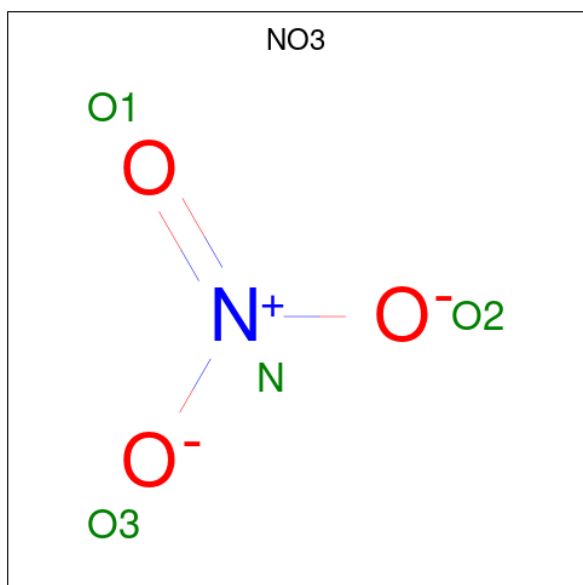
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	expression tag	UNP O73948
A	58	SER	-	expression tag	UNP O73948
A	59	HIS	-	expression tag	UNP O73948
A	60	MET	-	expression tag	UNP O73948
B	57	GLY	-	expression tag	UNP O73948
B	58	SER	-	expression tag	UNP O73948
B	59	HIS	-	expression tag	UNP O73948
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

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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 (CCD ID: 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		

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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		

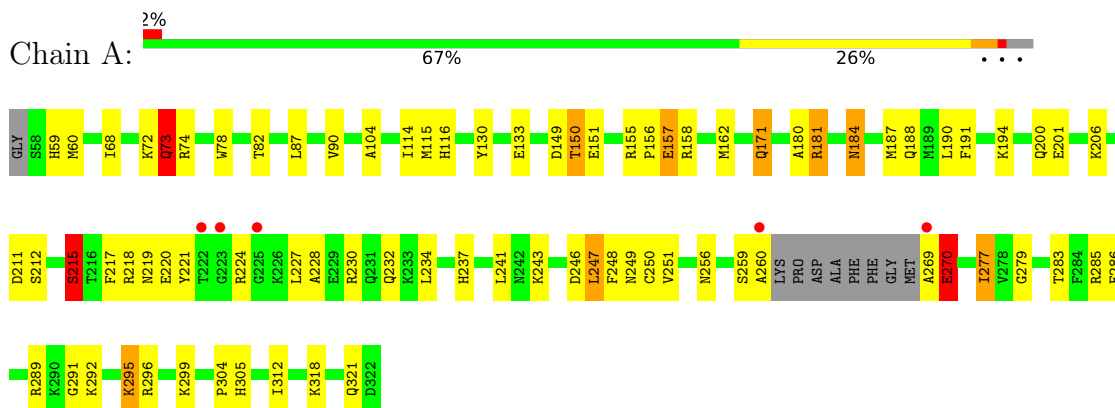
- Molecule 3 is water.

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		

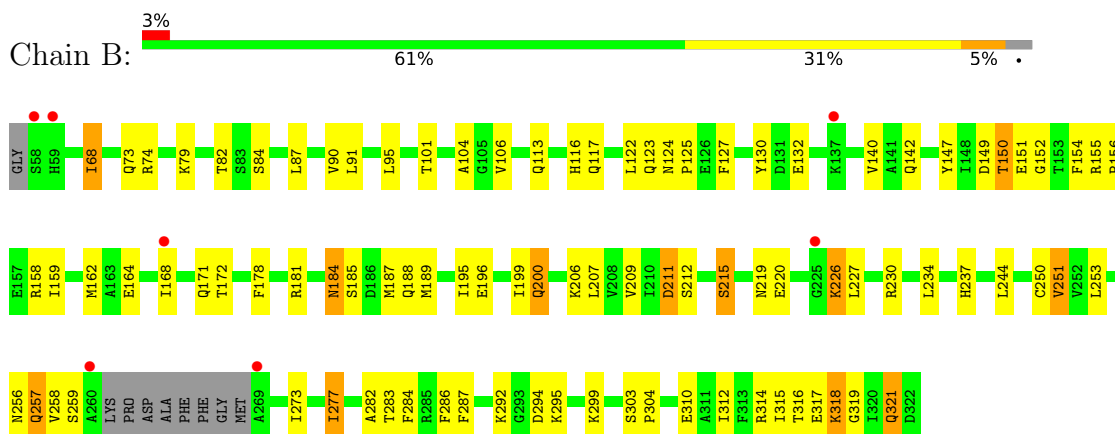
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: DNA repair and recombination protein radA

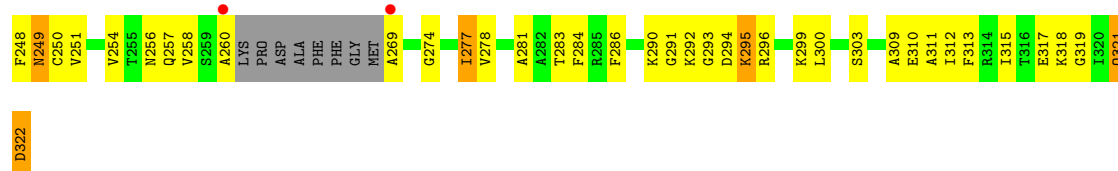


- Molecule 1: DNA repair and recombination protein radA



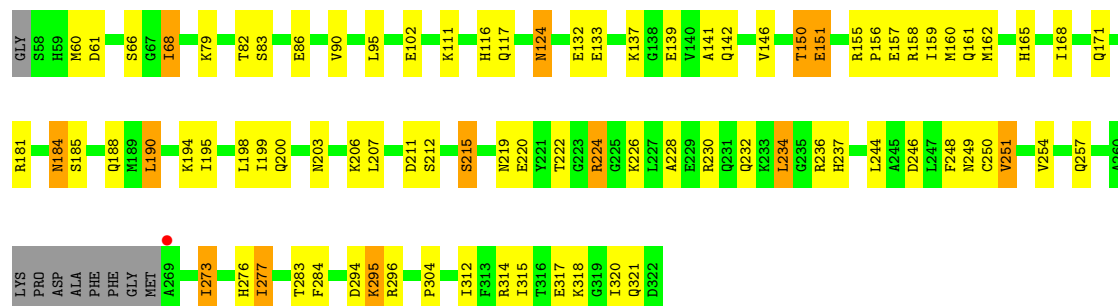
- Molecule 1: DNA repair and recombination protein radA





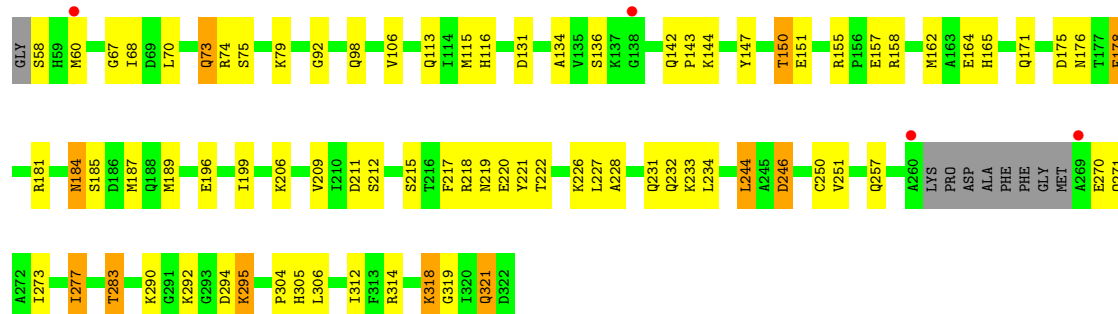
- Molecule 1: DNA repair and recombination protein radA

Chain D: 64% 27% 5% .



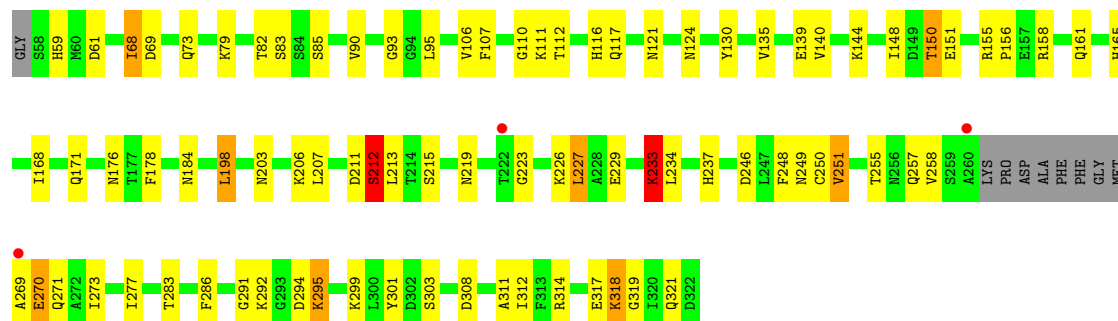
- Molecule 1: DNA repair and recombination protein radA

Chain E: 66% 26% 2% . .



- Molecule 1: DNA repair and recombination protein radA

Chain F: 65% 28% . . .



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 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.60) 90.3 (30.00-2.60)	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 , 0.263	Depositor DCC
R_{free} test set	2928 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h+2*l,-k,-l	Xtriage
F_o, F_c correlation	0.95	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, 0.333 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: 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	1.04	1/2028 (0.0%)	1.18	2/2727 (0.1%)
1	B	0.97	1/2028 (0.0%)	1.15	2/2727 (0.1%)
1	C	0.92	0/2028	1.08	4/2727 (0.1%)
1	D	0.93	0/2028	1.13	8/2727 (0.3%)
1	E	0.96	2/2028 (0.1%)	1.10	5/2727 (0.2%)
1	F	0.97	0/2028	1.16	8/2727 (0.3%)
All	All	0.97	4/12168 (0.0%)	1.13	29/16362 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	SER	CA-C	6.01	1.60	1.52
1	B	211	ASP	CA-C	-5.73	1.46	1.53
1	E	165	HIS	CG-CD2	5.46	1.41	1.35
1	E	165	HIS	ND1-CE1	5.21	1.37	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	321	GLN	N-CA-C	7.98	121.20	109.07
1	B	321	GLN	N-CA-C	7.77	119.81	108.86
1	D	321	GLN	N-CA-C	7.67	120.56	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	GLN	N-CA-C	7.49	120.12	108.96
1	E	270	GLU	N-CA-C	7.01	119.11	107.20
1	C	321	GLN	N-CA-C	6.86	118.93	109.18
1	F	61	ASP	CB-CG-OD2	6.86	134.17	118.40
1	D	273	ILE	N-CA-C	6.50	117.81	109.30
1	C	222	THR	N-CA-C	-6.17	101.80	110.50
1	F	61	ASP	OD1-CG-OD2	-5.98	108.54	122.90
1	D	124	ASN	CA-C-N	5.87	125.74	119.28
1	D	124	ASN	C-N-CA	5.87	125.74	119.28
1	E	271	GLN	N-CA-C	5.85	118.00	108.76
1	D	276	HIS	N-CA-C	5.80	118.39	111.71
1	E	222	THR	N-CA-C	-5.79	98.98	108.76
1	C	309	ALA	N-CA-C	5.71	117.53	108.79
1	E	321	GLN	N-CA-C	5.64	117.75	109.24
1	F	106	VAL	CB-CA-C	-5.61	105.42	111.59
1	B	259	SER	N-CA-C	5.43	116.51	108.86
1	C	227	LEU	N-CA-C	5.29	117.73	111.33
1	A	247	LEU	N-CA-C	5.19	116.94	111.28
1	F	212	SER	CB-CA-C	-5.13	100.35	110.10
1	D	190	LEU	N-CA-C	-5.12	105.39	111.69
1	F	233	LYS	N-CA-C	-5.11	105.79	111.36
1	E	244	LEU	N-CA-C	5.10	118.76	112.54
1	F	213	LEU	N-CA-C	5.08	116.82	111.28
1	F	148	ILE	CB-CA-C	5.03	116.66	111.23
1	D	249	ASN	CA-C-N	-5.02	114.39	122.82
1	D	249	ASN	C-N-CA	-5.02	114.39	122.82

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	58	1
1	B	1997	0	1976	65	0
1	C	1997	0	1976	81	0
1	D	1997	0	1976	54	0
1	E	1997	0	1976	60	1
1	F	1997	0	1976	61	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	2	0
3	A	13	0	0	2	0
3	B	10	0	0	1	0
3	C	5	0	0	3	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	362	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 15.

All (362) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:ASN:HB2	1:F:168:ILE:HD11	1.66	0.77
1:F:144:LYS:HE3	1:F:176:ASN:ND2	1.99	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
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:E:158:ARG:HE	1:E:162:MET:HE3	1.53	0.73
1:B:292:LYS:H	1:B:295:LYS:HE3	1.52	0.73
1:B:147:TYR:CE1	1:B:209:VAL:HG11	2.24	0.72
1:E:67:GLY:HA2	1:E:70:LEU:HD12	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:175:ASP:HB2	1:F:68:ILE:HD12	1.78	0.66
1:A:219:ASN:HB3	1:B:277:ILE:HG12	1.78	0.65
1:B:200:GLN:HA	1:B:200:GLN:OE1	1.95	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:A:157:GLU:CD	1:A:157:GLU:H	2.04	0.63
1:E:98:GLN:HG2	1:E:246:ASP:HA	1.77	0.63
1:A:270:GLU:OE2	1:A:270:GLU:HA	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:184:ASN:C	1:B:184:ASN:HD22	2.06	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
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: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:B:116:HIS:HE1	1:B:155:ARG:H	1.51	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:A:150:THR:C	1:A:151:GLU:HG3	2.26	0.59
1:A:292:LYS:O	1:A:295:LYS:HG3	2.03	0.59
1:B:294:ASP:OD1	1:B:314:ARG:HD2	2.02	0.59
1:F:90:VAL:HG21	1:F:311:ALA:HB2	1.84	0.59
1:B:207:LEU:HD13	1:B:251:VAL:HG22	1.84	0.58
1:F:111:LYS:HB2	2:F:402:NO3:O2	2.03	0.58
1:B:295:LYS:HD2	1:B:312:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:113:GLN:HG3	1:B:315:ILE:HG21	1.84	0.57
1:F:207:LEU:CD1	1:F:251:VAL:HG22	2.33	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:184:ASN:ND2	1:A:187:MET:H	2.03	0.57
1:A:228:ALA:O	1:A:232:GLN:HG3	2.04	0.57
1:E:115:MET:HE2	1:E:115:MET:N	2.20	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: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:C:248:PHE:O	1:C:249:ASN:C	2.47	0.56
1:A:171:GLN:HE21	1:A:171:GLN:CA	2.19	0.56
1:D:222:THR:OG1	1:E:227:LEU:HD21	2.05	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
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:C:291:GLY:HA3	1:C:295:LYS:HE3	1.88	0.56
1:D:158:ARG:O	1:D:162:MET:HG3	2.07	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: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: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:158:ARG:NE	1:A:162:MET:HE3	2.21	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:A:158:ARG:HE	1:A:162:MET:HE3	1.72	0.54
1:B:124:ASN:O	1:B:125:PRO:C	2.50	0.54
1:D:117:GLN:OE1	1:D:162:MET:HE2	2.07	0.54
1:B:219:ASN:HB3	1:C:277:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:260:ALA:HB1	1:A:269:ALA:HB1	1.90	0.53
1:C:147:TYR:CE1	1:C:209:VAL:HG11	2.44	0.53
1:C:269:ALA:CB	3:C:501:HOH:O	2.47	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:C:286:PHE:HA	1:C:299:LYS:O	2.09	0.53
1:F:158:ARG:NH1	1:F:319:GLY:HA2	2.23	0.53
1:F:301:TYR:HA	1:F:308:ASP:OD1	2.08	0.53
1:F:294:ASP:OD1	1:F:314:ARG:HD2	2.09	0.53
1:C:164:GLU:C	1:C:166:ALA:H	2.17	0.53
1:E:294:ASP:OD1	1:E:314:ARG:HD2	2.09	0.52
1:E:305:HIS:C	1:E:306:LEU:HD12	2.34	0.52
1:B:116:HIS:CE1	1:B:155:ARG:H	2.28	0.52
1:D:206:LYS:C	1:D:250:CYS:HB2	2.35	0.52
1:E:228:ALA:O	1:E:232:GLN:HG3	2.09	0.52
1:B:156:PRO:O	1:B:159:ILE:HB	2.10	0.52
1:C:206:LYS:O	1:C:250:CYS:HB2	2.10	0.52
1:D:198:LEU:O	1:D:203:ASN:HB2	2.10	0.52
1:E:199:ILE:O	1:E:199:ILE:HG22	2.09	0.52
1:A:295:LYS:HD2	1:A:312:ILE:HD11	1.91	0.51
1:C:238:MET:HE2	1:C:281:ALA:HB3	1.91	0.51
1:A:149:ASP:C	1:A:149:ASP:OD1	2.52	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:A:206:LYS:C	1:A:250:CYS:HB2	2.35	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:F:206:LYS:C	1:F:250:CYS:HB2	2.36	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
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: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:286:PHE:HA	1:F:299:LYS:O	2.11	0.50
1:F:295:LYS:HD2	1:F:312:ILE:HD11	1.93	0.50
1:A:243:LYS:HE2	1:A:247:LEU:CD1	2.42	0.50
1:F:211:ASP:HA	1:F:255:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HB3	1:C:64:PHE:HB3	1.94	0.49
1:B:303:SER:HB2	1:B:304:PRO:HD2	1.94	0.49
1:C:184:ASN:C	1:C:184:ASN:HD22	2.20	0.49
1:E:318:LYS:NZ	1:E:321:GLN:HE22	2.09	0.49
1:C:238:MET:CE	1:C:281:ALA:HB3	2.42	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:B:101:THR:HB	1:B:253:LEU:HD23	1.94	0.49
1:F:292:LYS:O	1:F:295:LYS:HG2	2.11	0.49
1:F:139:GLU:O	1:F:206:LYS:HE2	2.13	0.49
1:C:150:THR:HG23	1:C:216:THR:HG23	1.95	0.49
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.59	0.49
1:B:185:SER:OG	1:B:220:GLU:OE2	2.30	0.49
1:B:299:LYS:HD2	1:B:310:GLU:HG2	1.94	0.49
1:F:107:PHE:N	1:F:257:GLN:HE22	2.10	0.49
1:B:130:TYR:CE2	1:B:140:VAL:HG21	2.48	0.48
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: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:B:206:LYS:C	1:B:250:CYS:HB2	2.39	0.48
1:E:206:LYS:HA	1:E:250:CYS:HB3	1.94	0.48
1:E:150:THR:CG2	1:E:151:GLU:HG3	2.43	0.48
1:C:98:GLN:HG2	1:C:246:ASP:HA	1.95	0.47
1:D:206:LYS:HD3	1:D:206:LYS:HA	1.74	0.47
1:B:152:GLY:O	1:B:155:ARG:NH2	2.45	0.47
1:C:295:LYS:C	1:C:296:ARG:HG2	2.40	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
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:F:257:GLN:HG3	1:F:258:VAL:H	1.80	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:E:150:THR:HG21	1:E:212:SER:H	1.75	0.47
1:E:211:ASP:HA	1:E:212:SER:HA	1.57	0.47
1:F:151:GLU:OE2	1:F:212:SER:OG	2.33	0.47
1:A:304:PRO:HB2	1:A:305:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:O	1:A:249:ASN:C	2.57	0.47
1:A:291:GLY:CA	1:A:295:LYS:HE3	2.43	0.47
1:B:184:ASN:C	1:B:184:ASN:ND2	2.69	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:A:217:PHE:O	1:A:221:TYR:HD2	1.98	0.46
1:F:150:THR:HG23	1:F:151:GLU:HG3	1.96	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:B:106:VAL:HA	1:B:257:GLN:HE22	1.80	0.46
1:C:184:ASN:ND2	1:C:184:ASN:C	2.73	0.46
1:E:185:SER:OG	1:E:220:GLU:OE2	2.20	0.46
1:E:106:VAL:HA	1:E:257:GLN:HE22	1.79	0.46
1:E:147:TYR:HA	1:E:209:VAL:HB	1.97	0.46
1:B:82:THR:C	1:B:84:SER:H	2.23	0.46
1:C:80:LEU:HD11	1:C:121:ASN:HB3	1.97	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:158:ARG:HH11	1:C:319:GLY:HA2	1.81	0.46
1:E:178:PHE:CD1	1:E:178:PHE:N	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:B:104:ALA:HA	1:B:256:ASN:O	2.17	0.45
1:C:206:LYS:C	1:C:250:CYS:HB2	2.41	0.45
1:E:144:LYS:HE2	1:E:176:ASN:OD1	2.16	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:A:78:TRP:HB3	1:A:130:TYR:HB3	1.99	0.45
1:D:141:ALA:O	1:D:142:GLN:C	2.60	0.45
1:F:292:LYS:H	1:F:295:LYS:CE	2.20	0.45
1:D:294:ASP:OD1	1:D:314:ARG:HD2	2.16	0.44
1:F:59:HIS:HE1	1:F:69:ASP:OD2	2.00	0.44
1:F:291:GLY:HA3	1:F:295:LYS:HE2	1.98	0.44
1:E:158:ARG:HA	1:E:158:ARG:HD2	1.82	0.44
1:F:144:LYS:CE	1:F:176:ASN:ND2	2.73	0.44
1:C:180:ALA:HB1	1:C:191:PHE:CG	2.53	0.44
1:C:190:LEU:O	1:C:194:LYS:HD3	2.18	0.44
1:F:144:LYS:HG2	1:F:176:ASN:HB3	1.99	0.44
1:F:227:LEU:HD23	1:F:227:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HD13	1:B:277:ILE:HA	1.90	0.44
1:D:66:SER:C	1:D:68:ILE:N	2.73	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:C:164:GLU:C	1:C:166:ALA:N	2.76	0.44
1:D:102:GLU:HA	1:D:254:VAL:HG23	2.00	0.44
1:D:124:ASN:HB2	1:D:168:ILE:CD1	2.38	0.44
1:D:155:ARG:HD3	1:D:155:ARG:HA	1.78	0.44
1:D:156:PRO:O	1:D:159:ILE:HB	2.18	0.44
1:E:217:PHE:O	1:E:221:TYR:HD2	2.00	0.44
1:F:150:THR:HG21	1:F:212:SER:H	1.80	0.44
1:A:72:LYS:O	1:A:73:GLN:C	2.61	0.44
1:A:180:ALA:HB1	1:A:191:PHE:CD1	2.53	0.44
1:A:243:LYS:HE2	1:A:247:LEU:HD12	2.00	0.44
1:F:95:LEU:H	1:F:95:LEU:HG	1.71	0.44
1:B:226:LYS:HE3	1:C:228:ALA:HB3	2.00	0.43
1:C:213:LEU:HD13	1:C:254:VAL:HG11	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: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:A:78:TRP:CB	1:A:130:TYR:HB3	2.48	0.43
1:D:211:ASP:HA	1:D:212:SER:HA	1.64	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:D:185:SER:OG	1:D:220:GLU:OE2	2.18	0.43
1:A:74:ARG:HH12	1:F:156:PRO:HG2	1.84	0.43
1:D:222:THR:HG1	1:E:227:LEU:HD21	1.84	0.43
1:D:157:GLU:O	1:D:160:MET:HB2	2.19	0.43
1:F:90:VAL:CG2	1:F:311:ALA:HB2	2.48	0.43
1:D:82:THR:O	1:D:83:SER:HB2	2.19	0.43
1:D:284:PHE:CE2	1:D:304:PRO:HD2	2.54	0.43
1:E:150:THR:HG23	1:E:151:GLU:HG3	2.01	0.43
1:A:211:ASP:HA	1:A:212:SER:HA	1.79	0.43
1:B:124:ASN:HB3	1:B:127:PHE:HB2	2.01	0.43
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:E:157:GLU:CD	1:E:157:GLU:H	2.27	0.42
1:F:248:PHE:O	1:F:249:ASN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:82:THR:CB	1:A:87:LEU:HD23	2.50	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:C:312:ILE:HG12	1:C:313:PHE:N	2.35	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:C:144:LYS:HG3	1:C:176:ASN:HD22	1.84	0.42
1:C:260:ALA:HA	1:C:269:ALA:O	2.19	0.42
1:D:188:GLN:HE21	1:D:237:HIS:HE1	1.53	0.42
1:D:199:ILE:HD13	1:D:248:PHE:CD2	2.55	0.42
1:E:199:ILE:O	1:E:199:ILE:CG2	2.67	0.42
1:F:110:GLY:C	2:F:401:NO3:O2	2.62	0.42
1:F:116:HIS:HE1	1:F:155:ARG:N	2.06	0.42
1:A:59:HIS:CD2	1:F:178:PHE:HE2	2.38	0.42
1:A:279:GLY:HA2	1:A:285:ARG:CZ	2.50	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: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:D:146:VAL:HG11	1:D:195:ILE:HD11	2.03	0.41
1:D:190:LEU:HG	1:D:194:LYS:HE2	2.02	0.41
1:F:130:TYR:CD1	1:F:135:VAL:HB	2.54	0.41
1:F:79:LYS:HD3	1:F:93:GLY:HA3	2.02	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: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:F:229:GLU:O	1:F:233:LYS:HB2	2.21	0.41
1:B:195:ILE:O	1:B:196:GLU:C	2.63	0.41
1:E:189:MET:HE2	1:E:189:MET:HB3	1.93	0.41
1:F:161:GLN:O	1:F:165:HIS:HD2	2.03	0.41
1:B:116:HIS:O	1:B:117:GLN:C	2.62	0.41
1:B:122:LEU:HA	1:B:122:LEU:HD12	1.77	0.41
1:C:299:LYS:HD2	1:C:310:GLU:HG2	2.03	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:E:158:ARG:NE	1:E:162:MET:HE3	2.28	0.41
1:B:282:ALA:C	3:B:509:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:322:ASP:OD2	1:C:322:ASP:N	2.52	0.41
1:E:290:LYS:HE3	1:E:290:LYS:HB2	1.80	0.41
1:A:277:ILE:HG12	1:F:219:ASN:HB3	2.03	0.41
1:D:161:GLN:HE21	1:D:317:GLU:HB2	1.85	0.41
1:E:147:TYR:CD1	1:E:209:VAL:HG11	2.55	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:C:68:ILE:HG23	1:C:72:LYS:HE3	2.04	0.40
1:D:111:LYS:HB2	1:D:111:LYS:HE3	1.96	0.40
1:D:158:ARG:O	1:D:158:ARG:HG3	2.19	0.40
1:A:114:ILE:O	1:A:115:MET:C	2.63	0.40
1:B:284:PHE:CE2	1:B:304:PRO:HD2	2.56	0.40
1:C:111:LYS:NZ	3:C:505:HOH:O	2.54	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%)	10 23
1	B	253/266 (95%)	234 (92%)	18 (7%)	1 (0%)	30 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	253/266 (95%)	233 (92%)	16 (6%)	4 (2%)	7	16
1	D	253/266 (95%)	240 (95%)	12 (5%)	1 (0%)	30	51
1	E	253/266 (95%)	238 (94%)	14 (6%)	1 (0%)	30	51
1	F	253/266 (95%)	234 (92%)	17 (7%)	2 (1%)	16	34
All	All	1518/1596 (95%)	1417 (93%)	89 (6%)	12 (1%)	16	34

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%)	188 (87%)	27 (13%)	4	9
1	B	215/221 (97%)	187 (87%)	28 (13%)	4	8
1	C	215/221 (97%)	184 (86%)	31 (14%)	3	6
1	D	215/221 (97%)	188 (87%)	27 (13%)	4	9
1	E	215/221 (97%)	191 (89%)	24 (11%)	6	12
1	F	215/221 (97%)	193 (90%)	22 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1290/1326 (97%)	1131 (88%)	159 (12%)	4 9

All (159) 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	150	THR
1	A	157	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	251	VAL
1	A	259	SER
1	A	270	GLU
1	A	277	ILE
1	A	283	THR
1	A	289	ARG
1	A	295	LYS
1	A	318	LYS
1	B	68	ILE
1	B	73	GLN
1	B	74	ARG
1	B	87	LEU
1	B	90	VAL
1	B	91	LEU
1	B	132	GLU
1	B	142	GLN
1	B	150	THR
1	B	164	GLU

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Mol	Chain	Res	Type
1	B	168	ILE
1	B	171	GLN
1	B	172	THR
1	B	181	ARG
1	B	184	ASN
1	B	199	ILE
1	B	200	GLN
1	B	215	SER
1	B	226	LYS
1	B	227	LEU
1	B	230	ARG
1	B	234	LEU
1	B	244	LEU
1	B	251	VAL
1	B	257	GLN
1	B	277	ILE
1	B	317	GLU
1	B	318	LYS
1	C	58	SER
1	C	68	ILE
1	C	72	LYS
1	C	74	ARG
1	C	75	SER
1	C	85	SER
1	C	86	GLU
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	230	ARG
1	C	234	LEU
1	C	244	LEU
1	C	251	VAL
1	C	277	ILE

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Mol	Chain	Res	Type
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	60	MET
1	D	61	ASP
1	D	68	ILE
1	D	86	GLU
1	D	90	VAL
1	D	132	GLU
1	D	133	GLU
1	D	137	LYS
1	D	139	GLU
1	D	150	THR
1	D	151	GLU
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	D	320	ILE
1	E	58	SER
1	E	60	MET
1	E	68	ILE
1	E	73	GLN
1	E	74	ARG
1	E	75	SER
1	E	136	SER
1	E	150	THR

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Mol	Chain	Res	Type
1	E	171	GLN
1	E	178	PHE
1	E	181	ARG
1	E	184	ASN
1	E	196	GLU
1	E	215	SER
1	E	218	ARG
1	E	226	LYS
1	E	234	LEU
1	E	244	LEU
1	E	246	ASP
1	E	251	VAL
1	E	277	ILE
1	E	283	THR
1	E	295	LYS
1	E	318	LYS
1	F	68	ILE
1	F	73	GLN
1	F	85	SER
1	F	112	THR
1	F	140	VAL
1	F	150	THR
1	F	171	GLN
1	F	184	ASN
1	F	198	LEU
1	F	212	SER
1	F	215	SER
1	F	226	LYS
1	F	227	LEU
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	303	SER
1	F	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	171	GLN
1	A	184	ASN
1	A	232	GLN
1	A	237	HIS
1	A	257	GLN
1	A	276	HIS
1	A	305	HIS
1	B	59	HIS
1	B	98	GLN
1	B	116	HIS
1	B	142	GLN
1	B	171	GLN
1	B	184	ASN
1	B	188	GLN
1	B	237	HIS
1	B	257	GLN
1	B	280	HIS
1	B	321	GLN
1	C	116	HIS
1	C	161	GLN
1	C	171	GLN
1	C	176	ASN
1	C	184	ASN
1	C	200	GLN
1	C	203	ASN
1	C	237	HIS
1	C	242	ASN
1	C	280	HIS
1	C	305	HIS
1	D	73	GLN
1	D	116	HIS
1	D	161	GLN
1	D	184	ASN
1	D	203	ASN
1	D	232	GLN
1	D	237	HIS
1	D	257	GLN
1	D	276	HIS
1	E	113	GLN
1	E	116	HIS
1	E	171	GLN
1	E	184	ASN

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Mol	Chain	Res	Type
1	E	203	ASN
1	E	237	HIS
1	E	257	GLN
1	E	271	GLN
1	E	276	HIS
1	E	321	GLN
1	F	73	GLN
1	F	116	HIS
1	F	117	GLN
1	F	171	GLN
1	F	176	ASN
1	F	184	ASN
1	F	203	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 oligosaccharides 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	B	401	-	1,3,3	0.41	0	0,3,3	-	-
2	NO3	D	402	-	1,3,3	0.49	0	0,3,3	-	-
2	NO3	E	401	-	1,3,3	0.36	0	0,3,3	-	-
2	NO3	C	401	-	1,3,3	0.34	0	0,3,3	-	-
2	NO3	E	402	-	1,3,3	0.88	0	0,3,3	-	-
2	NO3	C	402	-	1,3,3	0.42	0	0,3,3	-	-
2	NO3	D	401	-	1,3,3	0.07	0	0,3,3	-	-
2	NO3	F	401	-	1,3,3	0.12	0	0,3,3	-	-
2	NO3	F	402	-	1,3,3	0.56	0	0,3,3	-	-
2	NO3	B	402	-	1,3,3	0.45	0	0,3,3	-	-
2	NO3	A	402	-	1,3,3	0.83	0	0,3,3	-	-
2	NO3	A	401	-	1,3,3	0.37	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.32	5 (1%) 66 61	22, 44, 79, 121	0
1	B	257/266 (96%)	0.04	7 (2%) 56 50	26, 52, 99, 122	0
1	C	257/266 (96%)	0.19	8 (3%) 51 45	35, 65, 99, 144	0
1	D	257/266 (96%)	-0.19	1 (0%) 88 86	28, 52, 81, 109	0
1	E	257/266 (96%)	-0.13	4 (1%) 70 66	26, 51, 96, 131	0
1	F	257/266 (96%)	-0.23	3 (1%) 76 73	27, 48, 77, 117	0
All	All	1542/1596 (96%)	-0.11	28 (1%) 67 63	22, 52, 94, 144	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	4.1
1	E	269	ALA	3.8
1	B	269	ALA	3.2
1	D	269	ALA	3.1
1	C	59	HIS	3.1
1	C	62	LEU	3.1
1	F	269	ALA	2.9
1	B	260	ALA	2.8
1	A	223	GLY	2.7
1	C	223	GLY	2.7
1	C	60	MET	2.6
1	C	226	LYS	2.6
1	B	58	SER	2.5
1	B	137	LYS	2.5
1	F	260	ALA	2.5
1	C	260	ALA	2.4
1	E	260	ALA	2.4
1	A	260	ALA	2.2
1	B	225	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	222	THR	2.2
1	B	168	ILE	2.2
1	E	60	MET	2.2
1	F	222	THR	2.1
1	C	269	ALA	2.1
1	C	127	PHE	2.1
1	E	138	GLY	2.1
1	B	59	HIS	2.0
1	A	225	GLY	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 oligosaccharides 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	NO3	F	402	4/4	0.90	0.10	45,46,51,52	0
2	NO3	F	401	4/4	0.94	0.11	34,43,44,45	0
2	NO3	C	401	4/4	0.94	0.08	47,51,56,57	0
2	NO3	B	402	4/4	0.95	0.07	39,39,42,43	0
2	NO3	D	401	4/4	0.95	0.11	38,43,46,50	0
2	NO3	B	401	4/4	0.96	0.09	34,38,39,39	0
2	NO3	D	402	4/4	0.97	0.05	49,50,50,53	0
2	NO3	E	401	4/4	0.97	0.05	37,39,39,43	0
2	NO3	C	402	4/4	0.97	0.05	45,49,50,53	0
2	NO3	A	402	4/4	0.97	0.05	39,40,43,44	0
2	NO3	A	401	4/4	0.98	0.08	37,37,39,39	0
2	NO3	E	402	4/4	0.98	0.05	32,35,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.