



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 08:04 AM EST

PDB ID : 1JR3
Title : Crystal Structure of the Processivity Clamp Loader Gamma Complex of E. coli DNA Polymerase III
Authors : Jeruzalmi, D.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2001-08-10
Resolution : 2.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

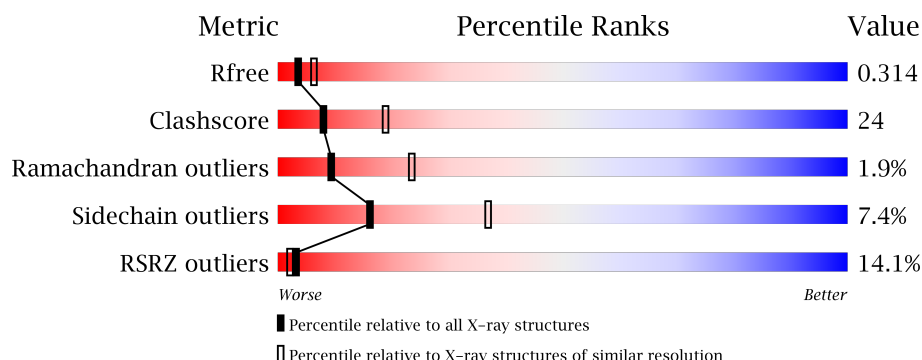
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	373	<div> <div>17%</div> <div>58%</div> <div>38%</div> <div>..</div> </div>
1	B	373	<div> <div>17%</div> <div>59%</div> <div>35%</div> <div>..</div> </div>
1	C	373	<div> <div>10%</div> <div>61%</div> <div>31%</div> <div>5% ..</div> </div>
2	D	343	<div> <div>8%</div> <div>56%</div> <div>36%</div> <div>5% ..</div> </div>
3	E	334	<div> <div>16%</div> <div>62%</div> <div>34%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1500	-	-	X	-
5	SO4	B	2500	-	-	X	-
5	SO4	C	5500	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13845 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 polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
1	B	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
1	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

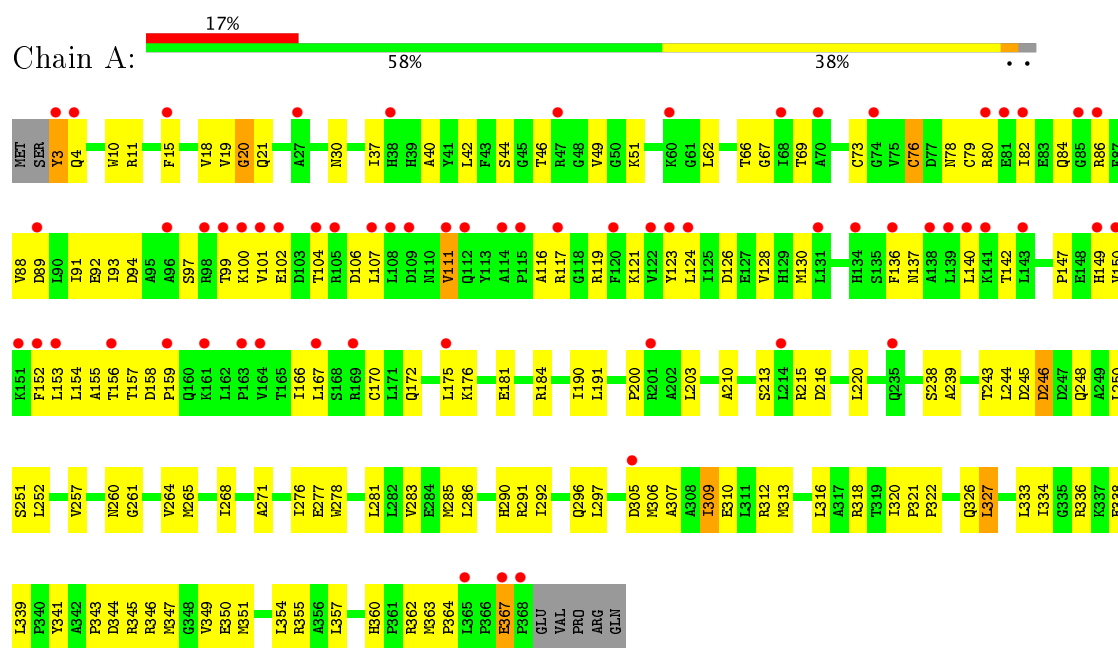


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

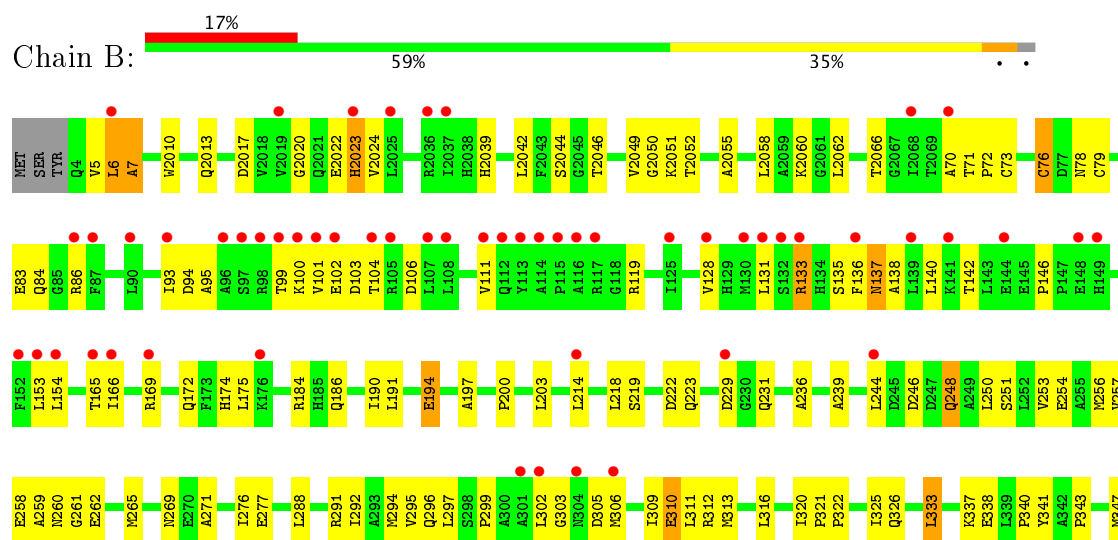
3 Residue-property plots

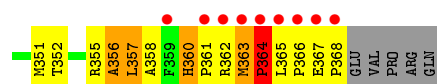
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 polymerase III subunit gamma

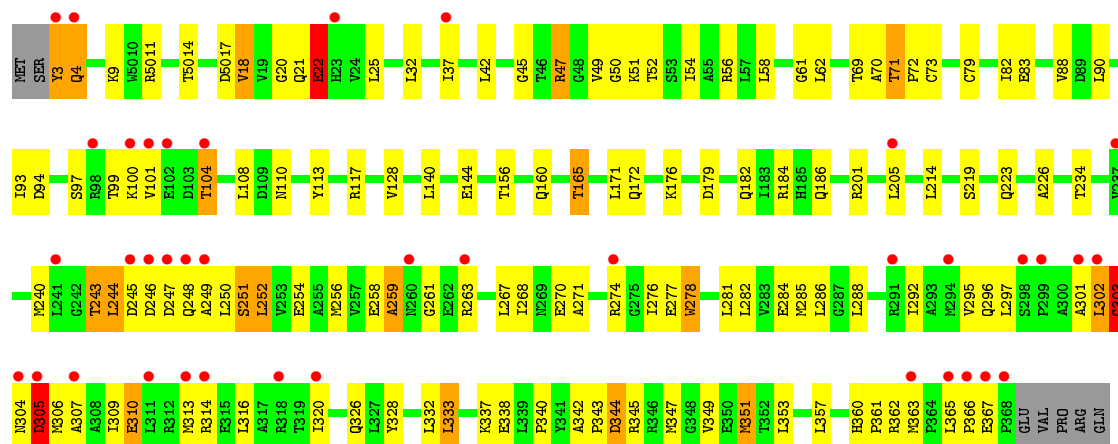


• Molecule 1: DNA polymerase III subunit gamma

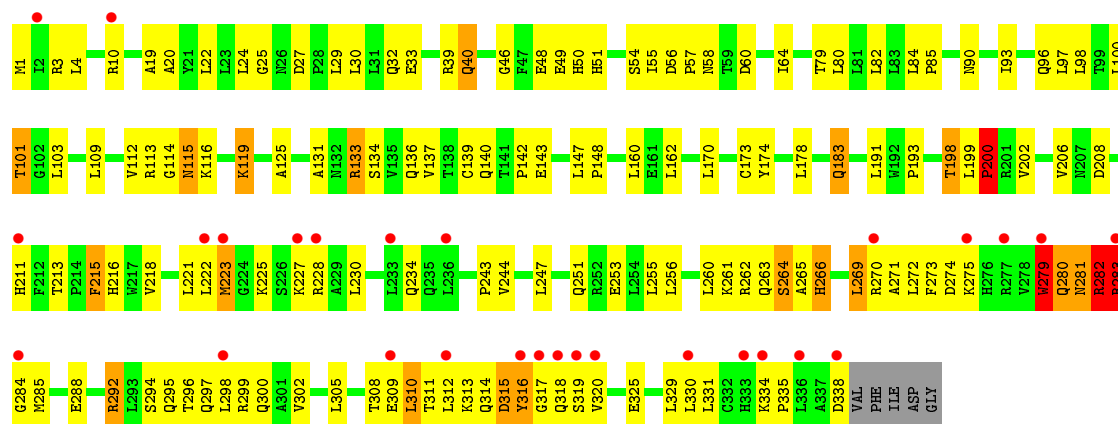




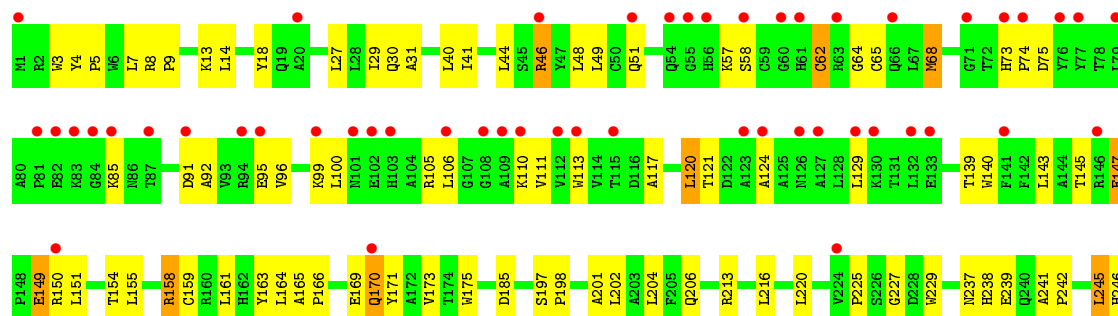
• Molecule 1: DNA polymerase III subunit gamma

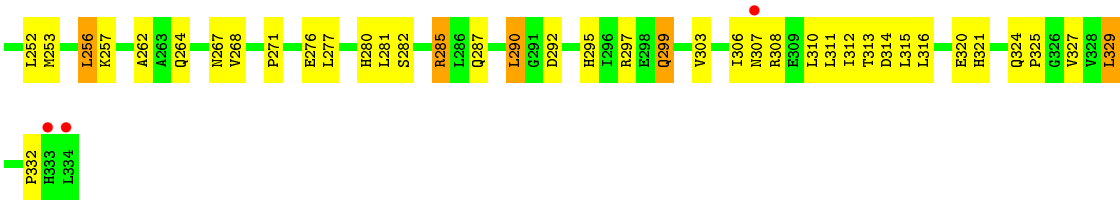


• Molecule 2: DNA polymerase III, delta subunit



• Molecule 3: DNA polymerase III, delta' subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.70 Å 95.86 Å 285.41 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70 90.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.70) 76.9 (90.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	13.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.69 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.304 0.286 , 0.314	Depositor DCC
R_{free} test set	2839 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13845	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: ZN, SO4

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	0/2898	0.74	2/3930 (0.1%)
1	B	0.66	7/2885 (0.2%)	0.95	14/3912 (0.4%)
1	C	0.57	0/2898	0.88	10/3930 (0.3%)
2	D	0.85	8/2735 (0.3%)	0.93	10/3716 (0.3%)
3	E	0.49	0/2666	0.70	0/3639
All	All	0.62	15/14082 (0.1%)	0.85	36/19127 (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	B	0	1
2	D	0	4
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	315	ASP	CB-CG	29.10	2.12	1.51
1	B	133	ARG	CZ-NH2	-10.95	1.18	1.33
2	D	310	LEU	CG-CD2	-9.05	1.18	1.51
1	B	363	MET	CG-SD	8.99	2.04	1.81
1	B	363	MET	SD-CE	8.90	2.27	1.77
2	D	316	TYR	CE1-CZ	6.79	1.47	1.38
2	D	283	ARG	CB-CG	6.61	1.70	1.52
1	B	360	HIS	CA-CB	5.72	1.66	1.53
1	B	356	ALA	C-O	-5.71	1.12	1.23
2	D	316	TYR	CZ-OH	5.62	1.47	1.37
2	D	200	PRO	N-CD	-5.57	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	ARG	CZ-NH1	-5.45	1.25	1.33
2	D	316	TYR	CG-CD1	5.22	1.46	1.39
1	B	360	HIS	CG-CD2	5.18	1.44	1.35
2	D	282	ARG	CB-CG	-5.11	1.38	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	MET	CG-SD-CE	17.06	127.49	100.20
2	D	283	ARG	C-N-CA	12.38	148.31	122.30
1	C	244	LEU	CB-CG-CD2	-11.83	90.88	111.00
2	D	280	GLN	C-N-CA	11.46	150.36	121.70
1	B	133	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	B	133	ARG	NE-CZ-NH2	10.89	125.75	120.30
2	D	315	ASP	CA-CB-CG	-10.71	89.84	113.40
1	B	133	ARG	NH1-CZ-NH2	-10.47	107.88	119.40
1	B	360	HIS	N-CA-CB	10.28	129.10	110.60
2	D	283	ARG	CA-C-N	-9.34	97.53	116.20
2	D	283	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	D	283	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	363	MET	CB-CG-SD	6.80	132.81	112.40
1	C	20	GLY	N-CA-C	6.75	129.97	113.10
1	C	305	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	302	LEU	C-N-CA	6.49	135.92	122.30
1	C	305	ASP	CB-CG-OD1	6.44	124.09	118.30
1	C	303	GLY	N-CA-C	6.36	129.01	113.10
1	A	20	GLY	N-CA-C	6.33	128.92	113.10
2	D	310	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	B	7	ALA	N-CA-C	-6.14	94.43	111.00
2	D	280	GLN	O-C-N	-6.04	113.04	122.70
1	B	360	HIS	CA-CB-CG	6.00	123.81	113.60
1	B	360	HIS	CB-CA-C	-5.99	98.41	110.40
1	B	364	PRO	CA-N-CD	-5.83	103.34	111.50
1	C	245	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	327	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	2020	GLY	N-CA-C	5.68	127.30	113.10
1	B	360	HIS	CB-CG-ND1	5.57	137.11	123.20
1	C	259	ALA	N-CA-C	5.40	125.59	111.00
2	D	282	ARG	CB-CG-CD	-5.28	97.88	111.60
1	C	243	THR	N-CA-C	5.21	125.06	111.00
1	B	303	GLY	N-CA-C	5.17	126.04	113.10
1	C	302	LEU	CA-C-N	-5.17	105.85	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	N-CA-C	5.10	124.77	111.00
2	D	264	SER	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2023	HIS	Sidechain
2	D	280	GLN	Peptide
2	D	281	ASN	Mainchain
2	D	282	ARG	Mainchain
2	D	319	SER	Mainchain

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	2850	0	2896	158	0
1	B	2838	0	2887	195	0
1	C	2850	0	2895	133	1
2	D	2687	0	2741	146	1
3	E	2601	0	2603	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	7	0
5	B	5	0	0	2	0
5	C	5	0	0	3	0
All	All	13845	0	14022	664	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 24.

All (664) 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:B:363:MET:SD	1:B:363:MET:CG	2.04	1.45
1:C:304:ASN:ND2	2:D:234:GLN:OE1	1.61	1.30
1:B:363:MET:SD	1:B:363:MET:CE	2.27	1.21
1:C:94:ASP:H	1:C:100:LYS:NZ	1.40	1.17
2:D:315:ASP:CB	2:D:315:ASP:CG	2.12	1.16
1:B:360:HIS:HB3	1:B:363:MET:CB	1.77	1.13
1:C:304:ASN:ND2	2:D:234:GLN:CD	2.02	1.12
1:B:360:HIS:HB3	1:B:363:MET:HB2	1.11	1.09
1:C:246:ASP:HB3	1:C:274:ARG:HD3	1.38	1.06
1:C:69:THR:HG22	1:C:71:THR:H	1.15	1.05
2:D:223:MET:SD	2:D:292:ARG:HB3	1.99	1.03
1:A:351:MET:HE1	1:B:326:GLN:HE22	1.23	1.03
1:B:363:MET:HB3	1:B:364:PRO:HD2	1.42	1.01
2:D:25:GLY:HA3	2:D:139:CYS:O	1.59	1.01
1:B:355:ARG:HH21	3:E:332:PRO:HD3	1.23	0.99
2:D:119:LYS:H	2:D:119:LYS:HD3	1.26	0.99
1:C:304:ASN:ND2	2:D:234:GLN:NE2	2.10	0.98
2:D:315:ASP:HB2	2:D:318:GLN:CG	1.94	0.98
1:A:239:ALA:HB1	1:B:2023:HIS:CE1	2.00	0.97
2:D:310:LEU:HD22	2:D:314:GLN:HE21	1.27	0.97
1:B:357:LEU:HA	1:B:363:MET:SD	2.05	0.97
1:C:18:VAL:HG22	1:C:25:LEU:HD11	1.47	0.94
1:C:94:ASP:N	1:C:100:LYS:HZ3	1.63	0.94
1:A:100:LYS:CD	1:B:133:ARG:HH21	1.82	0.93
1:A:100:LYS:HD3	1:B:133:ARG:NH2	1.82	0.93
1:A:239:ALA:HB1	1:B:2023:HIS:NE2	1.83	0.92
2:D:213:THR:H	2:D:216:HIS:HD2	1.13	0.90
1:C:94:ASP:N	1:C:100:LYS:NZ	2.21	0.89
1:B:357:LEU:O	1:B:363:MET:SD	2.31	0.88
1:B:363:MET:CB	1:B:364:PRO:HD2	2.04	0.87
1:A:271:ALA:HB1	1:A:276:ILE:HD11	1.57	0.86
1:B:309:ILE:CG2	1:B:313:MET:HG2	2.05	0.86
1:B:200:PRO:HB2	1:B:305:ASP:HB2	1.57	0.86
1:A:351:MET:CE	1:B:326:GLN:HE22	1.90	0.85
1:C:179:ASP:HB3	1:C:182:GLN:HB2	1.58	0.83
3:E:8:ARG:HG3	3:E:9:PRO:HD3	1.60	0.83
2:D:55:ILE:HD13	2:D:97:LEU:HD11	1.59	0.83
2:D:312:LEU:HB2	2:D:320:VAL:HG21	1.60	0.83
1:C:3:TYR:O	1:C:4:GLN:HG3	1.79	0.82
1:A:99:THR:HG22	1:A:99:THR:O	1.78	0.81
1:B:357:LEU:HA	1:B:363:MET:CE	2.09	0.81
1:B:360:HIS:HB3	1:B:363:MET:CG	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:HIS:ND1	1:B:363:MET:CE	2.44	0.81
1:B:360:HIS:ND1	1:B:363:MET:HE2	1.96	0.81
2:D:315:ASP:HB2	2:D:318:GLN:HG3	1.63	0.81
1:B:253:VAL:O	1:B:257:VAL:HG23	1.80	0.81
1:A:94:ASP:O	1:A:100:LYS:HE3	1.81	0.80
1:B:99:THR:O	1:B:99:THR:HG22	1.81	0.80
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.80
1:C:304:ASN:ND2	2:D:234:GLN:HE22	1.77	0.80
1:A:309:ILE:HG13	1:A:313:MET:HG2	1.62	0.80
1:C:259:ALA:HB3	1:C:363:MET:HE3	1.62	0.79
1:A:67:GLY:HA2	1:A:119:ARG:HH12	1.47	0.79
1:A:97:SER:OG	1:A:100:LYS:HE3	1.83	0.79
1:B:360:HIS:CB	1:B:363:MET:CG	2.61	0.78
1:C:94:ASP:C	1:C:100:LYS:HZ1	1.86	0.78
1:B:259:ALA:HB2	1:B:363:MET:CG	2.12	0.78
1:A:80:ARG:O	1:A:84:GLN:HG3	1.82	0.78
1:C:93:ILE:HG23	1:C:100:LYS:HZ2	1.48	0.78
1:C:99:THR:HG22	1:C:99:THR:O	1.83	0.78
2:D:310:LEU:HD22	2:D:314:GLN:NE2	1.98	0.78
1:A:281:LEU:HD23	1:A:285:MET:HE2	1.66	0.78
2:D:244:VAL:HG22	2:D:312:LEU:HD21	1.64	0.78
1:A:93:ILE:CG2	1:A:100:LYS:NZ	2.47	0.78
1:A:271:ALA:CB	1:A:276:ILE:HD11	2.13	0.78
1:C:45:GLY:O	1:C:51:LYS:HE2	1.84	0.77
1:C:94:ASP:H	1:C:100:LYS:HZ3	0.81	0.77
1:B:363:MET:HB3	1:B:364:PRO:CD	2.14	0.77
1:A:128:VAL:HG11	1:A:154:LEU:HD22	1.67	0.77
1:B:244:LEU:HD21	1:B:276:ILE:HG12	1.66	0.77
1:C:4:GLN:OE1	1:C:9:LYS:HD2	1.84	0.77
2:D:300:GLN:OE1	2:D:335:PRO:CG	2.32	0.76
1:B:360:HIS:HB2	1:B:363:MET:SD	2.26	0.76
1:A:111:VAL:HG11	1:A:142:THR:HG21	1.66	0.76
1:B:2042:LEU:HB3	1:B:172:GLN:HB3	1.67	0.76
1:C:248:GLN:HG3	1:C:267:LEU:HB3	1.65	0.76
2:D:222:LEU:O	2:D:223:MET:HB2	1.83	0.76
1:B:257:VAL:O	1:B:360:HIS:HE1	1.69	0.75
1:A:276:ILE:HD13	1:A:281:LEU:HD12	1.69	0.75
1:C:271:ALA:HB1	1:C:276:ILE:HD12	1.68	0.75
1:B:2013:GLN:HE22	1:B:83:GLU:HG2	1.49	0.75
1:B:259:ALA:CB	1:B:363:MET:HG2	2.17	0.74
3:E:5:PRO:O	3:E:8:ARG:HG2	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:O	1:A:100:LYS:CE	2.35	0.74
2:D:310:LEU:HD13	2:D:314:GLN:NE2	2.01	0.74
1:B:357:LEU:CA	1:B:363:MET:SD	2.75	0.74
2:D:147:LEU:HB3	2:D:148:PRO:HD3	1.69	0.74
1:A:156:THR:HG22	1:A:158:ASP:H	1.54	0.73
2:D:273:PHE:HB3	2:D:279:TRP:CB	2.18	0.73
1:B:355:ARG:NH2	3:E:332:PRO:HD3	2.01	0.73
1:A:93:ILE:HG22	1:A:100:LYS:NZ	2.03	0.73
1:A:100:LYS:CE	1:B:133:ARG:HH21	2.00	0.73
1:B:360:HIS:CG	1:B:363:MET:HG3	2.23	0.73
1:C:362:ARG:HE	1:C:363:MET:HE2	1.53	0.73
1:B:358:ALA:HA	1:B:364:PRO:HG2	1.71	0.72
2:D:82:LEU:HD21	2:D:100:LEU:HD12	1.70	0.72
1:B:271:ALA:HB1	1:B:276:ILE:CD1	2.19	0.72
3:E:49:LEU:HD23	3:E:68:MET:SD	2.29	0.72
3:E:117:ALA:O	3:E:120:LEU:HD22	1.89	0.72
1:B:259:ALA:HB1	1:B:363:MET:HG2	1.72	0.72
1:B:73:CYS:O	1:B:79:CYS:SG	2.48	0.71
2:D:223:MET:SD	2:D:292:ARG:CB	2.78	0.71
2:D:300:GLN:OE1	2:D:335:PRO:HG3	1.91	0.70
1:A:326:GLN:NE2	1:C:351:MET:SD	2.65	0.70
1:C:259:ALA:CB	1:C:363:MET:HE3	2.22	0.70
1:A:360:HIS:HB3	1:A:363:MET:O	1.91	0.70
2:D:313:LYS:O	2:D:316:TYR:CZ	2.44	0.70
1:A:276:ILE:HG22	1:A:277:GLU:H	1.56	0.70
2:D:222:LEU:HD12	2:D:285:MET:HG2	1.74	0.69
1:A:94:ASP:O	1:A:100:LYS:NZ	2.25	0.69
2:D:315:ASP:CG	2:D:315:ASP:CA	2.61	0.69
1:A:86:ARG:NH2	1:B:138:ALA:HA	2.08	0.69
2:D:213:THR:H	2:D:216:HIS:CD2	2.04	0.69
1:B:338:GLU:O	1:B:341:TYR:HB2	1.93	0.69
3:E:169:GLU:O	3:E:173:VAL:HG23	1.92	0.68
1:A:73:CYS:O	1:A:79:CYS:SG	2.50	0.68
2:D:202:VAL:O	2:D:206:VAL:HG23	1.92	0.68
2:D:55:ILE:O	2:D:85:PRO:HG3	1.93	0.68
1:C:93:ILE:CG2	1:C:100:LYS:NZ	2.57	0.68
1:A:93:ILE:CG2	1:A:100:LYS:HZ3	2.06	0.68
1:C:73:CYS:O	1:C:79:CYS:SG	2.51	0.68
3:E:111:VAL:HG12	3:E:140:TRP:HB2	1.75	0.68
1:A:367:GLU:HG3	1:B:322:PRO:HD2	1.74	0.68
1:B:357:LEU:HA	1:B:363:MET:HE1	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:LYS:HB3	2:D:140:GLN:HE21	1.59	0.68
1:A:67:GLY:HA2	1:A:119:ARG:NH1	2.07	0.68
1:B:93:ILE:HG22	1:B:100:LYS:HZ3	1.58	0.68
1:C:18:VAL:CG2	1:C:25:LEU:HD11	2.24	0.68
2:D:308:THR:HG23	2:D:320:VAL:HG13	1.75	0.67
1:A:11:ARG:HH22	1:B:165:THR:HG22	1.59	0.67
1:B:254:GLU:OE2	1:B:312:ARG:HD3	1.94	0.67
1:B:260:ASN:O	1:B:262:GLU:N	2.27	0.67
1:B:259:ALA:CB	1:B:363:MET:CG	2.72	0.67
1:C:93:ILE:HG23	1:C:100:LYS:NZ	2.09	0.67
1:C:73:CYS:O	1:C:73:CYS:SG	2.53	0.67
1:B:223:GLN:HE21	3:E:158:ARG:HE	1.43	0.67
1:B:358:ALA:HA	1:B:364:PRO:CG	2.25	0.67
3:E:31:ALA:HB2	3:E:164:LEU:HB3	1.76	0.67
1:C:165:THR:HG23	2:D:32:GLN:HE22	1.59	0.67
1:B:309:ILE:HG22	1:B:313:MET:HG2	1.74	0.66
1:C:110:ASN:HB3	1:C:113:TYR:HD1	1.58	0.66
1:B:271:ALA:HB1	1:B:276:ILE:HD12	1.75	0.66
3:E:64:GLY:O	3:E:68:MET:HB2	1.96	0.66
3:E:74:PRO:HB3	3:E:105:ARG:HD2	1.76	0.66
1:A:181:GLU:HG2	1:A:184:ARG:HD2	1.77	0.66
1:B:93:ILE:HG22	1:B:100:LYS:NZ	2.10	0.65
1:B:347:MET:O	1:B:351:MET:HG2	1.96	0.65
2:D:274:ASP:HA	2:D:279:TRP:CE3	2.32	0.65
1:B:2013:GLN:NE2	1:B:83:GLU:HG2	2.12	0.65
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	0.64
3:E:8:ARG:CG	3:E:9:PRO:HD3	2.25	0.64
1:A:111:VAL:HG11	1:A:142:THR:CG2	2.28	0.64
2:D:48:GLU:HG3	2:D:49:GLU:N	2.13	0.64
1:B:356:ALA:O	1:B:363:MET:CE	2.45	0.64
1:A:261:GLY:HA3	1:B:297:LEU:HD21	1.80	0.64
1:B:309:ILE:HG21	1:B:313:MET:HG2	1.77	0.64
2:D:273:PHE:HB3	2:D:279:TRP:CG	2.33	0.64
1:C:268:ILE:HD11	1:C:353:LEU:CD1	2.28	0.64
1:B:360:HIS:CG	1:B:363:MET:CG	2.80	0.64
1:C:254:GLU:O	1:C:258:GLU:HG3	1.98	0.64
1:A:73:CYS:SG	1:A:73:CYS:O	2.56	0.63
1:A:107:LEU:HD11	1:B:133:ARG:NH1	2.14	0.63
2:D:222:LEU:CD1	2:D:285:MET:HG2	2.29	0.63
3:E:329:LEU:HD23	3:E:329:LEU:H	1.63	0.63
1:A:94:ASP:C	1:A:100:LYS:HZ1	2.01	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:O	1:B:218:LEU:HB3	1.98	0.63
2:D:315:ASP:HB2	2:D:318:GLN:HG2	1.80	0.62
3:E:147:GLU:HG2	3:E:147:GLU:O	1.98	0.62
1:B:100:LYS:HB2	1:B:103:ASP:OD1	1.99	0.62
1:A:343:PRO:HG2	1:A:347:MET:SD	2.38	0.62
1:A:93:ILE:HG23	1:A:100:LYS:NZ	2.14	0.62
2:D:24:LEU:HA	2:D:114:GLY:O	2.00	0.62
2:D:256:LEU:O	2:D:260:LEU:HG	2.00	0.62
3:E:161:LEU:H	3:E:161:LEU:HD12	1.64	0.62
1:C:328:TYR:O	1:C:332:LEU:HD23	1.99	0.62
1:A:351:MET:HA	1:A:351:MET:HE3	1.82	0.62
1:C:263:ARG:O	1:C:267:LEU:HG	2.00	0.62
1:C:271:ALA:HB1	1:C:276:ILE:CD1	2.30	0.62
1:A:239:ALA:CB	1:B:2023:HIS:CE1	2.78	0.62
1:B:337:LYS:HG3	1:B:338:GLU:N	2.12	0.62
1:B:102:GLU:HB3	1:B:106:ASP:HB2	1.80	0.61
1:C:93:ILE:CG2	1:C:100:LYS:HZ2	2.12	0.61
1:C:246:ASP:HB3	1:C:274:ARG:CD	2.24	0.61
3:E:129:LEU:HD11	3:E:158:ARG:HH11	1.64	0.61
1:A:250:LEU:HD22	1:A:309:ILE:HD12	1.82	0.61
1:A:100:LYS:CD	1:B:133:ARG:NH2	2.48	0.61
1:A:86:ARG:HH21	1:B:138:ALA:HA	1.63	0.61
1:C:246:ASP:CB	1:C:274:ARG:HD3	2.24	0.61
1:A:351:MET:CE	1:A:351:MET:HA	2.30	0.61
1:B:316:LEU:HD22	1:B:320:ILE:HD11	1.81	0.61
3:E:73:HIS:CD2	3:E:75:ASP:H	2.18	0.61
1:A:100:LYS:HD3	1:B:133:ARG:HH21	1.44	0.61
2:D:281:ASN:C	2:D:283:ARG:H	2.02	0.61
1:B:363:MET:CG	1:B:364:PRO:HD2	2.31	0.60
1:C:268:ILE:HD11	1:C:353:LEU:HD12	1.83	0.60
1:C:94:ASP:O	1:C:100:LYS:HE3	1.99	0.60
1:B:338:GLU:OE2	3:E:295:HIS:NE2	2.34	0.60
1:A:30:ASN:HD22	1:C:226:ALA:HA	1.66	0.60
1:B:70:ALA:O	1:B:72:PRO:HD3	2.01	0.60
1:C:51:LYS:HB2	5:C:5500:SO4:O3	2.02	0.60
1:C:302:LEU:HD13	1:C:310:GLU:HG2	1.84	0.60
1:A:362:ARG:O	1:A:363:MET:HG3	2.02	0.60
1:C:284:GLU:O	1:C:288:LEU:HG	2.02	0.60
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	0.60
1:B:140:LEU:HD21	1:B:166:ILE:HG12	1.83	0.60
1:A:88:VAL:HG11	1:A:116:ALA:HB3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:TYR:O	1:A:4:GLN:HG3	2.01	0.59
2:D:269:LEU:HG	2:D:273:PHE:CE1	2.37	0.59
1:A:152:PHE:O	1:A:153:LEU:HD23	2.02	0.59
1:A:316:LEU:HD22	1:A:320:ILE:HD11	1.84	0.59
1:A:292:ILE:O	1:A:296:GLN:HG3	2.02	0.59
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.59
1:A:21:GLN:OE1	1:A:175:LEU:HD22	2.02	0.59
1:C:343:PRO:HG2	1:C:347:MET:SD	2.42	0.59
1:B:246:ASP:HB2	1:B:248:GLN:HG2	1.85	0.59
1:A:93:ILE:HG22	1:A:100:LYS:HZ3	1.65	0.59
1:C:47:ARG:O	1:C:47:ARG:HG3	2.03	0.59
1:B:363:MET:CB	1:B:364:PRO:CD	2.78	0.58
1:C:205:LEU:CD1	1:C:234:THR:HG23	2.33	0.58
2:D:263:GLN:HG2	2:D:266:HIS:HD2	1.68	0.58
1:A:30:ASN:ND2	1:C:226:ALA:HA	2.18	0.58
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.58
1:A:341:TYR:HB2	1:B:333:LEU:HD11	1.84	0.58
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
1:A:257:VAL:HG11	1:A:320:ILE:CD1	2.34	0.58
1:B:367:GLU:HB3	1:B:368:PRO:HD2	1.86	0.58
1:C:61:GLY:HA2	1:C:72:PRO:HG3	1.85	0.58
2:D:222:LEU:HD12	2:D:285:MET:SD	2.44	0.58
2:D:223:MET:HE1	2:D:292:ARG:HB2	1.86	0.58
1:B:2058:LEU:HD23	1:B:153:LEU:HD22	1.86	0.58
1:C:259:ALA:HB3	1:C:363:MET:CE	2.33	0.58
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.58
1:A:93:ILE:CG2	1:A:100:LYS:HZ2	2.17	0.57
1:B:94:ASP:O	1:B:100:LYS:HE2	2.03	0.57
1:B:360:HIS:CB	1:B:363:MET:SD	2.92	0.57
1:C:282:LEU:CD2	1:C:332:LEU:HD12	2.34	0.57
2:D:10:ARG:HH12	2:D:40:GLN:NE2	2.00	0.57
1:B:128:VAL:HG11	1:B:154:LEU:HD22	1.87	0.57
1:B:229:ASP:O	1:B:231:GLN:N	2.34	0.57
2:D:279:TRP:O	2:D:279:TRP:CG	2.57	0.57
1:A:291:ARG:HH11	1:A:306:MET:HG3	1.69	0.57
2:D:222:LEU:HD12	2:D:285:MET:CG	2.33	0.57
2:D:281:ASN:C	2:D:283:ARG:N	2.57	0.57
1:A:49:VAL:O	5:A:1500:SO4:S	2.63	0.57
1:C:304:ASN:OD1	1:C:305:ASP:N	2.37	0.57
2:D:10:ARG:HH22	2:D:40:GLN:HE22	1.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HG2	1:B:214:LEU:HD21	1.86	0.57
2:D:221:LEU:HD13	2:D:331:LEU:HD12	1.86	0.57
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.57
2:D:273:PHE:CE1	2:D:283:ARG:HG3	2.39	0.56
1:B:296:GLN:NE2	1:B:325:ILE:HD12	2.20	0.56
1:B:356:ALA:O	1:B:363:MET:HE3	2.05	0.56
1:C:205:LEU:HD11	1:C:234:THR:HG23	1.87	0.56
1:C:328:TYR:OH	1:C:361:PRO:HD2	2.05	0.56
2:D:170:LEU:O	2:D:173:CYS:O	2.24	0.56
1:B:194:GLU:HA	1:B:194:GLU:OE1	2.05	0.56
1:B:95:ALA:HA	1:B:100:LYS:HZ1	1.71	0.56
1:C:362:ARG:HH21	1:C:363:MET:CE	2.19	0.56
3:E:280:HIS:O	3:E:281:LEU:HD23	2.05	0.56
1:C:69:THR:HG22	1:C:71:THR:N	2.01	0.56
1:B:259:ALA:HB2	1:B:363:MET:SD	2.46	0.56
1:C:295:VAL:HG22	1:C:301:ALA:HB3	1.88	0.56
1:A:99:THR:CG2	1:A:99:THR:O	2.51	0.56
1:C:309:ILE:HG22	1:C:313:MET:HG2	1.88	0.56
1:A:156:THR:HG22	1:A:158:ASP:N	2.21	0.55
1:A:40:ALA:HB1	1:A:170:CYS:SG	2.46	0.55
1:C:362:ARG:HH21	1:C:363:MET:HE1	1.72	0.55
1:C:5011:ARG:HD3	1:C:83:GLU:OE2	2.07	0.55
2:D:218:VAL:HA	2:D:221:LEU:HB2	1.88	0.55
2:D:296:THR:HG22	2:D:299:ARG:NH1	2.21	0.55
2:D:39:ARG:NH2	2:D:50:HIS:HB3	2.21	0.55
1:B:360:HIS:HD2	1:B:361:PRO:O	1.90	0.55
2:D:308:THR:CG2	2:D:320:VAL:HG13	2.37	0.55
1:B:338:GLU:OE2	3:E:295:HIS:CE1	2.60	0.55
2:D:310:LEU:HD11	3:E:299:GLN:NE2	2.21	0.55
1:B:265:MET:HE3	3:E:257:LYS:HE2	1.89	0.55
1:B:355:ARG:NH1	3:E:287:GLN:HB3	2.22	0.55
2:D:313:LYS:O	2:D:316:TYR:CE2	2.60	0.55
1:B:259:ALA:HB2	1:B:363:MET:HG3	1.89	0.55
1:A:91:ILE:HD12	1:A:123:TYR:CE2	2.42	0.54
1:C:104:THR:O	1:C:108:LEU:HG	2.08	0.54
2:D:282:ARG:O	2:D:285:MET:HB3	2.07	0.54
1:C:297:LEU:HD23	2:D:334:LYS:O	2.06	0.54
1:C:3:TYR:O	1:C:3:TYR:CD2	2.60	0.54
1:A:281:LEU:HD23	1:A:285:MET:CE	2.36	0.54
1:A:97:SER:OG	1:A:100:LYS:CE	2.54	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:HA	1:C:310:GLU:HG3	1.89	0.54
1:A:346:ARG:O	1:A:350:GLU:HG3	2.07	0.54
1:B:360:HIS:CG	1:B:363:MET:CE	2.90	0.54
2:D:264:SER:O	2:D:265:ALA:HB3	2.07	0.54
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
1:C:248:GLN:O	1:C:252:LEU:N	2.39	0.54
1:C:49:VAL:O	5:C:5500:SO4:S	2.66	0.54
1:B:356:ALA:O	1:B:363:MET:HE1	2.07	0.54
2:D:1:MET:HA	2:D:134:SER:O	2.08	0.54
1:C:205:LEU:CD2	1:C:243:THR:HG23	2.38	0.54
2:D:48:GLU:HG3	2:D:49:GLU:H	1.73	0.54
1:B:244:LEU:HD11	1:B:276:ILE:HD13	1.90	0.54
2:D:271:ALA:O	2:D:275:LYS:HG2	2.07	0.53
1:C:276:ILE:HG22	1:C:277:GLU:N	2.24	0.53
2:D:262:ARG:NH2	3:E:320:GLU:OE1	2.42	0.53
1:A:94:ASP:C	1:A:100:LYS:NZ	2.62	0.53
1:B:296:GLN:HE22	1:B:325:ILE:HD12	1.73	0.53
1:B:302:LEU:HD22	1:B:306:MET:HG2	1.91	0.53
1:C:171:LEU:HA	2:D:183:GLN:HE22	1.73	0.53
2:D:119:LYS:CD	2:D:119:LYS:H	2.05	0.53
3:E:306:ILE:HG22	3:E:307:ASN:H	1.73	0.53
2:D:255:LEU:HD22	3:E:313:THR:HG21	1.91	0.53
1:A:307:ALA:HA	1:A:310:GLU:HB2	1.90	0.53
1:A:86:ARG:HE	1:B:137:ASN:HB2	1.73	0.53
1:B:244:LEU:HD21	1:B:276:ILE:CG1	2.37	0.53
1:A:261:GLY:CA	1:B:297:LEU:HD21	2.39	0.53
2:D:93:ILE:HG23	2:D:97:LEU:HD13	1.91	0.53
1:A:107:LEU:HD11	1:B:133:ARG:HH12	1.71	0.53
1:A:276:ILE:HG22	1:A:277:GLU:N	2.24	0.53
1:A:354:LEU:CD2	1:B:297:LEU:HD22	2.39	0.53
2:D:218:VAL:HG11	2:D:253:GLU:HG3	1.91	0.53
1:B:366:PRO:HB3	3:E:282:SER:HB2	1.91	0.53
1:B:259:ALA:CB	1:B:363:MET:SD	2.97	0.53
1:B:84:GLN:HB3	1:B:86:ARG:NH2	2.24	0.53
2:D:25:GLY:O	2:D:115:ASN:HA	2.08	0.53
1:A:191:LEU:HD12	1:A:203:LEU:HD21	1.91	0.52
1:B:360:HIS:HB2	1:B:363:MET:CE	2.39	0.52
1:B:271:ALA:HB1	1:B:276:ILE:HD11	1.90	0.52
2:D:309:GLU:O	2:D:313:LYS:HG3	2.09	0.52
1:A:100:LYS:HB3	1:B:133:ARG:CZ	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ARG:HD2	1:B:306:MET:SD	2.49	0.52
2:D:273:PHE:HB3	2:D:279:TRP:HB2	1.90	0.52
3:E:268:VAL:O	3:E:271:PRO:HD3	2.09	0.52
1:B:277:GLU:HB3	3:E:149:GLU:HG2	1.90	0.52
1:B:360:HIS:O	1:B:363:MET:HB2	2.09	0.52
3:E:238:HIS:ND1	3:E:239:GLU:N	2.56	0.52
1:A:360:HIS:HD2	1:A:363:MET:H	1.57	0.52
1:A:278:TRP:HB3	1:A:349:VAL:HG21	1.91	0.52
1:A:351:MET:HE1	1:B:326:GLN:NE2	2.08	0.52
1:B:360:HIS:CG	1:B:363:MET:SD	3.02	0.52
3:E:27:LEU:O	3:E:143:LEU:N	2.39	0.52
1:B:257:VAL:HG11	1:B:320:ILE:CD1	2.40	0.52
1:B:357:LEU:C	1:B:363:MET:SD	2.88	0.52
1:B:352:THR:O	1:B:355:ARG:HB3	2.10	0.52
2:D:310:LEU:O	2:D:314:GLN:HG3	2.11	0.52
1:B:250:LEU:HD23	1:B:312:ARG:HH11	1.75	0.51
1:A:252:LEU:HD13	1:A:281:LEU:HD21	1.92	0.51
1:C:93:ILE:HG22	1:C:100:LYS:NZ	2.25	0.51
2:D:10:ARG:HH22	2:D:40:GLN:NE2	2.08	0.51
1:A:213:SER:OG	1:A:216:ASP:HB2	2.11	0.51
1:A:334:ILE:O	1:A:338:GLU:HG3	2.09	0.51
1:C:343:PRO:CG	1:C:347:MET:SD	2.99	0.51
1:A:51:LYS:HE2	5:A:1500:SO4:O4	2.11	0.51
1:A:181:GLU:HA	1:A:184:ARG:HB3	1.93	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.11	0.51
1:C:243:THR:HG22	1:C:244:LEU:N	2.26	0.51
1:C:303:GLY:HA3	1:C:306:MET:HG2	1.93	0.51
1:C:304:ASN:HD22	2:D:234:GLN:CD	2.03	0.51
3:E:100:LEU:HD13	3:E:139:THR:HG21	1.93	0.51
2:D:261:LYS:HE3	2:D:295:GLN:HE21	1.76	0.51
2:D:300:GLN:OE1	2:D:335:PRO:HG2	2.09	0.51
3:E:139:THR:HG22	3:E:140:TRP:N	2.26	0.51
1:A:281:LEU:CD2	1:A:285:MET:HE2	2.40	0.50
1:C:201:ARG:O	1:C:205:LEU:HG	2.11	0.50
1:B:2049:VAL:O	5:B:2500:SO4:S	2.69	0.50
1:A:341:TYR:HB2	1:B:333:LEU:CD1	2.41	0.50
2:D:294:SER:H	2:D:297:GLN:NE2	2.08	0.50
3:E:151:LEU:HD21	3:E:155:LEU:HD12	1.93	0.50
1:B:2060:LYS:HE3	1:B:79:CYS:HB3	1.93	0.50
1:A:3:TYR:HB2	1:B:2039:HIS:CE1	2.46	0.50
1:C:302:LEU:HG	1:C:314:ARG:NH1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:HIS:CB	1:B:363:MET:CB	2.68	0.50
1:C:49:VAL:HG12	1:C:50:GLY:N	2.27	0.50
3:E:46:ARG:NH1	3:E:68:MET:HG3	2.27	0.50
1:A:102:GLU:HB3	1:A:106:ASP:CB	2.41	0.50
1:A:89:ASP:HB3	1:A:121:LYS:HA	1.92	0.50
2:D:96:GLN:O	2:D:100:LEU:HG	2.12	0.50
1:A:360:HIS:CD2	1:A:362:ARG:H	2.30	0.50
1:A:100:LYS:HG2	1:B:133:ARG:HE	1.77	0.50
1:B:288:LEU:O	1:B:292:ILE:HG13	2.12	0.50
2:D:312:LEU:HB2	2:D:320:VAL:CG2	2.35	0.50
1:A:107:LEU:CD1	1:B:133:ARG:HH12	2.25	0.49
1:A:297:LEU:HD21	1:C:261:GLY:HA3	1.93	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
1:A:244:LEU:HB3	1:A:248:GLN:HB2	1.95	0.49
1:A:44:SER:HB2	1:A:159:PRO:HG3	1.94	0.49
1:B:2052:THR:O	1:B:2055:ALA:HB3	2.13	0.49
1:C:51:LYS:HE3	5:C:5500:SO4:O3	2.12	0.49
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.94	0.49
2:D:274:ASP:HA	2:D:279:TRP:CZ3	2.47	0.49
1:B:276:ILE:HG22	1:B:277:GLU:N	2.28	0.49
1:C:366:PRO:C	1:C:367:GLU:HG3	2.32	0.49
1:A:92:GLU:HG2	1:A:124:LEU:HD23	1.94	0.49
2:D:22:LEU:HD22	2:D:112:VAL:HB	1.94	0.49
1:A:100:LYS:HE2	1:B:133:ARG:HH21	1.75	0.49
1:B:236:ALA:O	1:B:239:ALA:HB3	2.12	0.49
1:C:99:THR:CG2	1:C:99:THR:O	2.53	0.49
2:D:183:GLN:HA	2:D:183:GLN:HE21	1.78	0.49
2:D:282:ARG:HG2	2:D:285:MET:HE2	1.93	0.49
2:D:27:ASP:HB3	2:D:30:LEU:HB2	1.93	0.49
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.49
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.49
1:C:69:THR:HG22	1:C:70:ALA:N	2.28	0.49
2:D:20:ALA:O	2:D:134:SER:HB2	2.12	0.49
2:D:296:THR:HG22	2:D:299:ARG:HH12	1.77	0.49
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.49
1:A:238:SER:HB2	1:A:243:THR:O	2.13	0.49
1:A:354:LEU:HD11	1:B:294:MET:SD	2.53	0.49
1:B:360:HIS:HB2	1:B:363:MET:HE3	1.95	0.49
1:C:82:ILE:HG23	1:C:90:LEU:CD2	2.42	0.48
1:B:140:LEU:HD22	1:B:169:ARG:CZ	2.43	0.48
1:B:338:GLU:HA	1:B:341:TYR:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLU:HG2	1:C:274:ARG:NH1	2.28	0.48
1:B:302:LEU:HD11	1:B:313:MET:CB	2.43	0.48
1:C:244:LEU:HA	1:C:244:LEU:HD23	1.51	0.48
1:C:140:LEU:O	1:C:144:GLU:HG3	2.14	0.48
2:D:310:LEU:HD21	3:E:306:ILE:HD13	1.96	0.48
3:E:85:LYS:HB3	3:E:85:LYS:NZ	2.28	0.48
1:C:22:GLU:H	1:C:22:GLU:HG3	1.09	0.48
2:D:311:THR:HG23	2:D:318:GLN:CD	2.34	0.48
1:A:66:THR:HG22	1:A:66:THR:O	2.14	0.48
1:B:302:LEU:HD11	1:B:313:MET:HB2	1.94	0.48
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
1:A:101:VAL:HG12	1:A:102:GLU:HG3	1.96	0.48
2:D:10:ARG:NH2	2:D:40:GLN:HE22	2.11	0.48
1:B:260:ASN:O	1:B:260:ASN:OD1	2.32	0.48
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.48
1:C:205:LEU:HD22	1:C:243:THR:HG23	1.95	0.47
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
1:C:32:LEU:HD11	1:C:58:LEU:HD12	1.95	0.47
1:B:2013:GLN:HE22	1:B:83:GLU:CG	2.22	0.47
1:C:256:MET:CE	1:C:332:LEU:HD21	2.44	0.47
2:D:281:ASN:O	2:D:283:ARG:N	2.47	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
1:A:216:ASP:O	1:A:220:LEU:HG	2.15	0.47
1:A:291:ARG:NH1	1:A:306:MET:HG3	2.29	0.47
2:D:98:LEU:O	2:D:101:THR:HG22	2.14	0.47
2:D:48:GLU:CG	2:D:49:GLU:N	2.76	0.47
1:B:257:VAL:HG11	1:B:320:ILE:HD13	1.95	0.47
1:C:292:ILE:O	1:C:296:GLN:HG3	2.14	0.47
1:C:333:LEU:CD1	1:C:337:LYS:HE3	2.45	0.47
2:D:310:LEU:HD13	2:D:314:GLN:HE22	1.77	0.47
1:B:2024:VAL:HG11	1:B:175:LEU:HD21	1.96	0.47
1:A:271:ALA:HB1	1:A:276:ILE:CD1	2.36	0.47
1:C:286:LEU:HD11	1:C:333:LEU:HA	1.96	0.47
1:C:94:ASP:N	1:C:100:LYS:HZ1	2.07	0.47
1:A:316:LEU:HB3	1:A:320:ILE:HD12	1.96	0.47
1:A:126:ASP:HA	1:A:155:ALA:HB3	1.96	0.47
1:B:2044:SER:OG	1:B:174:HIS:HA	2.15	0.47
1:B:244:LEU:HD11	1:B:276:ILE:CG2	2.45	0.47
3:E:227:GLY:O	3:E:229:TRP:HD1	1.98	0.47
1:B:256:MET:HA	1:B:357:LEU:HD11	1.97	0.47
1:C:50:GLY:O	1:C:54:ILE:HG13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:GLN:HB2	2:D:272:LEU:HD21	1.97	0.47
2:D:60:ASP:O	2:D:64:ILE:HD12	2.15	0.47
1:A:147:PRO:HG2	1:A:150:VAL:HB	1.96	0.46
3:E:241:ALA:O	3:E:245:LEU:HD22	2.14	0.46
1:A:149:HIS:H	1:A:149:HIS:CD2	2.34	0.46
1:B:246:ASP:HB2	1:B:248:GLN:CG	2.45	0.46
1:B:343:PRO:HG3	1:B:347:MET:SD	2.56	0.46
1:C:362:ARG:HE	1:C:363:MET:CE	2.24	0.46
1:A:93:ILE:HG23	1:A:100:LYS:HZ3	1.76	0.46
1:B:165:THR:O	1:B:169:ARG:HG3	2.15	0.46
2:D:284:GLY:O	2:D:288:GLU:HB2	2.16	0.46
2:D:311:THR:HG23	2:D:318:GLN:OE1	2.15	0.46
1:A:246:ASP:O	1:A:250:LEU:HB2	2.16	0.46
1:B:2042:LEU:HB3	1:B:172:GLN:CB	2.42	0.46
1:B:316:LEU:HD22	1:B:320:ILE:CD1	2.45	0.46
1:B:338:GLU:HA	1:B:341:TYR:HD1	1.81	0.46
2:D:315:ASP:CB	2:D:318:GLN:HG2	2.45	0.46
1:A:257:VAL:HG11	1:A:320:ILE:HD13	1.97	0.46
1:B:2051:LYS:HE3	1:B:2051:LYS:HB2	1.76	0.46
2:D:213:THR:N	2:D:216:HIS:HD2	1.96	0.46
2:D:263:GLN:OE1	2:D:272:LEU:HD11	2.15	0.46
2:D:251:GLN:OE1	3:E:307:ASN:ND2	2.49	0.46
3:E:95:GLU:O	3:E:99:LYS:HB2	2.16	0.46
1:B:2042:LEU:HD12	1:B:172:GLN:OE1	2.16	0.46
1:A:257:VAL:O	1:A:360:HIS:HE1	1.99	0.46
1:C:94:ASP:O	1:C:100:LYS:CE	2.63	0.46
2:D:222:LEU:CD1	2:D:285:MET:SD	3.04	0.46
2:D:315:ASP:HB2	2:D:318:GLN:CD	2.36	0.46
3:E:257:LYS:HB3	3:E:262:ALA:HB3	1.98	0.46
1:A:21:GLN:HE22	1:A:49:VAL:HG13	1.81	0.46
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.54	0.46
1:C:186:GLN:HG2	1:C:214:LEU:HD21	1.98	0.46
1:C:56:ARG:NH1	1:C:82:ILE:O	2.49	0.46
2:D:174:TYR:CE2	2:D:211:HIS:CE1	3.04	0.46
1:B:338:GLU:CD	3:E:295:HIS:HE2	2.18	0.46
1:A:260:ASN:OD1	1:A:260:ASN:O	2.35	0.45
1:A:51:LYS:HB2	1:A:51:LYS:HE3	1.77	0.45
1:B:291:ARG:O	1:B:295:VAL:HG23	2.16	0.45
3:E:282:SER:OG	3:E:285:ARG:HB2	2.16	0.45
3:E:27:LEU:CD2	3:E:29:ILE:HD11	2.46	0.45
1:A:252:LEU:CD1	1:A:281:LEU:HD21	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:CD2	1:C:338:GLU:HB3	2.46	0.45
1:B:197:ALA:HB3	1:B:231:GLN:HG2	1.98	0.45
1:C:219:SER:O	1:C:223:GLN:HG3	2.17	0.45
1:A:265:MET:HE2	1:B:294:MET:SD	2.56	0.45
1:C:344:ASP:O	1:C:347:MET:HB3	2.16	0.45
2:D:19:ALA:CB	2:D:133:ARG:HD3	2.45	0.45
2:D:279:TRP:O	2:D:279:TRP:CD2	2.69	0.45
2:D:247:LEU:HD11	2:D:308:THR:HG22	1.98	0.45
1:B:2051:LYS:HB2	5:B:2500:SO4:O3	2.17	0.45
1:A:215:ARG:NH2	5:A:1500:SO4:O2	2.50	0.45
2:D:312:LEU:HG	2:D:312:LEU:O	2.15	0.45
3:E:14:LEU:HD13	3:E:44:LEU:HD11	1.98	0.45
2:D:222:LEU:HD11	2:D:285:MET:CE	2.47	0.45
2:D:48:GLU:CG	2:D:49:GLU:H	2.30	0.45
3:E:51:GLN:HB2	3:E:62:CYS:HB2	1.98	0.45
1:A:73:CYS:SG	1:A:76:CYS:HB3	2.56	0.45
1:C:270:GLU:HG2	1:C:274:ARG:CZ	2.46	0.45
2:D:315:ASP:HB2	2:D:318:GLN:NE2	2.31	0.45
1:B:361:PRO:O	1:B:362:ARG:HB2	2.15	0.45
2:D:198:THR:HB	2:D:200:PRO:HD2	1.98	0.45
3:E:253:MET:O	3:E:256:LEU:N	2.49	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.45
1:B:258:GLU:O	1:B:259:ALA:HB3	2.17	0.45
2:D:221:LEU:HD23	2:D:221:LEU:HA	1.47	0.45
2:D:225:LYS:HE3	2:D:227:LYS:HD2	1.99	0.45
2:D:27:ASP:OD2	2:D:178:LEU:HD12	2.17	0.45
2:D:298:LEU:O	2:D:302:VAL:HG23	2.16	0.45
1:B:2066:THR:O	1:B:2066:THR:HG22	2.17	0.45
1:A:21:GLN:NE2	1:A:176:LYS:O	2.49	0.44
1:A:86:ARG:HH21	1:B:138:ALA:CA	2.27	0.44
1:B:142:THR:O	1:B:146:PRO:N	2.50	0.44
1:B:140:LEU:HD11	1:B:165:THR:HB	1.99	0.44
1:B:2062:LEU:O	1:B:119:ARG:HD2	2.18	0.44
1:C:248:GLN:O	1:C:252:LEU:HB2	2.17	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
1:C:316:LEU:HD22	1:C:320:ILE:HD11	1.98	0.44
1:A:102:GLU:HB3	1:A:106:ASP:HB2	1.99	0.44
1:A:147:PRO:HB2	1:A:149:HIS:CD2	2.52	0.44
1:A:37:ILE:HD12	1:A:62:LEU:HD21	1.98	0.44
1:C:307:ALA:HA	1:C:310:GLU:CG	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD23	1:C:172:GLN:HG2	1.99	0.44
2:D:25:GLY:N	2:D:114:GLY:O	2.41	0.44
2:D:315:ASP:H	2:D:318:GLN:HE21	1.65	0.44
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.44
3:E:324:GLN:HA	3:E:325:PRO:HD3	1.86	0.44
2:D:57:PRO:HB3	2:D:90:ASN:ND2	2.33	0.44
1:B:343:PRO:HB2	3:E:246:HIS:ND1	2.33	0.44
1:A:215:ARG:CZ	5:A:1500:SO4:O1	2.65	0.44
1:B:2010:TRP:CE2	1:B:190:ILE:HG23	2.53	0.44
1:B:257:VAL:O	1:B:257:VAL:HG12	2.17	0.44
1:B:131:LEU:HB2	1:B:136:PHE:CD1	2.52	0.44
1:B:229:ASP:C	1:B:231:GLN:N	2.71	0.44
1:C:250:LEU:HD13	1:C:288:LEU:HD13	2.00	0.44
1:C:250:LEU:HD22	1:C:309:ILE:CG2	2.48	0.44
1:A:42:LEU:HD12	1:A:154:LEU:HB2	2.00	0.44
1:A:245:ASP:HB2	1:A:248:GLN:HG3	1.99	0.44
1:C:248:GLN:HA	1:C:251:SER:OG	2.17	0.44
1:C:360:HIS:CD2	1:C:361:PRO:HD2	2.52	0.44
2:D:315:ASP:CB	2:D:318:GLN:CG	2.82	0.44
1:A:290:HIS:CE1	1:C:347:MET:HG3	2.53	0.44
1:B:135:SER:O	1:B:138:ALA:HB3	2.17	0.44
1:B:191:LEU:HD12	1:B:203:LEU:HD21	1.99	0.44
1:A:167:LEU:HB3	1:A:172:GLN:NE2	2.33	0.43
1:B:94:ASP:O	1:B:100:LYS:CE	2.65	0.43
2:D:56:ASP:HB3	2:D:58:ASN:H	1.83	0.43
3:E:30:GLN:HG3	3:E:30:GLN:O	2.18	0.43
1:C:326:GLN:CD	2:D:338:ASP:OD2	2.56	0.43
2:D:100:LEU:O	2:D:103:LEU:HB3	2.18	0.43
2:D:3:ARG:HG2	2:D:136:GLN:NE2	2.33	0.43
1:C:104:THR:HG22	1:C:108:LEU:HG	1.99	0.43
1:C:243:THR:CG2	1:C:244:LEU:N	2.81	0.43
1:C:340:PRO:HB3	1:C:345:ARG:HH21	1.83	0.43
2:D:325:GLU:O	2:D:329:LEU:HG	2.18	0.43
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.43
1:C:244:LEU:HD23	1:C:247:ASP:OD2	2.17	0.43
1:C:42:LEU:HD11	1:C:156:THR:HG22	2.01	0.43
1:C:21:GLN:HE22	1:C:49:VAL:CG1	2.32	0.43
2:D:50:HIS:O	2:D:51:HIS:CD2	2.72	0.43
3:E:7:LEU:HD22	3:E:40:LEU:HB2	2.00	0.43
1:C:307:ALA:HA	1:C:310:GLU:CD	2.38	0.43
1:A:10:TRP:CZ2	1:A:190:ILE:HG23	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:O	1:A:268:ILE:HG13	2.18	0.43
1:A:345:ARG:O	1:A:349:VAL:HG23	2.19	0.43
1:B:358:ALA:C	1:B:360:HIS:H	2.22	0.43
2:D:29:LEU:O	2:D:33:GLU:HG3	2.19	0.43
3:E:165:ALA:HA	3:E:166:PRO:HD3	1.89	0.43
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.43
1:A:94:ASP:N	1:A:100:LYS:HZ3	2.17	0.43
1:B:337:LYS:O	1:B:340:PRO:HD2	2.19	0.43
2:D:191:LEU:O	2:D:193:PRO:HD3	2.18	0.43
1:B:269:ASN:ND2	3:E:264:GLN:HG3	2.34	0.43
2:D:119:LYS:N	2:D:119:LYS:HD3	2.11	0.43
1:B:265:MET:CE	3:E:257:LYS:HE2	2.49	0.43
1:B:5:VAL:HG13	1:B:222:ASP:CG	2.38	0.42
1:C:278:TRP:CE3	1:C:349:VAL:HG21	2.53	0.42
1:B:321:PRO:HA	1:B:322:PRO:HD2	1.92	0.42
1:C:37:ILE:HG12	1:C:62:LEU:HD21	2.02	0.42
1:A:136:PHE:CZ	1:A:166:ILE:HD12	2.54	0.42
1:B:131:LEU:HB2	1:B:136:PHE:HD1	1.85	0.42
1:C:276:ILE:CG2	1:C:277:GLU:N	2.82	0.42
1:B:76:CYS:SG	1:B:78:ASN:HB2	2.59	0.42
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.42
1:A:156:THR:HG22	1:A:157:THR:N	2.34	0.42
1:A:333:LEU:O	1:A:336:ARG:N	2.49	0.42
1:B:347:MET:O	1:B:351:MET:CG	2.65	0.42
1:C:104:THR:HG22	1:C:108:LEU:CD1	2.50	0.42
1:C:248:GLN:HA	1:C:251:SER:HG	1.85	0.42
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.42
1:A:362:ARG:C	1:A:363:MET:HG3	2.40	0.42
1:B:271:ALA:O	1:B:276:ILE:HG13	2.20	0.42
1:A:147:PRO:HB2	1:A:149:HIS:NE2	2.35	0.42
1:A:333:LEU:HD22	1:C:338:GLU:HB3	2.02	0.42
2:D:311:THR:O	2:D:318:GLN:NE2	2.53	0.42
1:B:119:ARG:H	1:B:119:ARG:HG3	1.65	0.42
3:E:18:TYR:HB3	3:E:48:LEU:HD21	2.00	0.42
1:A:200:PRO:HG2	1:A:305:ASP:CG	2.40	0.42
1:C:342:ALA:HB1	1:C:343:PRO:HD2	2.01	0.42
2:D:243:PRO:HG2	2:D:244:VAL:H	1.85	0.42
2:D:264:SER:O	2:D:265:ALA:CB	2.68	0.42
1:B:244:LEU:CD1	1:B:276:ILE:HD13	2.48	0.41
1:A:210:ALA:HB1	1:A:213:SER:OG	2.20	0.41
1:B:351:MET:SD	3:E:290:LEU:HD13	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:PRO:CD	2:D:178:LEU:HD11	2.50	0.41
2:D:79:THR:HG22	2:D:80:LEU:N	2.34	0.41
3:E:197:SER:HA	3:E:198:PRO:HD3	1.87	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:O1	2.53	0.41
2:D:64:ILE:HG12	2:D:96:GLN:HB3	2.02	0.41
1:B:351:MET:SD	3:E:290:LEU:HD22	2.60	0.41
1:A:320:ILE:HA	1:A:321:PRO:HD3	1.89	0.41
1:A:78:ASN:O	1:A:82:ILE:HG13	2.20	0.41
2:D:4:LEU:CD1	2:D:137:VAL:HG22	2.50	0.41
3:E:225:PRO:HB3	3:E:276:GLU:OE2	2.20	0.41
1:A:18:VAL:HG12	1:A:19:VAL:N	2.35	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:S	2.94	0.41
1:B:244:LEU:HD11	1:B:276:ILE:HG21	2.02	0.41
1:B:360:HIS:CB	1:B:363:MET:HE3	2.50	0.41
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.84	0.41
1:A:283:VAL:HA	1:A:286:LEU:HD12	2.03	0.41
1:A:250:LEU:HD23	1:A:312:ARG:CZ	2.51	0.41
1:B:343:PRO:CG	1:B:347:MET:SD	3.09	0.41
1:C:281:LEU:O	1:C:285:MET:HG3	2.20	0.41
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
1:B:302:LEU:HD13	1:B:310:GLU:HA	2.03	0.41
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.95	0.41
2:D:310:LEU:HA	2:D:310:LEU:HD23	1.61	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.21	0.41
3:E:170:GLN:HG2	3:E:170:GLN:H	1.65	0.41
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	0.41
2:D:310:LEU:HB3	2:D:314:GLN:NE2	2.35	0.41
1:A:257:VAL:HG12	1:A:257:VAL:O	2.21	0.40
2:D:270:ARG:HG2	2:D:283:ARG:NH2	2.36	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.22	0.40
3:E:73:HIS:HA	3:E:74:PRO:HD3	1.77	0.40
1:A:276:ILE:HG13	1:A:276:ILE:H	1.66	0.40
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.88	0.40
2:D:281:ASN:O	2:D:281:ASN:OD1	2.40	0.40
3:E:73:HIS:CE1	3:E:106:LEU:HD22	2.56	0.40
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.90	0.40
3:E:256:LEU:HD12	3:E:290:LEU:HD12	2.03	0.40
1:A:137:ASN:HA	1:A:140:LEU:HD12	2.02	0.40
1:B:250:LEU:CD2	1:B:309:ILE:HG23	2.51	0.40
1:C:82:ILE:HG23	1:C:90:LEU:HD23	2.03	0.40
2:D:213:THR:C	2:D:215:PHE:N	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ARG:CZ	2:D:50:HIS:HB3	2.51	0.40
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.57	0.40
1:A:322:PRO:HG3	1:C:365:LEU:HB2	2.03	0.40
1:A:49:VAL:O	5:A:1500:SO4:O1	2.40	0.40
1:B:365:LEU:HB3	1:B:366:PRO:HD2	2.04	0.40
1:C:32:LEU:HA	1:C:32:LEU:HD23	1.94	0.40
3:E:171:TYR:CD2	3:E:171:TYR:N	2.88	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:C:117:ARG:NH2	2:D:281:ASN:ND2[4_486]	1.70	0.50

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	364/373 (98%)	335 (92%)	23 (6%)	6 (2%)	11	28
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	6	14
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	8	20
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	8	21
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	28	56
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	9	23

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	104	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	VAL
1	A	364	PRO
1	B	2022	GLU
1	B	104	THR
1	B	261	GLY
1	B	310	GLU
1	C	310	GLU
2	D	279	TRP
1	B	2050	GLY
1	C	104	THR
1	C	303	GLY
2	D	131	ALA
2	D	282	ARG
1	B	111	VAL
1	C	4	GLN
2	D	46	GLY
2	D	269	LEU
3	E	62	CYS
1	C	249	ALA
2	D	125	ALA
3	E	150	ARG
1	A	339	LEU
1	B	7	ALA
1	B	364	PRO
1	C	22	GLU
1	C	278	TRP
1	A	246	ASP
1	B	101	VAL
1	B	299	PRO
2	D	317	GLY
1	C	101	VAL

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/310 (98%)	288 (95%)	15 (5%)	28	57
1	B	302/310 (97%)	289 (96%)	13 (4%)	33	64
1	C	303/310 (98%)	280 (92%)	23 (8%)	15	35
2	D	287/291 (99%)	261 (91%)	26 (9%)	11	25
3	E	270/270 (100%)	239 (88%)	31 (12%)	6	15
All	All	1465/1491 (98%)	1357 (93%)	108 (7%)	16	37

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	15	PHE
1	A	46	THR
1	A	69	THR
1	A	76	CYS
1	A	117	ARG
1	A	130	MET
1	A	251	SER
1	A	309	ILE
1	A	318	ARG
1	A	327	LEU
1	A	344	ASP
1	A	355	ARG
1	A	357	LEU
1	A	367	GLU
1	B	6	LEU
1	B	2017	ASP
1	B	2046	THR
1	B	71	THR
1	B	76	CYS
1	B	137	ASN
1	B	184	ARG
1	B	194	GLU
1	B	219	SER
1	B	248	GLN
1	B	251	SER
1	B	333	LEU
1	B	357	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3	TYR
1	C	5014	THR
1	C	5017	ASP
1	C	18	VAL
1	C	22	GLU
1	C	47	ARG
1	C	52	THR
1	C	71	THR
1	C	88	VAL
1	C	97	SER
1	C	128	VAL
1	C	160	GLN
1	C	165	THR
1	C	176	LYS
1	C	184	ARG
1	C	240	MET
1	C	251	SER
1	C	252	LEU
1	C	305	ASP
1	C	333	LEU
1	C	344	ASP
1	C	351	MET
1	C	357	LEU
2	D	40	GLN
2	D	54	SER
2	D	84	LEU
2	D	101	THR
2	D	109	LEU
2	D	113	ARG
2	D	115	ASN
2	D	119	LYS
2	D	133	ARG
2	D	143	GLU
2	D	160	LEU
2	D	162	LEU
2	D	183	GLN
2	D	198	THR
2	D	200	PRO
2	D	208	ASP
2	D	215	PHE
2	D	223	MET
2	D	228	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	230	LEU
2	D	266	HIS
2	D	279	TRP
2	D	283	ARG
2	D	292	ARG
2	D	305	LEU
2	D	330	LEU
3	E	3	TRP
3	E	13	LYS
3	E	46	ARG
3	E	68	MET
3	E	91	ASP
3	E	110	LYS
3	E	120	LEU
3	E	147	GLU
3	E	149	GLU
3	E	154	THR
3	E	158	ARG
3	E	159	CYS
3	E	170	GLN
3	E	175	TRP
3	E	185	ASP
3	E	202	LEU
3	E	206	GLN
3	E	216	LEU
3	E	220	LEU
3	E	237	ASN
3	E	245	LEU
3	E	252	LEU
3	E	256	LEU
3	E	277	LEU
3	E	285	ARG
3	E	290	LEU
3	E	292	ASP
3	E	299	GLN
3	E	310	LEU
3	E	315	LEU
3	E	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	198	HIS
1	A	360	HIS
1	B	2023	HIS
1	B	198	HIS
1	B	223	GLN
1	B	248	GLN
1	B	326	GLN
1	C	198	HIS
1	C	360	HIS
2	D	32	GLN
2	D	40	GLN
2	D	51	HIS
2	D	94	ASN
2	D	105	HIS
2	D	136	GLN
2	D	183	GLN
2	D	204	GLN
2	D	211	HIS
2	D	216	HIS
2	D	266	HIS
2	D	276	HIS
2	D	295	GLN
2	D	297	GLN
2	D	314	GLN
2	D	318	GLN
3	E	73	HIS
3	E	237	ASN
3	E	280	HIS
3	E	299	GLN
3	E	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	1500	-	4,4,4	1.82	2 (50%)	6,6,6	1.01	0
5	SO4	B	2500	-	4,4,4	1.86	1 (25%)	6,6,6	0.88	0
5	SO4	C	5500	-	4,4,4	1.83	2 (50%)	6,6,6	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	1500	-	-	0/0/0/0	0/0/0/0
5	SO4	B	2500	-	-	0/0/0/0	0/0/0/0
5	SO4	C	5500	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	SO4	O3-S	-2.16	1.28	1.47
5	C	5500	SO4	O3-S	-2.10	1.29	1.47
5	A	1500	SO4	O1-S	2.88	1.61	1.45
5	C	5500	SO4	O1-S	3.00	1.61	1.45
5	B	2500	SO4	O1-S	3.14	1.62	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	SO4	7	0
5	B	2500	SO4	2	0
5	C	5500	SO4	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	366/373 (98%)	1.06	64 (17%)	2 1	32, 76, 152, 173	0
1	B	365/373 (97%)	1.27	65 (17%)	2 1	27, 75, 159, 190	0
1	C	366/373 (98%)	0.85	39 (10%)	7 5	27, 62, 129, 156	0
2	D	338/343 (98%)	0.78	28 (8%)	12 9	38, 69, 121, 142	0
3	E	334/334 (100%)	1.10	54 (16%)	2 1	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.01	250 (14%)	3 2	27, 69, 151, 190	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	18.7
1	B	365	LEU	15.6
1	B	368	PRO	15.3
1	B	366	PRO	13.3
1	B	359	PHE	11.4
1	A	104	THR	11.0
1	B	367	GLU	8.4
3	E	82	GLU	8.3
3	E	103	HIS	8.1
1	B	100	LYS	7.6
1	A	152	PHE	7.6
1	C	241	LEU	7.5
1	B	101	VAL	7.3
3	E	108	GLY	7.2
1	B	2023	HIS	7.0
1	A	368	PRO	7.0
1	A	3	TYR	6.3
1	A	108	LEU	6.3
3	E	101	ASN	6.3
2	D	316	TYR	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	333	HIS	5.9
1	A	122	VAL	5.9
3	E	55	GLY	5.8
1	B	363	MET	5.7
3	E	61	HIS	5.6
1	C	248	GLN	5.4
1	A	74	GLY	5.4
1	A	101	VAL	5.4
1	B	108	LEU	5.3
3	E	109	ALA	5.3
1	B	136	PHE	5.3
1	A	112	GLN	5.3
1	C	302	LEU	5.2
3	E	74	PRO	5.2
2	D	338	ASP	5.2
3	E	127	ALA	5.0
3	E	77	TYR	5.0
1	B	70	ALA	5.0
3	E	102	GLU	4.9
1	A	70	ALA	4.9
1	B	362	ARG	4.9
1	B	111	VAL	4.8
1	A	102	GLU	4.7
1	A	86	ARG	4.6
1	C	294	MET	4.6
3	E	54	GLN	4.6
1	C	363	MET	4.6
1	C	245	ASP	4.5
3	E	76	TYR	4.5
1	B	104	THR	4.5
1	B	112	GLN	4.4
3	E	146	ARG	4.4
3	E	333	HIS	4.4
1	C	311	LEU	4.3
2	D	279	TRP	4.3
1	A	153	LEU	4.3
1	B	2068	ILE	4.2
2	D	277	ARG	4.2
1	A	124	LEU	4.2
1	B	90	LEU	4.2
2	D	317	GLY	4.2
1	C	247	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	112	VAL	4.2
1	B	98	ARG	4.1
3	E	95	GLU	4.1
3	E	79	LEU	4.0
1	B	133	ARG	4.0
1	B	361	PRO	4.0
1	C	101	VAL	4.0
1	A	100	LYS	3.9
3	E	83	LYS	3.9
2	D	283	ARG	3.8
1	B	302	LEU	3.8
1	B	86	ARG	3.8
1	B	102	GLU	3.8
3	E	63	ARG	3.8
1	A	89	ASP	3.8
1	B	113	TYR	3.7
1	B	99	THR	3.7
1	A	150	VAL	3.7
1	A	111	VAL	3.7
1	A	367	GLU	3.7
2	D	319	SER	3.7
1	A	99	THR	3.7
1	B	117	ARG	3.6
1	C	366	PRO	3.6
3	E	58	SER	3.5
2	D	334	LYS	3.5
2	D	275	LYS	3.5
3	E	106	LEU	3.5
1	B	149	HIS	3.4
1	B	244	LEU	3.4
2	D	233	LEU	3.4
1	B	125	ILE	3.4
3	E	85	LYS	3.4
1	C	313	MET	3.4
1	B	6	LEU	3.4
1	A	365	LEU	3.4
1	C	4	GLN	3.3
1	C	307	ALA	3.3
3	E	20	ALA	3.3
2	D	318	GLN	3.2
3	E	51	GLN	3.2
3	E	150	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	104	THR	3.2
1	B	114	ALA	3.2
1	A	117	ARG	3.2
1	C	100	LYS	3.2
1	A	138	ALA	3.2
1	B	229	ASP	3.2
2	D	2	ILE	3.2
1	B	115	PRO	3.2
2	D	330	LEU	3.1
1	B	87	PHE	3.1
1	A	159	PRO	3.1
1	A	134	HIS	3.1
2	D	320	VAL	3.1
2	D	227	LYS	3.0
1	C	314	ARG	3.0
1	C	299	PRO	3.0
1	A	60	LYS	3.0
1	A	81	GLU	3.0
1	A	235	GLN	3.0
1	A	140	LEU	3.0
3	E	84	GLY	3.0
1	B	301	ALA	2.9
1	A	149	HIS	2.9
1	C	298	SER	2.9
3	E	129	LEU	2.9
1	C	304	ASN	2.9
1	B	107	LEU	2.9
1	C	98	ARG	2.9
1	A	4	GLN	2.9
1	B	132	SER	2.9
1	A	98	ARG	2.8
1	A	139	LEU	2.8
2	D	336	LEU	2.8
3	E	113	TRP	2.8
1	A	161	LYS	2.8
1	A	141	LYS	2.7
1	C	274	ARG	2.7
1	A	115	PRO	2.7
1	A	175	LEU	2.7
1	A	85	GLY	2.7
1	B	2036	ARG	2.7
1	C	205	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	93	ILE	2.7
3	E	56	HIS	2.7
3	E	132	LEU	2.7
1	B	105	ARG	2.7
1	C	367	GLU	2.7
3	E	126	ASN	2.6
1	C	365	LEU	2.6
3	E	46	ARG	2.6
1	B	144	GLU	2.6
1	B	148	GLU	2.6
1	A	80	ARG	2.6
1	B	2025	LEU	2.6
1	A	47	ARG	2.6
3	E	133	GLU	2.6
3	E	224	VAL	2.6
1	A	82	ILE	2.6
1	A	123	TYR	2.6
1	C	291	ARG	2.6
1	B	153	LEU	2.5
1	A	107	LEU	2.5
1	A	15	PHE	2.5
1	B	2037	ILE	2.5
1	C	102	GLU	2.5
1	A	109	ASP	2.5
1	C	246	ASP	2.5
1	C	249	ALA	2.5
3	E	115	THR	2.5
1	B	152	PHE	2.5
2	D	223	MET	2.5
2	D	222	LEU	2.5
1	B	131	LEU	2.5
3	E	110	LYS	2.4
3	E	60	GLY	2.4
3	E	334	LEU	2.4
1	A	169	ARG	2.4
1	B	116	ALA	2.4
3	E	123	ALA	2.4
1	B	97	SER	2.4
1	A	305	ASP	2.4
1	A	151	LYS	2.4
1	A	143	LEU	2.4
1	A	167	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	305	ASP	2.4
1	A	27	ALA	2.4
3	E	1	MET	2.4
3	E	66	GLN	2.4
1	C	263	ARG	2.4
1	A	120	PHE	2.3
1	B	130	MET	2.3
1	C	3	TYR	2.3
1	C	368	PRO	2.3
1	A	96	ALA	2.3
1	B	154	LEU	2.3
1	B	214	LEU	2.3
1	A	131	LEU	2.3
3	E	99	LYS	2.3
1	A	164	VAL	2.3
1	B	306	MET	2.3
1	B	165	THR	2.3
1	A	163	PRO	2.3
3	E	87	THR	2.3
1	A	68	ILE	2.3
3	E	130	LYS	2.3
1	B	139	LEU	2.2
1	A	105	ARG	2.2
1	B	166	ILE	2.2
2	D	236	LEU	2.2
3	E	73	HIS	2.2
1	B	169	ARG	2.2
3	E	91	ASP	2.2
1	C	320	ILE	2.2
2	D	10	ARG	2.2
1	A	114	ALA	2.2
1	B	141	LYS	2.2
3	E	81	PRO	2.2
1	B	176	LYS	2.2
2	D	228	ARG	2.2
3	E	94	ARG	2.2
2	D	211	HIS	2.1
2	D	270	ARG	2.1
1	A	38	HIS	2.1
1	C	260	ASN	2.1
1	A	214	LEU	2.1
1	C	37	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	2.1
2	D	284	GLY	2.1
3	E	71	GLY	2.1
3	E	307	ASN	2.1
3	E	124	ALA	2.1
1	A	156	THR	2.1
1	C	237	VAL	2.1
1	C	301	ALA	2.1
1	B	128	VAL	2.1
1	C	23	HIS	2.0
3	E	170	GLN	2.0
1	A	201	ARG	2.0
1	B	304	ASN	2.0
1	B	2019	VAL	2.0
2	D	309	GLU	2.0
1	A	136	PHE	2.0
3	E	141	PHE	2.0
1	C	318	ARG	2.0
2	D	298	LEU	2.0
2	D	312	LEU	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
4	ZN	C	400	1/1	0.99	0.19	0.86	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	A	400	1/1	0.97	0.18	-0.39	130,130,130,130	0
4	ZN	B	400	1/1	0.98	0.15	-0.39	105,105,105,105	0
5	SO4	B	2500	5/5	0.95	0.17	-0.84	68,70,70,70	0
5	SO4	A	1500	5/5	0.97	0.14	-0.90	64,65,66,67	0
4	ZN	E	400	1/1	0.57	0.06	-1.96	156,156,156,156	0
5	SO4	C	5500	5/5	0.98	0.15	-2.66	36,36,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.