Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:19 PM GMT

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

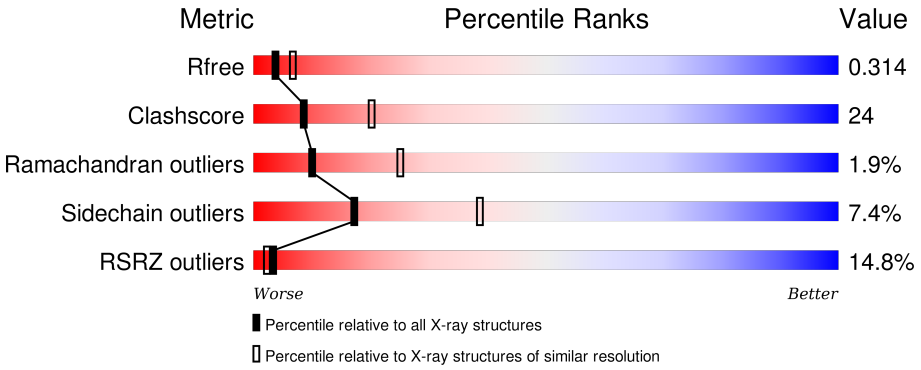
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 <=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	18% 58% 38%
1	B	373	18% 59% 35%
1	C	373	11% 61% 31% 5%
2	D	343	9% 56% 36% 5%
3	E	334	16% 62% 34%

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

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			

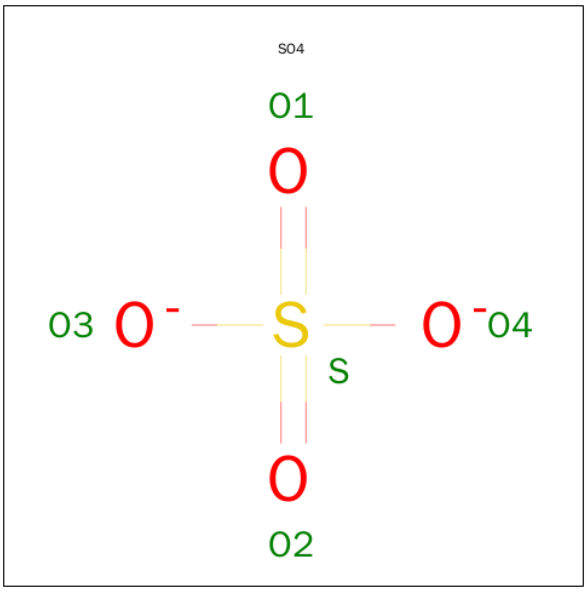
- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

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: O_4S).



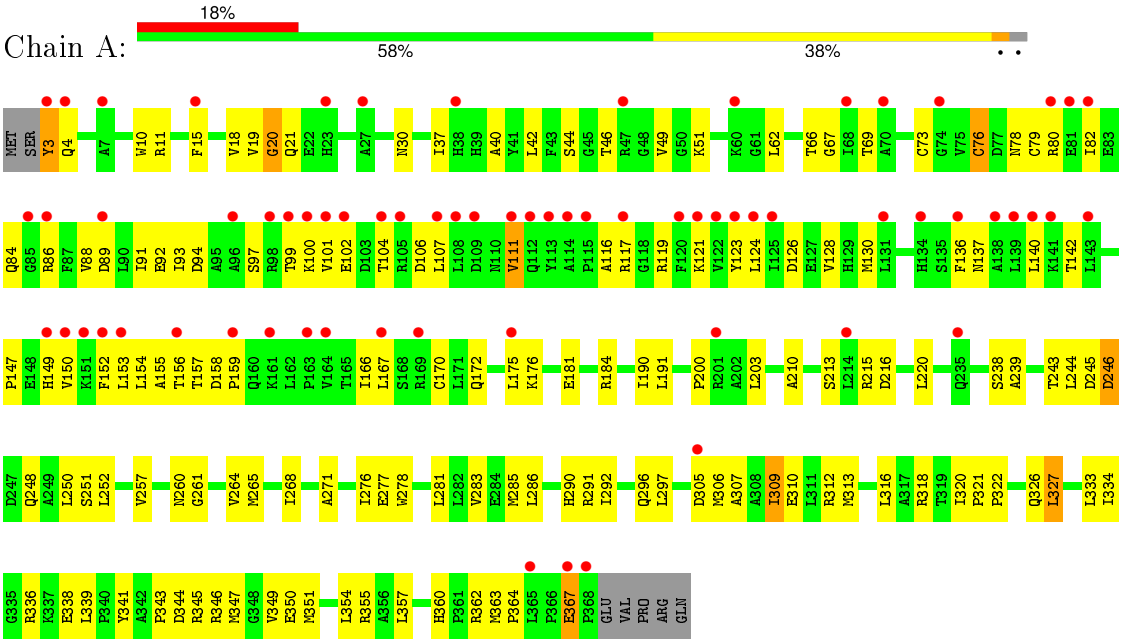
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

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

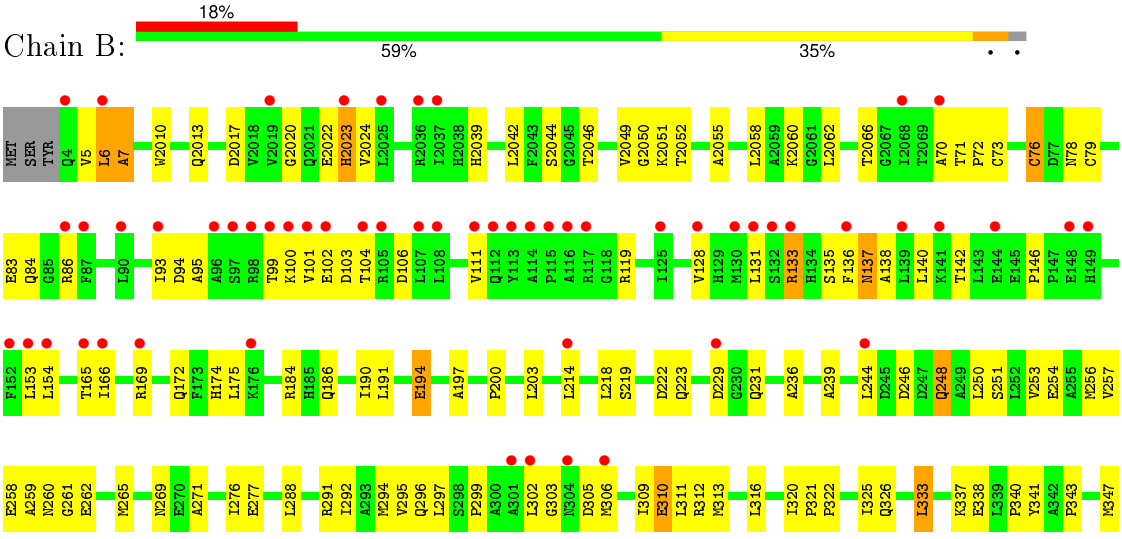
- Molecule 1: DNA polymerase III subunit gamma

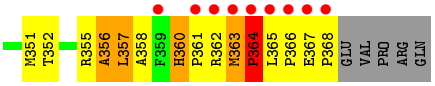
Chain A:



- Molecule 1: DNA polymerase III subunit gamma

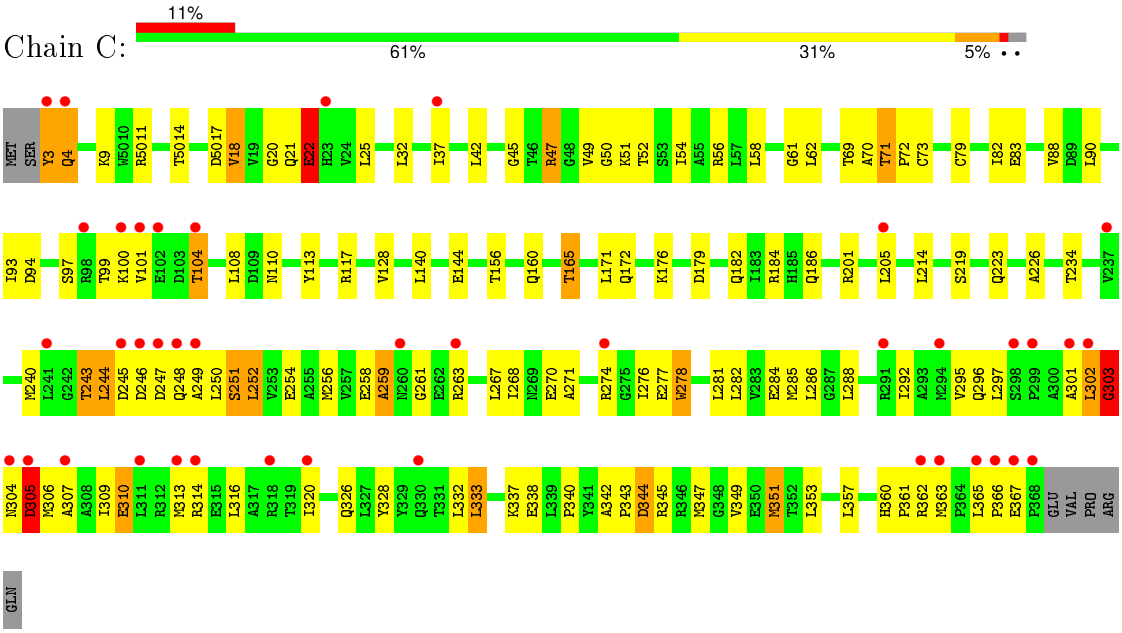
Chain B:





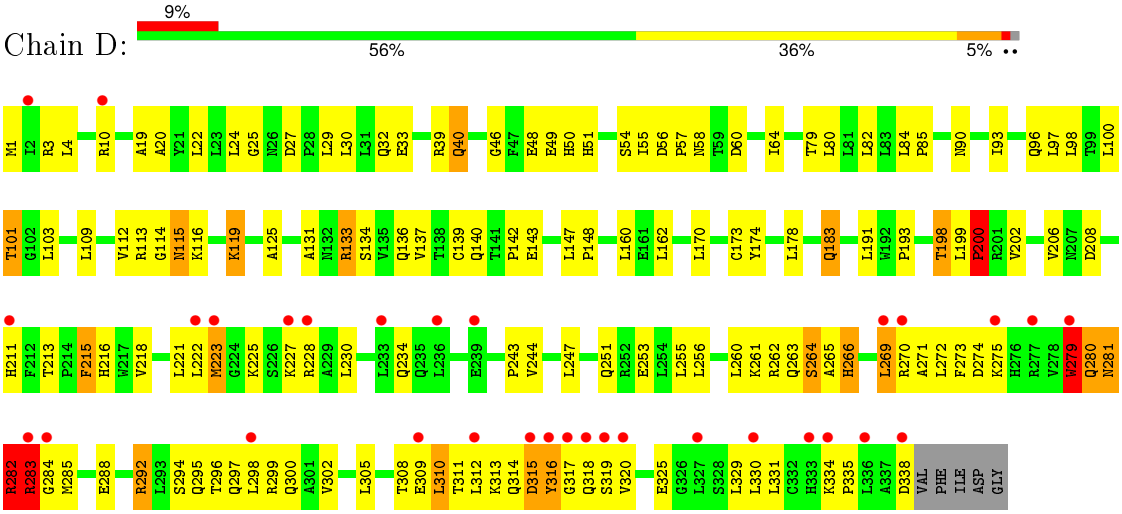
• Molecule 1: DNA polymerase III subunit gamma

Chain C:



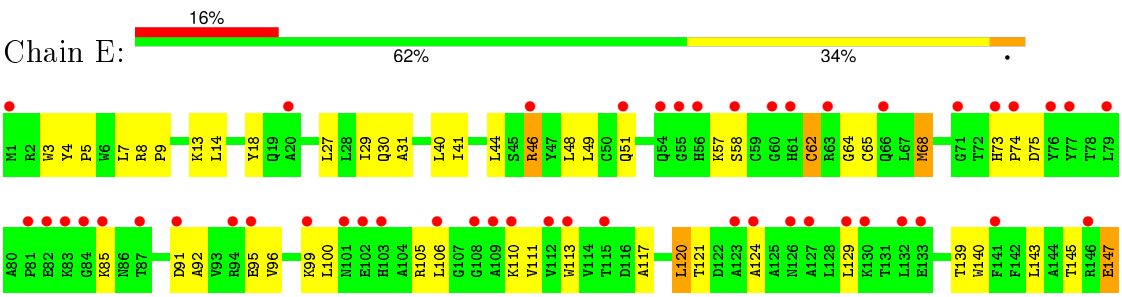
• Molecule 2: DNA polymerase III, delta subunit

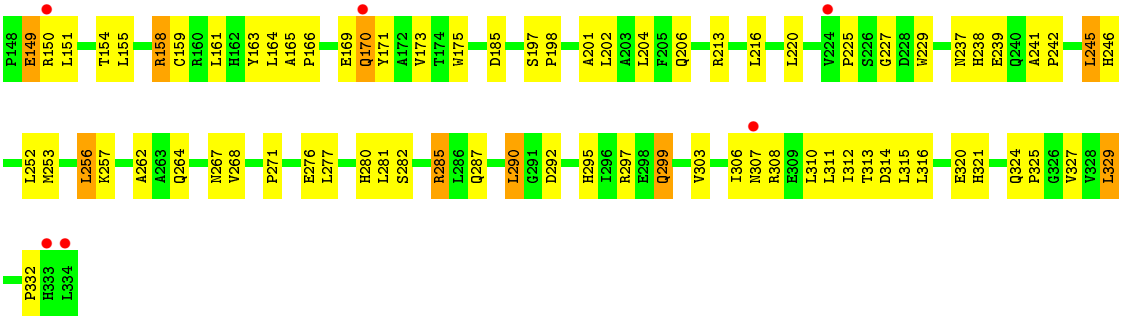
Chain D:



• Molecule 3: DNA polymerase III, delta' subunit

Chain E:




P148 E149 R150 L151 T154 L155 R158 C159 R160 L161 H162 Y163 L164 A165 P166 E169 Q170 Y171 A172 V173 T174 W175 D185 S197 P198 A201 L202 A203 L204 F205 Q206 R213 L216 L220 W224 P225 S226 G227 D228 W229 N237 H238 E239 Q240 A241 P242 L245 H246
L252 M253 L256 K257 A262 A263 Q264 N267 V268 P271 E276 L277 H280 L281 S282 R285 L286 Q287 L290 G291 D292 H295 I296 R297 E298 Q299 V303 I306 N307 R308 E309 L310 L311 I312 T313 D314 L315 L316 E320 H321 Q324 P325 G326 V327 V328 L329
P332 H333 L334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.70Å 95.86Å 285.41Å 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
$< I/\sigma(I) >$ [1]	2.18 (at 2.69Å)	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
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 60122 reflections (0.003%)	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2:D:310:LEU:HD22	2:D:314:GLN:HE21	1.27	0.97
1:A:239:ALA:HB1	1:B:2023:HIS:CE1	2.00	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

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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
3:E:58:SER:HB3	3:E:65:CYS:SG	2.21	0.80
1:B:99:THR:O	1:B:99:THR:HG22	1.81	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:97:SER:OG	1:A:100:LYS:HE3	1.83	0.79
1:A:67:GLY:HA2	1:A:119:ARG:HH12	1.47	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:C:93:ILE:HG23	1:C:100:LYS:HZ2	1.48	0.78
1:A:80:ARG:O	1:A:84:GLN:HG3	1.82	0.78
2:D:310:LEU:HD22	2:D:314:GLN:NE2	1.98	0.78
1:C:99:THR:HG22	1:C:99:THR:O	1.83	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:B:244:LEU:HD21	1:B:276:ILE:HG12	1.66	0.77
1:A:128:VAL:HG11	1:A:154:LEU:HD22	1.67	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
2:D:222:LEU:O	2:D:223:MET:HB2	1.83	0.76
1:C:248:GLN:HG3	1:C:267:LEU:HB3	1.65	0.76
1:B:2042:LEU:HB3	1:B:172:GLN:HB3	1.67	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

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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
2:D:273:PHE:HB3	2:D:279:TRP:CB	2.18	0.73
1:A:156:THR:HG22	1:A:158:ASP:H	1.54	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:B:360:HIS:CG	1:B:363:MET:HG3	2.23	0.73
1:A:100:LYS:CE	1:B:133:ARG:HH21	2.00	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
2:D:213:THR:H	2:D:216:HIS:CD2	2.04	0.69
1:A:86:ARG:NH2	1:B:138:ALA:HA	2.08	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
2:D:55:ILE:O	2:D:85:PRO:HG3	1.93	0.68
2:D:202:VAL:O	2:D:206:VAL:HG23	1.92	0.68
1:A:73:CYS:O	1:A:79:CYS:SG	2.50	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:B:357:LEU:HA	1:B:363:MET:HE1	1.76	0.68
2:D:116:LYS:HB3	2:D:140:GLN:HE21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:HG3	1:B:322:PRO:HD2	1.74	0.68
1:A:67:GLY:HA2	1:A:119:ARG:NH1	2.07	0.68
1:C:18:VAL:CG2	1:C:25:LEU:HD11	2.24	0.68
1:B:93:ILE:HG22	1:B:100:LYS:HZ3	1.58	0.68
2:D:308:THR:HG23	2:D:320:VAL:HG13	1.75	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:B:254:GLU:OE2	1:B:312:ARG:HD3	1.94	0.67
1:A:11:ARG:HH22	1:B:165:THR:HG22	1.59	0.67
1:B:260:ASN:O	1:B:262:GLU:N	2.27	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:8:ARG:CG	3:E:9:PRO:HD3	2.25	0.64
3:E:73:HIS:HD2	3:E:75:ASP:H	1.45	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: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:A:261:GLY:HA3	1:B:297:LEU:HD21	1.80	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
2:D:222:LEU:CD1	2:D:285:MET:HG2	2.29	0.63
1:A:107:LEU:HD11	1:B:133:ARG:NH1	2.14	0.63
1:A:73:CYS:SG	1:A:73:CYS:O	2.56	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

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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
2:D:24:LEU:HA	2:D:114:GLY:O	2.00	0.62
1:A:93:ILE:HG23	1:A:100:LYS:NZ	2.14	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: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:B:102:GLU:HB3	1:B:106:ASP:HB2	1.80	0.61
1:A:250:LEU:HD22	1:A:309:ILE:HD12	1.82	0.61
1:C:246:ASP:CB	1:C:274:ARG:HD3	2.24	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: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: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:C:268:ILE:HD11	1:C:353:LEU:HD12	1.83	0.60
1:A:30:ASN:HD22	1:C:226:ALA:HA	1.66	0.60
1:C:51:LYS:HB2	5:C:5500:SO4:O3	2.02	0.60
1:B:70:ALA:O	1:B:72:PRO:HD3	2.01	0.60
1:C:302:LEU:HD13	1:C:310:GLU:HG2	1.84	0.60
3:E:303:VAL:HB	3:E:306:ILE:HD11	1.83	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
1:B:140:LEU:HD21	1:B:166:ILE:HG12	1.83	0.60
2:D:269:LEU:HG	2:D:273:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:TYR:O	1:A:4:GLN:HG3	2.01	0.59
1:A:88:VAL:HG11	1:A:116:ALA:HB3	1.83	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
3:E:117:ALA:HB2	3:E:143:LEU:HD12	1.83	0.59
1:A:292:ILE:O	1:A:296:GLN:HG3	2.02	0.59
1:C:343:PRO:HG2	1:C:347:MET:SD	2.42	0.59
1:A:21:GLN:OE1	1:A:175:LEU:HD22	2.02	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
3:E:149:GLU:C	3:E:151:LEU:H	2.05	0.58
1:A:30:ASN:ND2	1:C:226:ALA:HA	2.18	0.58
1:A:341:TYR:HB2	1:B:333:LEU:HD11	1.84	0.58
3:E:46:ARG:CZ	3:E:68:MET:HG3	2.33	0.58
3:E:41:ILE:HG21	3:E:113:TRP:CD1	2.38	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: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
3:E:8:ARG:HG3	3:E:9:PRO:CD	2.33	0.58
1:C:259:ALA:HB3	1:C:363:MET:CE	2.33	0.58
1:B:2058:LEU:HD23	1:B:153:LEU:HD22	1.86	0.58
1:B:360:HIS:CB	1:B:363:MET:SD	2.92	0.57
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: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
2:D:279:TRP:O	2:D:279:TRP:CG	2.57	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: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:291:ARG:HH11	1:A:306:MET:HG3	1.69	0.57
1:C:304:ASN:OD1	1:C:305:ASP:N	2.37	0.57
1:A:49:VAL:O	5:A:1500:SO4:S	2.63	0.57
2:D:10:ARG:HH22	2:D:40:GLN:HE22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:308:ARG:O	3:E:312:ILE:HG13	2.04	0.57
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
2:D:273:PHE:CE1	2:D:283:ARG:HG3	2.39	0.56
1:B:356:ALA:O	1:B:363:MET:HE3	2.05	0.56
1:C:328:TYR:OH	1:C:361:PRO:HD2	2.05	0.56
1:C:205:LEU:HD11	1:C:234:THR:HG23	1.87	0.56
1:B:296:GLN:NE2	1:B:325:ILE:HD12	2.20	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:C:362:ARG:HH21	1:C:363:MET:CE	2.19	0.56
1:B:95:ALA:HA	1:B:100:LYS:HZ1	1.71	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
2:D:218:VAL:HA	2:D:221:LEU:HB2	1.88	0.55
1:C:5011:ARG:HD3	1:C:83:GLU:OE2	2.07	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
2:D:310:LEU:HD11	3:E:299:GLN:NE2	2.21	0.55
1:B:338:GLU:OE2	3:E:295:HIS:CE1	2.60	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:97:SER:OG	1:A:100:LYS:CE	2.54	0.54
1:A:281:LEU:HD23	1:A:285:MET:CE	2.36	0.54
3:E:213:ARG:NH2	3:E:267:ASN:OD1	2.39	0.54

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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:B:360:HIS:CG	1:B:363:MET:CE	2.90	0.54
3:E:4:TYR:HB3	3:E:5:PRO:HD2	1.89	0.54
1:A:346:ARG:O	1:A:350:GLU:HG3	2.07	0.54
3:E:201:ALA:O	3:E:204:LEU:HB2	2.06	0.54
2:D:264:SER:O	2:D:265:ALA:HB3	2.07	0.54
1:C:49:VAL:O	5:C:5500:SO4:S	2.66	0.54
1:C:248:GLN:O	1:C:252:LEU:N	2.39	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
2:D:48:GLU:HG3	2:D:49:GLU:H	1.73	0.54
1:C:205:LEU:CD2	1:C:243:THR:HG23	2.38	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:302:LEU:HD22	1:B:306:MET:HG2	1.91	0.53
1:B:296:GLN:HE22	1:B:325:ILE:HD12	1.73	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
2:D:93:ILE:HG23	2:D:97:LEU:HD13	1.91	0.53
1:B:244:LEU:HD21	1:B:276:ILE:CG1	2.37	0.53
1:A:86:ARG:HE	1:B:137:ASN:HB2	1.73	0.53
1:A:261:GLY:CA	1:B:297:LEU:HD21	2.39	0.53
1:A:307:ALA:HA	1:A:310:GLU:HB2	1.90	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
2:D:25:GLY:O	2:D:115:ASN:HA	2.08	0.53
1:B:84:GLN:HB3	1:B:86:ARG:NH2	2.24	0.53
1:B:360:HIS:HB2	1:B:363:MET:CE	2.39	0.52
1:A:191:LEU:HD12	1:A:203:LEU:HD21	1.91	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

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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:360:HIS:O	1:B:363:MET:HB2	2.09	0.52
1:B:277:GLU:HB3	3:E:149:GLU:HG2	1.90	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:351:MET:HE1	1:B:326:GLN:NE2	2.08	0.52
1:A:278:TRP:HB3	1:A:349:VAL:HG21	1.91	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:C:93:ILE:HG22	1:C:100:LYS:NZ	2.25	0.51
1:A:252:LEU:HD13	1:A:281:LEU:HD21	1.92	0.51
2:D:10:ARG:HH22	2:D:40:GLN:NE2	2.08	0.51
1:C:343:PRO:CG	1:C:347:MET:SD	2.99	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:A:181:GLU:HA	1:A:184:ARG:HB3	1.93	0.51
1:A:51:LYS:HE2	5:A:1500:SO4:O4	2.11	0.51
3:E:311:LEU:O	3:E:314:ASP:HB3	2.11	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
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
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
2:D:261:LYS:HE3	2:D:295:GLN:HE21	1.76	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:A:341:TYR:HB2	1:B:333:LEU:CD1	2.41	0.50
1:B:2049:VAL:O	5:B:2500:SO4:S	2.69	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:C:302:LEU:HG	1:C:314:ARG:NH1	2.26	0.50
1:A:3:TYR:HB2	1:B:2039:HIS:CE1	2.46	0.50

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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:89:ASP:HB3	1:A:121:LYS:HA	1.92	0.50
1:A:102:GLU:HB3	1:A:106:ASP:CB	2.41	0.50
2:D:96:GLN:O	2:D:100:LEU:HG	2.12	0.50
1:A:100:LYS:HG2	1:B:133:ARG:HE	1.77	0.50
2:D:312:LEU:HB2	2:D:320:VAL:CG2	2.35	0.50
1:A:360:HIS:CD2	1:A:362:ARG:H	2.30	0.50
1:B:288:LEU:O	1:B:292:ILE:HG13	2.12	0.50
1:A:107:LEU:CD1	1:B:133:ARG:HH12	2.25	0.49
3:E:312:ILE:O	3:E:316:LEU:HG	2.12	0.49
1:A:297:LEU:HD21	1:C:261:GLY:HA3	1.93	0.49
1:C:51:LYS:HE3	5:C:5500:SO4:O3	2.12	0.49
2:D:274:ASP:HA	2:D:279:TRP:CZ3	2.47	0.49
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.94	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:A:244:LEU:HB3	1:A:248:GLN:HB2	1.95	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
2:D:22:LEU:HD22	2:D:112:VAL:HB	1.94	0.49
1:A:92:GLU:HG2	1:A:124:LEU:HD23	1.94	0.49
2:D:282:ARG:HG2	2:D:285:MET:HE2	1.93	0.49
1:A:100:LYS:HE2	1:B:133:ARG:HH21	1.75	0.49
3:E:57:LYS:HG3	3:E:58:SER:H	1.78	0.49
1:C:99:THR:CG2	1:C:99:THR:O	2.53	0.49
3:E:41:ILE:HG21	3:E:113:TRP:CG	2.47	0.49
2:D:183:GLN:HA	2:D:183:GLN:HE21	1.78	0.49
2:D:27:ASP:HB3	2:D:30:LEU:HB2	1.93	0.49
1:B:236:ALA:O	1:B:239:ALA:HB3	2.12	0.49
1:C:69:THR:HG22	1:C:70:ALA:N	2.28	0.49
3:E:145:THR:HG22	3:E:147:GLU:N	2.27	0.49
2:D:296:THR:HG22	2:D:299:ARG:HH12	1.77	0.49
2:D:20:ALA:O	2:D:134:SER:HB2	2.12	0.49
1:B:360:HIS:HB2	1:B:363:MET:HE3	1.95	0.49
1:A:354:LEU:HD11	1:B:294:MET:SD	2.53	0.49
1:A:238:SER:HB2	1:A:243:THR:O	2.13	0.49
1:C:82:ILE:HG23	1:C:90:LEU:CD2	2.42	0.48
1:C:270:GLU:HG2	1:C:274:ARG:NH1	2.28	0.48
1:B:338:GLU:HA	1:B:341:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD22	1:B:169:ARG:CZ	2.43	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
2:D:310:LEU:HD21	3:E:306:ILE:HD13	1.96	0.48
1:C:140:LEU:O	1:C:144:GLU:HG3	2.14	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
3:E:306:ILE:HG22	3:E:307:ASN:N	2.29	0.48
1:B:302:LEU:HD11	1:B:313:MET:HB2	1.94	0.48
1:A:66:THR:HG22	1:A:66:THR:O	2.14	0.48
2:D:10:ARG:NH2	2:D:40:GLN:HE22	2.11	0.48
1:A:101:VAL:HG12	1:A:102:GLU:HG3	1.96	0.48
3:E:57:LYS:HA	3:E:57:LYS:HD2	1.67	0.48
1:B:260:ASN:O	1:B:260:ASN:OD1	2.32	0.48
3:E:145:THR:HG22	3:E:147:GLU:H	1.78	0.47
1:C:205:LEU:HD22	1:C:243:THR:HG23	1.95	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
2:D:281:ASN:O	2:D:283:ARG:N	2.47	0.47
1:C:256:MET:CE	1:C:332:LEU:HD21	2.44	0.47
3:E:241:ALA:N	3:E:242:PRO:HD2	2.29	0.47
2:D:48:GLU:CG	2:D:49:GLU:N	2.76	0.47
1:A:291:ARG:NH1	1:A:306:MET:HG3	2.29	0.47
1:A:216:ASP:O	1:A:220:LEU:HG	2.15	0.47
2:D:98:LEU:O	2:D:101:THR:HG22	2.14	0.47
1:B:257:VAL:HG11	1:B:320:ILE:HD13	1.95	0.47
2:D:310:LEU:HD13	2:D:314:GLN:HE22	1.77	0.47
1:C:333:LEU:CD1	1:C:337:LYS:HE3	2.45	0.47
1:C:292:ILE:O	1:C:296:GLN:HG3	2.14	0.47
1:B:2024:VAL:HG11	1:B:175:LEU:HD21	1.96	0.47
1:C:94:ASP:N	1:C:100:LYS:HZ1	2.07	0.47
1:A:271:ALA:HB1	1:A:276:ILE:CD1	2.36	0.47
1:A:316:LEU:HB3	1:A:320:ILE:HD12	1.96	0.47
1:C:286:LEU:HD11	1:C:333:LEU:HA	1.96	0.47
1:A:126:ASP:HA	1:A:155:ALA:HB3	1.96	0.47
1:B:244:LEU:HD11	1:B:276:ILE:CG2	2.45	0.47
1:B:2044:SER:OG	1:B:174:HIS:HA	2.15	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:HB3	1:B:231:GLN:HG2	1.98	0.45
1:A:333:LEU:CD2	1:C:338:GLU:HB3	2.46	0.45
1:C:219:SER:O	1:C:223:GLN:HG3	2.17	0.45
2:D:247:LEU:HD11	2:D:308:THR:HG22	1.98	0.45
2:D:279:TRP:O	2:D:279:TRP:CD2	2.69	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
1:B:2051:LYS:HB2	5:B:2500:SO4:O3	2.17	0.45
2:D:312:LEU:O	2:D:312:LEU:HG	2.15	0.45
1:A:215:ARG:NH2	5:A:1500:SO4:O2	2.50	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
2:D:315:ASP:HB2	2:D:318:GLN:NE2	2.31	0.45
1:C:270:GLU:HG2	1:C:274:ARG:CZ	2.46	0.45
1:A:73:CYS:SG	1:A:76:CYS:HB3	2.56	0.45
1:B:361:PRO:O	1:B:362:ARG:HB2	2.15	0.45
3:E:299:GLN:HE21	3:E:311:LEU:HD21	1.82	0.45
3:E:27:LEU:HG	3:E:29:ILE:CD1	2.47	0.45
3:E:253:MET:O	3:E:256:LEU:N	2.49	0.45
2:D:198:THR:HB	2:D:200:PRO:HD2	1.98	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:27:ASP:OD2	2:D:178:LEU:HD12	2.17	0.45
2:D:225:LYS:HE3	2:D:227:LYS:HD2	1.99	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:C:248:GLN:O	1:C:252:LEU:HB2	2.17	0.44
1:A:86:ARG:HH21	1:B:138:ALA:CA	2.27	0.44
1:B:140:LEU:HD11	1:B:165:THR:HB	1.99	0.44
3:E:30:GLN:HA	3:E:145:THR:O	2.17	0.44
1:A:21:GLN:NE2	1:A:176:LYS:O	2.49	0.44
1:B:2062:LEU:O	1:B:119:ARG:HD2	2.18	0.44
1:B:142:THR:O	1:B:146:PRO:N	2.50	0.44
1:C:316:LEU:HD22	1:C:320:ILE:HD11	1.98	0.44
2:D:315:ASP:H	2:D:318:GLN:HE21	1.65	0.44
2:D:25:GLY:N	2:D:114:GLY:O	2.41	0.44
3:E:149:GLU:C	3:E:151:LEU:N	2.71	0.44
1:C:307:ALA:HA	1:C:310:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:324:GLN:HA	3:E:325:PRO:HD3	1.86	0.44
1:C:42:LEU:HD23	1:C:172:GLN:HG2	1.99	0.44
1:B:343:PRO:HB2	3:E:246:HIS:ND1	2.33	0.44
2:D:57:PRO:HB3	2:D:90:ASN:ND2	2.33	0.44
1:B:257:VAL:O	1:B:257:VAL:HG12	2.17	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: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:B:229:ASP:C	1:B:231:GLN:N	2.71	0.44
1:B:131:LEU:HB2	1:B:136:PHE:CD1	2.52	0.44
1:A:42:LEU:HD12	1:A:154:LEU:HB2	2.00	0.44
1:C:248:GLN:HA	1:C:251:SER:OG	2.17	0.44
1:A:245:ASP:HB2	1:A:248:GLN:HG3	1.99	0.44
2:D:315:ASP:CB	2:D:318:GLN:CG	2.82	0.44
1:C:360:HIS:CD2	1:C:361:PRO:HD2	2.52	0.44
1:B:135:SER:O	1:B:138:ALA:HB3	2.17	0.44
1:A:290:HIS:CE1	1:C:347:MET:HG3	2.53	0.44
1:B:191:LEU:HD12	1:B:203:LEU:HD21	1.99	0.44
1:B:94:ASP:O	1:B:100:LYS:CE	2.65	0.43
3:E:30:GLN:HG3	3:E:30:GLN:O	2.18	0.43
1:A:167:LEU:HB3	1:A:172:GLN:NE2	2.33	0.43
2:D:56:ASP:HB3	2:D:58:ASN:H	1.83	0.43
2:D:100:LEU:O	2:D:103:LEU:HB3	2.18	0.43
1:C:326:GLN:CD	2:D:338:ASP:OD2	2.56	0.43
2:D:3:ARG:HG2	2:D:136:GLN:NE2	2.33	0.43
3:E:117:ALA:HB2	3:E:143:LEU:CD1	2.47	0.43
1:C:243:THR:CG2	1:C:244:LEU:N	2.81	0.43
1:C:104:THR:HG22	1:C:108:LEU:HG	1.99	0.43
2:D:325:GLU:O	2:D:329:LEU:HG	2.18	0.43
1:C:340:PRO:HB3	1:C:345:ARG:HH21	1.83	0.43
1:C:21:GLN:HE22	1:C:49:VAL:CG1	2.32	0.43
1:C:244:LEU:HD23	1:C:247:ASP:OD2	2.17	0.43
2:D:50:HIS:O	2:D:51:HIS:CD2	2.72	0.43
1:C:42:LEU:HD11	1:C:156:THR:HG22	2.01	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:345:ARG:O	1:A:349:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TRP:CZ2	1:A:190:ILE:HG23	2.54	0.43
1:A:264:VAL:O	1:A:268:ILE:HG13	2.18	0.43
1:B:358:ALA:C	1:B:360:HIS:H	2.22	0.43
3:E:51:GLN:HG2	3:E:62:CYS:SG	2.58	0.43
3:E:165:ALA:HA	3:E:166:PRO:HD3	1.89	0.43
2:D:29:LEU:O	2:D:33:GLU:HG3	2.19	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
1:B:269:ASN:ND2	3:E:264:GLN:HG3	2.34	0.43
2:D:191:LEU:O	2:D:193:PRO:HD3	2.18	0.43
2:D:119:LYS:HD3	2:D:119:LYS:N	2.11	0.43
1:B:265:MET:CE	3:E:257:LYS:HE2	2.49	0.43
1:C:278:TRP:CE3	1:C:349:VAL:HG21	2.53	0.42
1:B:5:VAL:HG13	1:B:222:ASP:CG	2.38	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:C:276:ILE:CG2	1:C:277:GLU:N	2.82	0.42
1:B:131:LEU:HB2	1:B:136:PHE:HD1	1.85	0.42
1:A:136:PHE:CZ	1:A:166:ILE:HD12	2.54	0.42
3:E:245:LEU:HB2	3:E:297:ARG:HG3	2.01	0.42
1:B:76:CYS:SG	1:B:78:ASN:HB2	2.59	0.42
1:C:248:GLN:HA	1:C:251:SER:HG	1.85	0.42
1:A:156:THR:HG22	1:A:157:THR:N	2.34	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:A:333:LEU:O	1:A:336:ARG:N	2.49	0.42
3:E:92:ALA:O	3:E:96:VAL:HG23	2.19	0.42
1:B:271:ALA:O	1:B:276:ILE:HG13	2.20	0.42
1:A:362:ARG:C	1:A:363:MET:HG3	2.40	0.42
2:D:311:THR:O	2:D:318:GLN:NE2	2.53	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
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
2:D:243:PRO:HG2	2:D:244:VAL:H	1.85	0.42
1:C:342:ALA:HB1	1:C:343:PRO:HD2	2.01	0.42
2:D:264:SER:O	2:D:265:ALA:CB	2.68	0.42
1:A:200:PRO:HG2	1:A:305:ASP:CG	2.40	0.42
1:B:244:LEU:CD1	1:B:276:ILE:HD13	2.48	0.41
1:B:351:MET:SD	3:E:290:LEU:HD13	2.59	0.41
1:A:210:ALA:HB1	1:A:213:SER:OG	2.20	0.41

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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
2:D:64:ILE:HG12	2:D:96:GLN:HB3	2.02	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:O1	2.53	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
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:78:ASN:O	1:A:82:ILE:HG13	2.20	0.41
1:B:360:HIS:CB	1:B:363:MET:HE3	2.50	0.41
1:B:244:LEU:HD11	1:B:276:ILE:HG21	2.02	0.41
1:A:215:ARG:NH2	5:A:1500:SO4:S	2.94	0.41
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.84	0.41
1:A:18:VAL:HG12	1:A:19:VAL:N	2.35	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
3:E:329:LEU:HD23	3:E:329:LEU:N	2.34	0.41
1:C:281:LEU:O	1:C:285:MET:HG3	2.20	0.41
2:D:310:LEU:HD23	2:D:310:LEU:HA	1.61	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
3:E:239:GLU:HA	3:E:308:ARG:CZ	2.51	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
2:D:310:LEU:HB3	2:D:314:GLN:NE2	2.35	0.41
2:D:270:ARG:HG2	2:D:283:ARG:NH2	2.36	0.40
1:A:257:VAL:HG12	1:A:257:VAL:O	2.21	0.40
3:E:73:HIS:HA	3:E:74:PRO:HD3	1.77	0.40
3:E:321:HIS:O	3:E:327:VAL:HG21	2.22	0.40
1:A:276:ILE:H	1:A:276:ILE:HG13	1.66	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:311:LEU:HA	1:B:311:LEU:HD12	1.88	0.40
3:E:256:LEU:HD12	3:E:290:LEU:HD12	2.03	0.40
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.90	0.40
2:D:213:THR:C	2:D:215:PHE:N	2.75	0.40
1:B:250:LEU:CD2	1:B:309:ILE:HG23	2.51	0.40
2:D:39:ARG:CZ	2:D:50:HIS:HB3	2.51	0.40
1:C:82:ILE:HG23	1:C:90:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:TYR:CE2	3:E:165:ALA:HB2	2.57	0.40
1:A:137:ASN:HA	1:A:140:LEU:HD12	2.02	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
1:A:322:PRO:HG3	1:C:365:LEU:HB2	2.03	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%)	12 30
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	6 15
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	8 22
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	9 23
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	30 59
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	10 25

All (33) Ramachandran outliers are listed below:

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

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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 (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	303/310 (98%)	288 (95%)	15 (5%)	30 60
1	B	302/310 (97%)	289 (96%)	13 (4%)	35 66
1	C	303/310 (98%)	280 (92%)	23 (8%)	16 37
2	D	287/291 (99%)	261 (91%)	26 (9%)	12 26
3	E	270/270 (100%)	239 (88%)	31 (12%)	7 16
All	All	1465/1491 (98%)	1357 (93%)	108 (7%)	17 39

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

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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

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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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	3.35	2 (50%)	6,6,6	0.97	1 (16%)
5	SO4	B	2500	-	4,4,4	3.29	2 (50%)	6,6,6	0.98	0
5	SO4	C	5500	-	4,4,4	3.32	2 (50%)	6,6,6	0.96	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	SO4	O3-S	-5.14	1.28	1.47
5	C	5500	SO4	O3-S	-4.99	1.29	1.47
5	B	2500	SO4	O3-S	-4.73	1.30	1.47
5	A	1500	SO4	O1-S	4.11	1.61	1.47
5	C	5500	SO4	O1-S	4.31	1.61	1.47
5	B	2500	SO4	O1-S	4.52	1.62	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1500	SO4	O4-S-O3	2.05	117.32	108.98

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	366/373 (98%)	1.10	69 (18%) 2 1	32, 76, 152, 173	0
1	B	365/373 (97%)	1.31	66 (18%) 2 1	27, 75, 159, 190	0
1	C	366/373 (98%)	0.89	41 (11%) 7 5	27, 62, 129, 156	0
2	D	338/343 (98%)	0.82	32 (9%) 10 8	38, 69, 121, 142	0
3	E	334/334 (100%)	1.14	54 (16%) 3 2	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.05	262 (14%) 3 2	27, 69, 151, 190	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	18.8
1	B	365	LEU	15.7
1	B	368	PRO	15.4
1	B	366	PRO	13.4
1	B	359	PHE	11.5
1	A	104	THR	11.1
1	B	367	GLU	8.6
3	E	82	GLU	8.5
3	E	103	HIS	8.2
1	B	100	LYS	7.8
1	A	152	PHE	7.7
1	C	241	LEU	7.6
1	B	101	VAL	7.4
3	E	108	GLY	7.3
1	B	2023	HIS	7.1
1	A	368	PRO	7.1
1	A	3	TYR	6.4
3	E	101	ASN	6.4
1	A	108	LEU	6.3
2	D	316	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	333	HIS	6.0
1	A	122	VAL	6.0
1	B	363	MET	5.9
3	E	55	GLY	5.9
3	E	61	HIS	5.7
1	C	248	GLN	5.6
1	A	74	GLY	5.5
1	A	101	VAL	5.4
3	E	109	ALA	5.4
1	B	108	LEU	5.4
1	A	112	GLN	5.4
2	D	338	ASP	5.3
1	B	136	PHE	5.3
3	E	74	PRO	5.3
1	C	302	LEU	5.3
3	E	127	ALA	5.1
3	E	77	TYR	5.1
1	B	70	ALA	5.1
3	E	102	GLU	5.0
1	A	70	ALA	5.0
1	B	362	ARG	4.9
1	B	111	VAL	4.9
1	A	102	GLU	4.8
1	C	294	MET	4.7
1	C	363	MET	4.7
1	C	245	ASP	4.7
1	A	86	ARG	4.7
3	E	54	GLN	4.7
3	E	76	TYR	4.6
1	B	104	THR	4.5
1	B	112	GLN	4.5
3	E	146	ARG	4.5
3	E	333	HIS	4.5
1	C	311	LEU	4.4
2	D	279	TRP	4.3
1	C	247	ASP	4.3
2	D	277	ARG	4.3
1	A	153	LEU	4.3
1	B	2068	ILE	4.3
1	A	124	LEU	4.3
2	D	317	GLY	4.3
3	E	95	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	4.2
3	E	112	VAL	4.2
1	B	98	ARG	4.2
1	B	133	ARG	4.1
1	C	101	VAL	4.0
1	B	361	PRO	4.0
3	E	79	LEU	4.0
1	A	100	LYS	4.0
3	E	83	LYS	4.0
1	A	89	ASP	3.9
1	B	102	GLU	3.9
2	D	283	ARG	3.9
1	B	86	ARG	3.9
1	B	302	LEU	3.9
3	E	63	ARG	3.9
1	B	113	TYR	3.8
1	B	99	THR	3.8
1	A	367	GLU	3.8
1	A	150	VAL	3.8
1	A	111	VAL	3.8
1	A	99	THR	3.7
2	D	319	SER	3.7
1	B	117	ARG	3.7
1	C	366	PRO	3.6
2	D	334	LYS	3.6
3	E	58	SER	3.6
2	D	275	LYS	3.6
1	C	313	MET	3.5
1	B	149	HIS	3.5
3	E	85	LYS	3.5
3	E	106	LEU	3.5
1	B	244	LEU	3.5
1	B	125	ILE	3.4
2	D	233	LEU	3.4
1	C	4	GLN	3.4
1	B	6	LEU	3.4
1	A	365	LEU	3.4
1	C	307	ALA	3.4
3	E	20	ALA	3.3
2	D	318	GLN	3.3
3	E	51	GLN	3.3
1	C	104	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	150	ARG	3.3
1	B	229	ASP	3.3
1	B	114	ALA	3.3
1	C	100	LYS	3.3
1	A	117	ARG	3.3
1	A	138	ALA	3.3
1	B	115	PRO	3.2
2	D	2	ILE	3.2
2	D	330	LEU	3.2
1	B	87	PHE	3.2
1	A	159	PRO	3.1
1	A	134	HIS	3.1
2	D	320	VAL	3.1
2	D	227	LYS	3.1
1	A	60	LYS	3.1
1	C	314	ARG	3.1
1	A	81	GLU	3.1
1	C	299	PRO	3.1
1	A	235	GLN	3.1
3	E	84	GLY	3.0
1	B	301	ALA	3.0
1	A	149	HIS	3.0
1	A	140	LEU	3.0
1	C	298	SER	3.0
1	C	304	ASN	3.0
3	E	129	LEU	3.0
1	A	4	GLN	2.9
1	C	98	ARG	2.9
1	B	107	LEU	2.9
1	B	132	SER	2.9
1	A	98	ARG	2.9
1	A	161	LYS	2.8
1	A	139	LEU	2.8
1	A	141	LYS	2.8
2	D	336	LEU	2.8
3	E	113	TRP	2.8
1	C	274	ARG	2.8
1	A	115	PRO	2.8
1	A	85	GLY	2.8
1	B	2036	ARG	2.8
1	A	175	LEU	2.7
1	C	367	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	56	HIS	2.7
1	B	105	ARG	2.7
1	C	205	LEU	2.7
1	B	93	ILE	2.7
3	E	132	LEU	2.7
3	E	126	ASN	2.7
1	B	144	GLU	2.7
1	B	148	GLU	2.7
3	E	46	ARG	2.7
1	C	365	LEU	2.7
3	E	133	GLU	2.7
1	A	80	ARG	2.7
1	A	47	ARG	2.7
1	B	2025	LEU	2.6
3	E	224	VAL	2.6
1	A	123	TYR	2.6
1	A	109	ASP	2.6
1	C	246	ASP	2.6
1	A	82	ILE	2.6
1	C	291	ARG	2.6
2	D	223	MET	2.6
1	C	102	GLU	2.6
1	B	153	LEU	2.6
1	A	15	PHE	2.6
1	C	249	ALA	2.6
1	A	107	LEU	2.6
3	E	115	THR	2.6
1	B	2037	ILE	2.6
1	B	152	PHE	2.5
3	E	110	LYS	2.5
1	A	305	ASP	2.5
2	D	222	LEU	2.5
3	E	60	GLY	2.5
1	C	305	ASP	2.5
1	B	131	LEU	2.5
1	A	169	ARG	2.5
3	E	1	MET	2.5
3	E	334	LEU	2.5
1	B	116	ALA	2.5
3	E	123	ALA	2.5
1	A	151	LYS	2.5
1	B	97	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	130	MET	2.4
1	A	27	ALA	2.4
3	E	66	GLN	2.4
1	A	143	LEU	2.4
1	A	167	LEU	2.4
1	C	263	ARG	2.4
1	B	306	MET	2.4
1	C	3	TYR	2.4
1	A	120	PHE	2.4
1	C	368	PRO	2.4
1	A	96	ALA	2.4
3	E	99	LYS	2.4
1	B	154	LEU	2.3
1	B	214	LEU	2.3
1	A	164	VAL	2.3
1	B	165	THR	2.3
1	A	131	LEU	2.3
3	E	130	LYS	2.3
3	E	91	ASP	2.3
3	E	87	THR	2.3
1	A	163	PRO	2.3
1	A	105	ARG	2.3
3	E	73	HIS	2.3
1	A	68	ILE	2.3
1	B	169	ARG	2.3
1	B	139	LEU	2.3
1	B	166	ILE	2.3
2	D	236	LEU	2.3
1	B	141	LYS	2.3
2	D	10	ARG	2.2
1	A	114	ALA	2.2
1	B	176	LYS	2.2
1	C	320	ILE	2.2
3	E	81	PRO	2.2
2	D	228	ARG	2.2
3	E	94	ARG	2.2
2	D	211	HIS	2.2
2	D	270	ARG	2.2
1	C	260	ASN	2.2
1	A	38	HIS	2.2
1	B	96	ALA	2.2
2	D	284	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	71	GLY	2.2
3	E	307	ASN	2.2
1	A	214	LEU	2.1
1	C	37	ILE	2.1
3	E	124	ALA	2.1
1	A	156	THR	2.1
1	C	301	ALA	2.1
1	C	237	VAL	2.1
3	E	170	GLN	2.1
1	B	128	VAL	2.1
1	B	304	ASN	2.1
2	D	309	GLU	2.1
1	C	23	HIS	2.1
1	A	201	ARG	2.1
1	B	2019	VAL	2.1
1	C	318	ARG	2.1
2	D	239	GLU	2.1
1	B	4	GLN	2.0
1	A	136	PHE	2.0
3	E	141	PHE	2.0
1	A	23	HIS	2.0
1	C	330	GLN	2.0
2	D	298	LEU	2.0
2	D	312	LEU	2.0
1	A	125	ILE	2.0
1	A	7	ALA	2.0
1	A	121	LYS	2.0
2	D	269	LEU	2.0
1	C	362	ARG	2.0
2	D	315	ASP	2.0
1	A	113	TYR	2.0
2	D	327	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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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
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

There are no such residues in this entry.