



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:26 pm GMT

PDB ID : 4N4R  
Title : Structure basis of lipopolysaccharide biogenesis  
Authors : Dong, H.; Xiang, Q.; Wang, Z.; Paterson, N.G.; He, C.; Zhang, Y.; Wang, W.;  
Dong, C.  
Deposited on : 2013-10-08  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

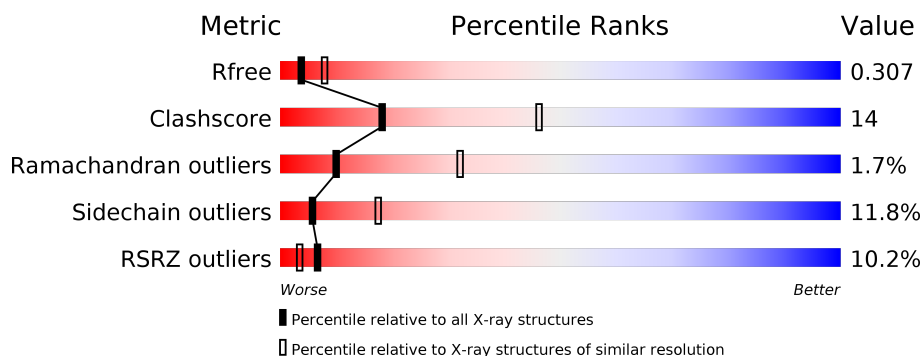
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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  $\geq 3$ , 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	786	<div> <div>5%</div> <div>47%</div> <div>17%</div> <div>• •</div> <div>32%</div> </div>
1	C	786	<div> <div>8%</div> <div>48%</div> <div>15%</div> <div>•</div> <div>32%</div> </div>
2	B	196	<div> <div>12%</div> <div>48%</div> <div>21%</div> <div>7%</div> <div>•</div> <div>23%</div> </div>
2	D	196	<div> <div>5%</div> <div>54%</div> <div>20%</div> <div>•</div> <div>23%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CAC	A	801	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11117 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.

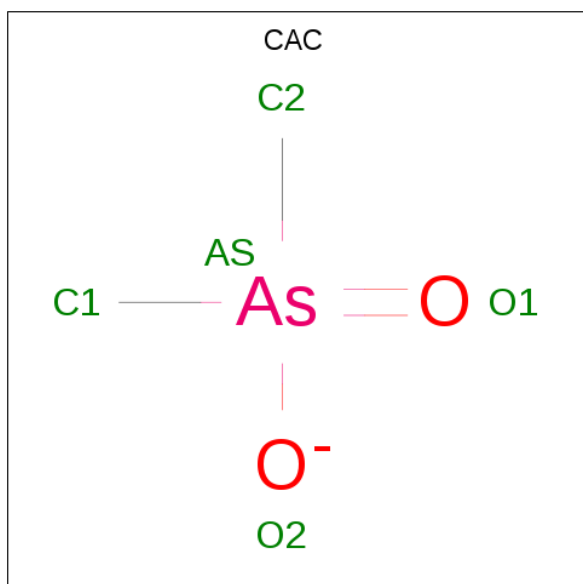
- Molecule 1 is a protein called LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	Se	0	0	0
			4370	2765	741	850	1	13			
1	C	533	Total	C	N	O	S	Se	0	0	0
			4373	2765	742	853	1	13			

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	151	Total	C	N	O	S	Se	0	0	0
			1176	731	209	228	1	7			
2	D	151	Total	C	N	O	S	Se	0	0	0
			1176	731	209	228	1	7			

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	As	C	O	0	0
			5	1	2	2		
3	C	1	Total	As	C	O	0	0
			5	1	2	2		

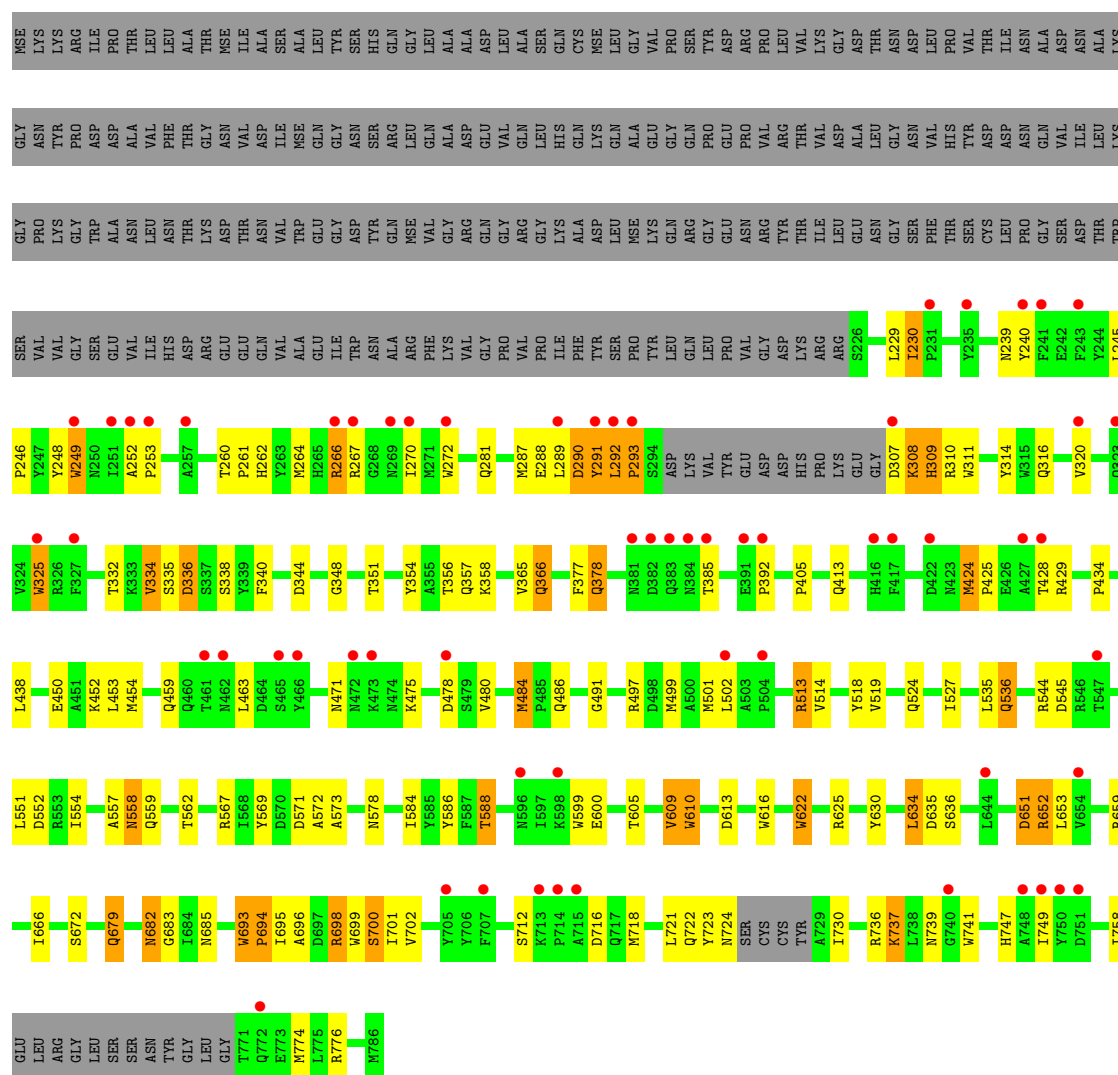
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

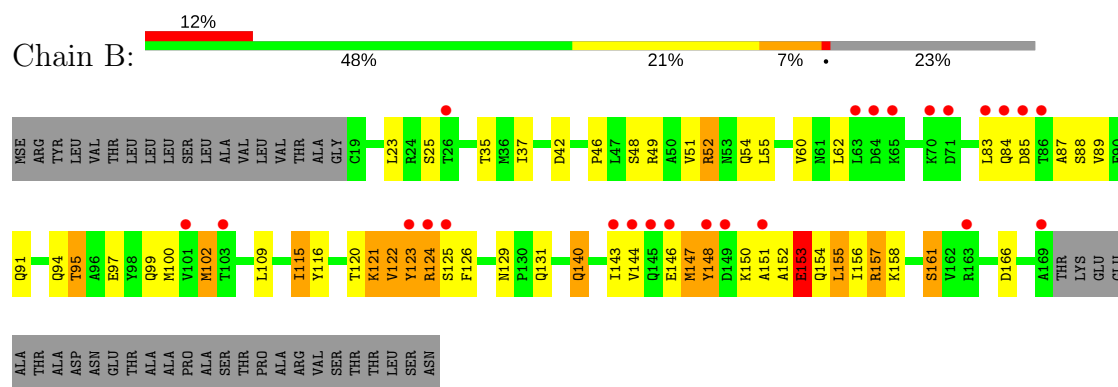
- Molecule 5 is water.

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



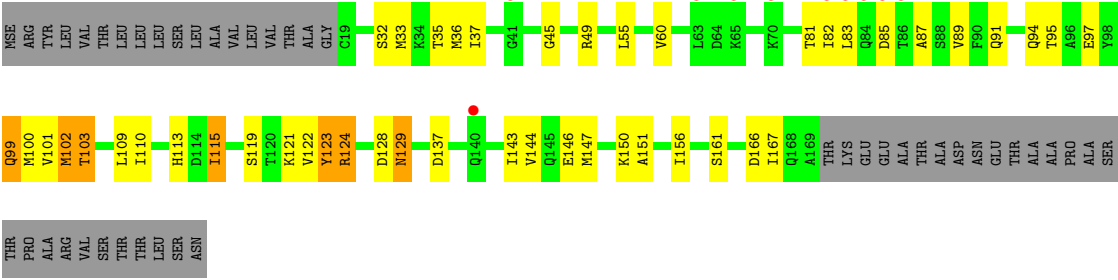


• Molecule 2: LPS-assembly lipoprotein LptE



• Molecule 2: LPS-assembly lipoprotein LptE







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.43Å 76.08Å 213.60Å 90.00° 111.52° 90.00°	Depositor
Resolution (Å)	107.49 – 2.80 43.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (107.49-2.80) 100.0 (43.92-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.285 , 0.305 0.286 , 0.307	Depositor DCC
$R_{free}$ test set	3253 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.96	24/4475 (0.5%)	0.91	11/6062 (0.2%)
1	C	0.67	8/4478 (0.2%)	0.76	2/6067 (0.0%)
2	B	1.36	10/1186 (0.8%)	1.14	8/1597 (0.5%)
2	D	0.84	1/1186 (0.1%)	0.94	1/1597 (0.1%)
All	All	0.90	43/11325 (0.4%)	0.88	22/15323 (0.1%)

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

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	TYR	CE1-CZ	20.71	1.65	1.38
2	B	122	VAL	CA-CB	11.37	1.78	1.54
1	A	578	ASN	CA-CB	10.72	1.81	1.53
1	A	625	ARG	CG-CD	9.03	1.74	1.51
1	A	645	GLU	CD-OE2	8.83	1.35	1.25
1	A	613	ASP	CA-CB	8.34	1.72	1.53
2	B	125	SER	CA-CB	8.06	1.65	1.52
2	B	153	GLU	CD-OE1	7.73	1.34	1.25
1	A	364	ALA	CA-CB	6.97	1.67	1.52
1	A	324	VAL	CA-CB	6.84	1.69	1.54
1	A	614	THR	CA-CB	6.68	1.70	1.53
2	D	123	TYR	CE1-CZ	6.30	1.46	1.38
1	A	615	TYR	CG-CD1	-6.23	1.31	1.39
1	C	610	TRP	CD2-CE2	6.22	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	148	TYR	CE1-CZ	-6.16	1.30	1.38
2	B	102	MSE	CG-SE	6.11	2.16	1.95
1	A	315	TRP	CD2-CE2	6.03	1.48	1.41
1	A	369	ASP	CA-CB	6.00	1.67	1.53
2	B	146	GLU	CD-OE1	5.93	1.32	1.25
1	A	691	ALA	CA-CB	5.74	1.64	1.52
1	A	539	TYR	CG-CD2	-5.65	1.31	1.39
1	A	615	TYR	CB-CG	-5.62	1.43	1.51
1	A	693	TRP	CD2-CE2	5.61	1.48	1.41
2	B	123	TYR	CG-CD2	5.55	1.46	1.39
1	A	643	SER	CB-OG	5.46	1.49	1.42
1	C	616	TRP	CD2-CE2	5.43	1.47	1.41
1	A	444	TRP	CD2-CE2	5.38	1.47	1.41
1	C	622	TRP	CD2-CE2	5.30	1.47	1.41
1	C	325	TRP	CD2-CE2	5.29	1.47	1.41
1	C	599	TRP	CD2-CE2	5.27	1.47	1.41
1	A	622	TRP	CD2-CE2	5.26	1.47	1.41
2	B	48	SER	N-CA	5.25	1.56	1.46
1	A	272	TRP	CD2-CE2	5.22	1.47	1.41
1	A	249	TRP	CD2-CE2	5.17	1.47	1.41
1	A	693	TRP	NE1-CE2	-5.15	1.30	1.37
2	B	121	LYS	CA-CB	5.14	1.65	1.53
1	C	693	TRP	CD2-CE2	5.13	1.47	1.41
1	C	249	TRP	CD2-CE2	5.12	1.47	1.41
1	A	599	TRP	CD2-CE2	5.12	1.47	1.41
1	A	693	TRP	CZ2-CH2	5.11	1.47	1.37
1	A	580	SER	CB-OG	5.10	1.48	1.42
1	C	569	TYR	CE1-CZ	-5.07	1.31	1.38
1	A	363	TYR	CE1-CZ	5.00	1.45	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	ARG	NE-CZ-NH2	-9.54	115.53	120.30
2	B	166	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	613	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	A	625	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	B	102	MSE	CB-CA-C	7.36	125.12	110.40
1	A	567	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	A	625	ARG	CG-CD-NE	-7.12	96.84	111.80
1	A	651	ASP	CB-CA-C	6.18	122.76	110.40
2	B	102	MSE	N-CA-C	-6.11	94.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	166	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	613	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	146	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	A	538	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	B	147	MSE	CB-CG-SE	-5.53	96.11	112.70
1	A	463	LEU	CA-CB-CG	5.40	127.71	115.30
2	B	157	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	634	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	510	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	C	513	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	634	LEU	CA-CB-CG	5.08	126.98	115.30
2	B	42	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	155	LEU	CB-CG-CD1	-5.07	102.38	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	ARG	Sidechain

## 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	4370	0	4073	124	0
1	C	4373	0	4075	117	0
2	B	1176	0	1186	55	0
2	D	1176	0	1186	37	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	0	0
5	C	5	0	0	0	0
5	D	1	0	0	0	0
All	All	11117	0	10520	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (311) 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:A:625:ARG:CG	1:A:625:ARG:CD	1.74	1.63
1:A:578:ASN:CA	1:A:578:ASN:CB	1.81	1.59
2:B:122:VAL:CA	2:B:122:VAL:CB	1.78	1.59
2:B:102:MSE:CG	2:B:102:MSE:SE	2.16	1.43
2:B:147:MSE:CE	2:B:147:MSE:SE	2.18	1.40
1:C:699:TRP:CE2	1:C:723:TYR:CD1	2.18	1.31
1:C:699:TRP:CE2	1:C:723:TYR:HD1	1.49	1.29
1:A:291:TYR:OH	1:A:309:HIS:HD2	1.18	1.25
1:A:291:TYR:OH	1:A:309:HIS:CD2	1.90	1.24
1:A:291:TYR:CD2	1:A:311:TRP:HB3	1.77	1.19
1:A:290:ASP:HB2	1:A:312:LEU:H	1.07	1.15
1:A:291:TYR:HD2	1:A:311:TRP:HB3	1.06	1.11
1:A:271:MSE:CE	1:A:292:LEU:HD13	1.81	1.06
1:A:272:TRP:HB2	1:A:291:TYR:O	1.54	1.05
1:A:271:MSE:HG3	1:A:292:LEU:HB2	1.34	1.04
1:C:699:TRP:CZ2	1:C:723:TYR:CD1	2.46	1.03
1:A:290:ASP:OD2	1:A:339:TYR:OH	1.75	1.03
1:C:699:TRP:NE1	1:C:723:TYR:CE1	2.28	1.02
1:A:290:ASP:HB2	1:A:312:LEU:N	1.76	1.01
1:C:700:SER:OG	1:C:722:GLN:HG2	1.60	1.00
1:C:308:LYS:H	1:C:308:LYS:HD2	1.25	1.00
1:C:699:TRP:NE1	1:C:723:TYR:CD1	2.32	0.96
1:C:291:TYR:CZ	1:C:309:HIS:HA	2.03	0.93
1:A:290:ASP:CB	1:A:312:LEU:H	1.82	0.92
1:A:308:LYS:O	1:A:309:HIS:HB2	1.68	0.92
2:B:84:GLN:OE1	2:B:100:MSE:HE3	1.69	0.92
1:C:699:TRP:HE1	1:C:723:TYR:HE1	1.17	0.90
1:C:700:SER:OG	1:C:722:GLN:CG	2.20	0.89
1:A:625:ARG:CG	1:A:625:ARG:NE	2.37	0.87
1:A:291:TYR:HE2	1:A:311:TRP:CD1	1.94	0.86
1:A:625:ARG:NH1	2:B:123:TYR:CZ	2.44	0.85
1:C:291:TYR:HB3	1:C:311:TRP:HB3	1.56	0.85
1:C:310:ARG:HA	1:C:335:SER:OG	1.80	0.82
2:B:122:VAL:CA	2:B:122:VAL:CG2	2.58	0.82
2:B:54:GLN:HG2	2:B:156:ILE:HD13	1.59	0.81
1:A:271:MSE:HE3	1:A:292:LEU:CD1	2.11	0.80
1:A:271:MSE:CE	1:A:292:LEU:CD1	2.59	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ILE:HG23	1:A:609:VAL:HG13	1.64	0.78
2:B:122:VAL:CA	2:B:122:VAL:CG1	2.61	0.78
1:A:271:MSE:HE3	1:A:292:LEU:HD13	1.65	0.78
2:B:102:MSE:HE1	2:B:148:TYR:CE1	2.20	0.76
1:A:514:VAL:HG12	1:A:562:THR:HG22	1.67	0.76
1:C:699:TRP:NE1	1:C:723:TYR:HE1	1.77	0.76
2:B:54:GLN:HG2	2:B:156:ILE:CD1	2.16	0.75
1:C:698:ARG:O	1:C:724:ASN:N	2.19	0.74
2:B:150:LYS:HE2	2:B:154:GLN:NE2	2.02	0.74
1:A:292:LEU:CD2	1:A:310:ARG:HB2	2.18	0.74
1:C:291:TYR:OH	1:C:309:HIS:HA	1.87	0.73
1:A:291:TYR:HH	1:A:309:HIS:HD2	1.33	0.73
1:A:291:TYR:CE2	1:A:311:TRP:CD1	2.77	0.73
2:B:156:ILE:HD12	2:B:156:ILE:N	2.04	0.72
1:A:292:LEU:HD23	1:A:310:ARG:HB2	1.71	0.71
1:A:651:ASP:OD1	1:A:651:ASP:O	2.08	0.71
1:C:289:LEU:HD13	1:C:289:LEU:O	1.91	0.70
1:C:292:LEU:HD22	1:C:293:PRO:HA	1.74	0.70
1:A:572:ALA:O	1:A:573:ALA:HB3	1.92	0.69
1:C:514:VAL:HG12	1:C:562:THR:HG22	1.74	0.69
1:C:308:LYS:H	1:C:308:LYS:CD	2.05	0.68
1:A:351:THR:O	2:B:95:THR:HG22	1.94	0.68
1:C:584:ILE:HG23	1:C:609:VAL:HG13	1.74	0.68
1:A:291:TYR:HE2	1:A:311:TRP:HD1	1.36	0.68
2:B:122:VAL:CB	2:B:122:VAL:HA	2.13	0.67
2:D:103:THR:HB	2:D:121:LYS:HG2	1.77	0.67
1:C:651:ASP:O	1:C:651:ASP:OD1	2.13	0.67
1:C:699:TRP:CD2	1:C:723:TYR:HD1	2.10	0.67
1:A:272:TRP:CB	1:A:291:TYR:O	2.40	0.67
1:A:730:ILE:HG22	1:A:758:ILE:HG22	1.75	0.67
1:C:699:TRP:CE2	1:C:723:TYR:CE1	2.76	0.66
1:C:291:TYR:CE2	1:C:309:HIS:HB2	2.30	0.66
1:C:291:TYR:HH	1:C:309:HIS:HA	1.60	0.66
1:A:288:GLU:HB3	1:A:314:TYR:HB3	1.78	0.66
1:A:314:TYR:OH	1:A:316:GLN:HG2	1.96	0.66
1:A:271:MSE:HG3	1:A:292:LEU:CB	2.08	0.65
1:C:586:TYR:O	1:C:605:THR:OG1	2.13	0.65
1:C:291:TYR:HE2	1:C:309:HIS:HB2	1.62	0.65
1:A:291:TYR:CE2	1:A:311:TRP:HB3	2.31	0.65
2:D:102:MSE:HB3	2:D:122:VAL:HB	1.78	0.65
1:A:722:GLN:HB2	1:A:730:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ILE:O	2:B:147:MSE:HG3	1.98	0.64
1:C:572:ALA:O	1:C:573:ALA:HB3	1.97	0.63
1:C:310:ARG:HA	1:C:335:SER:HG	1.62	0.63
1:C:311:TRP:H	1:C:335:SER:HB3	1.63	0.63
2:D:87:ALA:HB2	2:D:99:GLN:HB2	1.81	0.63
1:A:290:ASP:CG	1:A:312:LEU:HB3	2.19	0.63
2:D:124:ARG:HH11	2:D:143:ILE:HG23	1.63	0.63
1:A:454:MSE:HE2	1:A:486:GLN:HB2	1.81	0.61
1:A:578:ASN:CB	1:A:578:ASN:C	2.67	0.61
1:C:288:GLU:HB3	1:C:314:TYR:HB3	1.82	0.61
1:C:292:LEU:CD2	1:C:293:PRO:HA	2.30	0.61
1:A:291:TYR:CD2	1:A:311:TRP:CB	2.70	0.61
1:C:272:TRP:O	1:C:290:ASP:HA	2.01	0.61
1:A:292:LEU:HB3	1:A:310:ARG:O	2.00	0.60
1:A:625:ARG:CB	1:A:625:ARG:CD	2.73	0.60
2:B:150:LYS:HE2	2:B:154:GLN:HE22	1.64	0.60
1:A:482:ARG:NH2	1:A:551:LEU:O	2.30	0.60
2:B:156:ILE:HD12	2:B:156:ILE:H	1.67	0.60
2:B:55:LEU:HD13	2:B:62:LEU:HD21	1.84	0.60
1:A:271:MSE:HE2	1:A:292:LEU:HD22	1.83	0.60
1:C:334:VAL:H	1:C:378:GLN:HE22	1.50	0.59
1:C:730:ILE:HG22	1:C:758:ILE:CG2	2.32	0.59
1:A:290:ASP:HB2	1:A:312:LEU:CA	2.32	0.59
1:C:308:LYS:N	1:C:308:LYS:HD2	2.06	0.59
2:B:54:GLN:HG2	2:B:153:GLU:HA	1.84	0.59
1:A:776:ARG:NH1	2:B:85:ASP:OD2	2.36	0.59
1:A:499:MSE:HE2	1:A:508:GLN:HB2	1.86	0.58
1:C:229:LEU:HD11	1:C:248:TYR:HB2	1.85	0.58
2:D:102:MSE:O	2:D:121:LYS:HA	2.03	0.58
2:B:121:LYS:HB3	2:B:123:TYR:HE1	1.67	0.58
1:C:310:ARG:HD2	1:C:336:ASP:OD1	2.04	0.57
1:A:652:ARG:HG2	1:A:693:TRP:CZ3	2.39	0.57
2:D:87:ALA:HB2	2:D:99:GLN:CB	2.34	0.57
1:C:730:ILE:HG22	1:C:758:ILE:HG22	1.85	0.57
1:A:291:TYR:HA	1:A:292:LEU:C	2.24	0.57
1:C:245:LEU:O	1:C:261:PRO:HD2	2.04	0.56
2:B:124:ARG:HB2	2:B:147:MSE:HE3	1.86	0.56
1:A:711:SER:HB2	2:B:91:GLN:OE1	2.06	0.56
1:A:245:LEU:O	1:A:261:PRO:HD2	2.05	0.56
1:A:728:TYR:O	1:A:729:ALA:HB3	2.05	0.55
1:C:776:ARG:NH1	2:D:85:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:ARG:NH1	2:D:143:ILE:HG23	2.20	0.55
1:C:354:TYR:HE1	2:D:128:ASP:OD2	1.89	0.55
1:A:290:ASP:OD2	1:A:312:LEU:HB3	2.06	0.54
1:A:365:VAL:O	2:B:49:ARG:NH2	2.41	0.54
2:D:124:ARG:HB2	2:D:147:MSE:HE3	1.90	0.54
1:A:229:LEU:HD11	1:A:248:TYR:HB2	1.88	0.54
1:A:491:GLY:O	1:A:513:ARG:HG3	2.08	0.54
1:A:291:TYR:HH	1:A:309:HIS:CD2	2.14	0.54
1:A:368:PHE:CZ	1:A:370:ALA:HB2	2.43	0.54
2:B:140:GLN:O	2:B:144:VAL:HG23	2.07	0.54
1:C:700:SER:OG	1:C:722:GLN:HG3	2.04	0.54
1:C:291:TYR:CE2	1:C:309:HIS:HA	2.42	0.53
1:A:271:MSE:HE3	1:A:292:LEU:HD11	1.89	0.53
1:C:544:ARG:HH12	2:D:124:ARG:HH22	1.56	0.53
1:A:730:ILE:HG22	1:A:758:ILE:CG2	2.38	0.53
1:C:519:VAL:HG12	1:C:557:ALA:HB3	1.89	0.53
1:A:246:PRO:HA	1:A:260:THR:HB	1.91	0.53
1:A:723:TYR:HB3	1:A:730:ILE:HG13	1.90	0.53
1:C:776:ARG:HH12	2:D:85:ASP:CG	2.11	0.53
1:C:246:PRO:HA	1:C:260:THR:HB	1.91	0.53
1:A:567:ARG:NH1	2:B:157:ARG:NH1	2.57	0.53
1:A:694:PRO:O	1:A:696:ALA:N	2.43	0.52
1:A:723:TYR:O	1:A:724:ASN:HB2	2.08	0.52
2:B:153:GLU:HA	2:B:156:ILE:HD13	1.90	0.52
2:B:87:ALA:HB2	2:B:99:GLN:HB2	1.92	0.52
1:C:310:ARG:HA	1:C:335:SER:CB	2.39	0.52
1:A:518:TYR:HA	1:A:557:ALA:O	2.08	0.52
2:B:122:VAL:HG11	2:B:151:ALA:HB2	1.90	0.52
1:A:356:THR:HG23	1:A:377:PHE:CE1	2.45	0.52
1:C:314:TYR:OH	1:C:316:GLN:HG2	2.10	0.51
1:A:572:ALA:O	1:A:573:ALA:CB	2.55	0.51
1:A:291:TYR:HA	1:A:292:LEU:CB	2.40	0.51
2:B:102:MSE:HE1	2:B:148:TYR:CD1	2.45	0.51
1:C:291:TYR:CE2	1:C:309:HIS:CB	2.93	0.51
1:C:454:MSE:HE2	1:C:486:GLN:HB2	1.91	0.51
1:A:514:VAL:CG1	1:A:562:THR:HG22	2.40	0.51
1:C:625:ARG:NH1	2:D:123:TYR:CZ	2.79	0.51
2:D:143:ILE:O	2:D:147:MSE:HG3	2.11	0.51
1:C:702:VAL:HG21	1:C:774:MSE:HB3	1.92	0.50
1:A:290:ASP:O	1:A:311:TRP:HB2	2.12	0.50
2:B:156:ILE:CD1	2:B:156:ILE:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LYS:HB3	2:B:123:TYR:CE1	2.46	0.50
1:C:239:ASN:HB3	1:C:264:MSE:HB3	1.94	0.50
2:D:45:GLY:O	2:D:49:ARG:HG3	2.12	0.49
1:A:723:TYR:O	1:A:729:ALA:HA	2.11	0.49
1:C:310:ARG:HD2	1:C:336:ASP:CG	2.33	0.49
1:A:424:MSE:HG3	1:A:425:PRO:HD2	1.94	0.49
1:C:666:ILE:HG13	1:C:683:GLY:HA2	1.95	0.49
1:C:544:ARG:HH12	2:D:124:ARG:NH2	2.11	0.49
1:A:647:ARG:HB3	1:A:786:MSE:HE2	1.95	0.49
1:C:652:ARG:HG2	1:C:693:TRP:CZ3	2.48	0.49
1:A:290:ASP:CB	1:A:312:LEU:N	2.57	0.49
1:C:291:TYR:OH	1:C:308:LYS:O	2.31	0.49
2:D:110:ILE:O	2:D:113:HIS:HB2	2.12	0.48
1:A:239:ASN:HB3	1:A:264:MSE:HB3	1.95	0.48
2:B:54:GLN:NE2	2:B:153:GLU:HB3	2.27	0.48
1:A:486:GLN:HG3	1:A:519:VAL:HB	1.94	0.48
1:A:723:TYR:CB	1:A:730:ILE:HG13	2.42	0.48
2:B:102:MSE:HB3	2:B:122:VAL:HG13	1.96	0.48
2:B:46:PRO:HG2	2:B:148:TYR:CZ	2.48	0.48
1:C:434:PRO:HD2	1:C:453:LEU:O	2.13	0.48
1:A:781:PRO:HD2	2:B:85:ASP:HB3	1.96	0.48
1:A:434:PRO:HD2	1:A:453:LEU:O	2.14	0.48
1:C:518:TYR:HA	1:C:557:ALA:O	2.14	0.48
2:D:55:LEU:O	2:D:60:VAL:HB	2.14	0.48
1:A:480:VAL:HG21	1:A:527:ILE:HG22	1.95	0.48
1:C:424:MSE:HG3	1:C:425:PRO:CD	2.43	0.48
1:A:240:TYR:CD2	1:A:266:ARG:HB2	2.49	0.47
2:B:115:ILE:C	2:B:116:TYR:HD1	2.17	0.47
1:C:291:TYR:CE2	1:C:309:HIS:CA	2.97	0.47
1:C:698:ARG:HG2	1:C:699:TRP:CD1	2.48	0.47
1:A:578:ASN:CA	1:A:578:ASN:CG	2.70	0.47
1:A:584:ILE:CG2	1:A:609:VAL:HG13	2.40	0.47
1:A:666:ILE:HG13	1:A:683:GLY:HA2	1.97	0.47
2:B:140:GLN:HA	2:B:143:ILE:HD12	1.95	0.47
1:A:230:ILE:HB	1:A:758:ILE:CD1	2.45	0.47
1:A:240:TYR:HD2	1:A:266:ARG:HB2	1.80	0.47
1:A:610:TRP:HB2	1:A:630:TYR:HB3	1.96	0.47
2:B:156:ILE:H	2:B:156:ILE:CD1	2.25	0.47
1:A:310:ARG:NH1	1:A:336:ASP:OD1	2.37	0.47
1:A:291:TYR:CG	1:A:292:LEU:C	2.88	0.47
2:B:54:GLN:CG	2:B:153:GLU:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ARG:HG3	1:C:723:TYR:CE1	2.50	0.47
2:B:124:ARG:HH11	2:B:124:ARG:HG2	1.80	0.47
2:B:152:ALA:O	2:B:156:ILE:CD1	2.63	0.47
1:C:365:VAL:O	1:C:366:GLN:C	2.54	0.47
1:C:679:GLN:HG3	1:C:741:TRP:CE2	2.50	0.47
1:A:567:ARG:NH1	2:B:157:ARG:HH12	2.13	0.46
1:A:388:TYR:CD1	1:A:419:ASN:ND2	2.84	0.46
1:C:289:LEU:C	1:C:289:LEU:HD13	2.36	0.46
1:C:716:ASP:OD1	1:C:737:LYS:HB3	2.15	0.46
1:A:655:GLN:HG2	1:A:656:LEU:N	2.31	0.46
2:B:148:TYR:O	2:B:152:ALA:HB2	2.16	0.46
1:C:694:PRO:O	1:C:696:ALA:N	2.49	0.46
1:A:424:MSE:HG3	1:A:425:PRO:CD	2.46	0.46
2:B:158:LYS:O	2:B:161:SER:HB2	2.16	0.46
1:C:291:TYR:O	1:C:292:LEU:HG	2.16	0.46
2:D:101:VAL:HG13	2:D:101:VAL:O	2.15	0.46
2:D:167:ILE:HA	2:D:167:ILE:HD13	1.83	0.46
1:A:290:ASP:CB	1:A:312:LEU:HB3	2.46	0.46
1:C:340:PHE:CE1	1:C:348:GLY:HA3	2.51	0.46
2:B:88:SER:OG	2:B:97:GLU:HB2	2.15	0.45
1:C:659:ARG:HH11	2:D:97:GLU:CD	2.19	0.45
1:C:262:HIS:O	1:C:270:ILE:HA	2.16	0.45
1:C:351:THR:O	2:D:95:THR:HG22	2.17	0.45
1:A:260:THR:HG23	1:A:273:GLU:HB2	1.98	0.45
2:D:150:LYS:O	2:D:151:ALA:C	2.54	0.45
2:D:81:THR:HB	2:D:103:THR:HG23	1.99	0.45
1:A:290:ASP:HB2	1:A:312:LEU:HB3	1.99	0.45
1:A:625:ARG:NH1	2:B:123:TYR:CE1	2.85	0.45
1:C:454:MSE:HE3	1:C:484:MSE:HG3	1.98	0.45
1:A:252:ALA:HB1	1:A:253:PRO:CD	2.47	0.45
1:A:290:ASP:O	1:A:291:TYR:HB2	2.17	0.45
1:A:589:GLU:HB3	1:A:604:LYS:HB3	1.98	0.45
1:C:308:LYS:N	1:C:308:LYS:CD	2.75	0.45
1:C:701:ILE:O	1:C:701:ILE:HG23	2.17	0.45
2:D:33:MSE:HG2	2:D:36:MSE:HE3	1.98	0.44
1:C:309:HIS:O	1:C:311:TRP:CD1	2.70	0.44
2:D:82:ILE:HG13	2:D:102:MSE:HE2	1.98	0.44
1:C:290:ASP:N	1:C:290:ASP:OD1	2.49	0.44
1:C:429:ARG:NH1	1:C:552:ASP:OD1	2.51	0.44
1:C:491:GLY:O	1:C:513:ARG:HG3	2.18	0.44
1:A:608:LEU:HA	1:A:632:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ILE:O	2:D:144:VAL:C	2.54	0.44
2:D:82:ILE:CG1	2:D:102:MSE:HE2	2.48	0.44
2:D:100:MSE:N	2:D:124:ARG:O	2.41	0.43
1:A:271:MSE:CG	1:A:292:LEU:HB2	2.26	0.43
1:A:625:ARG:HG3	1:A:785:SER:OG	2.18	0.43
2:D:81:THR:CG2	2:D:83:LEU:HD13	2.48	0.43
1:C:700:SER:O	1:C:721:LEU:HA	2.18	0.43
1:C:551:LEU:HD23	1:C:554:ILE:HD11	2.01	0.43
1:A:519:VAL:HG12	1:A:557:ALA:HB3	1.99	0.43
1:C:572:ALA:O	1:C:573:ALA:CB	2.62	0.43
1:A:728:TYR:HB3	1:A:729:ALA:H	1.74	0.43
1:C:610:TRP:HB2	1:C:630:TYR:HB3	2.00	0.43
1:C:292:LEU:HA	1:C:293:PRO:HA	1.76	0.43
1:C:452:LYS:HB3	1:C:486:GLN:HB3	2.00	0.43
1:C:514:VAL:CG1	1:C:562:THR:HG22	2.44	0.43
1:A:290:ASP:O	1:A:311:TRP:CB	2.67	0.43
1:A:452:LYS:HB3	1:A:486:GLN:HB3	2.00	0.43
2:B:122:VAL:HG23	2:B:150:LYS:HD3	1.99	0.42
1:C:700:SER:HG	1:C:722:GLN:CG	2.28	0.42
1:A:527:ILE:HD11	1:A:552:ASP:O	2.19	0.42
2:B:51:VAL:O	2:B:52:ARG:C	2.56	0.42
2:B:55:LEU:O	2:B:60:VAL:HB	2.19	0.42
1:C:544:ARG:HD3	2:D:146:GLU:OE2	2.19	0.42
1:A:615:TYR:CE1	1:A:625:ARG:NH2	2.88	0.42
1:C:527:ILE:HD11	1:C:552:ASP:O	2.20	0.42
1:A:314:TYR:OH	1:A:316:GLN:HB3	2.20	0.42
1:A:429:ARG:NH1	1:A:552:ASP:OD1	2.52	0.42
1:C:252:ALA:HB1	1:C:253:PRO:CD	2.50	0.42
1:C:252:ALA:HB1	1:C:253:PRO:HD2	2.02	0.42
1:C:291:TYR:HB3	1:C:311:TRP:CB	2.40	0.42
1:C:480:VAL:HG21	1:C:527:ILE:HG22	2.02	0.42
2:B:115:ILE:O	2:B:116:TYR:HD1	2.03	0.42
1:C:659:ARG:NH1	2:D:97:GLU:OE2	2.51	0.42
2:B:131:GLN:OE1	2:B:131:GLN:N	2.53	0.41
1:C:536:GLN:O	1:C:544:ARG:NH2	2.52	0.41
1:A:291:TYR:CA	1:A:292:LEU:C	2.88	0.41
1:C:249:TRP:C	1:C:249:TRP:CD1	2.94	0.41
2:D:129:ASN:C	2:D:129:ASN:HD22	2.21	0.41
1:C:240:TYR:CD2	1:C:266:ARG:HB2	2.55	0.41
1:C:635:ASP:HA	1:C:636:SER:HA	1.73	0.41
2:B:120:THR:O	2:B:121:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:HE2	2:D:137:ASP:OD1	2.20	0.41
1:A:716:ASP:OD1	1:A:737:LYS:HB3	2.21	0.41
1:A:454:MSE:HE3	1:A:484:MSE:HG3	2.03	0.41
1:C:558:ASN:OD1	1:C:588:THR:OG1	2.30	0.41
1:A:499:MSE:CE	1:A:508:GLN:HB2	2.50	0.41
1:A:230:ILE:HB	1:A:758:ILE:HD12	2.03	0.41
1:C:307:ASP:O	1:C:309:HIS:ND1	2.54	0.41
1:A:694:PRO:C	1:A:696:ALA:H	2.23	0.41
1:C:291:TYR:CB	1:C:311:TRP:HB3	2.39	0.41
1:A:271:MSE:HE2	1:A:292:LEU:HD13	1.90	0.41
1:A:635:ASP:HA	1:A:636:SER:HA	1.75	0.41
2:B:124:ARG:NH1	2:B:124:ARG:HG2	2.35	0.41
1:C:230:ILE:HB	1:C:758:ILE:CD1	2.51	0.41
1:A:272:TRP:H	1:A:291:TYR:C	2.23	0.41
1:A:625:ARG:CG	1:A:625:ARG:CZ	2.98	0.41
1:C:486:GLN:HG3	1:C:519:VAL:HB	2.02	0.41
1:C:625:ARG:NH1	2:D:123:TYR:CE1	2.89	0.41
2:D:109:LEU:CD2	2:D:115:ILE:HD11	2.51	0.40
1:C:320:VAL:HA	1:C:325:TRP:O	2.21	0.40
1:C:524:GLN:O	1:C:527:ILE:HG13	2.21	0.40
1:C:682:ASN:ND2	2:D:91:GLN:OE1	2.53	0.40
2:B:109:LEU:HD23	2:B:115:ILE:HG13	2.03	0.40
1:C:240:TYR:HD2	1:C:266:ARG:HB2	1.86	0.40
1:C:314:TYR:OH	1:C:316:GLN:HB3	2.21	0.40
1:C:310:ARG:CA	1:C:335:SER:OG	2.62	0.40
1:C:356:THR:HG23	1:C:377:PHE:CE2	2.56	0.40
1:A:405:PRO:O	1:A:438:LEU:HD13	2.21	0.40
1:C:405:PRO:O	1:C:438:LEU:CD1	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/786 (67%)	470 (90%)	43 (8%)	11 (2%)	8	26
1	C	525/786 (67%)	473 (90%)	42 (8%)	10 (2%)	9	28
2	B	149/196 (76%)	140 (94%)	7 (5%)	2 (1%)	13	40
2	D	149/196 (76%)	141 (95%)	8 (5%)	0	100	100
All	All	1347/1964 (69%)	1224 (91%)	100 (7%)	23 (2%)	10	32

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	A	366	GLN
1	A	695	ILE
1	C	366	GLN
1	C	695	ILE
1	A	291	TYR
1	A	652	ARG
2	B	95	THR
1	C	694	PRO
1	A	685	ASN
1	A	694	PRO
1	A	728	TYR
1	C	291	TYR
1	C	685	ASN
2	B	52	ARG
1	C	293	PRO
1	C	499	MSE
1	C	652	ARG
1	A	573	ALA
1	C	292	LEU
1	A	324	VAL
1	A	392	PRO
1	C	392	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/665 (70%)	413 (88%)	56 (12%)	6	17
1	C	470/665 (71%)	413 (88%)	57 (12%)	5	16
2	B	132/160 (82%)	117 (89%)	15 (11%)	6	19
2	D	132/160 (82%)	118 (89%)	14 (11%)	7	22
All	All	1203/1650 (73%)	1061 (88%)	142 (12%)	6	17

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	A	266	ARG
1	A	267	ARG
1	A	277	ARG
1	A	281	GLN
1	A	287	MSE
1	A	291	TYR
1	A	292	LEU
1	A	308	LYS
1	A	334	VAL
1	A	336	ASP
1	A	338	SER
1	A	344	ASP
1	A	357	GLN
1	A	385	THR
1	A	413	GLN
1	A	424	MSE
1	A	428	THR
1	A	435	THR
1	A	450	GLU
1	A	459	GLN
1	A	463	LEU
1	A	471	ASN
1	A	483	VAL
1	A	484	MSE
1	A	497	ARG
1	A	501	MSE
1	A	502	LEU
1	A	510	LEU
1	A	535	LEU
1	A	536	GLN
1	A	545	ASP
1	A	558	ASN

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Mol	Chain	Res	Type
1	A	567	ARG
1	A	571	ASP
1	A	588	THR
1	A	600	GLU
1	A	609	VAL
1	A	613	ASP
1	A	622	TRP
1	A	634	LEU
1	A	651	ASP
1	A	653	LEU
1	A	669	THR
1	A	672	SER
1	A	679	GLN
1	A	682	ASN
1	A	698	ARG
1	A	712	SER
1	A	718	MSE
1	A	727	CYS
1	A	728	TYR
1	A	737	LYS
1	A	739	ASN
1	A	747	HIS
1	A	749	ILE
2	B	23	LEU
2	B	25	SER
2	B	35	THR
2	B	37	ILE
2	B	83	LEU
2	B	89	VAL
2	B	94	GLN
2	B	115	ILE
2	B	124	ARG
2	B	126	PHE
2	B	129	ASN
2	B	140	GLN
2	B	153	GLU
2	B	155	LEU
2	B	161	SER
1	C	230	ILE
1	C	266	ARG
1	C	267	ARG
1	C	281	GLN

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Mol	Chain	Res	Type
1	C	287	MSE
1	C	290	ASP
1	C	308	LYS
1	C	309	HIS
1	C	332	THR
1	C	334	VAL
1	C	336	ASP
1	C	338	SER
1	C	344	ASP
1	C	357	GLN
1	C	378	GLN
1	C	385	THR
1	C	413	GLN
1	C	424	MSE
1	C	428	THR
1	C	450	GLU
1	C	459	GLN
1	C	463	LEU
1	C	471	ASN
1	C	475	LYS
1	C	478	ASP
1	C	484	MSE
1	C	497	ARG
1	C	501	MSE
1	C	502	LEU
1	C	535	LEU
1	C	536	GLN
1	C	545	ASP
1	C	558	ASN
1	C	559	GLN
1	C	567	ARG
1	C	571	ASP
1	C	578	ASN
1	C	588	THR
1	C	600	GLU
1	C	609	VAL
1	C	613	ASP
1	C	622	TRP
1	C	634	LEU
1	C	651	ASP
1	C	653	LEU
1	C	672	SER

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Mol	Chain	Res	Type
1	C	679	GLN
1	C	682	ASN
1	C	698	ARG
1	C	700	SER
1	C	712	SER
1	C	718	MSE
1	C	736	ARG
1	C	737	LYS
1	C	739	ASN
1	C	747	HIS
1	C	749	ILE
2	D	32	SER
2	D	35	THR
2	D	37	ILE
2	D	89	VAL
2	D	94	GLN
2	D	99	GLN
2	D	102	MSE
2	D	103	THR
2	D	115	ILE
2	D	119	SER
2	D	124	ARG
2	D	129	ASN
2	D	156	ILE
2	D	161	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	281	GLN
1	A	309	HIS
1	A	471	ASN
1	A	486	GLN
1	A	657	ASN
1	A	722	GLN
1	A	724	ASN
2	B	129	ASN
2	B	154	GLN
1	C	281	GLN
1	C	357	GLN
1	C	459	GLN

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Mol	Chain	Res	Type
1	C	471	ASN
1	C	536	GLN
1	C	578	ASN
1	C	739	ASN
1	C	746	GLN
2	D	94	GLN
2	D	129	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
3	CAC	A	801	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	C	801	-	0,4,4	0.00	-	0,6,6	0.00	-

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
3	CAC	A	801	-	-	0/0/0/0	0/0/0/0
3	CAC	C	801	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	519/786 (66%)	0.38	40 (7%) 13 7	60, 111, 159, 201	0
1	C	520/786 (66%)	0.53	61 (11%) 4 2	80, 129, 182, 271	0
2	B	144/196 (73%)	0.92	24 (16%) 1 1	93, 104, 146, 163	0
2	D	144/196 (73%)	0.50	10 (6%) 17 9	70, 98, 131, 145	0
All	All	1327/1964 (67%)	0.51	135 (10%) 7 3	60, 115, 167, 271	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	748	ALA	9.2
1	C	266	ARG	8.8
1	C	749	ILE	8.3
1	C	240	TYR	8.2
1	C	267	ARG	7.3
1	C	428	THR	7.2
1	A	636	SER	7.1
2	B	65	LYS	7.1
1	C	292	LEU	6.3
1	C	253	PRO	6.1
1	A	502	LEU	5.9
2	B	70	LYS	5.4
1	A	384	ASN	5.4
1	A	478	ASP	5.3
1	C	502	LEU	5.2
1	A	229	LEU	5.0
1	C	291	TYR	4.8
1	A	713	LYS	4.8
2	B	26	THR	4.8
1	A	291	TYR	4.6
1	A	772	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	601	ASN	4.4
1	A	635	ASP	4.3
1	C	713	LYS	4.2
1	C	323	GLN	4.1
1	C	251	ILE	4.0
1	A	648	ARG	4.0
1	C	596	ASN	3.9
1	C	422	ASP	3.9
2	D	140	GLN	3.9
1	C	750	TYR	3.9
2	D	84	GLN	3.8
1	A	472	ASN	3.7
1	C	231	PRO	3.7
1	A	290	ASP	3.7
1	C	249	TRP	3.6
1	A	292	LEU	3.6
2	B	163	ARG	3.6
1	C	382	ASP	3.6
1	C	391	GLU	3.6
2	B	169	ALA	3.5
1	C	392	PRO	3.5
2	D	86	THR	3.5
2	B	84	GLN	3.5
1	C	241	PHE	3.4
1	A	610	TRP	3.4
2	D	70	LYS	3.4
1	A	650	GLN	3.3
2	B	64	ASP	3.3
1	A	479	SER	3.2
2	D	63	LEU	3.2
1	C	740	GLY	3.2
1	C	472	ASN	3.2
2	D	65	LYS	3.2
1	C	289	LEU	3.1
1	C	466	TYR	3.1
1	A	378	GLN	3.1
1	A	473	LYS	3.0
1	C	465	SER	3.0
1	A	707	PHE	3.0
1	A	241	PHE	3.0
2	D	82	ILE	3.0
2	D	83	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	707	PHE	2.9
1	C	416	HIS	2.9
1	A	333	LYS	2.9
1	C	461	THR	2.9
1	C	272	TRP	2.9
1	A	621	ARG	2.8
1	A	649	ASP	2.8
2	B	125	SER	2.8
1	A	750	TYR	2.8
1	C	705	TYR	2.8
1	A	335	SER	2.8
2	B	86	THR	2.7
1	C	473	LYS	2.7
2	D	85	ASP	2.7
1	C	235	TYR	2.7
1	A	381	ASN	2.6
2	B	103	THR	2.6
1	A	646	TYR	2.6
1	C	385	THR	2.6
1	C	383	GLN	2.6
1	C	644	LEU	2.5
1	A	714	PRO	2.5
1	C	381	ASN	2.5
2	B	63	LEU	2.5
1	C	462	ASN	2.5
1	A	359	PHE	2.5
1	C	751	ASP	2.5
2	B	83	LEU	2.5
1	A	480	VAL	2.4
1	A	343	PHE	2.4
1	C	547	THR	2.4
1	C	320	VAL	2.4
2	B	143	ILE	2.4
1	C	307	ASP	2.4
1	A	747	HIS	2.4
1	A	380	PHE	2.4
2	B	144	VAL	2.4
1	C	325	TRP	2.4
1	C	714	PRO	2.4
2	B	145	GLN	2.4
1	C	270	ILE	2.4
1	A	651	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	709	THR	2.3
1	C	384	ASN	2.3
1	A	602	ASP	2.3
1	C	478	ASP	2.3
2	B	85	ASP	2.3
1	A	383	GLN	2.3
2	B	101	VAL	2.3
2	B	149	ASP	2.2
2	D	41	GLY	2.2
1	C	327	PHE	2.2
1	A	477	GLU	2.2
1	C	243	PHE	2.2
1	C	252	ALA	2.2
1	C	427	ALA	2.2
1	C	598	LYS	2.2
1	C	257	ALA	2.2
1	A	334	VAL	2.2
1	C	293	PRO	2.2
1	C	269	ASN	2.2
1	C	417	PHE	2.2
1	C	772	GLN	2.1
2	B	151	ALA	2.1
1	C	504	PRO	2.1
2	B	148	TYR	2.1
1	C	654	VAL	2.1
1	C	715	ALA	2.1
2	B	124	ARG	2.0
2	B	123	TYR	2.0
2	B	146	GLU	2.0
2	B	71	ASP	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CAC	A	801	5/5	0.75	0.82	196,198,221,228	0
3	CAC	C	801	5/5	0.84	0.78	189,193,207,217	0
4	ZN	C	802	1/1	0.88	0.05	152,152,152,152	0
4	ZN	A	802	1/1	0.93	0.09	127,127,127,127	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.