



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:11 pm GMT

PDB ID : 2GMH  
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase in Complexed with Ubiquinone  
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.  
Deposited on : 2006-04-06  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

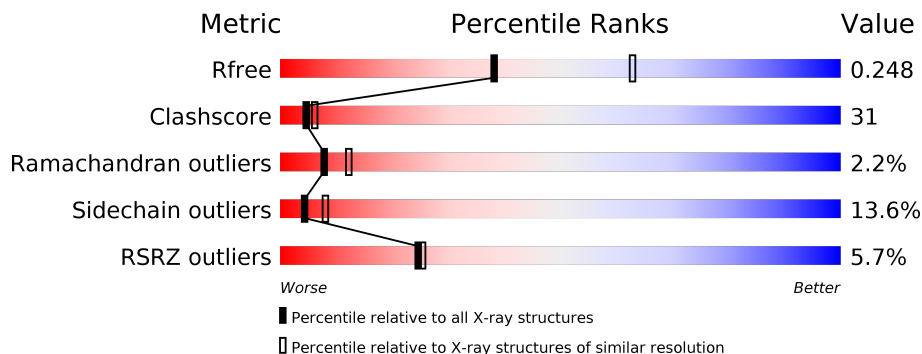
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	584	<div> <div>2%</div> <div>64%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
1	B	584	<div> <div>10%</div> <div>41%</div> <div>47%</div> <div>11%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BHG	A	616	X	-	-	X
2	BHG	A	617	X	-	-	X
2	BHG	B	618	X	-	-	-
6	UQ5	A	612	-	-	-	X
6	UQ5	B	615	-	-	-	X
7	EDO	A	619	-	-	-	X
7	EDO	A	621	-	-	-	X
7	EDO	A	622	-	-	-	X
7	EDO	A	623	-	-	X	X
7	EDO	A	624	-	-	-	X

## 2 Entry composition [i](#)

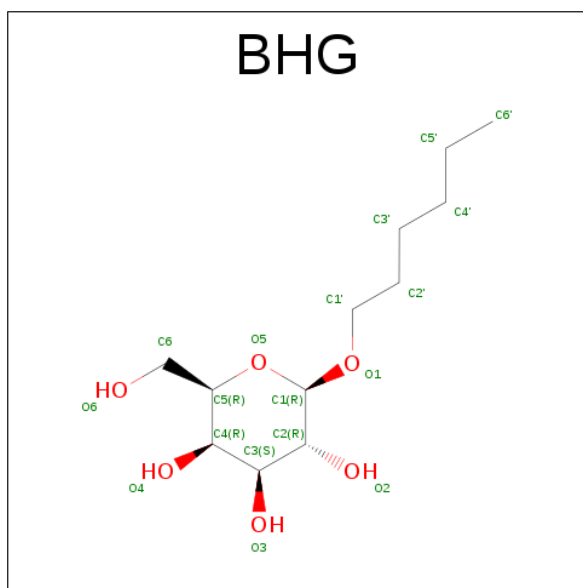
There are 8 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electron transfer flavoprotein-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4558	2910	792	836	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula:  $C_{12}H_{24}O_6$ ).

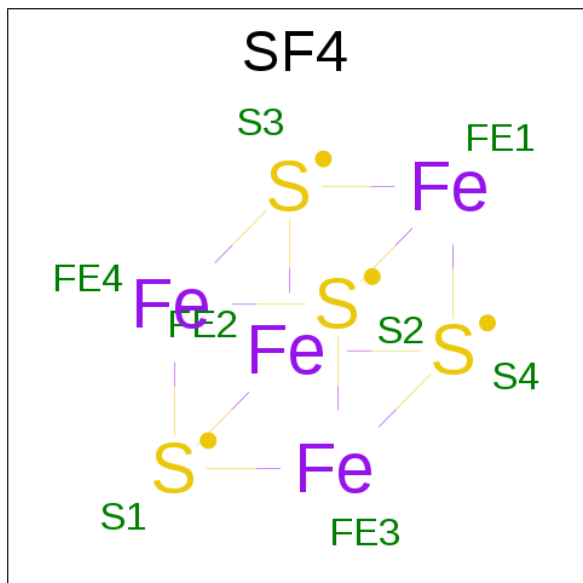


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

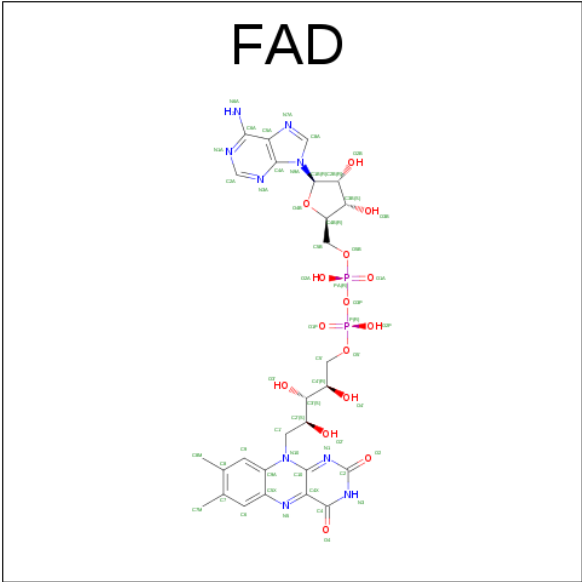
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



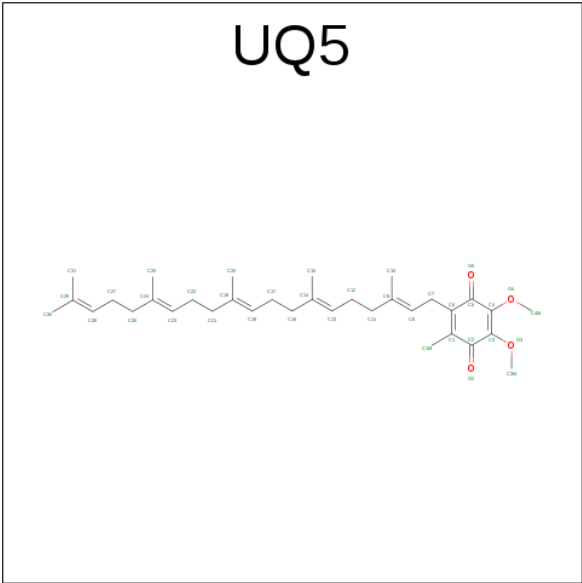
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>4</sub>).



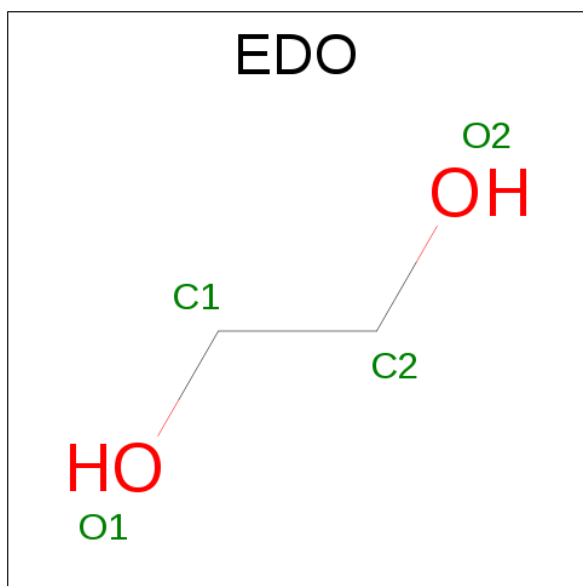
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			38	34	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			38	34	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

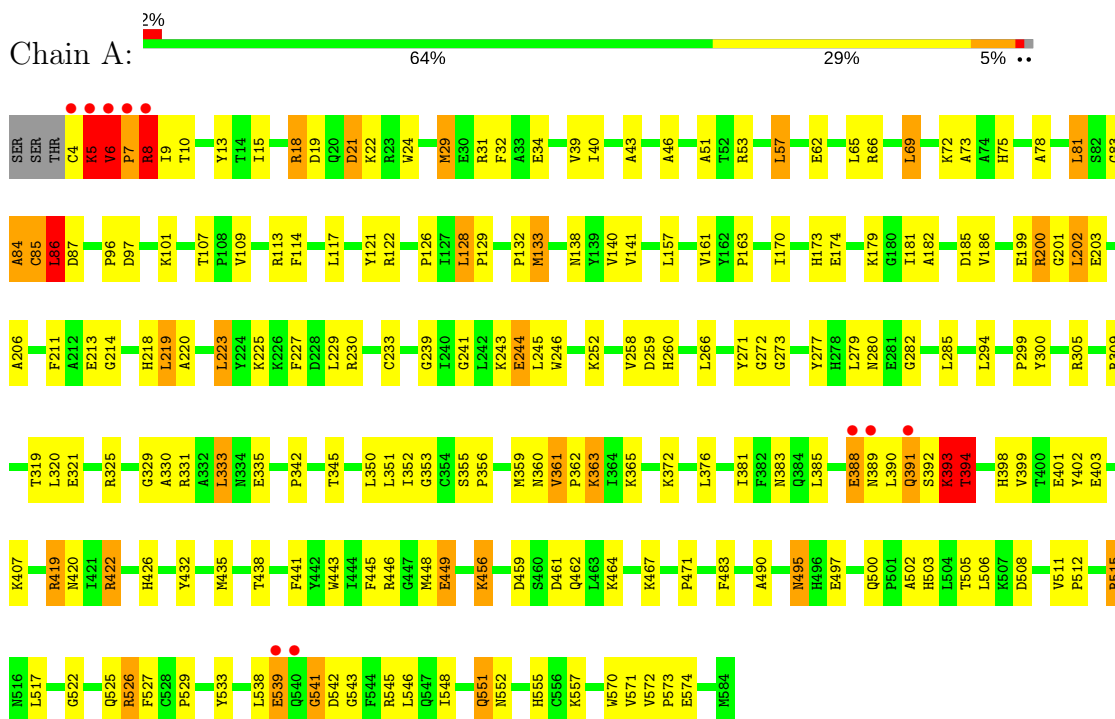
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	301	Total 301	O 301	0	0
8	B	68	Total 68	O 68	0	0



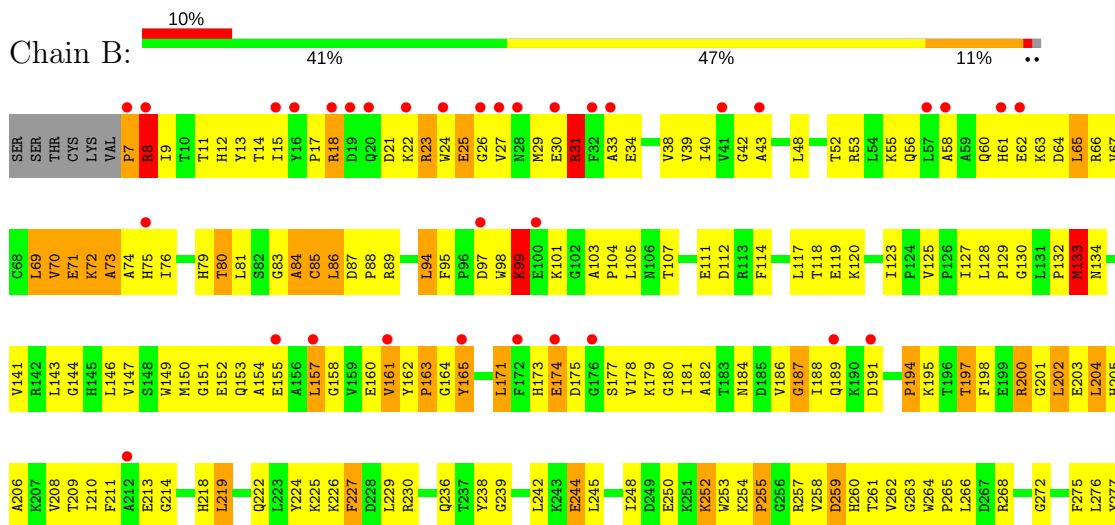
### 3 Residue-property plots

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

- Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase



- Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase



H278	V361	M448	P523
L279	P362	E449	E524
M280		P450	Q525
	K365	W451	R526
L286		T452	P527
L288	H368		V532
G289		K456	
	T375	G457	P535
L294		S458	V536
	E379	D459	P537
P299	S380	S460	L538
Y300	I381	D461	E539
L301	F382	Q462	Q540
S302	N383	L463	G541
	Q384		D542
F304	L385	K467	G543
R305	T386	P471	P544
E306	S387		R545
F307	E388	Y474	L546
	N389	P475	Q547
W310	L390	K476	T548
	Q391		N549
H313	S392	T481	A550
P314	K393	S482	Q551
S315	T394	F483	N552
I316	I395	D484	
K317	G396	L485	H555
P318	L397	L486	C556
T319	H398	S487	K557
L320	V399	S488	
	T400	V489	T561
R325	E401		K562
I326	Y402	T494	
A327	E403	M495	S565
		H496	Q566
R331	K407	E497	
A332		H498	N569
L333	W410	D499	W570
N334		Q500	V571
E335	V418	P501	V572
G336	R419	A502	P573
	M420	H503	E574
S340	I421	L504	G575
I341	R422	T505	
	P423	L506	G578
	V431	K507	P579
L344	Y432	D508	
T345		D509	N584
F346	M435	S510	
P347		V511	
G348	T438	P512	
G349		V513	
L350		N514	
L351	F441	R515	
I352	Y442	N516	
G353		L517	
C354			
S355	F445	D521	
P356	R446	G522	
G357	G447		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.32Å 154.32Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.50 29.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.67-2.50) 98.8 (29.66-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.94 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.254 0.216 , 0.248	Depositor DCC
$R_{free}$ test set	4358 reflections (8.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, EDO, BHG, UQ5, FAD

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	0.59	0/4687	0.96	18/6363 (0.3%)
1	B	0.50	0/4660	0.88	10/6326 (0.2%)
All	All	0.55	0/9347	0.92	28/12689 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	VAL	C-N-CD	-15.72	86.01	120.60
1	A	542	ASP	N-CA-C	9.67	137.11	111.00
1	A	5	LYS	N-CA-C	8.39	133.65	111.00
1	A	6	VAL	C-N-CA	8.38	157.20	122.00
1	A	8	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	B	396	GLY	N-CA-C	-7.82	93.55	113.10
1	A	388	GLU	N-CA-C	-7.63	90.40	111.00
1	A	393	LYS	CA-C-N	-7.17	101.42	117.20
1	A	541	GLY	N-CA-C	6.87	130.27	113.10
1	B	394	THR	N-CA-C	-6.85	92.51	111.00
1	A	83	GLY	N-CA-C	-6.30	97.36	113.10
1	A	393	LYS	C-N-CA	6.17	137.12	121.70
1	A	394	THR	N-CA-C	-5.79	95.38	111.00
1	B	31	ARG	N-CA-C	5.67	126.32	111.00
1	A	6	VAL	N-CA-C	5.67	126.31	111.00
1	A	84	ALA	N-CA-C	5.61	126.15	111.00
1	B	65	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	392	SER	CA-C-N	-5.54	105.02	117.20
1	B	8	ARG	N-CA-C	-5.51	96.13	111.00
1	B	541	GLY	N-CA-C	5.43	126.67	113.10
1	B	163	PRO	N-CA-C	5.36	126.03	112.10
1	B	508	ASP	N-CA-C	-5.22	96.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	SER	N-CA-C	5.16	124.94	111.00
1	B	7	PRO	C-N-CA	5.14	134.55	121.70
1	A	18	ARG	CG-CD-NE	-5.13	101.02	111.80
1	A	85	CYS	N-CA-C	-5.13	97.16	111.00
1	B	73	ALA	N-CA-C	5.11	124.79	111.00
1	A	86	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4558	0	4457	204	0
1	B	4531	0	4424	365	0
2	A	36	0	48	6	0
2	B	18	0	24	0	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	53	0	31	2	0
5	B	53	0	31	4	0
6	A	38	0	50	17	0
6	B	38	0	50	13	0
7	A	36	0	54	18	0
7	B	4	0	6	0	0
8	A	301	0	0	8	0
8	B	68	0	0	5	0
All	All	9751	0	9175	576	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 31.

All (576) 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:38:VAL:HG12	1:B:67:VAL:HG12	1.26	1.13
1:B:55:LYS:HB2	1:B:157:LEU:HD12	1.30	1.08
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.43	1.00
1:B:510:SER:O	1:B:514:ASN:HB2	1.62	0.99
1:B:203:GLU:HG2	1:B:205:HIS:CE1	1.97	0.99
1:B:43:ALA:HB3	1:B:71:GLU:HG2	1.46	0.98
1:B:31:ARG:HE	1:B:200:ARG:NH1	1.61	0.98
1:B:34:GLU:HG3	1:B:66:ARG:HH22	1.28	0.98
1:B:12:HIS:ND1	1:B:14:THR:HG23	1.81	0.95
1:A:345:THR:HG22	1:A:398:HIS:CD2	2.03	0.94
1:B:31:ARG:NE	1:B:200:ARG:HH12	1.64	0.93
1:B:208:VAL:HG13	1:B:349:GLY:HA2	1.48	0.93
1:B:55:LYS:HB2	1:B:157:LEU:CD1	1.99	0.92
1:B:203:GLU:HG2	1:B:205:HIS:HE1	1.34	0.92
1:A:361:VAL:HG21	1:A:422:ARG:HG3	1.53	0.91
1:B:188:ILE:HG22	1:B:189:GLN:N	1.84	0.90
1:B:209:THR:CG2	1:B:211:PHE:HE1	1.84	0.90
1:B:325:ARG:HH12	1:B:488:SER:HA	1.37	0.90
1:B:38:VAL:HG12	1:B:67:VAL:CG1	2.03	0.89
1:A:5:LYS:HD3	1:A:6:VAL:HG12	1.53	0.89
1:B:325:ARG:HH21	1:B:483:PHE:HB2	1.39	0.88
1:B:508:ASP:HB3	1:B:511:VAL:CG1	2.03	0.88
1:B:209:THR:HG23	1:B:211:PHE:HE1	1.35	0.88
1:B:496:HIS:CD2	1:B:578:GLY:H	1.90	0.88
1:B:43:ALA:CB	1:B:71:GLU:HG2	2.04	0.88
1:B:40:ILE:HB	1:B:69:LEU:HD23	1.56	0.88
1:A:351:LEU:HB3	1:A:356:PRO:HG3	1.53	0.87
1:B:503:HIS:HB2	1:B:571:VAL:O	1.72	0.87
1:B:325:ARG:HH21	1:B:483:PHE:CB	1.87	0.86
1:A:355:SER:HB3	1:A:356:PRO:HD3	1.57	0.86
1:A:551:GLN:HE21	1:A:551:GLN:H	1.23	0.86
1:B:114:PHE:CE1	6:B:615:UQ5:H4M3	2.10	0.86
1:B:188:ILE:HG22	1:B:189:GLN:H	1.38	0.86
1:B:133:MET:HG2	6:B:615:UQ5:H4M1	1.57	0.86
1:B:39:VAL:HG23	1:B:206:ALA:HB2	1.56	0.86
1:B:392:SER:HB2	1:B:394:THR:OG1	1.74	0.86
1:B:72:LYS:HE2	1:B:555:HIS:CD2	2.11	0.86
1:B:248:ILE:HG21	1:B:286:LEU:HD22	1.56	0.85
1:B:188:ILE:CG2	1:B:189:GLN:H	1.89	0.85
1:B:173:HIS:CE1	1:B:179:LYS:HG2	2.12	0.85
1:B:248:ILE:HD13	1:B:286:LEU:HD22	1.55	0.85
1:B:541:GLY:O	1:B:542:ASP:HB2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:HB3	1:A:449:GLU:OE2	1.76	0.84
1:B:508:ASP:O	1:B:511:VAL:HG13	1.78	0.84
1:B:361:VAL:HG11	1:B:422:ARG:HG3	1.58	0.83
1:A:353:GLY:O	1:A:356:PRO:HD2	1.77	0.83
1:B:114:PHE:HB2	1:B:127:ILE:HD11	1.61	0.83
1:B:325:ARG:NH2	1:B:483:PHE:HB2	1.94	0.82
1:B:209:THR:HG23	1:B:211:PHE:CE1	2.14	0.82
1:A:551:GLN:NE2	1:A:551:GLN:H	1.78	0.82
1:A:8:ARG:HE	1:A:8:ARG:H	1.28	0.81
1:A:490:ALA:HA	7:A:621:EDO:H21	1.62	0.81
1:B:21:ASP:HB3	1:B:24:TRP:HD1	1.46	0.81
1:B:72:LYS:HE2	1:B:555:HIS:HD2	1.45	0.81
1:B:171:LEU:HB2	1:B:179:LYS:HB2	1.63	0.81
1:A:117:LEU:CD2	1:A:122:ARG:HG3	2.11	0.80
1:B:498:HIS:CE1	1:B:551:GLN:HB3	2.16	0.80
1:B:81:LEU:HD22	1:B:331:ARG:HB2	1.64	0.80
7:A:621:EDO:H12	8:A:857:HOH:O	1.81	0.80
1:A:34:GLU:HG3	1:A:66:ARG:HH12	1.46	0.80
1:A:443:TRP:O	1:A:446:ARG:NH1	2.15	0.80
1:B:355:SER:HB3	1:B:356:PRO:HD3	1.63	0.79
1:B:15:ILE:HD13	1:B:506:LEU:O	1.83	0.79
1:B:132:PRO:HD3	1:B:442:TYR:CD2	2.18	0.79
1:B:127:ILE:HG22	1:B:127:ILE:O	1.83	0.79
1:A:114:PHE:HE1	6:A:612:UQ5:H4M2	1.48	0.79
1:B:353:GLY:O	1:B:356:PRO:HD2	1.84	0.78
1:B:275:PHE:CE2	1:B:289:GLY:HA3	2.18	0.78
1:B:517:LEU:HA	1:B:522:GLY:N	1.99	0.78
1:B:146:LEU:O	1:B:150:MET:HG3	1.83	0.78
1:A:445:PHE:O	1:A:448:MET:HG3	1.83	0.77
1:A:272:GLY:H	6:A:612:UQ5:H1M3	1.50	0.77
1:A:522:GLY:O	1:A:525:GLN:HG2	1.86	0.76
1:B:227:PHE:N	1:B:227:PHE:HD1	1.82	0.76
1:A:129:PRO:HG2	2:A:617:BHG:H62	1.66	0.76
1:B:73:ALA:CB	1:B:79:HIS:CE1	2.69	0.75
1:B:226:LYS:HB3	1:B:227:PHE:CD1	2.22	0.75
1:B:40:ILE:HB	1:B:69:LEU:CD2	2.16	0.75
1:B:15:ILE:CD1	1:B:505:THR:HB	2.17	0.74
1:B:132:PRO:HD3	1:B:442:TYR:CE2	2.23	0.74
1:B:84:ALA:HB3	1:B:141:VAL:O	1.87	0.73
1:B:334:ASN:HD21	1:B:354:CYS:HB3	1.54	0.73
1:A:361:VAL:HG22	1:A:362:PRO:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PRO:CB	1:B:546:LEU:HD22	2.19	0.73
1:B:508:ASP:HB3	1:B:511:VAL:HG12	1.71	0.72
1:B:227:PHE:N	1:B:227:PHE:CD1	2.55	0.72
1:B:73:ALA:HB3	1:B:79:HIS:CE1	2.24	0.72
1:B:15:ILE:HD11	1:B:505:THR:HB	1.72	0.72
1:B:72:LYS:NZ	1:B:79:HIS:ND1	2.37	0.72
1:B:538:LEU:HB2	1:B:543:GLY:O	1.90	0.72
1:B:522:GLY:O	1:B:525:GLN:HG2	1.89	0.72
1:A:117:LEU:HD23	1:A:122:ARG:HG3	1.72	0.71
6:B:615:UQ5:H4M2	6:B:615:UQ5:H153	1.70	0.71
1:A:345:THR:CG2	1:A:398:HIS:CD2	2.73	0.71
1:A:65:LEU:HD11	1:A:385:LEU:HD13	1.71	0.71
1:A:345:THR:HG22	1:A:398:HIS:HD2	1.54	0.71
1:B:76:ILE:HD11	1:B:161:VAL:HG21	1.71	0.71
1:A:345:THR:CG2	1:A:398:HIS:HD2	2.04	0.70
1:B:173:HIS:ND1	1:B:179:LYS:HG2	2.05	0.70
1:B:393:LYS:HE3	1:B:393:LYS:HA	1.72	0.70
1:B:512:PRO:HB3	1:B:546:LEU:HD22	1.73	0.70
1:B:260:HIS:HB3	6:B:615:UQ5:H3M2	1.73	0.70
1:B:186:VAL:HG12	1:B:187:GLY:N	2.07	0.70
1:A:32:PHE:HA	7:A:628:EDO:H21	1.73	0.70
1:B:21:ASP:OD1	1:B:23:ARG:HD3	1.90	0.70
6:A:612:UQ5:H3M2	6:A:612:UQ5:H4M3	1.74	0.70
1:B:344:LEU:HD12	1:B:403:GLU:OE1	1.92	0.70
1:B:97:ASP:OD2	1:B:101:LYS:HD2	1.92	0.70
1:A:8:ARG:H	1:A:8:ARG:NE	1.90	0.69
1:A:5:LYS:HZ2	1:A:8:ARG:NH1	1.89	0.69
1:B:403:GLU:HG2	1:B:407:LYS:HE3	1.74	0.69
1:B:310:TRP:CZ2	1:B:316:ILE:HD13	2.28	0.69
1:B:210:ILE:HG12	1:B:350:LEU:HD21	1.75	0.69
1:B:272:GLY:C	6:B:615:UQ5:H1M3	2.12	0.69
1:B:334:ASN:ND2	1:B:354:CYS:HB3	2.08	0.69
1:A:5:LYS:NZ	1:A:8:ARG:NH1	2.40	0.68
1:B:230:ARG:NH2	8:B:1009:HOH:O	2.18	0.68
1:A:490:ALA:HA	7:A:621:EDO:C2	2.22	0.68
1:A:8:ARG:CD	1:A:8:ARG:N	2.56	0.68
1:A:505:THR:HA	7:A:623:EDO:H12	1.74	0.68
1:B:394:THR:C	1:B:396:GLY:H	1.96	0.68
1:A:53:ARG:NH1	1:A:57:LEU:HD13	2.09	0.68
1:A:260:HIS:HB3	6:A:612:UQ5:C4M	2.24	0.67
1:A:272:GLY:O	6:A:612:UQ5:H1M3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:O	1:B:101:LYS:HB2	1.95	0.67
1:B:214:GLY:O	1:B:355:SER:HA	1.96	0.66
1:B:432:TYR:HA	1:B:435:MET:HE3	1.77	0.66
1:A:31:ARG:HG2	1:A:200:ARG:HD3	1.78	0.66
1:B:498:HIS:HE1	1:B:551:GLN:HB3	1.60	0.65
1:B:40:ILE:O	1:B:70:VAL:HG23	1.96	0.65
1:B:189:GLN:HB3	1:B:499:ASP:OD2	1.96	0.65
1:B:503:HIS:CD2	1:B:573:PRO:HD3	2.32	0.65
1:A:8:ARG:HD2	1:A:8:ARG:N	2.11	0.65
1:B:227:PHE:HD2	1:B:346:PHE:HB2	1.60	0.65
1:B:208:VAL:HA	1:B:348:GLY:O	1.96	0.65
1:B:394:THR:O	1:B:396:GLY:N	2.28	0.65
1:B:498:HIS:CE1	1:B:551:GLN:CB	2.80	0.65
1:B:34:GLU:CG	1:B:66:ARG:HH22	2.06	0.65
1:B:18:ARG:HG3	1:B:29:MET:HE1	1.77	0.64
1:B:252:LYS:HE2	1:B:318:PRO:O	1.97	0.64
1:B:276:LEU:O	1:B:277:TYR:HD1	1.81	0.64
1:B:512:PRO:O	1:B:516:ASN:HB2	1.97	0.64
1:A:132:PRO:O	1:A:363:LYS:HG3	1.98	0.64
1:B:242:LEU:N	1:B:242:LEU:HD12	2.13	0.64
1:B:70:VAL:HG12	1:B:165:TYR:O	1.99	0.63
1:B:79:HIS:CD2	1:B:579:PRO:HD2	2.33	0.63
1:A:272:GLY:H	6:A:612:UQ5:C1M	2.11	0.63
1:B:257:ARG:HD3	1:B:259:ASP:OD1	1.98	0.63
1:B:52:THR:HG21	1:B:95:PHE:CZ	2.33	0.63
1:A:128:LEU:HD23	2:A:617:BHG:O3	1.99	0.63
1:A:9:ILE:HG22	1:A:548:ILE:HD12	1.81	0.63
1:A:5:LYS:HE3	1:A:8:ARG:HD3	1.80	0.63
1:B:244:GLU:HG2	1:B:307:PHE:HZ	1.63	0.63
1:B:310:TRP:CE2	1:B:316:ILE:HD13	2.34	0.63
1:B:117:LEU:HD22	1:B:313:HIS:CE1	2.34	0.62
1:B:347:PRO:HB3	1:B:394:THR:HG21	1.80	0.62
1:A:6:VAL:HG13	1:A:8:ARG:CZ	2.29	0.62
1:A:350:LEU:HD12	1:A:381:ILE:HD11	1.81	0.62
1:A:6:VAL:HG13	1:A:8:ARG:NH2	2.14	0.62
1:A:5:LYS:HE3	1:A:8:ARG:CD	2.30	0.62
1:B:382:PHE:O	1:B:386:THR:HG23	2.00	0.62
1:A:170:ILE:HD13	1:A:223:LEU:HD13	1.82	0.62
1:B:393:LYS:CE	1:B:393:LYS:HA	2.29	0.62
1:B:242:LEU:HD22	1:B:304:PHE:HA	1.82	0.61
1:B:31:ARG:HE	1:B:200:ARG:HH12	0.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:HA3	1:B:204:LEU:O	2.00	0.61
1:B:242:LEU:CD2	1:B:304:PHE:HA	2.31	0.61
1:A:128:LEU:HD23	2:A:617:BHG:HO3	1.65	0.61
1:B:248:ILE:HD13	1:B:286:LEU:CD2	2.27	0.61
1:B:483:PHE:HD2	1:B:483:PHE:N	1.98	0.61
1:A:5:LYS:HD3	1:A:6:VAL:CG1	2.27	0.61
1:A:517:LEU:HA	1:A:522:GLY:H	1.66	0.61
1:A:39:VAL:HG23	1:A:206:ALA:HB2	1.81	0.61
1:B:365:LYS:HB3	1:B:368:HIS:CE1	2.36	0.61
1:B:352:ILE:HG22	1:B:402:TYR:OH	2.00	0.61
1:B:14:THR:HG21	1:B:571:VAL:HG11	1.82	0.60
1:B:485:LEU:O	1:B:489:VAL:HG23	2.01	0.60
1:A:173:HIS:CE1	1:A:179:LYS:HG3	2.36	0.60
1:B:517:LEU:O	1:B:521:ASP:HA	2.01	0.60
1:B:226:LYS:HB3	1:B:227:PHE:HD1	1.63	0.60
1:B:447:GLY:HA2	1:B:449:GLU:OE2	2.01	0.60
1:B:517:LEU:HA	1:B:522:GLY:H	1.65	0.60
1:A:426:HIS:CE1	1:A:456:LYS:HD2	2.36	0.59
1:B:299:PRO:HG3	1:B:463:LEU:HD22	1.84	0.59
1:B:483:PHE:CD2	1:B:483:PHE:N	2.68	0.59
1:A:401:GLU:H	1:A:401:GLU:CD	2.04	0.59
1:B:22:LYS:O	1:B:25:GLU:OE2	2.20	0.59
1:A:8:ARG:NE	1:A:8:ARG:N	2.51	0.59
1:B:244:GLU:HG2	1:B:307:PHE:CZ	2.38	0.59
1:B:325:ARG:NH2	1:B:483:PHE:CB	2.57	0.59
1:B:61:HIS:C	1:B:63:LYS:H	2.05	0.59
1:A:335:GLU:HA	1:A:361:VAL:CG1	2.33	0.59
1:B:276:LEU:C	1:B:277:TYR:HD1	2.07	0.59
1:B:84:ALA:CB	1:B:141:VAL:O	2.50	0.59
1:A:497:GLU:H	7:A:619:EDO:H12	1.68	0.59
1:B:375:THR:HG22	1:B:379:GLU:OE2	2.03	0.59
1:B:218:HIS:CD2	1:B:572:VAL:HG13	2.38	0.58
1:A:335:GLU:HA	1:A:361:VAL:HG11	1.84	0.58
1:B:160:GLU:HB3	1:B:162:TYR:CE1	2.39	0.58
1:B:499:ASP:O	1:B:500:GLN:HB3	2.01	0.58
1:A:352:ILE:HG22	1:A:402:TYR:OH	2.04	0.58
1:B:345:THR:HB	1:B:398:HIS:NE2	2.18	0.58
1:B:186:VAL:CG1	1:B:187:GLY:N	2.66	0.58
1:B:72:LYS:NZ	1:B:72:LYS:HB3	2.18	0.58
1:B:86:LEU:HD22	1:B:87:ASP:N	2.18	0.58
1:B:99:LYS:HD2	1:B:99:LYS:H	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LYS:H	1:B:476:LYS:CE	2.17	0.58
1:A:15:ILE:HD13	1:A:506:LEU:O	2.04	0.57
1:B:25:GLU:HG2	1:B:26:GLY:N	2.18	0.57
1:A:517:LEU:HA	1:A:522:GLY:N	2.19	0.57
1:B:60:GLN:HG3	1:B:61:HIS:CE1	2.40	0.57
1:A:40:ILE:HB	1:A:69:LEU:HD22	1.86	0.57
1:A:538:LEU:HB2	1:A:543:GLY:O	2.04	0.57
1:A:10:THR:HA	7:A:623:EDO:C2	2.34	0.57
1:B:348:GLY:N	1:B:397:LEU:O	2.34	0.57
1:A:107:THR:HG23	1:A:280:ASN:HB3	1.87	0.57
1:B:209:THR:CG2	1:B:211:PHE:CE1	2.75	0.56
1:B:226:LYS:HD2	1:B:227:PHE:CE1	2.39	0.56
1:B:294:LEU:O	1:B:459:ASP:HB3	2.06	0.56
1:B:224:TYR:HA	1:B:229:LEU:HD12	1.88	0.56
1:B:300:TYR:CE2	1:B:471:PRO:HG3	2.41	0.56
1:A:497:GLU:H	7:A:619:EDO:C1	2.17	0.56
1:B:317:LYS:HG3	1:B:481:ILE:HD13	1.87	0.56
1:B:300:TYR:CZ	1:B:471:PRO:HG3	2.41	0.56
1:A:107:THR:HB	1:A:140:VAL:HB	1.86	0.56
1:A:372:LYS:HE3	1:A:376:LEU:HD21	1.86	0.56
1:B:499:ASP:O	1:B:500:GLN:CB	2.53	0.56
1:B:260:HIS:HB3	6:B:615:UQ5:C3M	2.34	0.56
1:B:335:GLU:OE2	1:B:422:ARG:NH1	2.36	0.56
1:B:333:LEU:HD22	5:B:614:FAD:HM83	1.88	0.56
1:B:202:LEU:HD12	1:B:204:LEU:HG	1.88	0.55
1:B:85:CYS:HB3	1:B:365:LYS:HE3	1.89	0.55
1:A:260:HIS:HB3	6:A:612:UQ5:H4M1	1.89	0.55
1:B:317:LYS:HE3	1:B:481:ILE:HD12	1.87	0.55
1:B:218:HIS:NE2	1:B:219:LEU:HD13	2.21	0.55
1:B:25:GLU:HG2	1:B:26:GLY:H	1.72	0.55
1:B:83:GLY:O	1:B:84:ALA:HB3	2.06	0.55
1:A:551:GLN:HE21	1:A:551:GLN:N	1.98	0.55
1:B:422:ARG:N	1:B:423:PRO:HD2	2.21	0.55
1:B:445:PHE:O	1:B:448:MET:HG2	2.07	0.55
1:B:127:ILE:CG2	1:B:127:ILE:O	2.54	0.55
1:B:171:LEU:O	1:B:179:LYS:N	2.33	0.55
1:B:248:ILE:HG21	1:B:286:LEU:CD2	2.34	0.55
1:B:275:PHE:CZ	1:B:289:GLY:HA3	2.41	0.55
1:A:15:ILE:HD12	1:A:505:THR:HB	1.89	0.55
1:A:508:ASP:HB3	1:A:511:VAL:CG1	2.37	0.55
1:A:272:GLY:N	6:A:612:UQ5:H1M3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PHE:CE2	1:B:219:LEU:HD23	2.42	0.55
1:B:326:ILE:O	1:B:327:ALA:HB2	2.06	0.54
1:B:173:HIS:HB2	1:B:175:ASP:OD1	2.07	0.54
1:B:476:LYS:H	1:B:476:LYS:HE2	1.73	0.54
1:A:6:VAL:O	1:A:6:VAL:HG22	2.07	0.54
1:B:209:THR:HG21	1:B:211:PHE:HE1	1.67	0.54
1:B:272:GLY:O	6:B:615:UQ5:H1M3	2.08	0.54
1:A:218:HIS:CE1	1:A:219:LEU:HD13	2.43	0.54
1:A:31:ARG:CG	1:A:200:ARG:HD3	2.37	0.54
1:B:245:LEU:HB2	1:B:327:ALA:HB3	1.90	0.54
1:A:202:LEU:HD12	1:A:203:GLU:N	2.22	0.54
1:B:178:VAL:HG22	1:B:348:GLY:HA3	1.89	0.54
1:B:545:ARG:HH11	1:B:545:ARG:HG3	1.72	0.54
1:B:98:TRP:HB2	1:B:103:ALA:CB	2.38	0.54
1:B:226:LYS:HB3	1:B:227:PHE:CE1	2.42	0.54
1:B:389:ASN:H	1:B:389:ASN:ND2	2.04	0.54
1:B:347:PRO:HB3	1:B:394:THR:CG2	2.38	0.54
1:B:227:PHE:CD2	1:B:346:PHE:HB2	2.43	0.54
1:B:498:HIS:HE1	1:B:551:GLN:CB	2.19	0.54
1:B:73:ALA:HB2	1:B:79:HIS:CE1	2.42	0.54
1:B:81:LEU:CD2	1:B:331:ARG:HB2	2.36	0.53
1:B:341:ILE:HG12	1:B:357:GLY:O	2.08	0.53
1:B:38:VAL:CG1	1:B:67:VAL:CG1	2.84	0.53
1:B:151:GLY:O	1:B:154:ALA:HB3	2.07	0.53
1:B:344:LEU:HD12	1:B:403:GLU:CD	2.27	0.53
1:B:210:ILE:HD11	1:B:381:ILE:CD1	2.38	0.53
1:B:387:SER:O	1:B:388:GLU:HB2	2.07	0.53
1:A:350:LEU:CD1	1:A:381:ILE:HD11	2.38	0.53
1:B:55:LYS:NZ	1:B:158:GLY:O	2.42	0.53
1:B:177:SER:HB3	1:B:394:THR:HG22	1.90	0.53
1:B:435:MET:HG3	6:B:615:UQ5:H112	1.90	0.53
1:B:301:LEU:HD23	1:B:302:SER:N	2.23	0.53
1:B:43:ALA:HB3	1:B:71:GLU:CG	2.29	0.53
1:A:500:GLN:OE1	1:A:574:GLU:HG3	2.09	0.53
1:B:441:PHE:CD2	1:B:449:GLU:HG2	2.43	0.53
1:B:208:VAL:CG2	1:B:397:LEU:HB2	2.39	0.53
1:A:271:TYR:HE1	6:A:612:UQ5:H103	1.74	0.53
1:B:114:PHE:HD2	1:B:125:VAL:HB	1.75	0.52
1:B:15:ILE:HD12	1:B:505:THR:HB	1.90	0.52
1:B:385:LEU:HD21	1:B:397:LEU:CD1	2.39	0.52
1:A:230:ARG:HA	1:A:233:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HG22	1:A:398:HIS:NE2	2.25	0.52
1:A:355:SER:HB3	1:A:356:PRO:CD	2.35	0.52
1:B:335:GLU:HA	1:B:361:VAL:CG2	2.39	0.52
1:A:497:GLU:N	7:A:619:EDO:H12	2.24	0.52
1:B:85:CYS:H	5:B:614:FAD:C4	2.22	0.52
1:B:188:ILE:CG2	1:B:189:GLN:N	2.46	0.52
1:B:276:LEU:C	1:B:277:TYR:CD1	2.82	0.52
1:B:254:LYS:H	1:B:278:HIS:CE1	2.28	0.52
1:B:517:LEU:HD22	1:B:535:PHE:CD2	2.43	0.52
1:B:38:VAL:CG1	1:B:67:VAL:HG12	2.19	0.52
1:A:246:TRP:O	1:A:285:LEU:HD12	2.10	0.52
1:A:29:MET:CA	1:A:200:ARG:HD2	2.40	0.52
1:A:335:GLU:OE2	1:A:422:ARG:NH1	2.43	0.52
1:B:262:VAL:HG12	1:B:263:GLY:H	1.75	0.51
1:B:61:HIS:C	1:B:63:LYS:N	2.64	0.51
1:B:72:LYS:HZ3	1:B:72:LYS:HB3	1.74	0.51
1:B:76:ILE:HD11	1:B:161:VAL:CG2	2.40	0.51
1:A:8:ARG:C	1:A:10:THR:N	2.61	0.51
1:B:300:TYR:CD2	1:B:471:PRO:HA	2.46	0.51
1:B:302:SER:HB3	1:B:305:ARG:HB2	1.92	0.51
1:B:208:VAL:HG23	1:B:397:LEU:HB2	1.90	0.51
1:A:539:GLU:OE1	1:A:539:GLU:N	2.38	0.51
1:A:10:THR:HG23	7:A:623:EDO:H11	1.92	0.51
1:A:117:LEU:HD21	1:A:122:ARG:HG3	1.92	0.51
1:A:43:ALA:HB2	1:A:69:LEU:HD11	1.92	0.51
1:B:262:VAL:HG12	1:B:263:GLY:N	2.25	0.51
1:B:13:TYR:HB2	1:B:18:ARG:HD2	1.93	0.50
1:A:29:MET:HA	1:A:200:ARG:HD2	1.94	0.50
1:B:12:HIS:ND1	1:B:14:THR:CG2	2.65	0.50
1:B:40:ILE:O	1:B:69:LEU:CD2	2.60	0.50
1:A:393:LYS:O	1:A:394:THR:HG23	2.10	0.50
1:B:98:TRP:CZ3	1:B:105:LEU:HB2	2.46	0.50
1:B:335:GLU:HA	1:B:361:VAL:HG22	1.94	0.50
1:B:48:LEU:HD13	1:B:150:MET:HB2	1.93	0.50
1:B:143:LEU:O	1:B:144:GLY:C	2.50	0.50
1:A:420:ASN:ND2	1:A:449:GLU:OE1	2.45	0.50
1:B:33:ALA:HA	1:B:203:GLU:O	2.11	0.50
1:B:257:ARG:HG2	1:B:258:VAL:N	2.25	0.50
1:B:43:ALA:HB2	1:B:69:LEU:HD13	1.94	0.50
1:B:43:ALA:HB1	1:B:71:GLU:HG2	1.92	0.50
1:B:107:THR:OG1	1:B:280:ASN:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:LEU:O	1:B:540:GLN:N	2.45	0.50
1:A:282:GLY:HA2	7:A:627:EDO:H21	1.94	0.49
1:B:213:GLU:OE2	1:B:219:LEU:HB2	2.12	0.49
1:B:86:LEU:O	1:B:88:PRO:HD3	2.11	0.49
1:A:29:MET:C	1:A:200:ARG:HD2	2.33	0.49
1:A:34:GLU:HG3	1:A:66:ARG:NH1	2.23	0.49
1:A:5:LYS:HZ2	1:A:6:VAL:CG1	2.25	0.49
1:B:375:THR:O	1:B:379:GLU:HG3	2.12	0.49
1:B:505:THR:C	1:B:506:LEU:HD12	2.32	0.49
1:A:299:PRO:O	1:A:526:ARG:HD2	2.13	0.49
1:B:399:VAL:HG13	1:B:401:GLU:OE1	2.12	0.49
1:A:557:LYS:HE2	1:A:570:TRP:CE3	2.47	0.49
1:B:210:ILE:HA	1:B:350:LEU:HD23	1.95	0.49
1:B:545:ARG:NH1	1:B:545:ARG:HG3	2.27	0.49
1:B:203:GLU:CG	1:B:205:HIS:HE1	2.17	0.49
1:A:213:GLU:OE2	1:A:219:LEU:HB2	2.12	0.49
1:B:151:GLY:O	1:B:155:GLU:HG3	2.12	0.49
1:B:494:THR:HA	1:B:578:GLY:O	2.13	0.49
1:B:55:LYS:O	1:B:58:ALA:HB3	2.12	0.49
1:B:75:HIS:ND1	1:B:76:ILE:N	2.60	0.49
1:A:129:PRO:HG2	2:A:617:BHG:C6	2.42	0.49
1:A:333:LEU:H	1:A:333:LEU:HD23	1.76	0.49
1:A:333:LEU:N	1:A:333:LEU:HD23	2.27	0.49
1:A:65:LEU:HD11	1:A:385:LEU:CD1	2.39	0.49
1:B:24:TRP:CE2	1:B:194:PRO:HD3	2.48	0.49
1:B:31:ARG:HD2	1:B:203:GLU:OE1	2.13	0.48
1:B:257:ARG:NH1	8:B:1039:HOH:O	2.44	0.48
1:A:511:VAL:N	1:A:512:PRO:HD2	2.29	0.48
1:B:438:THR:CB	6:B:615:UQ5:H13	2.43	0.48
1:A:227:PHE:HB2	1:A:229:LEU:HD21	1.94	0.48
1:B:419:ARG:NH1	1:B:451:TRP:O	2.46	0.48
1:B:85:CYS:SG	1:B:258:VAL:HG11	2.53	0.48
1:A:5:LYS:HD2	1:A:7:PRO:HA	1.94	0.48
1:B:174:GLU:HA	1:B:174:GLU:OE1	2.13	0.48
1:B:557:LYS:HE2	1:B:570:TRP:CE3	2.49	0.48
1:B:161:VAL:HG23	1:B:163:PRO:HD3	1.94	0.48
1:B:385:LEU:HD21	1:B:397:LEU:HD11	1.95	0.48
1:A:72:LYS:HE3	5:A:611:FAD:O2B	2.14	0.48
1:A:5:LYS:NZ	1:A:6:VAL:HG12	2.28	0.48
1:B:61:HIS:O	1:B:63:LYS:N	2.47	0.48
1:A:73:ALA:HB1	1:A:78:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:TRP:CG	1:B:265:PRO:HA	2.49	0.48
1:B:236:GLN:OE1	1:B:336:GLY:HA3	2.14	0.48
1:B:362:PRO:HG3	1:B:418:VAL:HB	1.95	0.48
1:A:438:THR:CB	6:A:612:UQ5:H13	2.43	0.47
1:A:438:THR:OG1	6:A:612:UQ5:H13	2.14	0.47
1:B:210:ILE:HG12	1:B:350:LEU:CD2	2.43	0.47
1:A:46:ALA:HB1	1:A:352:ILE:HD12	1.96	0.47
1:B:160:GLU:HB3	1:B:162:TYR:HE1	1.78	0.47
1:A:243:LYS:HG2	1:A:244:GLU:N	2.29	0.47
1:A:186:VAL:HG12	1:A:199:GLU:HB2	1.96	0.47
1:B:494:THR:HG21	1:B:552:ASN:O	2.15	0.47
1:A:258:VAL:HG13	1:A:277:TYR:CE2	2.49	0.47
1:A:299:PRO:HG3	1:A:464:LYS:O	2.14	0.47
1:B:40:ILE:CG2	1:B:69:LEU:HD21	2.45	0.47
1:B:316:ILE:O	1:B:316:ILE:HG22	2.15	0.47
1:B:362:PRO:HG3	1:B:421:ILE:HD12	1.96	0.47
1:B:456:LYS:HE3	8:B:918:HOH:O	2.15	0.47
1:A:252:LYS:HD3	1:A:319:THR:HA	1.97	0.47
1:A:7:PRO:HD2	1:A:9:ILE:CG1	2.44	0.47
1:B:53:ARG:HD2	1:B:375:THR:HG23	1.97	0.47
1:A:515:ARG:HG3	8:A:1020:HOH:O	2.14	0.47
1:B:40:ILE:O	1:B:69:LEU:HD22	2.15	0.47
1:B:114:PHE:CZ	6:B:615:UQ5:H4M3	2.49	0.46
1:B:149:TRP:O	1:B:153:GLN:HG2	2.14	0.46
1:B:317:LYS:HB3	1:B:318:PRO:HD3	1.97	0.46
1:B:244:GLU:HA	1:B:327:ALA:O	2.15	0.46
1:A:29:MET:O	1:A:200:ARG:HD2	2.15	0.46
1:B:384:GLN:OE1	1:B:397:LEU:HD22	2.16	0.46
1:A:31:ARG:HG2	1:A:200:ARG:HB3	1.98	0.46
1:B:202:LEU:HD13	1:B:203:GLU:N	2.29	0.46
1:B:549:ASN:HB3	1:B:551:GLN:OE1	2.15	0.46
1:B:394:THR:C	1:B:396:GLY:N	2.65	0.46
1:B:538:LEU:HG	1:B:543:GLY:C	2.36	0.46
1:B:80:THR:HG21	1:B:147:VAL:HG21	1.98	0.46
1:A:181:ILE:HD12	1:A:181:ILE:C	2.36	0.46
1:A:239:GLY:O	1:A:333:LEU:HD23	2.16	0.46
1:A:40:ILE:HD12	1:A:51:ALA:HB2	1.98	0.46
1:B:505:THR:O	1:B:506:LEU:HD12	2.15	0.46
1:A:185:ASP:OD1	1:A:201:GLY:N	2.40	0.46
1:B:388:GLU:HA	1:B:388:GLU:OE1	2.16	0.46
1:B:72:LYS:CE	1:B:555:HIS:HD2	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:615:UQ5:H203	6:B:615:UQ5:H162	1.98	0.46
1:B:97:ASP:OD2	1:B:101:LYS:CD	2.63	0.46
1:B:186:VAL:CG1	1:B:187:GLY:H	2.29	0.46
1:B:210:ILE:HA	1:B:350:LEU:CD2	2.46	0.46
1:B:34:GLU:HG3	1:B:66:ARG:NH2	2.12	0.46
1:B:383:ASN:HA	1:B:383:ASN:HD22	1.51	0.46
1:A:399:VAL:HA	1:A:401:GLU:OE1	2.15	0.45
1:B:95:PHE:O	1:B:98:TRP:HD1	1.99	0.45
1:A:21:ASP:OD1	1:A:24:TRP:HD1	1.99	0.45
1:A:211:PHE:HB2	1:A:351:LEU:HD23	1.97	0.45
1:B:118:THR:O	1:B:119:GLU:C	2.55	0.45
1:A:182:ALA:HA	1:A:202:LEU:O	2.16	0.45
1:A:5:LYS:HE3	1:A:8:ARG:HD2	1.99	0.45
1:A:502:ALA:HB3	7:A:623:EDO:H21	1.98	0.45
1:A:97:ASP:OD2	1:A:101:LYS:HE3	2.15	0.45
1:B:175:ASP:OD2	1:B:394:THR:HA	2.16	0.45
1:A:72:LYS:HD3	1:A:572:VAL:HG12	1.98	0.45
6:A:612:UQ5:H272	6:A:612:UQ5:H251	1.45	0.45
1:B:261:THR:HG23	8:B:719:HOH:O	2.15	0.45
1:A:114:PHE:CE1	6:A:612:UQ5:H4M2	2.39	0.45
1:A:87:ASP:HA	1:A:138:ASN:OD1	2.16	0.45
1:B:210:ILE:HD11	1:B:381:ILE:HD12	1.98	0.45
1:B:460:SER:OG	1:B:566:GLN:HG2	2.17	0.45
1:B:344:LEU:HD12	1:B:344:LEU:H	1.82	0.45
1:B:361:VAL:HG11	1:B:422:ARG:CG	2.38	0.45
1:B:260:HIS:CD2	6:B:615:UQ5:H3M1	2.52	0.45
1:A:107:THR:HG23	1:A:280:ASN:CB	2.46	0.44
1:A:388:GLU:O	1:A:389:ASN:C	2.56	0.44
1:A:218:HIS:NE2	7:A:622:EDO:O1	2.49	0.44
1:B:188:ILE:HG21	1:B:501:PRO:HG3	1.99	0.44
1:A:407:LYS:NZ	8:A:806:HOH:O	2.50	0.44
1:A:502:ALA:O	7:A:623:EDO:H21	2.17	0.44
1:B:392:SER:CB	1:B:394:THR:OG1	2.56	0.44
1:A:230:ARG:HB3	8:A:1015:HOH:O	2.16	0.44
1:A:126:PRO:HB3	1:B:123:ILE:CG2	2.47	0.44
1:B:198:PHE:HZ	1:B:200:ARG:HD3	1.82	0.44
1:A:272:GLY:N	6:A:612:UQ5:C1M	2.79	0.44
1:A:443:TRP:HE1	2:A:617:BHG:HO3	1.65	0.44
1:B:189:GLN:NE2	1:B:191:ASP:OD1	2.41	0.44
1:B:182:ALA:HA	1:B:202:LEU:O	2.18	0.44
1:B:238:TYR:CG	1:B:561:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HB2	1:B:402:TYR:HE1	1.80	0.44
1:B:52:THR:HG21	1:B:95:PHE:HZ	1.82	0.44
1:A:360:ASN:ND2	1:A:363:LYS:HD3	2.32	0.44
1:B:307:PHE:O	1:B:307:PHE:CD1	2.70	0.44
1:A:273:GLY:C	6:A:612:UQ5:H3M3	2.38	0.44
1:B:394:THR:O	1:B:395:ILE:HG23	2.17	0.44
1:A:15:ILE:CD1	1:A:506:LEU:O	2.65	0.44
1:A:557:LYS:HE2	1:A:570:TRP:CZ3	2.53	0.44
1:A:391:GLN:HB3	8:A:805:HOH:O	2.18	0.44
1:A:8:ARG:HD3	1:A:8:ARG:HH11	1.55	0.44
1:B:214:GLY:O	1:B:355:SER:CA	2.65	0.44
1:B:331:ARG:HD2	1:B:332:ALA:H	1.83	0.44
1:A:5:LYS:HD3	1:A:6:VAL:N	2.32	0.44
1:B:129:PRO:HA	1:B:134:ASN:ND2	2.33	0.44
1:B:239:GLY:O	1:B:333:LEU:HD23	2.17	0.44
1:A:5:LYS:NZ	1:A:8:ARG:HH11	2.15	0.43
1:B:55:LYS:HA	1:B:58:ALA:CB	2.48	0.43
1:B:165:TYR:HD2	1:B:165:TYR:HA	1.49	0.43
1:B:390:LEU:HA	1:B:390:LEU:HD13	1.56	0.43
1:B:516:ASN:HB3	1:B:524:GLU:OE2	2.18	0.43
1:A:113:ARG:HB2	1:A:259:ASP:OD1	2.19	0.43
1:A:161:VAL:HG12	1:A:163:PRO:HD3	2.00	0.43
1:A:214:GLY:O	1:A:355:SER:HA	2.18	0.43
1:B:325:ARG:NH2	1:B:483:PHE:CD1	2.87	0.43
1:B:547:GLN:HG2	1:B:547:GLN:O	2.19	0.43
1:B:556:CYS:O	1:B:557:LYS:HB2	2.18	0.43
1:A:361:VAL:CG2	1:A:362:PRO:HD3	2.46	0.43
1:A:572:VAL:HG23	7:A:622:EDO:O2	2.18	0.43
1:B:181:ILE:HG23	1:B:182:ALA:N	2.33	0.43
1:A:29:MET:HG3	1:A:200:ARG:NE	2.32	0.43
1:A:419:ARG:HG2	1:A:420:ASN:N	2.34	0.43
1:B:157:LEU:HD22	1:B:157:LEU:HA	1.78	0.43
1:B:181:ILE:HD11	1:B:211:PHE:CZ	2.54	0.43
1:B:236:GLN:NE2	1:B:340:SER:CB	2.82	0.43
1:B:387:SER:OG	1:B:389:ASN:ND2	2.51	0.43
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.90	0.43
1:A:403:GLU:HG2	1:A:407:LYS:NZ	2.34	0.43
1:B:253:TRP:CD2	1:B:255:PRO:HD3	2.54	0.43
1:A:81:LEU:CD1	1:A:329:GLY:HA3	2.49	0.43
1:A:432:TYR:CD2	1:A:435:MET:CE	3.02	0.42
1:A:128:LEU:CD2	2:A:617:BHG:O3	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HZ1	1:A:8:ARG:NH1	2.15	0.42
1:B:130:GLY:O	1:B:446:ARG:NH1	2.46	0.42
1:A:13:TYR:OH	7:A:622:EDO:H22	2.18	0.42
1:B:99:LYS:C	1:B:101:LYS:H	2.22	0.42
1:B:365:LYS:HA	5:B:614:FAD:C2	2.49	0.42
1:A:241:GLY:O	1:A:330:ALA:HA	2.20	0.42
1:A:503:HIS:HB2	1:A:571:VAL:O	2.20	0.42
1:A:5:LYS:CE	1:A:8:ARG:HD3	2.46	0.42
1:B:387:SER:O	1:B:388:GLU:CB	2.68	0.42
1:A:300:TYR:CG	1:A:471:PRO:HA	2.54	0.42
1:A:552:ASN:ND2	8:A:857:HOH:O	2.52	0.42
1:B:120:LYS:HE3	8:B:913:HOH:O	2.18	0.42
1:B:7:PRO:HG2	1:B:9:ILE:HD11	2.02	0.42
1:A:533:TYR:HB3	1:A:546:LEU:HD11	2.01	0.42
1:A:555:HIS:N	1:A:555:HIS:CD2	2.88	0.42
1:B:31:ARG:NH1	1:B:203:GLU:OE1	2.49	0.42
1:A:325:ARG:HD3	1:A:483:PHE:CE1	2.55	0.42
6:A:612:UQ5:H203	6:A:612:UQ5:H162	2.01	0.42
1:B:395:ILE:CG1	1:B:395:ILE:O	2.68	0.42
1:A:5:LYS:HZ2	1:A:8:ARG:CZ	2.33	0.42
1:A:7:PRO:HD2	1:A:9:ILE:HG13	2.02	0.42
1:B:99:LYS:C	1:B:101:LYS:N	2.71	0.42
1:A:96:PRO:HD2	1:A:97:ASP:OD1	2.20	0.42
1:B:155:GLU:HG2	1:B:161:VAL:HG11	2.01	0.42
1:B:268:ARG:O	1:B:431:VAL:HG13	2.19	0.42
1:A:220:ALA:HA	1:A:223:LEU:HB2	2.02	0.41
1:B:103:ALA:HA	1:B:104:PRO:HD2	1.87	0.41
1:B:128:LEU:HB3	1:B:129:PRO:HD2	2.01	0.41
1:A:539:GLU:CD	1:A:539:GLU:H	2.09	0.41
1:B:306:GLU:CD	1:B:474:TYR:HE2	2.23	0.41
1:A:449:GLU:H	1:A:449:GLU:HG2	1.51	0.41
1:B:111:GLU:HG2	1:B:257:ARG:HG3	2.02	0.41
1:A:335:GLU:CA	1:A:361:VAL:HG11	2.48	0.41
1:B:188:ILE:CG2	1:B:501:PRO:HG3	2.50	0.41
1:B:226:LYS:C	1:B:227:PHE:HD1	2.23	0.41
1:B:224:TYR:OH	1:B:355:SER:O	2.38	0.41
1:B:89:ARG:HD3	1:B:410:TRP:CE2	2.55	0.41
1:A:86:LEU:HD22	1:A:87:ASP:N	2.36	0.41
1:A:573:PRO:HA	8:A:1028:HOH:O	2.21	0.41
6:A:612:UQ5:H71	6:A:612:UQ5:H1M1	1.72	0.41
1:A:10:THR:HA	7:A:623:EDO:H22	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG23	1:A:138:ASN:O	2.21	0.41
1:A:21:ASP:OD1	1:A:24:TRP:CD1	2.73	0.41
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.91	0.41
1:B:200:ARG:HB3	1:B:201:GLY:H	1.57	0.41
1:B:516:ASN:ND2	1:B:565:SER:OG	2.48	0.41
1:B:569:ASN:O	1:B:571:VAL:HG23	2.20	0.41
1:A:84:ALA:HB3	1:A:141:VAL:O	2.21	0.41
1:B:536:VAL:HA	1:B:537:PRO:HD3	1.68	0.41
1:B:184:ASN:ND2	1:B:575:GLY:H	2.19	0.41
6:B:615:UQ5:H251	6:B:615:UQ5:H272	1.73	0.41
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.72	0.41
1:B:236:GLN:NE2	1:B:340:SER:HB2	2.36	0.41
1:B:355:SER:N	1:B:356:PRO:CD	2.83	0.41
1:B:99:LYS:O	1:B:101:LYS:N	2.54	0.41
1:A:495:ASN:HD22	1:A:495:ASN:C	2.25	0.41
1:A:5:LYS:HZ2	1:A:6:VAL:HG12	1.85	0.41
1:A:8:ARG:HE	1:A:8:ARG:N	2.01	0.41
1:B:294:LEU:O	1:B:562:LYS:NZ	2.43	0.41
1:B:392:SER:HB2	1:B:394:THR:HG1	1.80	0.41
1:A:305:ARG:O	1:A:309:ARG:HB3	2.20	0.40
1:A:388:GLU:HB3	1:A:389:ASN:H	1.63	0.40
1:A:5:LYS:HD3	1:A:6:VAL:H	1.87	0.40
1:B:258:VAL:HG12	1:B:277:TYR:CD1	2.57	0.40
1:B:42:GLY:O	1:B:43:ALA:HB3	2.21	0.40
1:B:562:LYS:O	1:B:562:LYS:HG3	2.21	0.40
1:B:94:LEU:HD13	1:B:95:PHE:CE1	2.56	0.40
1:A:5:LYS:HZ1	1:A:8:ARG:HH11	1.69	0.40
1:B:56:GLN:O	1:B:60:GLN:HG2	2.21	0.40
1:B:72:LYS:HB2	5:B:614:FAD:C4A	2.50	0.40
1:A:294:LEU:O	1:A:459:ASP:HB3	2.21	0.40
1:A:365:LYS:HA	5:A:611:FAD:C2	2.52	0.40
1:B:129:PRO:HA	1:B:134:ASN:HD22	1.85	0.40
1:B:200:ARG:HH11	1:B:200:ARG:HB3	1.87	0.40
1:B:21:ASP:HB3	1:B:24:TRP:CD1	2.37	0.40
1:A:133:MET:HA	8:A:710:HOH:O	2.20	0.40
1:A:15:ILE:CD1	1:A:505:THR:HB	2.52	0.40
1:A:538:LEU:N	1:A:543:GLY:O	2.43	0.40
1:B:198:PHE:CZ	1:B:200:ARG:HD3	2.56	0.40
1:B:244:GLU:CG	1:B:307:PHE:HZ	2.32	0.40
1:A:10:THR:OG1	7:A:623:EDO:H11	2.22	0.40
1:B:195:LYS:HB3	1:B:197:THR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LYS:H	1:B:467:LYS:HG2	1.58	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	579/584 (99%)	544 (94%)	31 (5%)	4 (1%)	25	43
1	B	576/584 (99%)	493 (86%)	62 (11%)	21 (4%)	4	5
All	All	1155/1168 (99%)	1037 (90%)	93 (8%)	25 (2%)	8	12

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	B	74	ALA
1	B	84	ALA
1	B	99	LYS
1	B	391	GLN
1	B	395	ILE
1	B	500	GLN
1	B	532	VAL
1	B	539	GLU
1	B	62	GLU
1	B	187	GLY
1	B	385	LEU
1	A	6	VAL
1	A	394	THR
1	A	541	GLY
1	B	314	PRO
1	A	7	PRO

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Mol	Chain	Res	Type
1	B	23	ARG
1	B	164	GLY
1	B	542	ASP
1	B	17	PRO
1	B	133	MET
1	B	573	PRO
1	B	537	PRO
1	B	194	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	483/486 (99%)	428 (89%)	55 (11%)	7	12
1	B	479/486 (99%)	403 (84%)	76 (16%)	3	5
All	All	962/972 (99%)	831 (86%)	131 (14%)	4	8

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	5	LYS
1	A	8	ARG
1	A	18	ARG
1	A	19	ASP
1	A	21	ASP
1	A	22	LYS
1	A	29	MET
1	A	57	LEU
1	A	62	GLU
1	A	69	LEU
1	A	75	HIS
1	A	81	LEU
1	A	85	CYS
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	121	TYR
1	A	128	LEU
1	A	133	MET
1	A	157	LEU
1	A	174	GLU
1	A	200	ARG
1	A	202	LEU
1	A	219	LEU
1	A	223	LEU
1	A	225	LYS
1	A	244	GLU
1	A	266	LEU
1	A	279	LEU
1	A	320	LEU
1	A	321	GLU
1	A	331	ARG
1	A	333	LEU
1	A	342	PRO
1	A	359	MET
1	A	361	VAL
1	A	363	LYS
1	A	383	ASN
1	A	390	LEU
1	A	391	GLN
1	A	393	LYS
1	A	419	ARG
1	A	422	ARG
1	A	449	GLU
1	A	456	LYS
1	A	461	ASP
1	A	462	GLN
1	A	467	LYS
1	A	495	ASN
1	A	515	ARG
1	A	526	ARG
1	A	527	PHE
1	A	529	PRO
1	A	539	GLU
1	A	545	ARG
1	A	551	GLN
1	B	8	ARG
1	B	11	THR

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Mol	Chain	Res	Type
1	B	18	ARG
1	B	25	GLU
1	B	27	VAL
1	B	30	GLU
1	B	31	ARG
1	B	64	ASP
1	B	65	LEU
1	B	69	LEU
1	B	70	VAL
1	B	71	GLU
1	B	72	LYS
1	B	80	THR
1	B	85	CYS
1	B	86	LEU
1	B	94	LEU
1	B	99	LYS
1	B	112	ASP
1	B	133	MET
1	B	152	GLU
1	B	157	LEU
1	B	161	VAL
1	B	165	TYR
1	B	171	LEU
1	B	174	GLU
1	B	197	THR
1	B	200	ARG
1	B	202	LEU
1	B	204	LEU
1	B	219	LEU
1	B	222	GLN
1	B	225	LYS
1	B	227	PHE
1	B	244	GLU
1	B	250	GLU
1	B	252	LYS
1	B	255	PRO
1	B	259	ASP
1	B	266	LEU
1	B	279	LEU
1	B	286	LEU
1	B	288	LEU
1	B	320	LEU

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Mol	Chain	Res	Type
1	B	331	ARG
1	B	333	LEU
1	B	335	GLU
1	B	344	LEU
1	B	350	LEU
1	B	380	SER
1	B	383	ASN
1	B	389	ASN
1	B	393	LYS
1	B	394	THR
1	B	402	TYR
1	B	419	ARG
1	B	422	ARG
1	B	452	THR
1	B	458	SER
1	B	461	ASP
1	B	467	LYS
1	B	476	LYS
1	B	483	PHE
1	B	485	LEU
1	B	486	LEU
1	B	495	ASN
1	B	500	GLN
1	B	510	SER
1	B	513	VAL
1	B	515	ARG
1	B	524	GLU
1	B	527	PHE
1	B	538	LEU
1	B	539	GLU
1	B	540	GLN
1	B	551	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	106	ASN
1	A	173	HIS
1	A	222	GLN
1	A	384	GLN
1	A	495	ASN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	551	GLN
1	B	106	ASN
1	B	205	HIS
1	B	383	ASN
1	B	389	ASN
1	B	462	GLN
1	B	498	HIS
1	B	516	ASN
1	B	525	GLN
1	B	582	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z  > 2$
4	SF4	A	610	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	A	611	-	51,58,58	2.72	19 (37%)	54,89,89	2.62	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	UQ5	A	612	-	38,38,38	2.54	15 (39%)	46,49,49	2.33	14 (30%)
2	BHG	A	616	-	18,18,18	1.07	2 (11%)	23,23,23	3.54	4 (17%)
2	BHG	A	617	-	18,18,18	1.40	3 (16%)	23,23,23	2.35	6 (26%)
7	EDO	A	619	-	3,3,3	0.60	0	2,2,2	0.45	0
7	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.45	0
7	EDO	A	622	-	3,3,3	0.72	0	2,2,2	0.08	0
7	EDO	A	623	-	3,3,3	0.52	0	2,2,2	0.64	0
7	EDO	A	624	-	3,3,3	0.64	0	2,2,2	0.62	0
7	EDO	A	625	-	3,3,3	0.71	0	2,2,2	0.48	0
7	EDO	A	626	-	3,3,3	0.77	0	2,2,2	0.52	0
7	EDO	A	627	-	3,3,3	0.82	0	2,2,2	0.46	0
7	EDO	A	628	-	3,3,3	0.84	0	2,2,2	0.35	0
4	SF4	B	613	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	B	614	-	51,58,58	2.39	17 (33%)	54,89,89	2.94	15 (27%)
6	UQ5	B	615	-	38,38,38	2.57	17 (44%)	46,49,49	2.16	18 (39%)
2	BHG	B	618	-	18,18,18	1.04	1 (5%)	23,23,23	2.81	3 (13%)
7	EDO	B	620	-	3,3,3	0.63	0	2,2,2	0.59	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
4	SF4	A	610	1	-	0/0/48/48	0/6/5/5
5	FAD	A	611	-	-	0/28/50/50	0/6/6/6
6	UQ5	A	612	-	-	0/33/57/57	0/1/1/1
2	BHG	A	616	-	1/1/5/5	0/9/29/29	0/1/1/1
2	BHG	A	617	-	1/1/5/5	1/9/29/29	0/1/1/1
7	EDO	A	619	-	-	0/1/1/1	0/0/0/0
7	EDO	A	621	-	-	0/1/1/1	0/0/0/0
7	EDO	A	622	-	-	0/1/1/1	0/0/0/0
7	EDO	A	623	-	-	0/1/1/1	0/0/0/0
7	EDO	A	624	-	-	0/1/1/1	0/0/0/0
7	EDO	A	625	-	-	0/1/1/1	0/0/0/0
7	EDO	A	626	-	-	0/1/1/1	0/0/0/0
7	EDO	A	627	-	-	0/1/1/1	0/0/0/0
7	EDO	A	628	-	-	0/1/1/1	0/0/0/0
4	SF4	B	613	1	-	0/0/48/48	0/6/5/5
5	FAD	B	614	-	-	0/28/50/50	0/6/6/6
6	UQ5	B	615	-	-	0/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BHG	B	618	-	1/1/5/5	0/9/29/29	0/1/1/1
7	EDO	B	620	-	-	0/1/1/1	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	FAD	C1'-N10	-10.01	1.38	1.48
5	B	614	FAD	C1'-N10	-6.45	1.41	1.48
6	B	615	UQ5	C7-C8	-4.84	1.43	1.50
6	A	612	UQ5	C7-C8	-3.61	1.45	1.50
5	B	614	FAD	C2-N1	-3.52	1.31	1.38
6	B	615	UQ5	C22-C23	-3.47	1.38	1.50
5	B	614	FAD	C8A-N7A	-3.42	1.28	1.34
5	A	611	FAD	C5'-C4'	-3.32	1.46	1.51
5	A	611	FAD	P-O5'	-3.16	1.45	1.59
6	A	612	UQ5	C22-C23	-3.01	1.40	1.50
6	A	612	UQ5	C20-C19	-2.81	1.43	1.50
6	A	612	UQ5	O3-C3M	-2.76	1.38	1.45
6	B	615	UQ5	C20-C19	-2.73	1.43	1.50
5	A	611	FAD	O4B-C4B	-2.52	1.39	1.45
5	A	611	FAD	C8A-N7A	-2.42	1.30	1.34
6	A	612	UQ5	C11-C9	-2.27	1.46	1.51
2	A	616	BHG	O1-C1	-2.25	1.36	1.40
6	B	615	UQ5	C11-C9	-2.22	1.46	1.51
5	B	614	FAD	P-O5'	-2.14	1.50	1.59
6	B	615	UQ5	O3-C3M	-2.06	1.40	1.45
5	A	611	FAD	C2-N1	-2.05	1.34	1.38
2	A	616	BHG	C1-C2	2.04	1.58	1.52
6	B	615	UQ5	C30-C29	2.05	1.56	1.50
6	A	612	UQ5	C25-C24	2.07	1.56	1.50
5	B	614	FAD	C10-N1	2.09	1.36	1.33
6	A	612	UQ5	C4-C3	2.11	1.44	1.35
5	A	611	FAD	C9-C9A	2.11	1.45	1.40
5	A	611	FAD	C4A-N3A	2.14	1.38	1.35
6	B	615	UQ5	C23-C24	2.16	1.38	1.33
5	B	614	FAD	C5X-N5	2.18	1.38	1.35
2	B	618	BHG	O5-C1	2.35	1.47	1.41
6	A	612	UQ5	C6-C5	2.43	1.53	1.46
2	A	617	BHG	O5-C5	2.43	1.50	1.44
6	B	615	UQ5	C7-C6	2.44	1.55	1.51
5	B	614	FAD	C2-N3	2.47	1.43	1.38
5	A	611	FAD	C2-N3	2.55	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	615	UQ5	O4-C4	2.62	1.43	1.36
6	B	615	UQ5	C21-C19	2.75	1.57	1.51
2	A	617	BHG	O1-C1'	2.76	1.50	1.43
5	B	614	FAD	C9A-C5X	2.79	1.48	1.42
6	B	615	UQ5	O3-C3	2.82	1.43	1.36
5	B	614	FAD	C8-C7	2.83	1.48	1.41
5	B	614	FAD	C4X-C10	2.84	1.46	1.41
2	A	617	BHG	O5-C1	2.96	1.49	1.41
5	A	611	FAD	C2A-N3A	2.99	1.37	1.32
6	A	612	UQ5	C13-C14	3.05	1.40	1.33
6	B	615	UQ5	C13-C14	3.10	1.40	1.33
5	B	614	FAD	O4B-C1B	3.12	1.45	1.41
5	A	611	FAD	C4-C4X	3.21	1.47	1.41
6	B	615	UQ5	C6-C5	3.29	1.55	1.46
6	A	612	UQ5	C23-C24	3.38	1.41	1.33
5	A	611	FAD	C9A-N10	3.57	1.43	1.38
6	A	612	UQ5	C21-C19	3.61	1.59	1.51
5	B	614	FAD	C6-C5X	3.80	1.47	1.41
5	B	614	FAD	C5'-C4'	3.84	1.57	1.51
5	A	611	FAD	C8-C7	3.88	1.50	1.41
5	A	611	FAD	C10-N1	3.93	1.38	1.33
5	A	611	FAD	C5X-N5	4.09	1.41	1.35
6	B	615	UQ5	C25-C24	4.13	1.61	1.50
5	A	611	FAD	C4X-N5	4.38	1.39	1.33
5	B	614	FAD	C4A-N3A	4.44	1.42	1.35
5	B	614	FAD	C4-N3	4.61	1.41	1.33
6	B	615	UQ5	C8-C9	4.86	1.45	1.33
6	B	615	UQ5	C18-C19	4.96	1.45	1.33
5	A	611	FAD	O4B-C1B	5.02	1.48	1.41
6	A	612	UQ5	O3-C3	5.08	1.49	1.36
6	A	612	UQ5	C18-C19	5.09	1.45	1.33
5	A	611	FAD	C6-C5X	5.20	1.49	1.41
6	A	612	UQ5	C8-C9	5.25	1.46	1.33
5	B	614	FAD	C9A-N10	5.79	1.46	1.38
5	A	611	FAD	C4-N3	6.05	1.44	1.33
5	B	614	FAD	C4X-N5	6.33	1.42	1.33
6	A	612	UQ5	C28-C29	7.25	1.53	1.32
6	B	615	UQ5	C28-C29	7.56	1.54	1.32

All (71) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	614	FAD	C4X-C4-N3	-7.50	112.80	123.48
5	A	611	FAD	C4X-C4-N3	-7.08	113.40	123.48
5	B	614	FAD	C4X-C10-N10	-6.87	115.75	120.52
5	A	611	FAD	C4X-C10-N10	-5.30	116.84	120.52
6	A	612	UQ5	C12-C11-C9	-5.09	95.72	112.93
6	B	615	UQ5	C12-C11-C9	-4.79	96.73	112.93
6	A	612	UQ5	O2-C2-C3	-3.59	113.31	120.95
2	A	616	BHG	O5-C1-O1	-3.47	101.78	110.02
6	B	615	UQ5	O2-C2-C3	-3.47	113.57	120.95
5	A	611	FAD	C4-C4X-C10	-3.37	117.23	119.96
5	B	614	FAD	C4-C4X-N5	-3.25	115.11	118.68
5	B	614	FAD	N3A-C2A-N1A	-3.18	126.09	128.86
6	A	612	UQ5	O5-C5-C6	-3.14	116.04	121.82
6	A	612	UQ5	C1M-C1-C6	-2.98	118.16	124.20
5	A	611	FAD	C5X-C9A-N10	-2.86	115.53	117.66
6	B	615	UQ5	C1M-C1-C6	-2.74	118.65	124.20
6	B	615	UQ5	C10-C9-C8	-2.66	116.60	123.69
5	B	614	FAD	C4X-N5-C5X	-2.66	113.96	116.76
5	B	614	FAD	C4-C4X-C10	-2.65	117.82	119.96
2	A	617	BHG	C1'-O1-C1	-2.64	109.33	113.87
6	A	612	UQ5	C31-C29-C30	-2.64	108.44	114.60
5	B	614	FAD	C6-C5X-N5	-2.47	116.06	118.97
6	B	615	UQ5	O5-C5-C6	-2.42	117.35	121.82
6	B	615	UQ5	C31-C29-C30	-2.23	109.38	114.60
5	A	611	FAD	O3B-C3B-C4B	-2.18	104.73	111.09
6	B	615	UQ5	O4-C4-C3	-2.13	115.44	123.62
2	A	617	BHG	C1-C2-C3	-2.09	106.09	109.98
6	B	615	UQ5	C25-C24-C23	-2.02	118.31	123.69
6	B	615	UQ5	C4M-O4-C4	2.10	123.94	116.44
5	B	614	FAD	C1'-N10-C9A	2.11	120.28	118.35
5	B	614	FAD	C4B-O4B-C1B	2.11	112.01	109.77
2	A	617	BHG	C4'-C3'-C2'	2.14	125.46	114.45
2	A	617	BHG	O5-C1-O1	2.31	115.51	110.02
2	B	618	BHG	C4'-C3'-C2'	2.44	127.01	114.45
6	A	612	UQ5	O4-C4-C5	2.57	124.59	116.60
5	A	611	FAD	O4'-C4'-C3'	2.59	115.51	109.09
5	A	611	FAD	C4A-C5A-N7A	2.59	111.91	109.41
6	A	612	UQ5	C17-C18-C19	2.59	134.19	127.68
6	B	615	UQ5	C25-C24-C26	2.67	119.92	115.29
5	A	611	FAD	C1'-N10-C9A	2.77	120.89	118.35
2	A	617	BHG	O1-C1-C2	2.88	112.94	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	614	FAD	C4A-C5A-N7A	3.04	112.35	109.41
5	B	614	FAD	C9A-C5X-N5	3.08	126.83	122.24
6	B	615	UQ5	C16-C17-C18	3.10	122.61	111.97
6	A	612	UQ5	C26-C27-C28	3.11	122.63	111.97
6	B	615	UQ5	C10-C9-C11	3.13	120.72	115.29
6	B	615	UQ5	C15-C14-C16	3.14	120.74	115.29
6	B	615	UQ5	O4-C4-C5	3.27	126.75	116.60
6	A	612	UQ5	C10-C9-C11	3.30	121.01	115.29
6	B	615	UQ5	C26-C27-C28	3.32	123.34	111.97
6	A	612	UQ5	C11-C12-C13	3.37	123.52	111.97
6	B	615	UQ5	C8-C7-C6	3.45	121.54	111.85
6	A	612	UQ5	C20-C19-C21	3.46	121.29	115.29
6	B	615	UQ5	C20-C19-C21	3.63	121.58	115.29
6	A	612	UQ5	C16-C17-C18	3.75	124.82	111.97
6	A	612	UQ5	C15-C14-C16	3.85	121.97	115.29
5	A	611	FAD	O3'-C3'-C2'	3.91	118.50	108.82
5	B	614	FAD	O4'-C4'-C3'	4.04	119.12	109.09
5	A	611	FAD	C10-C4X-N5	4.78	126.09	120.59
6	B	615	UQ5	C11-C12-C13	4.82	128.50	111.97
5	B	614	FAD	C10-C4X-N5	5.59	127.02	120.59
2	B	618	BHG	C1'-O1-C1	5.73	123.71	113.87
2	A	616	BHG	O1-C1-C2	6.62	119.03	108.23
5	B	614	FAD	O3'-C3'-C2'	6.76	125.55	108.82
6	A	612	UQ5	C8-C7-C6	6.78	130.88	111.85
2	A	617	BHG	O1-C1'-C2'	9.28	142.78	109.68
2	A	616	BHG	O1-C1'-C2'	9.83	144.74	109.68
2	A	616	BHG	C1'-O1-C1	11.02	132.78	113.87
2	B	618	BHG	O1-C1'-C2'	11.51	150.73	109.68
5	A	611	FAD	C4-N3-C2	12.77	126.33	115.16
5	B	614	FAD	C4-N3-C2	13.15	126.66	115.16

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	618	BHG	C4
2	A	616	BHG	C4
2	A	617	BHG	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	617	BHG	C1-O1-C1'-C2'

There are no ring outliers.

11 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	FAD	2	0
6	A	612	UQ5	17	0
2	A	617	BHG	6	0
7	A	619	EDO	3	0
7	A	621	EDO	3	0
7	A	622	EDO	3	0
7	A	623	EDO	7	0
7	A	627	EDO	1	0
7	A	628	EDO	1	0
5	B	614	FAD	4	0
6	B	615	UQ5	13	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<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	581/584 (99%)	-0.25	10 (1%) 70 72	13, 30, 57, 84	0
1	B	578/584 (98%)	0.62	56 (9%) 8 8	38, 64, 79, 86	0
All	All	1159/1168 (99%)	0.19	66 (5%) 24 25	13, 49, 77, 86	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	CYS	7.8
1	B	176	GLY	5.4
1	B	540	GLN	5.4
1	B	390	LEU	5.2
1	A	540	GLN	5.0
1	A	7	PRO	5.0
1	A	6	VAL	5.0
1	A	389	ASN	4.9
1	B	502	ALA	4.6
1	B	7	PRO	4.6
1	B	389	ASN	4.4
1	B	27	VAL	4.3
1	B	538	LEU	4.1
1	B	61	HIS	3.8
1	B	388	GLU	3.8
1	B	382	PHE	3.7
1	A	5	LYS	3.5
1	B	100	GLU	3.5
1	B	26	GLY	3.5
1	B	32	PHE	3.4
1	B	499	ASP	3.4
1	B	537	PRO	3.4
1	B	8	ARG	3.3
1	B	24	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	539	GLU	3.2
1	B	541	GLY	3.0
1	B	30	GLU	2.9
1	B	498	HIS	2.9
1	B	174	GLU	2.8
1	B	28	ASN	2.8
1	B	395	ILE	2.7
1	B	22	LYS	2.7
1	B	536	VAL	2.7
1	B	386	THR	2.7
1	B	19	ASP	2.7
1	B	20	GLN	2.7
1	B	43	ALA	2.7
1	B	212	ALA	2.7
1	A	8	ARG	2.6
1	B	191	ASP	2.6
1	B	62	GLU	2.6
1	B	391	GLN	2.6
1	B	535	PHE	2.5
1	A	391	GLN	2.5
1	B	501	PRO	2.4
1	B	172	PHE	2.4
1	B	165	TYR	2.4
1	B	396	GLY	2.4
1	B	155	GLU	2.4
1	B	542	ASP	2.4
1	B	33	ALA	2.4
1	A	388	GLU	2.3
1	B	495	ASN	2.3
1	B	15	ILE	2.3
1	B	496	HIS	2.3
1	B	41	VAL	2.3
1	B	75	HIS	2.2
1	B	57	LEU	2.2
1	B	16	TYR	2.2
1	A	539	GLU	2.2
1	B	161	VAL	2.1
1	B	58	ALA	2.1
1	B	97	ASP	2.1
1	B	157	LEU	2.1
1	B	18	ARG	2.1
1	B	189	GLN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BHG	A	617	18/18	0.59	0.57	16.72	55,75,78,79	0
7	EDO	A	623	4/4	0.92	0.45	15.56	48,49,49,53	0
2	BHG	A	616	18/18	0.59	0.38	14.60	52,76,78,79	0
7	EDO	A	622	4/4	0.84	0.38	11.07	51,55,55,57	0
7	EDO	A	621	4/4	0.94	0.27	8.76	45,47,48,49	0
7	EDO	A	624	4/4	0.95	0.32	7.81	35,41,42,42	0
7	EDO	A	619	4/4	0.89	0.20	4.70	37,37,38,43	0
6	UQ5	A	612	38/38	0.88	0.26	3.08	39,48,62,63	0
6	UQ5	B	615	38/38	0.85	0.27	2.28	51,56,68,71	0
7	EDO	B	620	4/4	0.88	0.15	0.34	49,53,54,56	0
5	FAD	A	611	53/53	0.98	0.17	-0.02	16,20,24,26	0
5	FAD	B	614	53/53	0.92	0.19	-0.31	44,60,68,69	0
4	SF4	A	610	8/8	0.99	0.11	-0.35	16,19,22,22	0
4	SF4	B	613	8/8	0.98	0.09	-2.33	55,58,59,59	0
7	EDO	A	626	4/4	0.89	0.16	-	43,45,45,46	0
7	EDO	A	628	4/4	0.77	0.34	-	53,54,55,55	0
3	NA	A	1070	1/1	0.95	0.07	-	37,37,37,37	0
7	EDO	A	627	4/4	0.81	0.56	-	57,58,58,58	0
2	BHG	B	618	18/18	0.53	0.36	-	61,76,78,78	0
7	EDO	A	625	4/4	0.90	0.15	-	49,55,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.