



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:35 AM GMT

PDB ID : 2GMH
Title : Structure of Porcine Electron Transfer Flavoprotein-UbiquinoneOxidoreduc-
tase 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

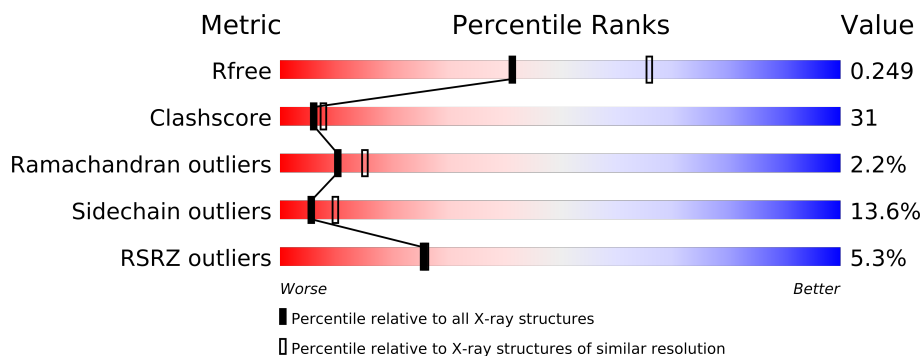
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BHG	A	616	-	X
2	BHG	A	617	-	X
2	BHG	B	618	-	X
6	UQ5	A	612	-	X
6	UQ5	B	615	-	X
7	EDO	A	619	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	EDO	A	621	-	X
7	EDO	A	622	-	X
7	EDO	A	623	-	X
7	EDO	A	624	-	X
7	EDO	A	627	-	X
7	EDO	A	628	-	X

2 Entry composition i

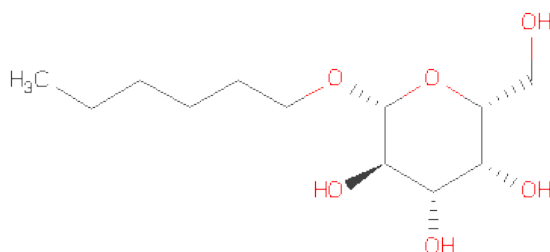
There are 8 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogen and 0 are deuterium.

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-ubiquinoneoxidoreductase.

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: C₁₂H₂₄O₆).

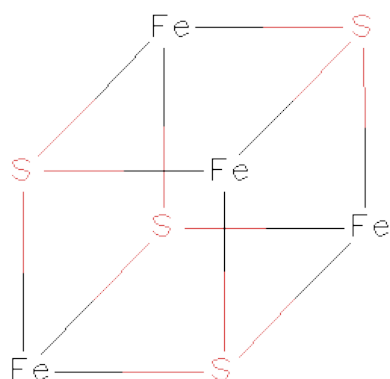


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

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

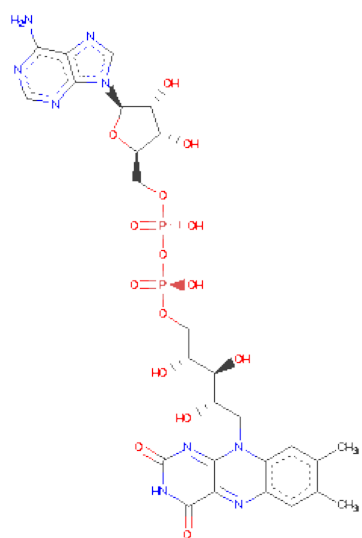
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



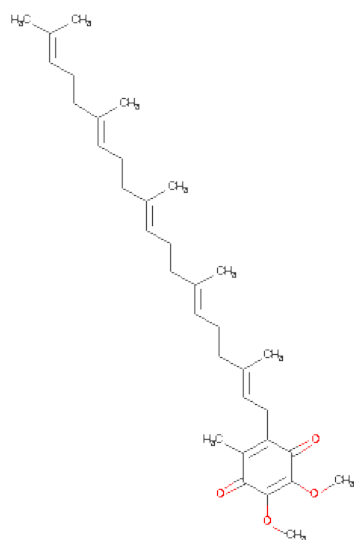
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- 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: C₃₄H₅₀O₄).



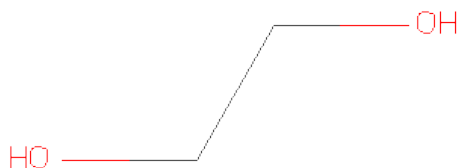
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C	O	0
			38	34	4	

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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.

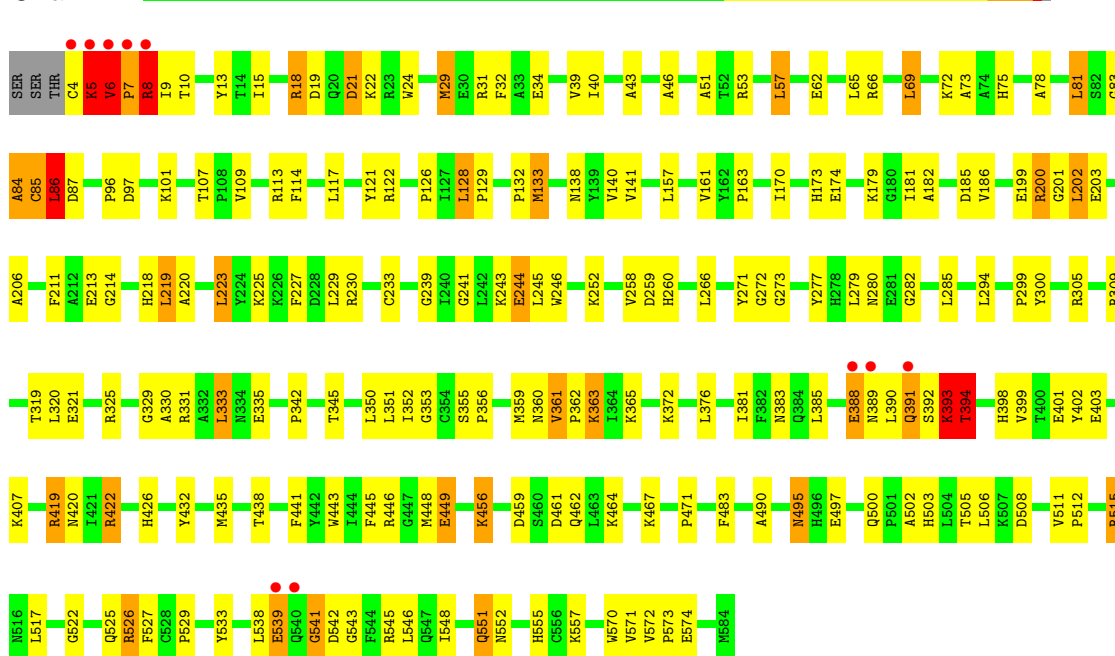
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	301	Total 301	O 301	0	0
8	B	68	Total 68	O 68	0	0

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

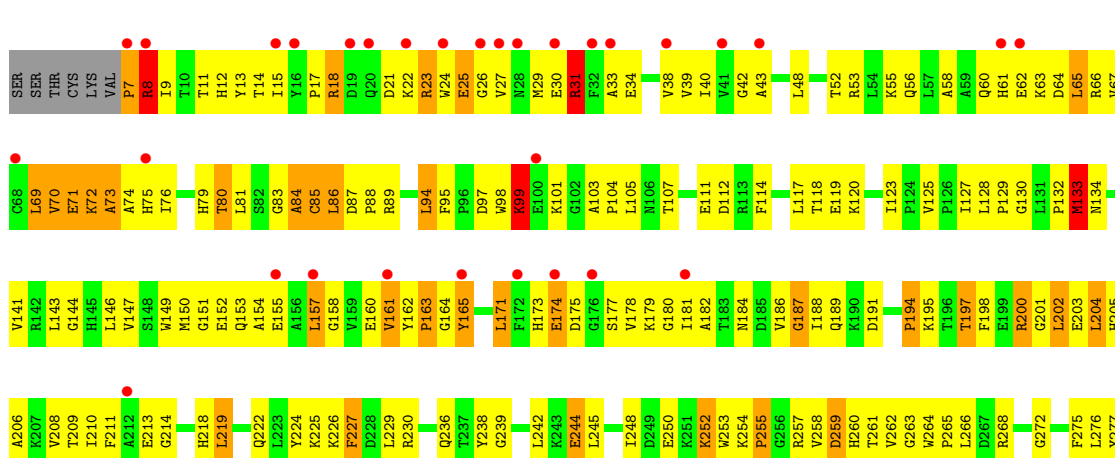
- Molecule 1: Electron transfer flavoprotein-ubiquinoneoxidoreductase

Chain A:



- Molecule 1: Electron transfer flavoprotein-ubiquinoneoxidoreductase

Chain B:



H278	V361	M448	P523
L279	P362	E449	E524
M280		P450	Q525
	K365	W451	R526
L286		T452	P527
A287	H368		V532
L288		K456	
G289	T375	G457	P535
		S458	V536
L294	E379	D459	P537
	S380	S460	L538
P299	I381	D461	E539
Y300	F382	Q462	Q540
L301	N383	L463	Q541
S302	Q384		D542
P303	L385	K467	G543
F304	T386	P471	P544
R305	S387		R545
E306	E388	Y474	L546
F307	N389	P475	Q547
	L390	K476	T548
W310	Q391		N549
	S392	T481	A550
H313	K393	S482	Q551
P314	T394	F483	N552
S315	I395	D484	
I316	G396	L485	H555
K317	L397	L486	C556
P318	H398	S487	K557
T319	V399	S488	
L320	T400	V489	T561
	E401		K562
R325	Y402	T494	S565
I326	E403	M495	Q566
A327		H496	
	K407	E497	N569
R331		H498	W570
A332	W410	D499	V571
L333		Q500	V572
N334	V418	P501	P573
E335	R419	A502	E574
G336	N420	H503	G575
	I421	L504	
S340	R422	T505	
I341	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	F445		
S355	R446	D521	
P356	G447	G522	
G357			

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	6.94 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.254 0.216 , 0.249	Depositor DCC
R_{free} test set	4358 reflections (8.87%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 53524 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (576) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:43:ALA:CB	1:B:71:GLU:HG2	2.04	0.88
1:B:496:HIS:CD2	1:B:578:GLY:H	1.90	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:H	1:A:551:GLN:HE21	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
1:A:441:PHE:HB3	1:A:449:GLU:OE2	1.76	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:H	1:A:551:GLN:NE2	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:72:LYS:HE2	1:B:555:HIS:HD2	1.45	0.81
1:B:21:ASP:HB3	1:B:24:TRP:HD1	1.46	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:73:ALA:HB3	1:B:79:HIS:CE1	2.24	0.72
1:B:227:PHE:N	1:B:227:PHE:CD1	2.55	0.72
1:B:72:LYS:NZ	1:B:79:HIS:ND1	2.37	0.72
1:B:15:ILE:HD11	1:B:505:THR:HB	1.72	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:512:PRO:HB3	1:B:546:LEU:HD22	1.73	0.70
1:B:393:LYS:HE3	1:B:393:LYS:HA	1.72	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:97:ASP:OD2	1:B:101:LYS:HD2	1.92	0.70
1:B:344:LEU:HD12	1:B:403:GLU:OE1	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:210:ILE:HG12	1:B:350:LEU:HD21	1.75	0.69
1:B:310:TRP:CZ2	1:B:316:ILE:HD13	2.28	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:8:ARG:CD	1:A:8:ARG:N	2.56	0.68
1:A:490:ALA:HA	7:A:621:EDO:C2	2.22	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:503:HIS:CD2	1:B:573:PRO:HD3	2.32	0.65
1:B:189:GLN:HB3	1:B:499:ASP:OD2	1.96	0.65
1:A:8:ARG:HD2	1:A:8:ARG:N	2.11	0.65
1:B:208:VAL:HA	1:B:348:GLY:O	1.96	0.65
1:B:227:PHE:HD2	1:B:346:PHE:HB2	1.60	0.65
1:B:394:THR:O	1:B:396:GLY:N	2.28	0.65
1:B:34:GLU:CG	1:B:66:ARG:HH22	2.06	0.65
1:B:498:HIS:CE1	1:B:551:GLN:CB	2.80	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:B:257:ARG:HD3	1:B:259:ASP:OD1	1.98	0.63
1:A:272:GLY:H	6:A:612:UQ5:C1M	2.11	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:310:TRP:CE2	1:B:316:ILE:HD13	2.34	0.63
1:B:244:GLU:HG2	1:B:307:PHE:HZ	1.63	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:6:VAL:HG13	1:A:8:ARG:NH2	2.14	0.62
1:A:350:LEU:HD12	1:A:381:ILE:HD11	1.81	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:B:393:LYS:CE	1:B:393:LYS:HA	2.29	0.62
1:A:170:ILE:HD13	1:A:223:LEU:HD13	1.82	0.62
1:B:31:ARG:HE	1:B:200:ARG:HH12	0.79	0.61
1:B:242:LEU:HD22	1:B:304:PHE:HA	1.82	0.61
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:B:248:ILE:HD13	1:B:286:LEU:CD2	2.27	0.61
1:A:128:LEU:HD23	2:A:617:BHG:HO3	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:39:VAL:HG23	1:A:206:ALA:HB2	1.81	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:517:LEU:HA	1:B:522:GLY:H	1.65	0.60
1:B:447:GLY:HA2	1:B:449:GLU:OE2	2.01	0.60
1:B:299:PRO:HG3	1:B:463:LEU:HD22	1.84	0.59
1:A:426:HIS:CE1	1:A:456:LYS:HD2	2.36	0.59
1:B:483:PHE:CD2	1:B:483:PHE:N	2.68	0.59
1:A:401:GLU:CD	1:A:401:GLU:H	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:B:375:THR:HG22	1:B:379:GLU:OE2	2.03	0.59
1:A:497:GLU:H	7:A:619:EDO:H12	1.68	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:499:ASP:O	1:B:500:GLN:HB3	2.01	0.58
1:B:160:GLU:HB3	1:B:162:TYR:CE1	2.39	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:72:LYS:NZ	1:B:72:LYS:HB3	2.18	0.58
1:B:186:VAL:CG1	1:B:187:GLY:N	2.66	0.58
1:B:99:LYS:H	1:B:99:LYS:HD2	1.66	0.58
1:B:86:LEU:HD22	1:B:87:ASP:N	2.18	0.58
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:348:GLY:N	1:B:397:LEU:O	2.34	0.57
1:A:10:THR:HA	7:A:623:EDO:C2	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:224:TYR:HA	1:B:229:LEU:HD12	1.88	0.56
1:B:294:LEU:O	1:B:459:ASP:HB3	2.06	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:B:499:ASP:O	1:B:500:GLN:CB	2.53	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: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:83:GLY:O	1:B:84:ALA:HB3	2.06	0.55
1:B:25:GLU:HG2	1:B:26:GLY:H	1.72	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
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:B:209:THR:HG21	1:B:211:PHE:HE1	1.67	0.54
1:A:6:VAL:O	1:A:6:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:272:GLY:O	6:B:615:UQ5:H1M3	2.08	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:218:HIS:CE1	1:A:219:LEU:HD13	2.43	0.54
1:B:178:VAL:HG22	1:B:348:GLY:HA3	1.89	0.54
1:A:202:LEU:HD12	1:A:203:GLU:N	2.22	0.54
1:B:545:ARG:HH11	1:B:545:ARG:HG3	1.72	0.54
1:B:347:PRO:HB3	1:B:394:THR:CG2	2.38	0.54
1:B:226:LYS:HB3	1:B:227:PHE:CE1	2.42	0.54
1:B:98:TRP:HB2	1:B:103:ALA:CB	2.38	0.54
1:B:389:ASN:H	1:B:389:ASN:ND2	2.04	0.54
1:B:73:ALA:HB2	1:B:79:HIS:CE1	2.42	0.54
1:B:498:HIS:HE1	1:B:551:GLN:CB	2.19	0.54
1:B:227:PHE:CD2	1:B:346:PHE:HB2	2.43	0.54
1:B:38:VAL:CG1	1:B:67:VAL:CG1	2.84	0.53
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: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:435:MET:HG3	6:B:615:UQ5:H112	1.90	0.53
1:B:177:SER:HB3	1:B:394:THR:HG22	1.90	0.53
1:B:43:ALA:HB3	1:B:71:GLU:CG	2.29	0.53
1:B:301:LEU:HD23	1:B:302:SER:N	2.23	0.53
1:B:441:PHE:CD2	1:B:449:GLU:HG2	2.43	0.53
1:A:500:GLN:OE1	1:A:574:GLU:HG3	2.09	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: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:230:ARG:HA	1:A:233:CYS:SG	2.49	0.52
1:B:85:CYS:H	5:B:614:FAD:C4	2.22	0.52
1:A:497:GLU:N	7:A:619:EDO:H12	2.24	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:38:VAL:CG1	1:B:67:VAL:HG12	2.19	0.52
1:B:517:LEU:HD22	1:B:535:PHE:CD2	2.43	0.52
1:B:254:LYS:H	1:B:278:HIS:CE1	2.28	0.52
1:A:246:TRP:O	1:A:285:LEU:HD12	2.10	0.52
1:A:335:GLU:OE2	1:A:422:ARG:NH1	2.43	0.52
1:A:29:MET:CA	1:A:200:ARG:HD2	2.40	0.52
1:B:262:VAL:HG12	1:B:263:GLY:H	1.75	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:B:61:HIS:C	1:B:63:LYS:N	2.64	0.51
1:B:208:VAL:HG23	1:B:397:LEU:HB2	1.90	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:A:10:THR:HG23	7:A:623:EDO:H11	1.92	0.51
1:A:539:GLU:OE1	1:A:539:GLU:N	2.38	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:40:ILE:O	1:B:69:LEU:CD2	2.60	0.50
1:B:12:HIS:ND1	1:B:14:THR:CG2	2.65	0.50
1:B:335:GLU:HA	1:B:361:VAL:HG22	1.94	0.50
1:B:98:TRP:CZ3	1:B:105:LEU:HB2	2.46	0.50
1:A:393:LYS:O	1:A:394:THR:HG23	2.10	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: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:A:420:ASN:ND2	1:A:449:GLU:OE1	2.45	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:538:LEU:O	1:B:540:GLN:N	2.45	0.50
1:B:107:THR:OG1	1:B:280:ASN:HB3	2.12	0.50
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:282:GLY:HA2	7:A:627:EDO:H21	1.94	0.49
1:A:5:LYS:HZ2	1:A:6:VAL:CG1	2.25	0.49
1:A:34:GLU:HG3	1:A:66:ARG:NH1	2.23	0.49
1:B:505:THR:C	1:B:506:LEU:HD12	2.32	0.49
1:A:29:MET:C	1:A:200:ARG:HD2	2.33	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:375:THR:O	1:B:379:GLU:HG3	2.12	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: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:A:557:LYS:HE2	1:A:570:TRP:CE3	2.47	0.49
1:B:203:GLU:CG	1:B:205:HIS:HE1	2.17	0.49
1:B:55:LYS:O	1:B:58:ALA:HB3	2.12	0.49
1:B:494:THR:HA	1:B:578:GLY:O	2.13	0.49
1:B:151:GLY:O	1:B:155:GLU:HG3	2.12	0.49
1:B:75:HIS:ND1	1:B:76:ILE:N	2.60	0.49
1:A:213:GLU:OE2	1:A:219:LEU:HB2	2.12	0.49
1:A:129:PRO:HG2	2:A:617:BHG:C6	2.42	0.49
1:B:24:TRP:CE2	1:B:194:PRO:HD3	2.48	0.49
1:A:65:LEU:HD11	1:A:385:LEU:CD1	2.39	0.49
1:A:333:LEU:H	1:A:333:LEU:HD23	1.76	0.49
1:A:333:LEU:HD23	1:A:333:LEU:N	2.27	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:B:438:THR:CB	6:B:615:UQ5:H13	2.43	0.48
1:A:511:VAL:N	1:A:512:PRO:HD2	2.29	0.48
1:B:85:CYS:SG	1:B:258:VAL:HG11	2.53	0.48
1:B:419:ARG:NH1	1:B:451:TRP:O	2.46	0.48
1:A:227:PHE:HB2	1:A:229:LEU:HD21	1.94	0.48
1:A:5:LYS:HD2	1:A:7:PRO:HA	1.94	0.48
1:B:557:LYS:HE2	1:B:570:TRP:CE3	2.49	0.48
1:B:174:GLU:HA	1:B:174:GLU:OE1	2.13	0.48
1:B:385:LEU:HD21	1:B:397:LEU:HD11	1.95	0.48
1:B:161:VAL:HG23	1:B:163:PRO:HD3	1.94	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:72:LYS:HE3	5:A:611:FAD:O2B	2.14	0.48
1:B:264:TRP:CG	1:B:265:PRO:HA	2.49	0.48
1:A:73:ALA:HB1	1:A:78:ALA:HB3	1.96	0.48
1:B:362:PRO:HG3	1:B:418:VAL:HB	1.95	0.48
1:B:236:GLN:OE1	1:B:336:GLY:HA3	2.14	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:B:160:GLU:HB3	1:B:162:TYR:HE1	1.78	0.47
1:A:46:ALA:HB1	1:A:352:ILE:HD12	1.96	0.47
1:A:243:LYS:HG2	1:A:244:GLU:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:494:THR:HG21	1:B:552:ASN:O	2.15	0.47
1:A:186:VAL:HG12	1:A:199:GLU:HB2	1.96	0.47
1:B:40:ILE:CG2	1:B:69:LEU:HD21	2.45	0.47
1:A:299:PRO:HG3	1:A:464:LYS:O	2.14	0.47
1:A:258:VAL:HG13	1:A:277:TYR:CE2	2.49	0.47
1:A:7:PRO:HD2	1:A:9:ILE:CG1	2.44	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:B:53:ARG:HD2	1:B:375:THR:HG23	1.97	0.47
1:B:40:ILE:O	1:B:69:LEU:HD22	2.15	0.47
1:A:515:ARG:HG3	8:A:1020:HOH:O	2.14	0.47
1:B:114:PHE:CZ	6:B:615:UQ5:H4M3	2.49	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:B:149:TRP:O	1:B:153:GLN:HG2	2.14	0.46
1:B:384:GLN:OE1	1:B:397:LEU:HD22	2.16	0.46
1:A:29:MET:O	1:A:200:ARG:HD2	2.15	0.46
1:B:202:LEU:HD13	1:B:203:GLU:N	2.29	0.46
1:A:31:ARG:HG2	1:A:200:ARG:HB3	1.98	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:239:GLY:O	1:A:333:LEU:HD23	2.16	0.46
1:A:181:ILE:HD12	1:A:181:ILE:C	2.36	0.46
1:B:505:THR:O	1:B:506:LEU:HD12	2.15	0.46
1:A:40:ILE:HD12	1:A:51:ALA:HB2	1.98	0.46
6:B:615:UQ5:H203	6:B:615:UQ5:H162	1.98	0.46
1:B:72:LYS:CE	1:B:555:HIS:HD2	2.23	0.46
1:B:97:ASP:OD2	1:B:101:LYS:CD	2.63	0.46
1:B:388:GLU:HA	1:B:388:GLU:OE1	2.16	0.46
1:A:185:ASP:OD1	1:A:201:GLY:N	2.40	0.46
1:B:34:GLU:HG3	1:B:66:ARG:NH2	2.12	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:383:ASN:HA	1:B:383:ASN:HD22	1.51	0.46
1:B:95:PHE:O	1:B:98:TRP:HD1	1.99	0.45
1:A:399:VAL:HA	1:A:401:GLU:OE1	2.15	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:ASP:OD1	1:A:24:TRP:HD1	1.99	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:B:175:ASP:OD2	1:B:394:THR:HA	2.16	0.45
1:A:182:ALA:HA	1:A:202:LEU:O	2.16	0.45
1:A:97:ASP:OD2	1:A:101:LYS:HE3	2.15	0.45
1:A:72:LYS:HD3	1:A:572:VAL:HG12	1.98	0.45
6:A:612:UQ5:H251	6:A:612:UQ5:H272	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:B:210:ILE:HD11	1:B:381:ILE:HD12	1.98	0.45
1:A:87:ASP:HA	1:A:138:ASN:OD1	2.16	0.45
1:B:460:SER:OG	1:B:566:GLN:HG2	2.17	0.45
1:B:260:HIS:CD2	6:B:615:UQ5:H3M1	2.52	0.45
1:B:361:VAL:HG11	1:B:422:ARG:CG	2.38	0.45
1:B:344:LEU:HD12	1:B:344:LEU:H	1.82	0.45
1:B:188:ILE:HG21	1:B:501:PRO:HG3	1.99	0.44
1:A:107:THR:HG23	1:A:280:ASN:CB	2.46	0.44
1:A:218:HIS:NE2	7:A:622:EDO:O1	2.49	0.44
1:A:388:GLU:O	1:A:389:ASN:C	2.56	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:407:LYS:NZ	8:A:806:HOH:O	2.50	0.44
1:B:198:PHE:HZ	1:B:200:ARG:HD3	1.82	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:182:ALA:HA	1:B:202:LEU:O	2.18	0.44
1:B:189:GLN:NE2	1:B:191:ASP:OD1	2.41	0.44
1:A:443:TRP:HE1	2:A:617:BHG:HO3	1.65	0.44
1:A:272:GLY:N	6:A:612:UQ5:C1M	2.79	0.44
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:B:238:TYR:CG	1:B:561:ILE:HD13	2.53	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:B:394:THR:O	1:B:395:ILE:HG23	2.17	0.44
1:A:273:GLY:C	6:A:612:UQ5:H3M3	2.38	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:B:214:GLY:O	1:B:355:SER:CA	2.65	0.44
1:A:8:ARG:HD3	1:A:8:ARG:HH11	1.55	0.44
1:B:331:ARG:HD2	1:B:332:ALA:H	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:391:GLN:HB3	8:A:805:HOH:O	2.18	0.44
1:A:5:LYS:HD3	1:A:6:VAL:N	2.32	0.44
1:B:239:GLY:O	1:B:333:LEU:HD23	2.17	0.44
1:B:129:PRO:HA	1:B:134:ASN:ND2	2.33	0.44
1:B:55:LYS:HA	1:B:58:ALA:CB	2.48	0.43
1:A:5:LYS:NZ	1:A:8:ARG:HH11	2.15	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:B:325:ARG:NH2	1:B:483:PHE:CD1	2.87	0.43
1:A:214:GLY:O	1:A:355:SER:HA	2.18	0.43
1:B:556:CYS:O	1:B:557:LYS:HB2	2.18	0.43
1:B:547:GLN:HG2	1:B:547:GLN:O	2.19	0.43
1:A:161:VAL:HG12	1:A:163:PRO:HD3	2.00	0.43
1:A:113:ARG:HB2	1:A:259:ASP:OD1	2.19	0.43
1:B:181:ILE:HG23	1:B:182:ALA:N	2.33	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:157:LEU:HA	1:B:157:LEU:HD22	1.78	0.43
1:B:181:ILE:HD11	1:B:211:PHE:CZ	2.54	0.43
1:A:419:ARG:HG2	1:A:420:ASN:N	2.34	0.43
1:A:29:MET:HG3	1:A:200:ARG:NE	2.32	0.43
1:B:387:SER:OG	1:B:389:ASN:ND2	2.51	0.43
1:B:236:GLN:NE2	1:B:340:SER:CB	2.82	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:5:LYS:HZ1	1:A:8:ARG:NH1	2.15	0.42
1:A:128:LEU:CD2	2:A:617:BHG:O3	2.67	0.42
1:B:130:GLY:O	1:B:446:ARG:NH1	2.46	0.42
1:A:432:TYR:CD2	1:A:435:MET:CE	3.02	0.42
1:B:365:LYS:HA	5:B:614:FAD:C2	2.49	0.42
1:B:99:LYS:C	1:B:101:LYS:H	2.22	0.42
1:A:13:TYR:OH	7:A:622:EDO:H22	2.18	0.42
1:A:5:LYS:CE	1:A:8:ARG:HD3	2.46	0.42
1:A:503:HIS:HB2	1:A:571:VAL:O	2.20	0.42
1:A:241:GLY:O	1:A:330:ALA:HA	2.20	0.42
1:B:387:SER:O	1:B:388:GLU:CB	2.68	0.42
1:A:552:ASN:ND2	8:A:857:HOH:O	2.52	0.42
1:B:7:PRO:HG2	1:B:9:ILE:HD11	2.02	0.42
1:A:300:TYR:CG	1:A:471:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:LYS:HE3	8:B:913:HOH:O	2.18	0.42
1:B:31:ARG:NH1	1:B:203:GLU:OE1	2.49	0.42
1:A:555:HIS:N	1:A:555:HIS:CD2	2.88	0.42
1:A:533:TYR:HB3	1:A:546:LEU:HD11	2.01	0.42
1:B:395:ILE:CG1	1:B:395:ILE:O	2.68	0.42
6:A:612:UQ5:H162	6:A:612:UQ5:H203	2.01	0.42
1:A:325:ARG:HD3	1:A:483:PHE:CE1	2.55	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:B:155:GLU:HG2	1:B:161:VAL:HG11	2.01	0.42
1:A:96:PRO:HD2	1:A:97:ASP:OD1	2.20	0.42
1:B:268:ARG:O	1:B:431:VAL:HG13	2.19	0.42
1:B:103:ALA:HA	1:B:104:PRO:HD2	1.87	0.41
1:A:220:ALA:HA	1:A:223:LEU:HB2	2.02	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:B:111:GLU:HG2	1:B:257:ARG:HG3	2.02	0.41
1:A:449:GLU:H	1:A:449:GLU:HG2	1.51	0.41
1:B:224:TYR:OH	1:B:355:SER:O	2.38	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: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:B:200:ARG:HB3	1:B:201:GLY:H	1.57	0.41
1:B:569:ASN:O	1:B:571:VAL:HG23	2.20	0.41
1:A:10:THR:HA	7:A:623:EDO:H22	2.00	0.41
1:B:516:ASN:ND2	1:B:565:SER:OG	2.48	0.41
1:A:538:LEU:HD12	1:A:538:LEU:HA	1.91	0.41
1:A:21:ASP:OD1	1:A:24:TRP:CD1	2.73	0.41
1:A:109:VAL:HG23	1:A:138:ASN:O	2.21	0.41
1:B:355:SER:N	1:B:356:PRO:CD	2.83	0.41
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.72	0.41
6:B:615:UQ5:H251	6:B:615:UQ5:H272	1.73	0.41
1:B:99:LYS:O	1:B:101:LYS:N	2.54	0.41
1:B:236:GLN:NE2	1:B:340:SER:HB2	2.36	0.41
1:B:536:VAL:HA	1:B:537:PRO:HD3	1.68	0.41
1:A:84:ALA:HB3	1:A:141:VAL:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:ASN:ND2	1:B:575:GLY:H	2.19	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:392:SER:HB2	1:B:394:THR:HG1	1.80	0.41
1:B:294:LEU:O	1:B:562:LYS:NZ	2.43	0.41
1:A:495:ASN:C	1:A:495:ASN:HD22	2.25	0.41
1:B:42:GLY:O	1:B:43:ALA:HB3	2.21	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:94:LEU:HD13	1:B:95:PHE:CE1	2.56	0.40
1:B:562:LYS:O	1:B:562:LYS:HG3	2.21	0.40
1:A:388:GLU:HB3	1:A:389:ASN:H	1.63	0.40
1:A:305:ARG:O	1:A:309:ARG:HB3	2.20	0.40
1:A:5:LYS:HZ1	1:A:8:ARG:HH11	1.69	0.40
1:B:72:LYS:HB2	5:B:614:FAD:C4A	2.50	0.40
1:B:56:GLN:O	1:B:60:GLN:HG2	2.21	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: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:A:294:LEU:O	1:A:459:ASP:HB3	2.21	0.40
1:B:198:PHE:CZ	1:B:200:ARG:HD3	2.56	0.40
1:A:15:ILE:CD1	1:A:505:THR:HB	2.52	0.40
1:B:244:GLU:CG	1:B:307:PHE:HZ	2.32	0.40
1:A:538:LEU:N	1:A:543:GLY:O	2.43	0.40
1:A:133:MET:HA	8:A:710:HOH:O	2.20	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
1:B:467:LYS:H	1:B:467:LYS:HG2	1.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	30	50
1	B	576/584 (99%)	493 (86%)	62 (11%)	21 (4%)	5	6
All	All	1155/1168 (99%)	1037 (90%)	93 (8%)	25 (2%)	10	15

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
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%)	8	15
1	B	479/486 (99%)	403 (84%)	76 (16%)	4	6
All	All	962/972 (99%)	831 (86%)	131 (14%)	5	10

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains 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 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	12,12,12	13.09	12 (100%)	0,24,24	0.00	-
5	FAD	A	611	-	58,58,58	2.57	21 (36%)	85,89,89	1.96	15 (17%)
6	UQ5	A	612	-	38,38,38	2.68	16 (42%)	49,49,49	2.43	17 (34%)
2	BHG	A	616	-	18,18,18	1.02	1 (5%)	23,23,23	3.53	4 (17%)
2	BHG	A	617	-	18,18,18	1.34	3 (16%)	23,23,23	2.24	6 (26%)
7	EDO	A	619	-	3,3,3	0.68	0	2,2,2	0.47	0
7	EDO	A	621	-	3,3,3	0.70	0	2,2,2	0.46	0
7	EDO	A	622	-	3,3,3	0.82	0	2,2,2	0.09	0
7	EDO	A	623	-	3,3,3	0.62	0	2,2,2	0.66	0
7	EDO	A	624	-	3,3,3	0.74	0	2,2,2	0.64	0
7	EDO	A	625	-	3,3,3	0.80	0	2,2,2	0.49	0
7	EDO	A	626	-	3,3,3	0.85	0	2,2,2	0.54	0
7	EDO	A	627	-	3,3,3	0.90	0	2,2,2	0.48	0
7	EDO	A	628	-	3,3,3	0.93	0	2,2,2	0.36	0
4	SF4	B	613	1	12,12,12	13.03	10 (83%)	0,24,24	0.00	-
5	FAD	B	614	-	58,58,58	2.30	20 (34%)	85,89,89	2.30	17 (20%)
6	UQ5	B	615	-	38,38,38	2.68	15 (39%)	49,49,49	2.37	20 (40%)
2	BHG	B	618	-	18,18,18	1.00	1 (5%)	23,23,23	2.60	4 (17%)
7	EDO	B	620	-	3,3,3	0.72	0	2,2,2	0.61	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	0/0/5/5
5	FAD	A	611	-	-	0/34/50/50	0/1/6/6
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	0/0/5/5
5	FAD	B	614	-	-	0/34/50/50	0/1/6/6
6	UQ5	B	615	-	-	0/33/57/57	0/1/1/1
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 (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	613	SF4	S1-FE4	-22.51	2.18	2.33
4	B	613	SF4	S4-FE3	-22.11	2.18	2.33
4	A	610	SF4	S2-FE4	-22.05	2.18	2.33
4	A	610	SF4	S1-FE4	-21.77	2.18	2.33
4	B	613	SF4	S2-FE4	-21.58	2.18	2.33
4	A	610	SF4	S3-FE4	-20.79	2.19	2.33
4	B	613	SF4	S3-FE4	-20.09	2.19	2.33
4	A	610	SF4	S4-FE3	-19.85	2.19	2.33
4	A	610	SF4	S2-FE1	-9.27	2.27	2.33
5	A	611	FAD	C1'-N10	-8.90	1.38	1.48
4	A	610	SF4	S1-FE2	-8.47	2.27	2.33
4	B	613	SF4	S2-FE1	-8.45	2.27	2.33
4	B	613	SF4	S1-FE2	-7.77	2.28	2.33
6	B	615	UQ5	C28-C29	6.77	1.54	1.32
5	A	611	FAD	C6-C5X	6.59	1.49	1.41
6	A	612	UQ5	C8-C9	6.52	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	612	UQ5	C28-C29	6.49	1.53	1.32
6	A	612	UQ5	C18-C19	6.32	1.45	1.32
6	B	615	UQ5	C18-C19	6.16	1.45	1.32
6	B	615	UQ5	C8-C9	6.04	1.45	1.32
5	A	611	FAD	PA-O3P	-5.94	1.49	1.59
5	B	614	FAD	C1'-N10	-5.66	1.41	1.48
5	B	614	FAD	C1'-C2'	-5.65	1.46	1.51
4	A	610	SF4	S4-FE2	-5.38	2.29	2.33
4	A	610	SF4	S4-FE1	-5.14	2.29	2.33
5	B	614	FAD	C9A-N10	5.06	1.46	1.38
5	B	614	FAD	PA-O3P	-5.03	1.50	1.59
6	A	612	UQ5	O3-C3	5.03	1.49	1.36
5	A	611	FAD	C1'-C2'	-5.01	1.46	1.51
5	B	614	FAD	C6-C5X	4.82	1.47	1.41
5	B	614	FAD	C10-N10	4.66	1.48	1.38
6	B	615	UQ5	C7-C8	-4.66	1.43	1.50
5	A	611	FAD	O4B-C1B	4.46	1.48	1.41
4	A	610	SF4	S2-FE3	-4.44	2.30	2.33
5	B	614	FAD	C4A-N3A	4.25	1.42	1.35
6	A	612	UQ5	C23-C24	4.21	1.41	1.32
6	B	615	UQ5	C25-C24	4.17	1.61	1.50
6	B	615	UQ5	C22-C23	-4.12	1.38	1.50
5	A	611	FAD	C5X-N5	4.07	1.41	1.35
5	A	611	FAD	C4-N3	4.05	1.44	1.37
4	A	610	SF4	S3-FE2	-4.01	2.30	2.33
4	B	613	SF4	S4-FE1	-3.89	2.30	2.33
6	B	615	UQ5	C13-C14	3.86	1.40	1.32
5	A	611	FAD	C4-C4X	3.82	1.47	1.41
6	A	612	UQ5	C13-C14	3.79	1.40	1.32
4	B	613	SF4	S3-FE2	-3.79	2.30	2.33
5	B	614	FAD	C5'-C4'	3.66	1.57	1.51
6	A	612	UQ5	C22-C23	-3.57	1.40	1.50
6	A	612	UQ5	C7-C8	-3.48	1.45	1.50
5	A	611	FAD	C8-C7	3.44	1.50	1.40
4	A	610	SF4	S1-FE3	-3.39	2.31	2.33
6	A	612	UQ5	C21-C19	3.33	1.59	1.51
5	B	614	FAD	C8A-N7A	-3.22	1.28	1.34
6	B	615	UQ5	C6-C5	3.20	1.55	1.46
5	A	611	FAD	C9A-N10	3.11	1.43	1.38
5	A	611	FAD	C10-N10	3.09	1.45	1.38
5	A	611	FAD	C5'-C4'	-3.05	1.46	1.51
5	A	611	FAD	C2-N3	3.03	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	614	FAD	C4X-N5	3.01	1.42	1.36
5	A	611	FAD	P-O5'	-2.98	1.45	1.59
5	B	614	FAD	C2-N3	2.95	1.43	1.37
5	B	614	FAD	C4X-C10	2.93	1.46	1.40
6	A	612	UQ5	C20-C19	-2.91	1.43	1.50
2	A	617	BHG	O5-C1	2.87	1.49	1.41
4	A	610	SF4	S3-FE1	-2.86	2.31	2.33
6	B	615	UQ5	C20-C19	-2.83	1.43	1.50
6	B	615	UQ5	O3-C3	2.81	1.43	1.36
5	B	614	FAD	C9A-C5X	2.80	1.48	1.42
5	B	614	FAD	C8A-N9A	2.80	1.40	1.36
5	B	614	FAD	O4B-C1B	2.75	1.45	1.41
6	B	615	UQ5	C23-C24	2.70	1.38	1.32
6	A	612	UQ5	O3-C3M	-2.66	1.38	1.45
6	B	615	UQ5	O4-C4	2.61	1.43	1.36
2	A	617	BHG	O1-C1'	2.60	1.50	1.42
6	B	615	UQ5	C21-C19	2.52	1.57	1.51
5	A	611	FAD	C2A-N3A	2.52	1.37	1.32
5	B	614	FAD	C8-C7	2.51	1.48	1.40
5	B	614	FAD	C4-N3	2.49	1.41	1.37
5	A	611	FAD	O4B-C4B	-2.44	1.39	1.45
2	A	617	BHG	O5-C5	2.36	1.50	1.44
6	A	612	UQ5	C6-C5	2.35	1.53	1.46
4	B	613	SF4	S4-FE2	-2.32	2.31	2.33
5	A	611	FAD	C9-C9A	2.28	1.45	1.40
2	B	618	BHG	O5-C1	2.28	1.47	1.41
5	A	611	FAD	C8A-N7A	-2.26	1.30	1.34
4	B	613	SF4	S2-FE3	-2.25	2.31	2.33
5	B	614	FAD	C5X-N5	2.19	1.38	1.35
6	B	615	UQ5	C7-C6	2.16	1.55	1.51
6	A	612	UQ5	C12-C13	-2.13	1.44	1.50
6	A	612	UQ5	C11-C9	-2.11	1.46	1.51
2	A	616	BHG	O1-C1	-2.10	1.36	1.40
5	B	614	FAD	C9-C9A	2.09	1.44	1.40
6	B	615	UQ5	C11-C9	-2.07	1.46	1.51
5	A	611	FAD	C2B-C1B	-2.07	1.50	1.53
6	A	612	UQ5	C25-C24	2.07	1.56	1.50
5	A	611	FAD	PA-O2A	-2.06	1.45	1.55
5	A	611	FAD	C4A-N3A	2.03	1.38	1.35
6	A	612	UQ5	C4-C3	2.02	1.44	1.35
5	B	614	FAD	P-O5'	-2.02	1.50	1.59

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	BHG	O1-C1'-C2'	10.46	150.73	109.87
2	A	616	BHG	C1'-O1-C1	10.46	132.78	113.96
5	B	614	FAD	C4X-C10-N10	-9.55	115.75	120.51
2	A	616	BHG	O1-C1'-C2'	8.93	144.74	109.87
5	B	614	FAD	C2'-C1'-N10	8.69	123.98	112.45
2	A	616	BHG	O1-C1-C2	8.52	119.03	108.18
2	A	617	BHG	O1-C1'-C2'	8.43	142.78	109.87
5	A	611	FAD	C4X-C10-N10	-7.35	116.84	120.51
5	A	611	FAD	C2'-C1'-N10	6.98	121.71	112.45
5	B	614	FAD	O3'-C3'-C2'	6.65	125.55	108.74
5	B	614	FAD	O4B-C1B-C2B	-6.36	97.02	106.77
6	A	612	UQ5	C8-C7-C6	6.04	130.88	111.61
6	B	615	UQ5	C11-C12-C13	5.91	128.50	111.62
2	B	618	BHG	C1'-O1-C1	5.42	123.71	113.96
5	B	614	FAD	C10-C4X-N5	5.40	127.02	120.45
5	A	611	FAD	O4B-C1B-C2B	-5.34	98.58	106.77
6	A	612	UQ5	C12-C11-C9	-5.14	95.72	112.74
5	A	611	FAD	C2-N1-C10	4.96	119.98	114.98
6	B	615	UQ5	C12-C11-C9	-4.83	96.73	112.74
5	A	611	FAD	C10-C4X-N5	4.64	126.09	120.45
6	A	612	UQ5	C16-C17-C18	4.62	124.82	111.62
6	A	612	UQ5	C15-C14-C16	4.33	121.97	115.39
5	A	611	FAD	P-O3P-PA	4.17	143.92	131.68
6	A	612	UQ5	C11-C12-C13	4.17	123.52	111.62
5	B	614	FAD	C2-N1-C10	4.14	119.15	114.98
6	B	615	UQ5	C26-C27-C28	4.10	123.34	111.62
6	B	615	UQ5	C20-C19-C21	4.07	121.58	115.39
5	B	614	FAD	O4'-C4'-C3'	4.05	119.12	109.05
5	B	614	FAD	P-O5'-C5'	3.91	150.18	122.03
6	A	612	UQ5	C20-C19-C21	3.88	121.29	115.39
5	A	611	FAD	O3'-C3'-C2'	3.86	118.50	108.74
6	A	612	UQ5	C26-C27-C28	3.85	122.63	111.62
6	B	615	UQ5	C16-C17-C18	3.85	122.61	111.62
2	A	617	BHG	O1-C1-C2	3.74	112.94	108.18
6	A	612	UQ5	C10-C9-C11	3.70	121.01	115.39
6	B	615	UQ5	C15-C14-C16	3.52	120.74	115.39
6	B	615	UQ5	C10-C9-C11	3.50	120.72	115.39
6	B	615	UQ5	C10-C9-C8	-3.50	116.60	123.52
2	A	616	BHG	O5-C1-O1	-3.49	101.78	109.98
6	A	612	UQ5	O2-C2-C3	-3.45	113.31	120.96
6	B	615	UQ5	C1-C6-C5	-3.42	115.96	120.26
5	A	611	FAD	C3B-C2B-C1B	3.38	106.20	100.91
6	B	615	UQ5	O2-C2-C3	-3.33	113.57	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	614	FAD	C4A-C5A-N7A	3.30	112.35	109.52
6	B	615	UQ5	O4-C4-C5	3.26	126.75	116.54
5	B	614	FAD	N3A-C2A-N1A	-3.13	126.09	128.71
6	B	615	UQ5	C8-C7-C6	3.11	121.54	111.61
6	A	612	UQ5	O5-C5-C6	-3.06	116.04	121.67
6	A	612	UQ5	C1M-C1-C6	-3.04	118.16	124.20
6	B	615	UQ5	C25-C24-C26	2.98	119.92	115.39
6	A	612	UQ5	C17-C18-C19	2.96	134.19	127.80
5	A	611	FAD	C4X-C10-N1	2.92	125.65	122.73
5	B	614	FAD	C9A-C5X-N5	2.91	126.83	122.37
5	B	614	FAD	P-O3P-PA	2.89	140.15	131.68
5	B	614	FAD	C3B-C2B-C1B	2.80	105.29	100.91
6	B	615	UQ5	C1M-C1-C6	-2.80	118.65	124.20
5	A	611	FAD	P-O5'-C5'	2.79	142.10	122.03
5	A	611	FAD	C4A-C5A-N7A	2.79	111.91	109.52
6	B	615	UQ5	C25-C24-C23	-2.63	118.31	123.52
5	B	614	FAD	C8A-N9A-C4A	-2.61	104.91	106.90
5	A	611	FAD	O4'-C4'-C3'	2.59	115.51	109.05
2	A	617	BHG	C1'-O1-C1	-2.57	109.33	113.96
6	A	612	UQ5	O4-C4-C5	2.57	124.59	116.54
5	B	614	FAD	C6-C5X-N5	-2.50	116.06	118.97
6	A	612	UQ5	C1-C6-C5	-2.48	117.14	120.26
5	B	614	FAD	C4X-N5-C5X	-2.43	113.96	116.69
6	A	612	UQ5	C31-C29-C30	-2.42	108.44	114.62
6	A	612	UQ5	C10-C9-C8	-2.40	118.76	123.52
5	A	611	FAD	O4B-C1B-N9A	-2.40	106.20	108.44
2	A	617	BHG	O5-C1-O1	2.36	115.51	109.98
6	B	615	UQ5	O5-C5-C6	-2.35	117.35	121.67
6	B	615	UQ5	C4-C5-C6	2.32	123.47	117.35
2	B	618	BHG	C4'-C3'-C2'	2.29	127.01	114.61
6	B	615	UQ5	C4M-O4-C4	2.19	123.94	116.48
2	B	618	BHG	O1-C1-C2	2.18	110.96	108.18
5	A	611	FAD	O3B-C3B-C4B	-2.15	104.73	111.08
6	B	615	UQ5	O4-C4-C3	-2.11	115.44	123.80
5	B	614	FAD	C4B-O4B-C1B	2.08	112.01	109.75
5	A	611	FAD	C1'-N10-C9A	2.07	120.89	118.87
6	B	615	UQ5	C31-C29-C30	-2.05	109.38	114.62
6	A	612	UQ5	C17-C16-C14	2.02	119.43	112.74
2	A	617	BHG	C1-C2-C3	-2.01	106.09	110.00
2	A	617	BHG	C4'-C3'-C2'	2.01	125.46	114.61

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/584 (99%)	-0.22	10 (1%) 67 69	13, 30, 57, 84	0
1	B	578/584 (98%)	0.61	51 (8%) 10 9	38, 64, 79, 86	0
All	All	1159/1168 (99%)	0.20	61 (5%) 25 26	13, 49, 77, 86	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	CYS	7.5
1	B	176	GLY	5.1
1	B	540	GLN	5.0
1	A	540	GLN	4.8
1	B	390	LEU	4.7
1	A	6	VAL	4.6
1	A	7	PRO	4.4
1	B	7	PRO	4.4
1	A	389	ASN	4.3
1	B	389	ASN	4.2
1	B	502	ALA	4.2
1	B	27	VAL	3.8
1	B	537	PRO	3.5
1	B	100	GLU	3.5
1	B	538	LEU	3.4
1	B	61	HIS	3.4
1	A	5	LYS	3.4
1	B	388	GLU	3.4
1	B	8	ARG	3.3
1	B	32	PHE	3.3
1	B	499	ASP	3.2
1	B	498	HIS	3.1
1	B	24	TRP	3.1
1	B	382	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	535	PHE	3.0
1	B	22	LYS	3.0
1	B	212	ALA	2.9
1	B	539	GLU	2.9
1	B	172	PHE	2.8
1	B	26	GLY	2.7
1	B	19	ASP	2.7
1	B	395	ILE	2.5
1	B	541	GLY	2.5
1	A	391	GLN	2.5
1	B	20	GLN	2.5
1	B	496	HIS	2.5
1	B	43	ALA	2.5
1	B	62	GLU	2.5
1	B	536	VAL	2.4
1	A	388	GLU	2.4
1	B	391	GLN	2.4
1	B	165	TYR	2.4
1	B	495	ASN	2.4
1	B	155	GLU	2.3
1	A	8	ARG	2.3
1	B	157	LEU	2.3
1	B	16	TYR	2.3
1	B	501	PRO	2.2
1	B	15	ILE	2.2
1	B	75	HIS	2.2
1	B	174	GLU	2.2
1	A	539	GLU	2.2
1	B	68	CYS	2.2
1	B	33	ALA	2.1
1	B	161	VAL	2.1
1	B	28	ASN	2.1
1	B	551	GLN	2.1
1	B	38	VAL	2.1
1	B	30	GLU	2.1
1	B	181	ILE	2.1
1	B	41	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	EDO	A	627	4/4	0.52	19.46	57,58,58,58	0
2	BHG	A	617	18/18	0.56	19.34	55,75,78,79	0
2	BHG	A	616	18/18	0.39	18.21	52,76,78,79	0
7	EDO	A	622	4/4	0.40	14.27	51,55,55,57	0
2	BHG	B	618	18/18	0.35	12.96	61,76,78,78	0
7	EDO	A	623	4/4	0.43	12.67	48,49,49,53	0
7	EDO	A	621	4/4	0.28	8.19	45,47,48,49	0
7	EDO	A	624	4/4	0.31	7.40	35,41,42,42	0
7	EDO	A	619	4/4	0.23	6.70	37,37,38,43	0
7	EDO	A	628	4/4	0.34	3.85	53,54,55,55	0
6	UQ5	A	612	38/38	0.25	3.10	39,48,62,63	0
6	UQ5	B	615	38/38	0.27	2.32	51,56,68,71	0
4	SF4	A	610	8/8	0.13	1.48	16,19,22,22	0
7	EDO	A	626	4/4	0.15	1.28	43,45,45,46	0
7	EDO	A	625	4/4	0.16	1.07	49,55,55,57	0
7	EDO	B	620	4/4	0.17	0.80	49,53,54,56	0
5	FAD	A	611	53/53	0.16	-0.05	16,20,24,26	0
5	FAD	B	614	53/53	0.19	-0.25	44,60,68,69	0
3	NA	A	1070	1/1	0.07	-1.43	37,37,37,37	0
4	SF4	B	613	8/8	0.12	-1.74	55,58,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.