



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 1L8X / pdb_00001l8x
Title : Crystal Structure of Ferrochelatase from the Yeast, *Saccharomyces cerevisiae*, with Cobalt(II) as the Substrate Ion
Authors : Karlberg, T.; Lecerof, D.; Gora, M.; Silvegren, G.; Labbe-Bois, R.; Hansson, M.; Al-Karadaghi, S.
Deposited on : 2002-03-22
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

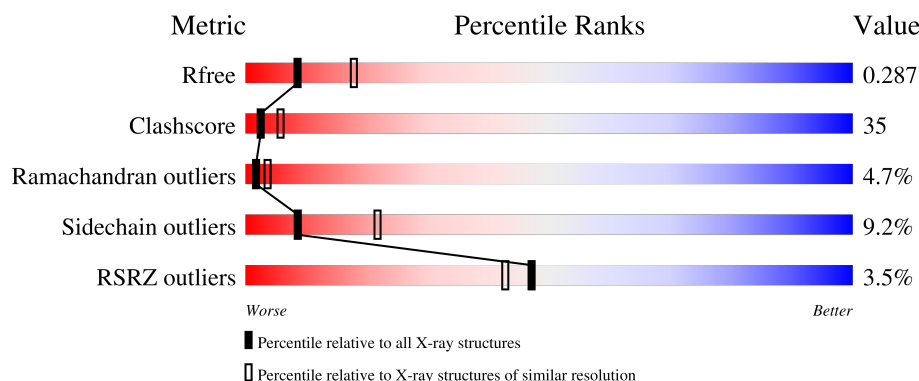
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	362	
1	B	362	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5675 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 Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2835	1828	468	529	10			
1	B	354	Total	C	N	O	S	0	0	0
			2829	1825	467	527	10			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		

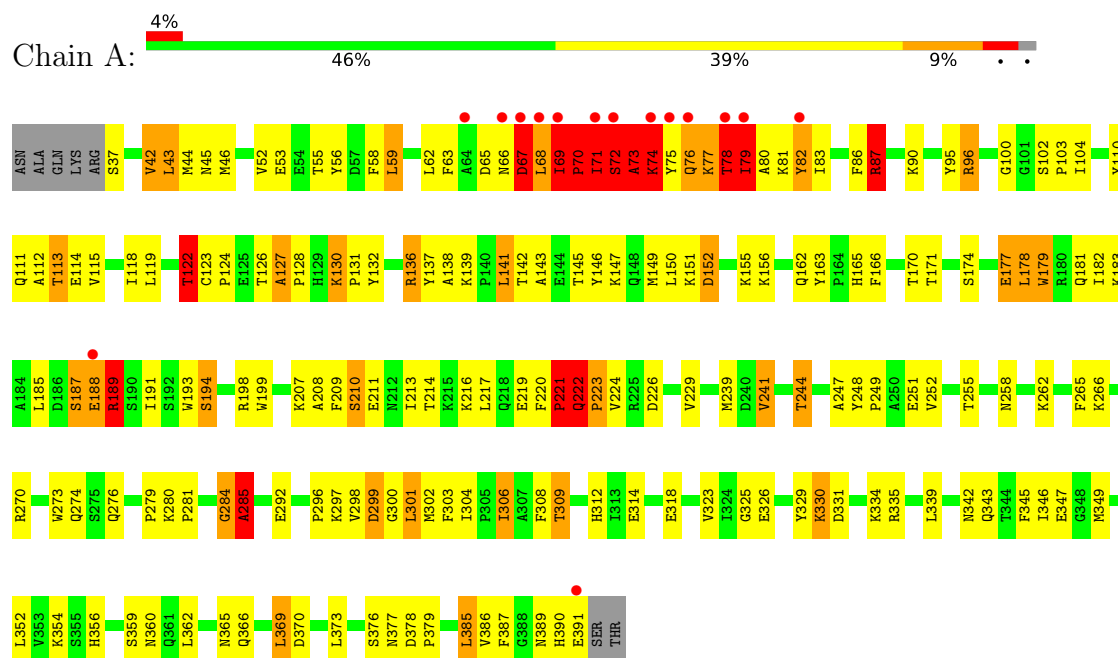
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	9	Total	O	0	0
			9	9		

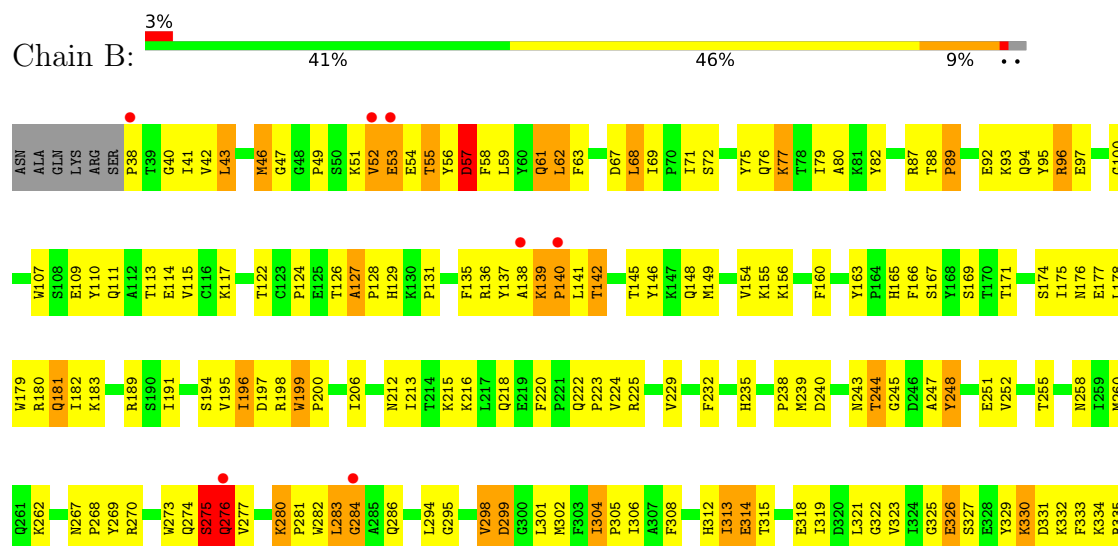
3 Residue-property plots

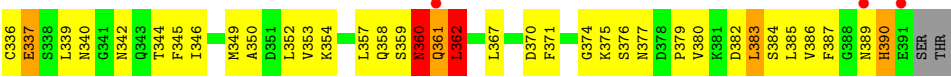
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Ferrochelatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.38Å 96.66Å 120.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.9 (15.00-2.70) 98.8 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.287 0.236 , 0.287	Depositor DCC
R_{free} test set	2235 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5675	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 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.68	8/2908 (0.3%)	1.32	49/3941 (1.2%)
1	B	0.62	4/2902 (0.1%)	1.16	26/3932 (0.7%)
All	All	0.65	12/5810 (0.2%)	1.24	75/7873 (1.0%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ILE	CA-C	11.35	1.64	1.52
1	A	70	PRO	N-CA	10.59	1.60	1.47
1	B	314	GLU	N-CA	-10.07	1.33	1.46
1	B	314	GLU	CA-CB	-9.98	1.38	1.53
1	B	313	ILE	C-N	-9.01	1.21	1.33
1	A	79	ILE	N-CA	7.38	1.55	1.46
1	A	70	PRO	CA-C	6.18	1.61	1.52
1	A	78	THR	CA-C	5.80	1.60	1.52
1	A	68	LEU	C-N	5.30	1.39	1.33
1	A	78	THR	C-N	5.30	1.40	1.33
1	A	78	THR	N-CA	-5.27	1.39	1.46
1	B	315	THR	N-CA	-5.23	1.40	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLU	N-CA-C	-16.05	90.41	114.16
1	A	77	LYS	N-CA-C	-14.43	94.00	112.90
1	A	71	ILE	CA-C-N	-13.29	96.15	121.54
1	A	71	ILE	C-N-CA	-13.29	96.15	121.54
1	A	75	TYR	N-CA-C	-11.45	100.05	113.21
1	A	210	SER	N-CA-C	-10.60	97.05	110.19
1	B	314	GLU	N-CA-CB	-10.11	95.71	110.47
1	B	274	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	B	276	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	A	284	GLY	N-CA-C	9.38	122.65	112.33
1	A	76	GLN	OE1-CD-NE2	-9.31	113.29	122.60
1	A	241	VAL	N-CA-C	-9.06	104.51	112.12
1	A	74	LYS	CA-C-N	-8.70	104.89	122.55
1	A	74	LYS	C-N-CA	-8.70	104.89	122.55
1	B	283	LEU	N-CA-C	8.62	121.01	110.41
1	A	75	TYR	N-CA-CB	8.42	122.77	110.57
1	A	75	TYR	CA-CB-CG	-8.20	99.15	113.90
1	A	187	SER	N-CA-C	-8.17	100.36	110.41
1	A	72	SER	CA-C-N	8.13	137.06	121.54
1	A	72	SER	C-N-CA	8.13	137.06	121.54
1	A	70	PRO	N-CA-C	7.89	128.73	112.47
1	B	362	LEU	N-CA-C	-7.43	104.22	113.28
1	B	244	THR	N-CA-C	-7.39	104.06	113.23
1	A	71	ILE	CB-CA-C	7.25	123.18	111.29
1	A	76	GLN	CG-CD-NE2	7.03	126.95	116.40
1	B	274	GLN	CG-CD-NE2	6.84	126.66	116.40
1	B	275	SER	N-CA-C	6.84	125.36	110.80
1	B	199	TRP	CA-C-N	6.69	126.94	119.32
1	B	199	TRP	C-N-CA	6.69	126.94	119.32
1	A	309	THR	N-CA-C	6.62	120.67	112.59
1	A	70	PRO	CA-N-CD	-6.55	102.82	112.00
1	A	306	ILE	N-CA-C	6.50	118.03	110.62
1	A	37	SER	CA-C-N	6.43	126.38	119.76
1	A	37	SER	C-N-CA	6.43	126.38	119.76
1	B	57	ASP	N-CA-C	-6.19	97.61	110.80
1	A	126	THR	N-CA-C	-6.17	103.05	111.56
1	A	189	ARG	N-CA-C	6.16	123.92	110.80
1	B	248	TYR	N-CA-C	6.13	120.83	112.55
1	B	252	VAL	N-CA-C	-6.10	104.40	110.62
1	A	223	PRO	N-CA-C	-6.09	106.89	114.20
1	B	276	GLN	CG-CD-NE2	6.08	125.53	116.40
1	A	152	ASP	N-CA-C	-6.06	104.52	113.61
1	A	87	ARG	N-CA-C	6.00	119.86	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	VAL	N-CA-C	5.95	118.26	108.99
1	A	42	VAL	N-CA-C	5.94	116.36	107.51
1	A	285	ALA	N-CA-C	-5.93	98.17	110.80
1	A	130	LYS	CA-C-N	5.87	127.45	120.23
1	A	130	LYS	C-N-CA	5.87	127.45	120.23
1	A	67	ASP	N-CA-C	-5.87	104.71	112.34
1	A	72	SER	N-CA-C	5.78	123.10	110.80
1	A	78	THR	N-CA-C	-5.68	98.69	110.80
1	A	194	SER	N-CA-C	-5.50	101.00	109.52
1	B	196	ILE	N-CA-C	-5.46	98.58	106.88
1	B	195	VAL	N-CA-C	5.46	117.25	108.85
1	B	145	THR	N-CA-C	5.36	117.20	111.36
1	A	122	THR	N-CA-C	5.32	116.89	111.14
1	A	96	ARG	N-CA-C	-5.32	105.48	111.28
1	A	76	GLN	N-CA-C	5.29	118.80	111.71
1	B	314	GLU	CB-CA-C	5.27	118.46	109.24
1	B	304	ILE	CA-C-N	5.27	126.42	119.84
1	B	304	ILE	C-N-CA	5.27	126.42	119.84
1	B	344	THR	N-CA-C	-5.23	105.58	111.28
1	A	77	LYS	CA-C-N	-5.22	111.58	121.54
1	A	77	LYS	C-N-CA	-5.22	111.58	121.54
1	A	326	GLU	N-CA-C	5.20	118.76	112.93
1	A	214	THR	N-CA-C	-5.18	105.72	111.36
1	A	77	LYS	CA-C-O	5.15	125.63	119.60
1	B	299	ASP	N-CA-C	-5.15	106.16	112.90
1	A	74	LYS	CB-CA-C	5.15	120.66	110.42
1	B	377	ASN	N-CA-C	-5.15	106.85	113.23
1	A	76	GLN	CA-CB-CG	-5.14	103.81	114.10
1	A	73	ALA	CA-C-N	5.14	131.36	121.54
1	A	73	ALA	C-N-CA	5.14	131.36	121.54
1	B	42	VAL	N-CA-C	5.06	114.89	107.15
1	A	314	GLU	N-CA-C	5.04	116.77	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2835	0	2828	187	0
1	B	2829	0	2824	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	9	0	0	3	0
All	All	5675	0	5652	394	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 35.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:O	1:A:72:SER:CB	1.79	1.19
1:A:76:GLN:CG	1:A:79:ILE:HG22	1.79	1.11
1:B:46:MET:HG3	1:B:163:TYR:OH	1.50	1.11
1:B:308:PHE:CD2	1:B:312:HIS:CD2	2.40	1.10
1:B:139:LYS:HB3	1:B:140:PRO:HD3	1.28	1.08
1:A:284:GLY:HA3	1:B:243:ASN:OD1	1.58	1.03
1:A:76:GLN:HG3	1:A:79:ILE:CG2	1.87	1.02
1:A:127:ALA:HB3	1:A:128:PRO:HD3	1.41	1.01
1:B:362:LEU:H	1:B:362:LEU:HD12	1.21	1.00
1:A:298:VAL:HG12	1:A:300:GLY:H	1.28	0.98
1:A:76:GLN:HG3	1:A:79:ILE:HG22	1.38	0.97
1:B:127:ALA:HB1	1:B:128:PRO:CD	1.96	0.95
1:B:46:MET:CG	1:B:163:TYR:OH	2.14	0.95
1:B:68:LEU:HD13	1:B:69:ILE:HG13	1.47	0.94
1:A:71:ILE:O	1:A:72:SER:HB3	1.13	0.94
1:A:274:GLN:HA	1:A:276:GLN:HE22	1.32	0.94
1:B:127:ALA:HB1	1:B:128:PRO:HD3	1.47	0.92
1:B:139:LYS:HB3	1:B:140:PRO:CD	2.00	0.92
1:B:308:PHE:CE2	1:B:312:HIS:HD2	1.87	0.91
1:B:308:PHE:CE2	1:B:312:HIS:CD2	2.58	0.91
1:A:70:PRO:CG	1:A:76:GLN:OE1	2.20	0.90
1:A:78:THR:O	1:A:80:ALA:N	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:MET:HE3	1:B:336:CYS:HB2	1.56	0.87
1:B:308:PHE:CD2	1:B:312:HIS:NE2	2.42	0.86
1:A:127:ALA:CB	1:A:128:PRO:HD3	2.08	0.84
1:B:283:LEU:HD12	1:B:284:GLY:H	1.44	0.81
1:B:325:GLY:HA2	1:B:330:LYS:HD2	1.61	0.80
1:A:70:PRO:HG2	1:A:76:GLN:OE1	1.79	0.80
1:A:155:LYS:HG3	1:A:156:LYS:H	1.48	0.79
1:B:43:LEU:HD22	1:B:160:PHE:HD2	1.47	0.78
1:B:139:LYS:O	1:B:141:LEU:N	2.16	0.77
1:B:176:ASN:HD22	1:B:380:VAL:HG23	1.49	0.77
1:A:229:VAL:HG12	1:A:301:LEU:HD12	1.65	0.77
1:A:221:PRO:O	1:A:222:GLN:HB3	1.84	0.76
1:A:210:SER:O	1:A:211:GLU:HB2	1.85	0.75
1:A:155:LYS:HG3	1:A:156:LYS:N	2.02	0.75
1:A:43:LEU:HG	1:A:112:ALA:HB2	1.69	0.74
1:A:69:ILE:HB	1:A:70:PRO:HD2	1.69	0.74
1:B:176:ASN:ND2	1:B:380:VAL:HG23	2.03	0.73
1:A:130:LYS:HB3	1:A:132:TYR:HE2	1.54	0.72
1:A:189:ARG:HG3	1:A:390:HIS:HB2	1.69	0.72
1:A:296:PRO:HG3	1:A:329:TYR:OH	1.90	0.72
1:B:149:MET:O	1:B:154:VAL:HG22	1.90	0.72
1:A:229:VAL:CG1	1:A:301:LEU:HD12	2.20	0.72
1:B:224:VAL:HG11	1:B:299:ASP:HB3	1.72	0.72
1:B:283:LEU:CD1	1:B:284:GLY:H	2.04	0.71
1:A:132:TYR:CE1	1:A:149:MET:HG2	2.25	0.71
1:A:70:PRO:HG3	1:A:76:GLN:OE1	1.88	0.71
1:B:181:GLN:HA	1:B:181:GLN:OE1	1.89	0.71
1:B:361:GLN:OE1	1:B:361:GLN:HA	1.90	0.71
1:A:76:GLN:CD	1:A:79:ILE:HG22	2.15	0.71
1:B:198:ARG:NH2	1:B:370:ASP:OD2	2.23	0.70
1:A:187:SER:C	1:A:188:GLU:HG3	2.14	0.70
1:B:376:SER:HB3	1:B:379:PRO:HG3	1.72	0.70
1:A:248:TYR:HB3	1:A:249:PRO:HD3	1.72	0.70
1:B:136:ARG:HG3	1:B:137:TYR:CE2	2.27	0.70
1:A:389:ASN:ND2	1:A:391:GLU:H	1.89	0.70
1:B:224:VAL:CG1	1:B:299:ASP:HB3	2.22	0.70
1:A:122:THR:HG23	1:A:354:LYS:HD2	1.74	0.69
1:A:77:LYS:C	1:A:78:THR:O	2.35	0.69
1:B:127:ALA:CB	1:B:128:PRO:CD	2.71	0.69
1:B:38:PRO:O	1:B:155:LYS:HG2	1.92	0.69
1:A:69:ILE:HG22	1:A:70:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB3	1:B:154:VAL:HG21	1.74	0.69
1:B:273:TRP:CD1	1:B:284:GLY:HA3	2.28	0.68
1:A:74:LYS:C	1:A:76:GLN:H	2.01	0.68
1:B:308:PHE:HD2	1:B:312:HIS:CD2	2.09	0.68
1:A:165:HIS:HE1	1:A:255:THR:OG1	1.75	0.68
1:B:329:TYR:CD2	1:B:332:LYS:HD2	2.29	0.68
1:A:132:TYR:CD1	1:A:149:MET:HG2	2.28	0.68
1:B:312:HIS:ND1	1:B:314:GLU:HB2	2.10	0.67
1:B:53:GLU:HG2	1:B:92:GLU:OE2	1.93	0.67
1:A:221:PRO:HB2	1:A:224:VAL:HG12	1.78	0.66
1:B:283:LEU:HG	1:B:284:GLY:N	2.10	0.66
1:B:52:VAL:HG21	1:B:96:ARG:HG3	1.78	0.66
1:B:46:MET:HG3	1:B:163:TYR:HH	1.58	0.65
1:A:66:ASN:C	1:A:68:LEU:N	2.53	0.65
1:B:277:VAL:O	1:B:280:LYS:HE2	1.96	0.65
1:B:362:LEU:H	1:B:362:LEU:CD1	1.95	0.64
1:B:260:MET:HE2	1:B:269:TYR:CD2	2.32	0.64
1:B:308:PHE:CD2	1:B:312:HIS:HD2	1.97	0.64
1:A:179:TRP:CE2	1:A:183:LYS:HD2	2.33	0.64
1:A:76:GLN:O	1:A:76:GLN:HG2	1.97	0.63
1:A:74:LYS:C	1:A:76:GLN:N	2.51	0.63
1:A:122:THR:HG22	1:A:123:CYS:SG	2.39	0.63
1:A:221:PRO:O	1:A:222:GLN:CB	2.46	0.63
1:B:367:LEU:HG	1:B:383:LEU:HD21	1.81	0.63
1:B:312:HIS:CE1	1:B:314:GLU:OE1	2.52	0.62
1:B:382:ASP:OD2	1:B:384:SER:HB3	2.00	0.62
1:A:122:THR:CG2	1:A:354:LYS:HD2	2.29	0.62
1:B:283:LEU:CG	1:B:284:GLY:N	2.63	0.62
1:A:111:GLN:HB3	1:A:349:MET:HE1	1.81	0.62
1:A:136:ARG:HG3	1:A:137:TYR:CE2	2.35	0.62
1:B:177:GLU:HG2	1:B:180:ARG:NH2	2.15	0.62
1:B:327:SER:C	1:B:329:TYR:H	2.08	0.62
1:B:342:ASN:HD22	1:B:345:PHE:H	1.48	0.61
1:A:274:GLN:CA	1:A:276:GLN:HE22	2.11	0.61
1:B:374:GLY:O	1:B:375:LYS:HD3	2.00	0.61
1:A:366:GLN:OE1	1:B:268:PRO:HA	2.00	0.61
1:B:222:GLN:HB3	1:B:223:PRO:HD3	1.83	0.61
1:B:165:HIS:HE1	1:B:255:THR:OG1	1.83	0.61
1:A:123:CYS:SG	1:A:354:LYS:HG3	2.41	0.61
1:A:247:ALA:O	1:A:251:GLU:HG3	2.01	0.61
1:B:280:LYS:H	1:B:280:LYS:HD3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:O	1:B:175:ILE:HG13	2.00	0.60
1:B:262:LYS:O	1:B:262:LYS:HD3	2.02	0.60
1:B:52:VAL:HG21	1:B:96:ARG:HD2	1.81	0.60
1:B:72:SER:H	1:B:76:GLN:NE2	2.00	0.60
1:B:212:ASN:ND2	1:B:337:GLU:HB3	2.16	0.60
1:A:77:LYS:O	1:A:78:THR:O	2.19	0.60
1:B:199:TRP:N	1:B:200:PRO:HD3	2.17	0.60
1:A:44:MET:HE2	1:A:174:SER:HB3	1.84	0.59
1:B:46:MET:HG2	1:B:163:TYR:OH	2.02	0.59
1:B:51:LYS:O	1:B:53:GLU:N	2.36	0.59
1:A:274:GLN:HA	1:A:276:GLN:NE2	2.10	0.59
1:B:49:PRO:HD2	1:B:95:TYR:CE1	2.37	0.59
1:B:68:LEU:HD22	1:B:169:SER:HB3	1.84	0.59
1:A:373:LEU:HD11	1:B:294:LEU:HD21	1.83	0.59
1:B:312:HIS:HE1	1:B:314:GLU:OE1	1.84	0.59
1:B:329:TYR:HD2	1:B:332:LYS:HD2	1.67	0.59
1:A:222:GLN:C	1:A:224:VAL:H	2.09	0.58
1:A:70:PRO:HG2	1:A:76:GLN:HE22	1.68	0.58
1:B:276:GLN:HE22	1:B:286:GLN:HG2	1.69	0.58
1:A:369:LEU:CD2	1:A:373:LEU:HD13	2.33	0.58
1:B:43:LEU:HD22	1:B:160:PHE:CD2	2.33	0.58
1:B:360:ASN:H	1:B:360:ASN:ND2	2.02	0.58
1:B:362:LEU:HD22	1:B:387:PHE:O	2.04	0.58
1:A:127:ALA:HB3	1:A:128:PRO:CD	2.24	0.57
1:B:235:HIS:CE1	1:B:275:SER:HB3	2.39	0.57
1:B:47:GLY:HA3	1:B:138:ALA:HB3	1.86	0.57
1:A:70:PRO:HG2	1:A:76:GLN:NE2	2.19	0.57
1:B:53:GLU:OE1	1:B:53:GLU:C	2.47	0.57
1:B:67:ASP:O	1:B:169:SER:HA	2.04	0.57
1:B:94:GLN:HE21	1:B:313:ILE:HD11	1.70	0.57
1:A:142:THR:HG22	1:A:181:GLN:HG3	1.87	0.57
1:A:194:SER:OG	1:A:356:HIS:HE1	1.88	0.57
1:A:389:ASN:HD22	1:A:390:HIS:N	2.03	0.57
1:A:136:ARG:NH1	1:A:177:GLU:HG2	2.21	0.56
1:B:275:SER:HA	1:B:318:GLU:OE2	2.05	0.56
1:A:376:SER:HB3	1:A:379:PRO:HG3	1.87	0.56
1:A:69:ILE:CB	1:A:70:PRO:HD2	2.36	0.56
1:B:52:VAL:HG11	1:B:96:ARG:HD2	1.88	0.56
1:A:56:TYR:OH	1:A:81:LYS:HD2	2.06	0.56
1:B:213:ILE:HA	1:B:302:MET:HE1	1.88	0.56
1:A:224:VAL:HG21	1:A:299:ASP:CG	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LEU:HD22	1:B:137:TYR:CD1	2.41	0.55
1:B:38:PRO:HB2	1:B:155:LYS:HD2	1.87	0.55
1:B:40:GLY:C	1:B:41:ILE:HD12	2.31	0.55
1:B:113:THR:HG22	1:B:131:PRO:HG3	1.88	0.55
1:A:255:THR:CG2	1:A:306:ILE:HD11	2.36	0.55
1:A:110:TYR:O	1:A:113:THR:HG22	2.07	0.55
1:A:343:GLN:O	1:A:347:GLU:HG3	2.07	0.55
1:B:113:THR:HG22	1:B:131:PRO:CG	2.36	0.55
1:B:213:ILE:HG23	1:B:302:MET:HE1	1.89	0.55
1:B:197:ASP:O	1:B:198:ARG:HB3	2.06	0.55
1:A:55:THR:HG22	1:A:59:LEU:HD22	1.89	0.55
1:A:111:GLN:O	1:A:115:VAL:HG23	2.07	0.55
1:A:71:ILE:HD13	1:A:72:SER:H	1.72	0.54
1:A:66:ASN:C	1:A:68:LEU:H	2.15	0.54
1:A:217:LEU:O	1:A:220:PHE:HB2	2.06	0.54
1:B:49:PRO:HD2	1:B:95:TYR:CZ	2.41	0.54
1:A:378:ASP:N	1:A:379:PRO:HD3	2.23	0.54
1:A:65:ASP:OD2	1:A:67:ASP:HB2	2.08	0.54
1:A:303:PHE:CE2	1:A:323:VAL:HG11	2.43	0.54
1:B:179:TRP:CE3	1:B:386:VAL:HG22	2.43	0.53
1:B:71:ILE:H	1:B:76:GLN:HE22	1.56	0.53
1:B:182:ILE:HG21	1:B:189:ARG:NH1	2.24	0.53
1:A:141:LEU:N	1:A:141:LEU:HD22	2.24	0.53
1:A:70:PRO:HG2	1:A:76:GLN:CD	2.34	0.53
1:A:198:ARG:NH2	1:A:370:ASP:OD2	2.37	0.53
1:A:222:GLN:HB3	1:A:223:PRO:HD3	1.91	0.53
1:A:247:ALA:HB2	1:B:270:ARG:NH1	2.24	0.53
1:B:206:ILE:HG13	1:B:258:ASN:ND2	2.23	0.53
1:A:222:GLN:C	1:A:224:VAL:N	2.67	0.52
1:B:49:PRO:HD2	1:B:95:TYR:OH	2.09	0.52
1:A:373:LEU:CD1	1:B:294:LEU:HD21	2.38	0.52
1:B:206:ILE:HG13	1:B:258:ASN:HD22	1.74	0.52
1:A:69:ILE:HG22	1:A:70:PRO:CD	2.40	0.52
1:A:76:GLN:HG2	1:A:79:ILE:HG22	1.85	0.52
1:A:229:VAL:CG1	1:A:301:LEU:CD1	2.87	0.52
1:B:283:LEU:CG	1:B:284:GLY:H	2.22	0.52
1:B:337:GLU:HA	3:B:8:HOH:O	2.08	0.52
1:B:342:ASN:HB3	1:B:345:PHE:HB3	1.92	0.52
1:B:52:VAL:HG21	1:B:96:ARG:CD	2.40	0.52
1:B:149:MET:HB3	1:B:154:VAL:CG2	2.40	0.51
1:B:319:ILE:HG21	1:B:335:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PHE:CE2	1:A:87:ARG:NH1	2.78	0.51
1:B:280:LYS:HG2	1:B:282:TRP:HE1	1.75	0.51
1:B:322:GLY:O	1:B:326:GLU:HB2	2.11	0.51
1:A:309:THR:HG22	1:A:339:LEU:HD12	1.93	0.51
1:B:167:SER:HB2	1:B:248:TYR:HB2	1.91	0.51
1:A:298:VAL:HG12	1:A:299:ASP:N	2.26	0.51
1:A:181:GLN:HA	1:A:181:GLN:NE2	2.25	0.51
1:A:339:LEU:HD13	1:A:345:PHE:CD2	2.46	0.51
1:A:298:VAL:HG12	1:A:300:GLY:N	2.12	0.51
1:B:318:GLU:O	1:B:323:VAL:HG23	2.11	0.50
1:B:213:ILE:CD1	1:B:304:ILE:HD13	2.41	0.50
1:B:77:LYS:O	1:B:80:ALA:HB3	2.12	0.50
1:B:273:TRP:NE1	1:B:284:GLY:HA3	2.25	0.50
1:A:284:GLY:O	1:A:285:ALA:HB3	2.11	0.50
1:A:325:GLY:O	1:A:330:LYS:HE2	2.12	0.50
1:B:114:GLU:OE1	1:B:117:LYS:HE3	2.11	0.50
1:B:122:THR:CG2	1:B:354:LYS:HD2	2.42	0.50
1:B:160:PHE:CD1	1:B:196:ILE:HD12	2.47	0.50
1:B:314:GLU:O	1:B:318:GLU:HB2	2.12	0.50
1:B:329:TYR:O	1:B:331:ASP:N	2.45	0.50
1:A:362:LEU:N	1:A:362:LEU:HD12	2.27	0.50
1:B:47:GLY:HA3	1:B:138:ALA:CB	2.42	0.49
1:B:206:ILE:HG21	1:B:258:ASN:HD22	1.77	0.49
1:A:131:PRO:C	1:A:132:TYR:HD2	2.20	0.49
1:A:217:LEU:HG	1:A:302:MET:HE1	1.94	0.49
1:A:377:ASN:C	1:A:379:PRO:HD3	2.36	0.49
1:B:52:VAL:HG21	1:B:96:ARG:CG	2.42	0.49
1:A:146:TYR:HB3	1:A:185:LEU:HD12	1.93	0.49
1:A:209:PHE:C	1:A:210:SER:O	2.50	0.49
1:B:75:TYR:O	1:B:79:ILE:HG13	2.12	0.49
1:A:76:GLN:HG3	1:A:79:ILE:CB	2.43	0.49
1:A:179:TRP:CE3	1:A:179:TRP:HA	2.48	0.49
1:A:138:ALA:O	1:A:141:LEU:HD13	2.13	0.49
1:A:179:TRP:HA	1:A:179:TRP:HE3	1.76	0.49
1:B:57:ASP:O	1:B:61:GLN:HB2	2.13	0.49
1:B:276:GLN:NE2	1:B:286:GLN:HG2	2.28	0.49
1:B:213:ILE:HD11	1:B:304:ILE:HD13	1.95	0.49
1:B:385:LEU:HD23	1:B:385:LEU:O	2.13	0.49
1:B:122:THR:HG21	1:B:354:LYS:HD2	1.94	0.49
1:A:127:ALA:CB	1:A:128:PRO:CD	2.78	0.48
1:A:81:LYS:O	1:A:83:ILE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TRP:CZ3	1:B:340:ASN:HB3	2.48	0.48
1:B:189:ARG:CB	1:B:390:HIS:O	2.61	0.48
1:B:225:ARG:O	1:B:267:ASN:ND2	2.45	0.48
1:A:53:GLU:H	1:A:53:GLU:CD	2.21	0.48
1:A:229:VAL:O	1:A:229:VAL:HG13	2.14	0.48
1:B:38:PRO:HB2	1:B:155:LYS:CD	2.43	0.48
1:A:122:THR:C	1:A:124:PRO:HD3	2.38	0.48
1:B:122:THR:C	1:B:124:PRO:HD3	2.38	0.48
1:B:238:PRO:HG3	1:B:282:TRP:CZ2	2.48	0.48
1:B:298:VAL:HG21	1:B:301:LEU:HG	1.95	0.48
1:B:367:LEU:O	1:B:370:ASP:HB2	2.14	0.48
1:A:81:LYS:O	1:A:82:TYR:C	2.55	0.48
1:A:147:LYS:HG3	1:A:185:LEU:HD13	1.96	0.48
1:B:43:LEU:HD23	1:B:43:LEU:N	2.29	0.48
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.78	0.48
1:B:178:LEU:O	1:B:182:ILE:HG13	2.14	0.47
1:B:327:SER:O	1:B:330:LYS:HG2	2.14	0.47
1:A:220:PHE:CE1	1:A:334:LYS:HD2	2.49	0.47
1:A:239:MET:HE2	1:B:239:MET:SD	2.54	0.47
1:B:88:THR:O	1:B:92:GLU:HB2	2.15	0.47
1:B:107:TRP:O	1:B:111:GLN:HG3	2.15	0.47
1:A:142:THR:CG2	1:A:181:GLN:HG3	2.45	0.47
1:B:312:HIS:CE1	1:B:314:GLU:HB2	2.50	0.47
1:B:321:LEU:O	1:B:325:GLY:O	2.33	0.47
1:A:131:PRO:C	1:A:132:TYR:CD2	2.92	0.46
1:A:274:GLN:HB2	1:A:318:GLU:OE2	2.14	0.46
1:A:145:THR:O	1:A:149:MET:HG3	2.15	0.46
1:A:273:TRP:N	1:A:273:TRP:CD1	2.84	0.46
1:B:194:SER:HB2	1:B:362:LEU:HA	1.96	0.46
1:A:141:LEU:HD22	1:A:141:LEU:H	1.80	0.46
1:A:276:GLN:NE2	1:A:276:GLN:H	2.14	0.46
1:A:342:ASN:O	1:A:346:ILE:HG12	2.15	0.46
1:B:59:LEU:O	1:B:63:PHE:HD1	1.98	0.46
1:B:179:TRP:CD2	1:B:386:VAL:HG22	2.51	0.46
1:A:69:ILE:CB	1:A:70:PRO:CD	2.93	0.46
1:A:86:PHE:CE2	1:A:87:ARG:CZ	2.99	0.46
1:A:389:ASN:HD22	1:A:389:ASN:C	2.24	0.46
1:B:52:VAL:O	1:B:52:VAL:CG1	2.64	0.46
1:B:224:VAL:HG13	1:B:299:ASP:HB3	1.97	0.46
1:A:165:HIS:CE1	1:A:252:VAL:HA	2.50	0.46
1:B:362:LEU:HD12	1:B:362:LEU:N	2.06	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:C	1:A:83:ILE:N	2.73	0.46
1:A:69:ILE:H	1:A:69:ILE:HG12	1.32	0.46
1:B:56:TYR:C	1:B:56:TYR:CD2	2.94	0.46
1:A:146:TYR:CE2	1:A:191:ILE:HD12	2.51	0.46
1:A:284:GLY:HA3	1:B:243:ASN:CG	2.37	0.46
1:A:330:LYS:HB2	1:A:330:LYS:HE3	1.64	0.46
1:B:69:ILE:HG22	1:B:71:ILE:HG12	1.98	0.46
1:B:360:ASN:O	1:B:361:GLN:O	2.34	0.46
1:B:136:ARG:HG3	1:B:137:TYR:CD2	2.51	0.45
1:A:189:ARG:NH1	1:A:385:LEU:O	2.47	0.45
1:A:224:VAL:HG22	1:A:224:VAL:O	2.16	0.45
1:B:327:SER:C	1:B:329:TYR:N	2.72	0.45
1:A:43:LEU:HD12	1:A:162:GLN:NE2	2.32	0.45
1:B:294:LEU:O	1:B:295:GLY:C	2.59	0.45
1:B:332:LYS:C	1:B:333:PHE:HD1	2.24	0.45
1:A:166:PHE:CD1	1:A:171:THR:HB	2.51	0.45
1:A:79:ILE:O	1:A:83:ILE:HG13	2.16	0.45
1:A:226:ASP:OD1	1:A:266:LYS:HD3	2.16	0.45
1:A:292:GLU:OE1	1:A:292:GLU:HA	2.15	0.45
1:B:95:TYR:O	1:B:100:GLY:N	2.49	0.45
1:B:220:PHE:CE1	1:B:334:LYS:HD2	2.51	0.45
1:A:46:MET:HE2	1:A:46:MET:N	2.32	0.45
1:A:76:GLN:HG3	1:A:79:ILE:HG21	1.91	0.45
1:A:143:ALA:HB2	1:A:181:GLN:CD	2.42	0.45
1:A:385:LEU:O	1:A:385:LEU:HD23	2.17	0.45
1:B:109:GLU:O	1:B:113:THR:HG23	2.16	0.45
1:B:325:GLY:HA2	1:B:330:LYS:CD	2.39	0.45
1:B:389:ASN:O	1:B:390:HIS:C	2.60	0.45
1:A:72:SER:OG	1:A:73:ALA:N	2.35	0.45
1:A:76:GLN:CG	1:A:76:GLN:O	2.57	0.45
1:B:166:PHE:CD2	1:B:167:SER:N	2.85	0.45
1:B:229:VAL:HB	1:B:301:LEU:HD23	1.99	0.45
1:A:42:VAL:HA	1:A:132:TYR:O	2.18	0.44
1:B:72:SER:H	1:B:76:GLN:HE22	1.62	0.44
1:B:213:ILE:HG12	1:B:302:MET:CE	2.47	0.44
1:A:187:SER:O	1:A:188:GLU:HG3	2.16	0.44
1:A:102:SER:OG	1:A:104:ILE:HG13	2.16	0.44
1:A:151:LYS:HD2	1:A:151:LYS:HA	1.72	0.44
1:A:189:ARG:NH2	1:A:386:VAL:O	2.50	0.44
1:B:93:LYS:HE3	1:B:97:GLU:OE1	2.18	0.44
1:B:166:PHE:CD2	1:B:166:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HG22	1:A:306:ILE:HD11	1.99	0.44
1:B:139:LYS:CB	1:B:140:PRO:CD	2.82	0.44
1:A:222:GLN:CB	1:A:223:PRO:HD3	2.48	0.44
1:A:213:ILE:HD11	1:A:304:ILE:HD13	1.98	0.44
1:B:154:VAL:HG23	1:B:191:ILE:HG12	2.00	0.43
1:A:208:ALA:O	1:A:210:SER:O	2.36	0.43
1:A:241:VAL:O	1:A:244:THR:HB	2.18	0.43
1:A:44:MET:CE	1:A:174:SER:HB3	2.47	0.43
1:A:219:GLU:O	1:A:334:LYS:HE3	2.18	0.43
1:B:41:ILE:HD12	1:B:41:ILE:N	2.33	0.43
1:A:297:LYS:HB3	1:A:297:LYS:HE2	1.86	0.43
1:B:224:VAL:HG13	1:B:299:ASP:CB	2.48	0.43
1:B:380:VAL:HG11	1:B:383:LEU:HD12	2.00	0.43
1:A:136:ARG:CZ	1:A:177:GLU:HG2	2.47	0.43
1:A:199:TRP:CD1	1:A:199:TRP:N	2.85	0.43
1:A:362:LEU:HD23	1:A:387:PHE:C	2.44	0.43
1:B:276:GLN:H	1:B:276:GLN:HG3	1.32	0.43
1:B:304:ILE:C	1:B:306:ILE:H	2.27	0.43
1:A:308:PHE:CD2	1:A:312:HIS:CE1	3.07	0.43
1:B:136:ARG:HG3	1:B:136:ARG:NH1	2.33	0.43
1:B:215:LYS:HD2	3:B:6:HOH:O	2.18	0.43
1:B:232:PHE:HE1	1:B:269:TYR:HB2	1.84	0.43
1:A:115:VAL:O	1:A:119:LEU:HG	2.18	0.43
1:B:55:THR:O	1:B:58:PHE:N	2.48	0.43
1:B:189:ARG:HB3	1:B:390:HIS:O	2.18	0.43
1:A:298:VAL:CG1	1:A:299:ASP:N	2.82	0.43
1:A:359:SER:O	1:A:360:ASN:HB2	2.18	0.43
1:B:52:VAL:O	1:B:92:GLU:HG3	2.18	0.43
1:B:138:ALA:O	1:B:139:LYS:C	2.62	0.43
1:B:357:LEU:C	1:B:359:SER:H	2.27	0.43
1:B:367:LEU:CG	1:B:383:LEU:HD21	2.49	0.43
1:B:51:LYS:C	1:B:53:GLU:N	2.77	0.42
1:B:126:THR:OG1	1:B:129:HIS:NE2	2.43	0.42
1:B:141:LEU:O	1:B:142:THR:C	2.62	0.42
1:A:86:PHE:CD2	1:A:87:ARG:HD3	2.54	0.42
1:A:198:ARG:HD3	1:A:251:GLU:OE2	2.19	0.42
1:A:76:GLN:OE1	1:A:79:ILE:CG2	2.67	0.42
1:B:135:PHE:HB3	1:B:138:ALA:HB3	2.00	0.42
1:B:280:LYS:H	1:B:280:LYS:CD	2.31	0.42
1:A:193:TRP:O	1:A:387:PHE:HB3	2.19	0.42
1:B:182:ILE:CG2	1:B:189:ARG:NH1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:CZ	1:B:114:GLU:HG3	2.55	0.42
1:B:216:LYS:HD3	3:B:9:HOH:O	2.20	0.42
1:B:360:ASN:O	1:B:361:GLN:C	2.63	0.42
1:A:178:LEU:HD13	1:A:182:ILE:HD11	2.01	0.42
1:B:55:THR:O	1:B:58:PHE:HB3	2.20	0.42
1:B:166:PHE:HB3	1:B:198:ARG:NH1	2.35	0.42
1:A:216:LYS:HE3	1:A:335:ARG:O	2.20	0.42
1:B:95:TYR:O	1:B:100:GLY:CA	2.68	0.42
1:B:136:ARG:CG	1:B:137:TYR:CE2	3.02	0.42
1:A:95:TYR:O	1:A:100:GLY:N	2.53	0.41
1:A:189:ARG:HH12	1:A:385:LEU:CD2	2.32	0.41
1:B:165:HIS:CE1	1:B:255:THR:OG1	2.69	0.41
1:B:206:ILE:HG21	1:B:258:ASN:ND2	2.34	0.41
1:A:163:TYR:CD1	1:A:170:THR:HB	2.55	0.41
1:A:239:MET:C	1:A:241:VAL:H	2.27	0.41
1:B:53:GLU:OE1	1:B:53:GLU:O	2.38	0.41
1:B:139:LYS:O	1:B:140:PRO:C	2.57	0.41
1:B:146:TYR:CE2	1:B:191:ILE:HD12	2.55	0.41
1:B:215:LYS:O	1:B:218:GLN:HB2	2.20	0.41
1:B:240:ASP:O	1:B:244:THR:HG23	2.20	0.41
1:A:222:GLN:HE21	1:A:222:GLN:HB2	1.57	0.41
1:B:247:ALA:O	1:B:251:GLU:HG3	2.20	0.41
1:A:178:LEU:HD13	1:A:182:ILE:CD1	2.50	0.41
1:B:176:ASN:HD21	1:B:371:PHE:HE2	1.67	0.41
1:B:68:LEU:CD2	1:B:169:SER:HB3	2.49	0.41
1:A:150:LEU:C	1:A:152:ASP:H	2.27	0.41
1:B:349:MET:O	1:B:353:VAL:HG23	2.21	0.41
1:A:270:ARG:HD2	1:B:245:GLY:O	2.20	0.41
1:B:136:ARG:HD3	1:B:174:SER:HA	2.03	0.41
1:B:115:VAL:HG13	1:B:350:ALA:HA	2.02	0.41
1:B:342:ASN:O	1:B:346:ILE:HG13	2.20	0.41
1:B:52:VAL:CG2	1:B:100:GLY:HA2	2.51	0.41
1:B:339:LEU:HB3	1:B:345:PHE:CD1	2.55	0.41
1:A:42:VAL:HG22	1:A:132:TYR:HB2	2.03	0.41
1:A:114:GLU:O	1:A:118:ILE:HG13	2.21	0.41
1:A:102:SER:HA	1:A:103:PRO:HD3	1.85	0.40
1:A:207:LYS:HE2	1:A:207:LYS:HB3	1.90	0.40
1:A:58:PHE:CE1	1:A:137:TYR:HB2	2.57	0.40
1:A:66:ASN:O	1:A:67:ASP:C	2.64	0.40
1:B:280:LYS:HA	1:B:281:PRO:HD3	1.98	0.40
1:A:280:LYS:HA	1:A:281:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PHE:CZ	1:A:323:VAL:HG11	2.57	0.40
1:B:113:THR:HA	1:B:131:PRO:HG3	2.03	0.40
1:B:304:ILE:HA	1:B:305:PRO:HD3	1.78	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	353/362 (98%)	297 (84%)	38 (11%)	18 (5%)	1	3
1	B	352/362 (97%)	296 (84%)	41 (12%)	15 (4%)	2	4
All	All	705/724 (97%)	593 (84%)	79 (11%)	33 (5%)	2	3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ILE
1	A	72	SER
1	A	78	THR
1	A	79	ILE
1	A	127	ALA
1	A	222	GLN
1	B	52	VAL
1	B	127	ALA
1	B	139	LYS
1	B	140	PRO
1	B	276	GLN
1	B	326	GLU
1	B	361	GLN
1	A	71	ILE
1	A	73	ALA

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Mol	Chain	Res	Type
1	B	55	THR
1	B	57	ASP
1	B	284	GLY
1	B	330	LYS
1	B	360	ASN
1	B	390	HIS
1	A	63	PHE
1	A	70	PRO
1	A	82	TYR
1	A	221	PRO
1	A	285	ALA
1	A	330	LYS
1	B	89	PRO
1	B	358	GLN
1	A	189	ARG
1	A	265	PHE
1	A	52	VAL
1	A	279	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	311/317 (98%)	277 (89%)	34 (11%)	6	16
1	B	310/317 (98%)	287 (93%)	23 (7%)	13	32
All	All	621/634 (98%)	564 (91%)	57 (9%)	8	22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	45	ASN
1	A	59	LEU
1	A	62	LEU
1	A	67	ASP

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Mol	Chain	Res	Type
1	A	69	ILE
1	A	71	ILE
1	A	74	LYS
1	A	79	ILE
1	A	87	ARG
1	A	90	LYS
1	A	96	ARG
1	A	113	THR
1	A	122	THR
1	A	136	ARG
1	A	139	LYS
1	A	141	LEU
1	A	177	GLU
1	A	178	LEU
1	A	179	TRP
1	A	188	GLU
1	A	189	ARG
1	A	221	PRO
1	A	222	GLN
1	A	244	THR
1	A	258	ASN
1	A	262	LYS
1	A	299	ASP
1	A	301	LEU
1	A	331	ASP
1	A	352	LEU
1	A	365	ASN
1	A	369	LEU
1	A	385	LEU
1	B	43	LEU
1	B	46	MET
1	B	53	GLU
1	B	61	GLN
1	B	62	LEU
1	B	68	LEU
1	B	77	LYS
1	B	82	TYR
1	B	89	PRO
1	B	96	ARG
1	B	142	THR
1	B	148	GLN
1	B	156	LYS

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Mol	Chain	Res	Type
1	B	181	GLN
1	B	183	LYS
1	B	275	SER
1	B	276	GLN
1	B	280	LYS
1	B	337	GLU
1	B	352	LEU
1	B	360	ASN
1	B	362	LEU
1	B	383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	181	GLN
1	A	222	GLN
1	A	276	GLN
1	A	286	GLN
1	A	356	HIS
1	A	358	GLN
1	A	360	ASN
1	A	365	ASN
1	A	389	ASN
1	B	45	ASN
1	B	61	GLN
1	B	66	ASN
1	B	76	GLN
1	B	94	GLN
1	B	148	GLN
1	B	162	GLN
1	B	165	HIS
1	B	176	ASN
1	B	212	ASN
1	B	222	GLN
1	B	258	ASN
1	B	274	GLN
1	B	312	HIS
1	B	342	ASN
1	B	358	GLN
1	B	365	ASN
1	B	377	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	355/362 (98%)	0.04	15 (4%)	40 37	18, 43, 75, 99	0
1	B	354/362 (97%)	0.06	10 (2%)	55 51	19, 48, 70, 88	0
All	All	709/724 (97%)	0.05	25 (3%)	47 43	18, 46, 74, 99	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	5.6
1	A	68	LEU	5.4
1	A	82	TYR	5.0
1	A	72	SER	4.3
1	A	75	TYR	4.1
1	A	69	ILE	3.9
1	B	138	ALA	3.9
1	B	361	GLN	3.6
1	A	79	ILE	3.6
1	B	53	GLU	3.4
1	A	71	ILE	3.3
1	A	66	ASN	3.3
1	A	76	GLN	3.2
1	A	78	THR	3.1
1	B	284	GLY	3.0
1	B	140	PRO	2.8
1	B	389	ASN	2.8
1	B	276	GLN	2.7
1	B	391	GLU	2.6
1	A	188	GLU	2.5
1	B	38	PRO	2.4
1	B	52	VAL	2.2
1	A	74	LYS	2.2
1	A	391	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CO	A	501	1/1	0.87	0.07	38,38,38,38	1
2	CO	B	502	1/1	0.90	0.06	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.