



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 PM UTC

PDB ID : 6FC7 / pdb_00006fc7
Title : Crystal Structure of Two-Domain Laccase mutant H165F from *Streptomyces griseoflavus* with high copper ions occupancy
Authors : Gabdulkhakov, A.G.; Tishchenko, T.V.
Deposited on : 2017-12-20
Resolution : 1.95 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

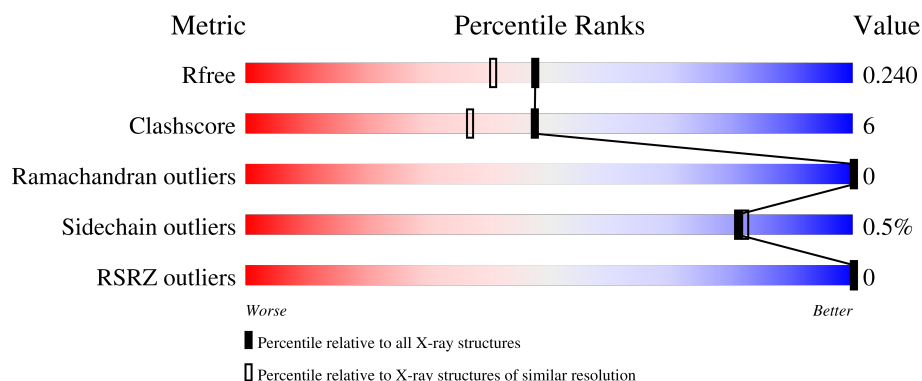
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	

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Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	

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	CU	D	401	-	-	X	-
3	PER	G	406	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26455 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 Two-domain laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2159	1347	393	407	12			
1	B	281	Total	C	N	O	S	0	2	0
			2171	1356	396	407	12			
1	C	277	Total	C	N	O	S	0	1	0
			2134	1333	387	401	13			
1	D	278	Total	C	N	O	S	0	1	0
			2140	1336	388	404	12			
1	E	278	Total	C	N	O	S	1	1	0
			2134	1333	387	401	13			
1	F	277	Total	C	N	O	S	1	2	0
			2143	1338	389	403	13			
1	G	281	Total	C	N	O	S	0	1	0
			2168	1352	394	410	12			
1	H	278	Total	C	N	O	S	0	0	0
			2131	1331	387	401	12			
1	I	281	Total	C	N	O	S	0	1	0
			2167	1352	394	408	13			
1	J	281	Total	C	N	O	S	0	1	0
			2168	1352	394	410	12			
1	K	282	Total	C	N	O	S	0	0	0
			2164	1350	394	408	12			
1	L	276	Total	C	N	O	S	0	1	0
			2124	1327	386	398	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	PHE	HIS	conflict	UNP A0A0M4FJ81
B	165	PHE	HIS	conflict	UNP A0A0M4FJ81
C	165	PHE	HIS	conflict	UNP A0A0M4FJ81
D	165	PHE	HIS	conflict	UNP A0A0M4FJ81
E	165	PHE	HIS	conflict	UNP A0A0M4FJ81

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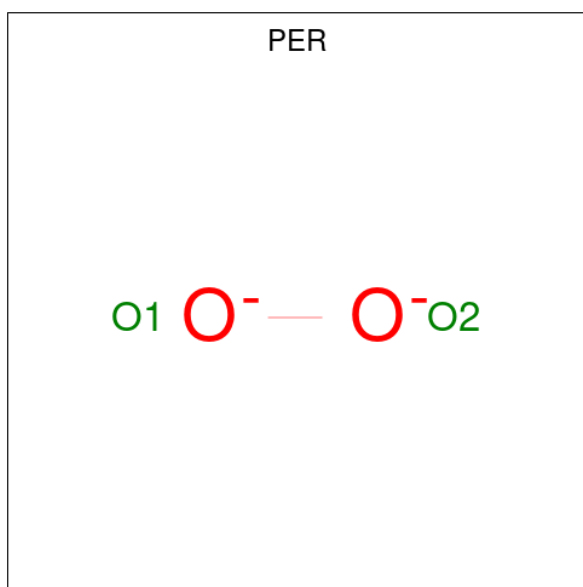
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Chain	Residue	Modelled	Actual	Comment	Reference
F	165	PHE	HIS	conflict	UNP A0A0M4FJ81
G	165	PHE	HIS	conflict	UNP A0A0M4FJ81
H	165	PHE	HIS	conflict	UNP A0A0M4FJ81
I	165	PHE	HIS	conflict	UNP A0A0M4FJ81
J	165	PHE	HIS	conflict	UNP A0A0M4FJ81
K	165	PHE	HIS	conflict	UNP A0A0M4FJ81
L	165	PHE	HIS	conflict	UNP A0A0M4FJ81

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Cu	0	0
			7	7		
2	B	4	Total	Cu	0	0
			4	4		
2	C	1	Total	Cu	0	0
			1	1		
2	D	7	Total	Cu	0	0
			7	7		
2	E	4	Total	Cu	0	0
			4	4		
2	F	1	Total	Cu	0	0
			1	1		
2	G	7	Total	Cu	0	0
			7	7		
2	H	4	Total	Cu	0	0
			4	4		
2	I	1	Total	Cu	0	0
			1	1		
2	J	7	Total	Cu	0	0
			7	7		
2	K	4	Total	Cu	0	0
			4	4		
2	L	1	Total	Cu	0	0
			1	1		

- Molecule 3 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



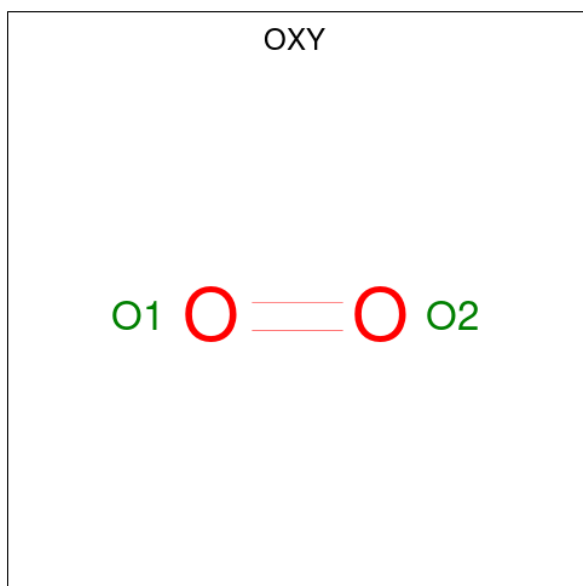
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0
3	E	1	Total O 2 2	0	0
3	G	1	Total O 2 2	0	0
3	J	1	Total O 2 2	0	0
3	K	1	Total O 2 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

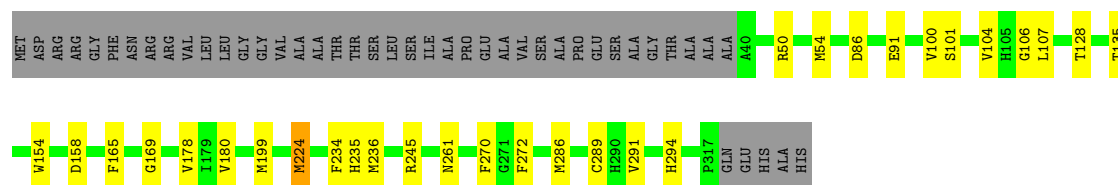
- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	O	0	0
			2	2		
5	J	1	Total	O	0	0
			2	2		

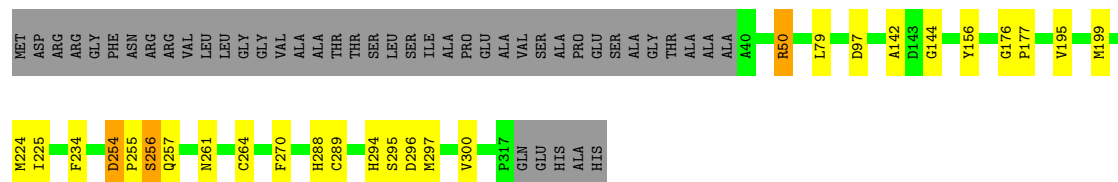
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total 53	O 53	0	0
6	B	57	Total 57	O 57	0	0
6	C	43	Total 43	O 43	0	0
6	D	49	Total 49	O 49	0	0
6	E	70	Total 70	O 70	0	0
6	F	40	Total 40	O 40	0	0
6	G	43	Total 43	O 43	0	0
6	H	44	Total 44	O 44	0	0
6	I	42	Total 42	O 42	0	0
6	J	53	Total 53	O 53	0	0
6	K	50	Total 50	O 50	0	0
6	L	38	Total 38	O 38	0	0



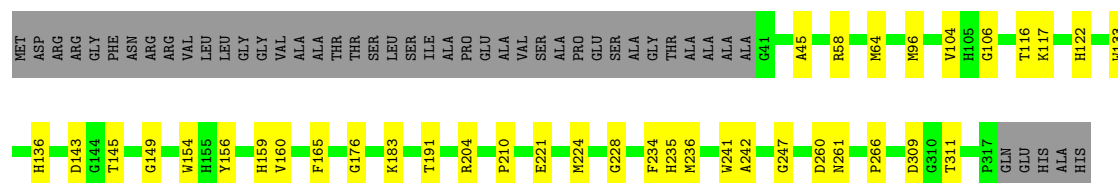
- Molecule 1: Two-domain laccase

Chain E: 78% 7% 14%



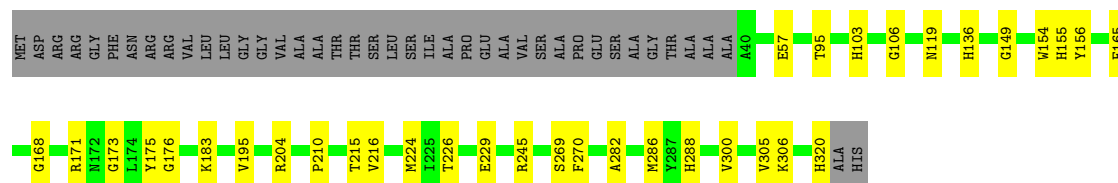
- Molecule 1: Two-domain laccase

Chain F: 74% 12% 14%



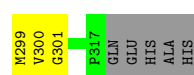
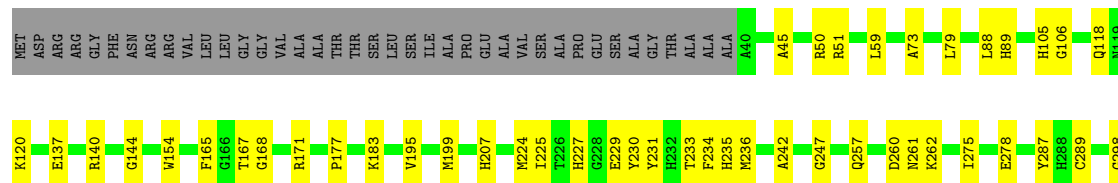
- Molecule 1: Two-domain laccase

Chain G: 76% 11% 13%



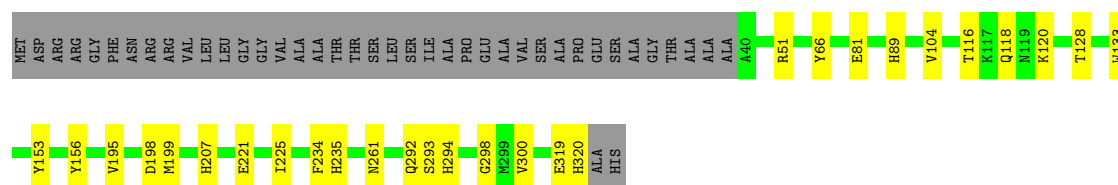
- Molecule 1: Two-domain laccase

Chain H: 71% 15% 14%



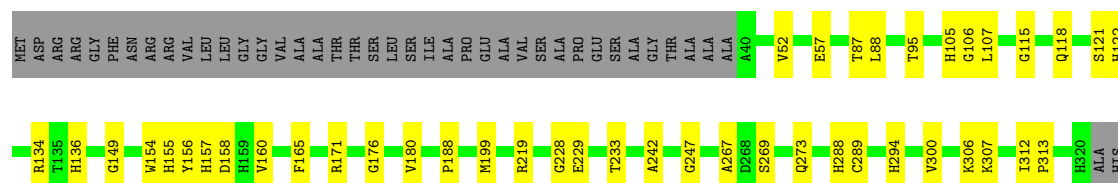
- Molecule 1: Two-domain laccase

Chain I:  79% 9% 13%



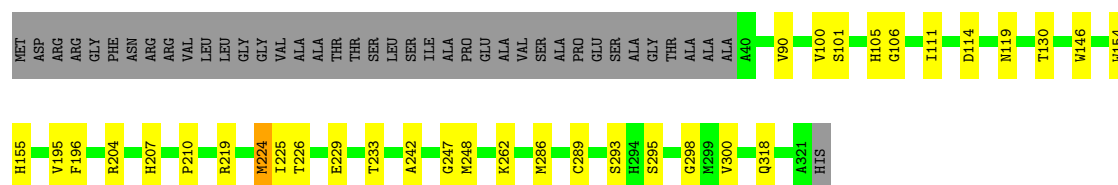
- Molecule 1: Two-domain laccase

Chain J:  74% 14% 13%



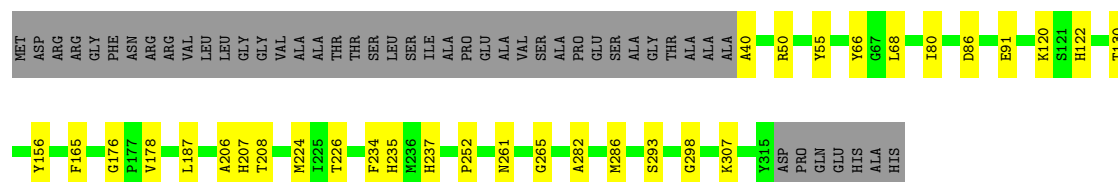
- Molecule 1: Two-domain laccase

Chain K:  77% 10% 12%



- Molecule 1: Two-domain laccase

Chain L:  76% 10% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.03Å 94.58Å 115.93Å 90.00° 90.00° 92.01°	Depositor
Resolution (Å)	49.41 – 1.95 49.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.41-1.95) 94.7 (49.41-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.195 , 0.231 0.204 , 0.240	Depositor DCC
R_{free} test set	11831 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l 0.095 for -h,k,-l 0.116 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26455	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, PER, OXY, GOL

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	0.43	0/2222	0.61	0/3018
1	B	0.49	1/2240 (0.0%)	0.67	0/3042
1	C	0.50	4/2196 (0.2%)	0.67	2/2982 (0.1%)
1	D	0.43	0/2202	0.65	0/2992
1	E	0.49	2/2199 (0.1%)	0.68	3/2987 (0.1%)
1	F	0.41	0/2205	0.61	1/2994 (0.0%)
1	G	0.38	0/2231	0.59	0/3031
1	H	0.41	0/2193	0.63	0/2979
1	I	0.36	0/2230	0.58	1/3028 (0.0%)
1	J	0.39	0/2231	0.59	1/3031 (0.0%)
1	K	0.44	1/2227 (0.0%)	0.58	0/3025
1	L	0.35	0/2185	0.58	0/2966
All	All	0.43	8/26561 (0.0%)	0.62	8/36075 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	254	ASP	C-N	7.48	1.40	1.33
1	K	224	MET	C-O	-7.30	1.15	1.24
1	C	70	LYS	CA-C	-5.86	1.45	1.53
1	C	136	HIS	C-O	-5.79	1.16	1.23
1	C	70	LYS	C-O	-5.63	1.16	1.23
1	B	316	ASP	C-N	5.39	1.41	1.33
1	E	255	PRO	N-CD	5.11	1.54	1.47
1	C	137	GLU	CA-C	-5.05	1.45	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	PRO	CB-CA-C	-7.87	101.72	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	254	ASP	CA-C-N	-6.86	113.83	120.83
1	E	254	ASP	C-N-CA	-6.86	113.83	120.83
1	F	228	GLY	N-CA-C	5.97	118.79	111.45
1	J	228	GLY	N-CA-C	5.40	118.09	111.45
1	I	198	ASP	CB-CA-C	-5.32	110.42	116.54
1	C	125	PRO	N-CA-C	5.13	118.92	111.03
1	E	254	ASP	O-C-N	5.07	125.34	121.23

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	2159	0	2024	31	0
1	B	2171	0	2047	31	0
1	C	2134	0	2006	30	0
1	D	2140	0	2010	23	0
1	E	2134	0	2008	23	0
1	F	2143	0	2013	22	0
1	G	2168	0	2030	25	0
1	H	2131	0	2003	38	0
1	I	2167	0	2032	21	0
1	J	2168	0	2031	27	0
1	K	2164	0	2029	25	0
1	L	2124	0	2000	20	0
2	A	7	0	0	0	0
2	B	4	0	0	0	0
2	C	1	0	0	0	0
2	D	7	0	0	2	0
2	E	4	0	0	0	0
2	F	1	0	0	0	0
2	G	7	0	0	0	0
2	H	4	0	0	0	0
2	I	1	0	0	0	0
2	J	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	4	0	0	0	0
2	L	1	0	0	0	0
3	B	2	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	2	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
4	B	6	0	8	0	0
5	D	2	0	0	0	0
5	J	2	0	0	0	0
6	A	53	0	0	0	0
6	B	57	0	0	0	0
6	C	43	0	0	0	0
6	D	49	0	0	0	0
6	E	70	0	0	0	0
6	F	40	0	0	0	0
6	G	43	0	0	1	0
6	H	44	0	0	2	0
6	I	42	0	0	1	0
6	J	53	0	0	1	0
6	K	50	0	0	0	0
6	L	38	0	0	0	0
All	All	26455	0	24241	282	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 6.

All (282) 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:C:70:LYS:HE3	1:C:95:THR:HG21	1.37	1.04
1:K:196:PHE:HB2	1:K:226:THR:HG22	1.64	0.79
1:B:250:THR:HG22	1:B:254:ASP:HB2	1.64	0.78
1:I:120:LYS:O	1:I:120:LYS:HD3	1.84	0.78
1:E:288:HIS:HB3	1:E:300:VAL:HG12	1.66	0.77
1:D:107:LEU:HD12	1:D:135:THR:HG22	1.68	0.76
1:C:70:LYS:HG3	1:C:71:GLY:H	1.53	0.73
1:D:91:GLU:OE2	1:D:128:THR:CG2	2.37	0.73
1:C:70:LYS:HG3	1:C:71:GLY:N	2.03	0.72
1:C:70:LYS:HE3	1:C:95:THR:CG2	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:ARG:HH12	1:K:248:MET:HE3	1.56	0.70
1:D:291:VAL:HG22	1:F:266:PRO:HG2	1.74	0.68
1:L:50:ARG:NH2	1:L:86:ASP:OD2	2.27	0.68
1:B:59:LEU:HD21	1:B:73:ALA:HB3	1.77	0.67
1:H:51:ARG:HG2	1:H:89:HIS:HB2	1.76	0.67
1:I:207:HIS:NE2	6:I:502:HOH:O	2.28	0.67
1:F:64:MET:SD	1:F:96:MET:HE1	2.34	0.67
1:C:50:ARG:NH1	1:C:86:ASP:OD2	2.29	0.66
1:I:199:MET:HE1	1:I:294:HIS:CD2	2.30	0.66
1:C:48:GLU:HG2	1:C:50:ARG:HG2	1.78	0.65
1:L:120:LYS:HD3	1:L:122:HIS:HE1	1.60	0.65
1:D:289:CYS:HG	2:D:401:CU:CU	1.11	0.65
1:H:45:ALA:HA	1:H:183:LYS:HG2	1.79	0.65
1:D:165:PHE:CZ	1:E:300:VAL:HG11	2.32	0.64
1:F:58:ARG:HG2	1:F:96:MET:HE3	1.79	0.63
1:B:224:MET:HE1	1:B:264:CYS:SG	2.39	0.62
1:A:288:HIS:HB3	1:A:300:VAL:HG13	1.81	0.62
1:D:289:CYS:SG	2:D:401:CU:CU	1.88	0.62
1:E:50:ARG:NH2	1:E:50:ARG:HG3	2.13	0.62
1:F:45:ALA:HB2	1:F:183:LYS:HE3	1.81	0.62
1:A:165:PHE:CZ	1:B:300[B]:VAL:HG21	2.35	0.62
1:D:107:LEU:HD11	1:D:180:VAL:HG21	1.82	0.61
1:E:50:ARG:HH21	1:E:50:ARG:CG	2.14	0.61
1:C:293:SER:O	1:C:297:MET:HG2	2.01	0.61
1:A:156:TYR:CZ	1:A:176:GLY:HA3	2.36	0.61
1:B:318:GLN:HA	1:B:318:GLN:OE1	2.01	0.60
1:E:224:MET:HE1	1:E:264[B]:CYS:SG	2.41	0.60
1:G:286:MET:HE2	1:G:300:VAL:HG21	1.83	0.60
1:D:199:MET:HE1	1:D:294:HIS:CD2	2.37	0.60
1:G:204:ARG:HD3	1:G:210:PRO:HD3	1.85	0.59
1:E:50:ARG:HG3	1:E:50:ARG:HH21	1.68	0.59
1:A:68:LEU:HD13	1:A:78:PRO:HG3	1.84	0.59
1:H:120:LYS:HE3	1:I:319:GLU:HG2	1.83	0.59
1:K:114:ASP:OD2	1:K:119:ASN:ND2	2.35	0.59
1:D:286:MET:HE1	1:F:116:THR:HG21	1.85	0.59
1:H:118:GLN:HB3	1:I:320:HIS:CE1	2.38	0.59
1:D:199:MET:HE1	1:D:294:HIS:CG	2.38	0.58
1:H:45:ALA:HA	1:H:183:LYS:CG	2.34	0.58
1:A:297:MET:HE3	1:H:168:GLY:HA2	1.85	0.58
1:J:300:VAL:HG21	1:L:165:PHE:CZ	2.39	0.57
1:C:50:ARG:HH22	1:C:82:LEU:HA	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:HIS:CB	1:E:300:VAL:HG12	2.34	0.57
1:E:199:MET:HE1	1:E:294:HIS:CD2	2.40	0.56
1:K:195:VAL:HG22	1:K:225:ILE:HB	1.86	0.56
1:B:106:GLY:HA3	1:B:154:TRP:CD2	2.40	0.56
1:J:199:MET:HE1	1:J:294:HIS:CD2	2.41	0.56
1:H:229:GLU:OE2	1:I:293:SER:N	2.24	0.56
1:A:79:LEU:HA	1:A:177:PRO:HG2	1.88	0.55
1:E:264[A]:CYS:SG	1:E:270:PHE:HE1	2.29	0.55
1:G:175:TYR:CE1	1:G:195:VAL:HG11	2.42	0.55
1:K:286:MET:HE2	1:K:300:VAL:HG11	1.89	0.55
1:E:224:MET:HE3	1:E:270:PHE:CE1	2.40	0.55
1:B:224:MET:HE3	1:B:270:PHE:CE1	2.42	0.55
3:B:403:PER:O1	1:C:290:HIS:NE2	2.38	0.55
1:F:136:HIS:CD2	1:F:149:GLY:HA2	2.42	0.55
1:G:155:HIS:CD2	1:G:269:SER:HB3	2.42	0.55
1:H:199:MET:HE2	1:H:230:TYR:CE2	2.41	0.55
1:C:286:MET:HE2	1:C:300:VAL:HG21	1.88	0.55
1:H:195:VAL:HG22	1:H:225:ILE:HB	1.90	0.54
1:E:142:ALA:C	1:E:144:GLY:H	2.15	0.54
1:H:50:ARG:HB2	1:H:88:LEU:HD12	1.90	0.54
1:I:207:HIS:CD2	1:I:298:GLY:HA2	2.44	0.53
1:J:229:GLU:OE2	1:K:293:SER:OG	2.26	0.53
1:J:52:VAL:HG22	1:J:88:LEU:HD11	1.91	0.53
1:J:156:TYR:CZ	1:J:176:GLY:HA3	2.44	0.52
1:F:204:ARG:HD3	1:F:210:PRO:HD3	1.90	0.52
1:A:300:VAL:HG21	1:C:165:PHE:CZ	2.44	0.52
1:J:136:HIS:CD2	1:J:149:GLY:HA2	2.45	0.51
1:C:70:LYS:CE	1:C:95:THR:HG21	2.26	0.51
1:G:183:LYS:HD3	1:G:183:LYS:C	2.35	0.51
1:J:307:LYS:HE2	1:J:313:PRO:HD3	1.92	0.51
1:E:156:TYR:CZ	1:E:176:GLY:HA3	2.46	0.51
1:G:155:HIS:HD2	1:G:269:SER:HB3	1.75	0.51
1:H:137:GLU:CD	1:H:183:LYS:HE2	2.35	0.50
1:I:120:LYS:O	1:I:120:LYS:CD	2.58	0.50
1:A:220:VAL:HG13	1:A:274:ILE:HG13	1.94	0.50
1:A:319:GLU:HG3	1:C:120:LYS:HD2	1.92	0.50
1:G:229:GLU:O	1:H:231:TYR:OH	2.30	0.50
1:C:288:HIS:HB3	1:C:300:VAL:HG23	1.93	0.50
1:G:103:HIS:CD2	3:G:406:PER:O1	2.64	0.50
1:A:155:HIS:CD2	1:A:269:SER:HB3	2.47	0.50
1:H:199:MET:HE2	1:H:230:TYR:CD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:156:TYR:CZ	1:L:176:GLY:HA3	2.47	0.50
1:A:118:GLN:HB3	1:B:320:HIS:CE1	2.47	0.50
1:H:207:HIS:CE1	1:H:298:GLY:HA2	2.46	0.49
1:B:286:MET:HE2	1:B:300[A]:VAL:HG21	1.94	0.49
1:C:79:LEU:HD23	1:C:177:PRO:HG2	1.95	0.49
1:G:216:VAL:HG23	1:G:306:LYS:O	2.12	0.49
1:K:219:ARG:NH1	1:K:248:MET:HE3	2.27	0.49
1:C:195:VAL:HA	1:C:225:ILE:O	2.13	0.49
1:G:119:ASN:ND2	6:G:504:HOH:O	2.46	0.49
1:K:207:HIS:CD2	1:K:298:GLY:HA2	2.48	0.49
1:L:187:LEU:HD12	1:L:187:LEU:H	1.77	0.49
1:B:224:MET:HE3	1:B:270:PHE:HE1	1.77	0.49
1:J:106:GLY:HA3	1:J:154:TRP:CD2	2.48	0.49
1:J:288:HIS:HB3	1:J:300:VAL:HG13	1.95	0.48
1:A:297:MET:HE1	1:H:167:THR:HG22	1.95	0.48
1:C:289:CYS:O	1:C:295:SER:HB3	2.13	0.48
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.49	0.48
1:I:51:ARG:HG2	1:I:89:HIS:HB2	1.95	0.48
1:L:91:GLU:OE2	1:L:130:THR:OG1	2.32	0.48
1:D:50:ARG:NH1	1:D:86:ASP:OD2	2.40	0.48
1:G:168:GLY:HA2	1:G:171:ARG:HD2	1.96	0.48
1:J:118:GLN:NE2	1:K:286:MET:HE1	2.29	0.48
1:B:114:ASP:HB3	1:B:119:ASN:OD1	2.13	0.48
1:H:275:ILE:HB	1:H:278:GLU:HB2	1.96	0.48
1:K:146:TRP:CZ2	1:L:252:PRO:HB3	2.49	0.48
1:B:236:MET:HE2	1:B:236:MET:HB3	1.79	0.48
1:E:224:MET:HE2	1:E:234:PHE:HB2	1.94	0.48
1:B:122:HIS:HB3	1:B:160:VAL:HG21	1.96	0.47
1:B:286:MET:HE2	1:B:300[B]:VAL:HG11	1.95	0.47
1:C:234:PHE:O	1:C:261:ASN:HA	2.15	0.47
1:E:289:CYS:O	1:E:295:SER:HB3	2.13	0.47
1:D:100:VAL:HG22	1:D:101:SER:H	1.80	0.47
1:L:40:ALA:HB1	1:L:187:LEU:HB2	1.95	0.47
1:D:224:MET:HB3	1:D:270:PHE:CE1	2.50	0.47
1:B:51[B]:ARG:HG2	1:B:89:HIS:HB2	1.97	0.47
1:G:103:HIS:NE2	3:G:406:PER:O1	2.48	0.47
1:I:235:HIS:HB2	1:I:261:ASN:OD1	2.15	0.47
1:J:87:THR:OG1	1:J:134:ARG:HG2	2.15	0.47
1:C:307:LYS:NZ	1:C:311:THR:OG1	2.47	0.47
1:H:79:LEU:HA	1:H:177:PRO:HG2	1.97	0.47
1:K:105:HIS:CD2	1:K:155:HIS:CE1	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLY:HA3	1:B:154:TRP:CE3	2.50	0.46
1:F:143:ASP:OD1	1:F:145:THR:OG1	2.28	0.46
1:L:234:PHE:O	1:L:261:ASN:HA	2.15	0.46
1:B:233:THR:HB	1:B:261:ASN:HD21	1.80	0.46
1:K:106:GLY:HA3	1:K:154:TRP:CD2	2.50	0.46
1:A:118:GLN:NE2	1:B:286:MET:HE1	2.30	0.46
1:C:79:LEU:CD1	1:C:81:GLU:HG2	2.46	0.46
1:E:195:VAL:HG22	1:E:225:ILE:HB	1.97	0.46
1:F:122:HIS:HB3	1:F:160:VAL:HG11	1.98	0.46
1:F:156:TYR:CZ	1:F:176:GLY:HA3	2.51	0.46
1:A:195:VAL:HG22	1:A:225:ILE:HB	1.97	0.46
1:E:142:ALA:C	1:E:144:GLY:N	2.73	0.46
1:J:107:LEU:HD21	1:J:180:VAL:HG21	1.97	0.46
1:J:115:GLY:N	1:J:121:SER:OG	2.49	0.46
1:L:55:TYR:O	1:L:66:TYR:HA	2.15	0.46
1:B:249:LEU:HD22	1:B:254:ASP:HB3	1.98	0.46
1:H:207:HIS:CG	1:H:298:GLY:HA2	2.50	0.46
1:L:207:HIS:CE1	1:L:298:GLY:HA2	2.51	0.46
1:E:296:ASP:O	1:E:297:MET:HE2	2.16	0.45
1:K:229:GLU:OE2	1:L:293:SER:OG	2.23	0.45
1:D:107:LEU:HD21	1:D:178:VAL:HG11	1.98	0.45
1:G:224:MET:HE1	1:G:226:THR:OG1	2.16	0.45
1:J:165:PHE:CZ	1:K:300:VAL:HG21	2.51	0.45
1:C:220:VAL:O	1:C:273:GLN:HA	2.15	0.45
1:E:195:VAL:HA	1:E:225:ILE:O	2.17	0.45
1:I:195:VAL:HA	1:I:225:ILE:O	2.17	0.45
1:D:235:HIS:HB2	1:D:261:ASN:OD1	2.17	0.45
1:F:58:ARG:CG	1:F:96:MET:HE3	2.45	0.45
1:C:235:HIS:HB2	1:C:261:ASN:OD1	2.15	0.45
1:J:219:ARG:HD3	1:J:273:GLN:OE1	2.17	0.45
1:B:254:ASP:OD1	1:B:256:SER:OG	2.28	0.44
1:C:79:LEU:HD23	1:C:177:PRO:CG	2.47	0.44
1:A:118:GLN:HE21	1:B:286:MET:HE1	1.82	0.44
1:A:234:PHE:O	1:A:261:ASN:HA	2.17	0.44
1:G:215:THR:O	1:G:216:VAL:C	2.61	0.44
1:C:45:ALA:HB2	1:C:183:LYS:HD3	1.98	0.44
1:G:173:GLY:HA2	1:G:175:TYR:CE2	2.52	0.44
1:A:204:ARG:HE	1:A:204:ARG:HB3	1.64	0.44
1:B:319:GLU:O	1:B:319:GLU:HG3	2.18	0.44
1:B:233:THR:HA	1:B:262:LYS:O	2.18	0.44
1:C:214:ALA:O	1:C:306:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:TYR:CE1	1:H:301:GLY:HA3	2.53	0.44
1:D:54:MET:HE2	1:D:54:MET:HB3	1.82	0.44
1:G:57:GLU:HG2	1:G:95:THR:OG1	2.17	0.44
1:H:242:ALA:O	1:H:247:GLY:HA2	2.18	0.44
1:I:104:VAL:HB	1:I:133:TRP:CZ2	2.53	0.44
1:K:111:ILE:HD12	1:K:111:ILE:HA	1.85	0.44
1:A:242:ALA:O	1:A:247:GLY:HA2	2.18	0.44
1:D:234:PHE:O	1:D:261:ASN:HA	2.18	0.44
1:F:224[A]:MET:HE2	1:F:234:PHE:HB2	1.99	0.44
1:K:105:HIS:CE1	1:L:235:HIS:CE1	3.06	0.44
1:B:242:ALA:O	1:B:247:GLY:HA2	2.18	0.43
1:E:254:ASP:OD1	1:E:256:SER:OG	2.22	0.43
1:L:237:HIS:CE1	1:L:286:MET:HE3	2.54	0.43
1:A:159:HIS:CE1	1:A:165:PHE:HA	2.53	0.43
1:B:207:HIS:CD2	1:B:298:GLY:HA2	2.53	0.43
1:C:122:HIS:HB3	1:C:160:VAL:HG11	2.00	0.43
1:I:153:TYR:OH	1:I:221:GLU:OE1	2.25	0.43
1:B:79:LEU:HA	1:B:177:PRO:HG2	1.99	0.43
1:J:155:HIS:CD2	1:J:269:SER:HB3	2.54	0.43
1:H:105:HIS:CE1	1:I:235:HIS:CE1	3.06	0.43
1:B:224:MET:HE2	1:B:234:PHE:HB2	2.00	0.43
1:D:245:ARG:HA	1:E:257:GLN:HG3	1.99	0.43
1:J:122:HIS:HB3	1:J:160:VAL:HG11	1.99	0.43
1:A:68:LEU:HD13	1:A:78:PRO:CG	2.47	0.43
1:F:191:THR:HA	1:F:221:GLU:O	2.19	0.43
1:J:171:ARG:NH2	6:J:503:HOH:O	2.33	0.43
1:A:106:GLY:HA3	1:A:154:TRP:CD2	2.54	0.43
1:C:97:ASP:OD1	1:C:98:VAL:HG13	2.19	0.43
1:K:195:VAL:HA	1:K:225:ILE:O	2.19	0.43
1:H:140:ARG:NH2	1:H:144:GLY:O	2.52	0.43
1:H:298:GLY:O	1:H:300:VAL:N	2.51	0.43
1:A:122:HIS:HB3	1:A:160:VAL:HG11	2.01	0.42
1:B:245:ARG:HA	1:C:257:GLN:HG3	1.99	0.42
1:F:104:VAL:HB	1:F:133:TRP:CZ2	2.54	0.42
1:J:57:GLU:HG2	1:J:95:THR:OG1	2.19	0.42
1:B:121:SER:O	1:B:131:TYR:OH	2.31	0.42
1:E:234:PHE:O	1:E:261:ASN:HA	2.19	0.42
1:F:236:MET:HE2	1:F:236:MET:HB3	1.95	0.42
1:J:233:THR:O	1:J:289:CYS:HA	2.19	0.42
1:K:242:ALA:O	1:K:247:GLY:HA2	2.20	0.42
1:F:235:HIS:HB2	1:F:261:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:HA	1:A:221:GLU:O	2.19	0.42
1:H:59:LEU:HD21	1:H:73:ALA:HB3	2.02	0.42
1:H:233:THR:HA	1:H:262:LYS:O	2.19	0.42
1:J:157:HIS:ND1	1:J:158:ASP:O	2.40	0.42
1:J:306:LYS:CG	1:J:312:ILE:HD11	2.49	0.42
1:F:309:ASP:OD1	1:F:311:THR:OG1	2.33	0.42
1:I:116:THR:HB	1:I:118:GLN:OE1	2.19	0.42
1:A:155:HIS:HD2	1:A:269:SER:HB3	1.84	0.42
1:J:118:GLN:HE21	1:K:286:MET:HE1	1.85	0.42
1:A:209:GLY:HA3	1:A:210:PRO:HA	1.89	0.42
1:G:282:ALA:HB1	1:G:305:VAL:O	2.20	0.42
1:H:289:CYS:HB2	1:H:299:MET:HE2	2.01	0.42
1:L:282:ALA:HB2	1:L:307:LYS:HE3	2.02	0.42
1:A:173:GLY:HA2	1:A:175:TYR:CE2	2.54	0.42
1:G:320:HIS:CE1	1:I:118:GLN:HB3	2.55	0.42
1:K:204:ARG:HD3	1:K:210:PRO:HD3	2.01	0.42
1:F:242:ALA:O	1:F:247:GLY:HA2	2.20	0.42
1:G:156:TYR:CZ	1:G:176:GLY:HA3	2.54	0.42
6:H:541:HOH:O	1:I:292:GLN:HG3	2.19	0.42
1:A:120:LYS:HB3	1:A:120:LYS:HE3	1.84	0.41
1:F:159:HIS:CE1	1:F:165:PHE:HA	2.55	0.41
1:K:233:THR:HA	1:K:262:LYS:O	2.20	0.41
1:L:206:ALA:O	1:L:208:THR:HG23	2.20	0.41
1:L:226:THR:HB	1:L:265:GLY:O	2.20	0.41
1:D:236:MET:HE1	1:D:272:PHE:CZ	2.55	0.41
1:F:106:GLY:HA3	1:F:154:TRP:CE3	2.55	0.41
1:G:165:PHE:CZ	1:H:300:VAL:HG21	2.55	0.41
1:K:233:THR:O	1:K:289:CYS:HA	2.19	0.41
1:B:114:ASP:OD2	1:B:116:THR:OG1	2.32	0.41
1:G:224:MET:SD	1:G:270:PHE:CE1	3.14	0.41
1:H:106:GLY:HA3	1:H:154:TRP:CD2	2.55	0.41
1:J:188:PRO:HA	1:J:219:ARG:HG2	2.01	0.41
1:K:100:VAL:HG22	1:K:101:SER:H	1.85	0.41
1:H:165:PHE:CZ	1:I:300:VAL:HG21	2.56	0.41
1:C:204:ARG:NH1	1:C:210:PRO:HB3	2.36	0.41
1:D:158:ASP:OD2	1:D:169:GLY:HA3	2.21	0.41
1:E:97:ASP:OD1	1:E:97:ASP:N	2.53	0.41
1:F:241:TRP:CZ3	1:F:260:ASP:HA	2.55	0.41
1:H:227:HIS:NE2	6:H:505:HOH:O	2.37	0.41
1:J:105:HIS:CE1	1:J:267:ALA:HB1	2.55	0.41
1:L:68:LEU:HD23	1:L:68:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:OG1	1:A:254:ASP:HB2	2.21	0.41
1:A:297:MET:HE3	1:H:168:GLY:CA	2.49	0.41
1:F:117:LYS:HD2	1:F:122:HIS:CE1	2.56	0.41
1:H:106:GLY:HA3	1:H:154:TRP:CE3	2.56	0.41
1:J:242:ALA:O	1:J:247:GLY:HA2	2.20	0.41
1:K:289:CYS:O	1:K:295:SER:HB3	2.21	0.41
1:A:69:GLU:OE2	1:A:72:LYS:HD2	2.21	0.41
1:H:234:PHE:O	1:H:261:ASN:HA	2.20	0.41
1:H:236:MET:HE2	1:H:236:MET:HB3	1.93	0.41
1:A:297:MET:HE2	1:H:171:ARG:NH1	2.36	0.40
1:D:104:VAL:CG2	1:D:107:LEU:HD23	2.50	0.40
1:E:79:LEU:HA	1:E:177:PRO:HG2	2.03	0.40
1:G:106:GLY:HA3	1:G:154:TRP:CD2	2.56	0.40
1:G:245:ARG:HA	1:H:257:GLN:HG3	2.03	0.40
1:I:66:TYR:CD2	1:I:156:TYR:HE2	2.39	0.40
1:I:234:PHE:O	1:I:261:ASN:HA	2.20	0.40
1:C:66:TYR:CD2	1:C:156:TYR:HE1	2.39	0.40
1:G:288:HIS:HB3	1:G:300:VAL:HG23	2.02	0.40
1:L:80:ILE:HB	1:L:178:VAL:HG13	2.03	0.40
1:B:118:GLN:OE1	1:B:118:GLN:N	2.54	0.40
1:D:91:GLU:OE2	1:D:128:THR:HG23	2.20	0.40
1:G:136:HIS:CD2	1:G:149:GLY:HA2	2.56	0.40
1:H:229:GLU:OE1	1:I:293:SER:OG	2.33	0.40
1:H:235:HIS:ND1	1:H:260:ASP:O	2.39	0.40
1:J:300:VAL:HG21	1:L:165:PHE:HZ	1.87	0.40
1:K:90:VAL:O	1:K:130:THR:HA	2.21	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	279/322 (87%)	273 (98%)	6 (2%)	0	100	100
1	B	281/322 (87%)	268 (95%)	13 (5%)	0	100	100
1	C	276/322 (86%)	268 (97%)	8 (3%)	0	100	100
1	D	277/322 (86%)	271 (98%)	6 (2%)	0	100	100
1	E	277/322 (86%)	270 (98%)	7 (2%)	0	100	100
1	F	277/322 (86%)	268 (97%)	9 (3%)	0	100	100
1	G	280/322 (87%)	271 (97%)	9 (3%)	0	100	100
1	H	276/322 (86%)	266 (96%)	10 (4%)	0	100	100
1	I	280/322 (87%)	273 (98%)	7 (2%)	0	100	100
1	J	280/322 (87%)	271 (97%)	9 (3%)	0	100	100
1	K	280/322 (87%)	272 (97%)	8 (3%)	0	100	100
1	L	275/322 (85%)	266 (97%)	9 (3%)	0	100	100
All	All	3338/3864 (86%)	3237 (97%)	101 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	222/249 (89%)	221 (100%)	1 (0%)	81	82
1	B	224/249 (90%)	223 (100%)	1 (0%)	84	85
1	C	220/249 (88%)	219 (100%)	1 (0%)	81	82
1	D	220/249 (88%)	219 (100%)	1 (0%)	81	82
1	E	220/249 (88%)	218 (99%)	2 (1%)	70	70
1	F	221/249 (89%)	221 (100%)	0	100	100
1	G	223/249 (90%)	223 (100%)	0	100	100
1	H	219/249 (88%)	218 (100%)	1 (0%)	81	82
1	I	223/249 (90%)	221 (99%)	2 (1%)	70	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	223/249 (90%)	223 (100%)	0	100	100
1	K	222/249 (89%)	220 (99%)	2 (1%)	70	70
1	L	218/249 (88%)	216 (99%)	2 (1%)	70	70
All	All	2655/2988 (89%)	2642 (100%)	13 (0%)	81	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	MET
1	B	318	GLN
1	C	70	LYS
1	D	224	MET
1	E	50	ARG
1	E	256	SER
1	H	224	MET
1	I	81	GLU
1	I	128	THR
1	K	224	MET
1	K	318	GLN
1	L	224[A]	MET
1	L	224[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	ASN
1	B	292	GLN
1	C	119	ASN
1	D	292	GLN
1	E	119	ASN
1	F	83	ASN
1	F	292	GLN
1	G	83	ASN
1	G	292	GLN
1	H	83	ASN
1	H	292	GLN
1	I	318	GLN
1	J	257	GLN
1	K	83	ASN
1	L	83	ASN

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Mol	Chain	Res	Type
1	L	207	HIS

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 57 ligands modelled in this entry, 48 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PER	G	406	2	1,1,1	0.17	0	-		
5	OXY	J	405	2	1,1,1	0.10	0	-		
3	PER	D	409	2	1,1,1	0.20	0	-		
3	PER	J	406	2	1,1,1	0.18	0	-		
3	PER	B	403	2	1,1,1	0.20	0	-		
4	GOL	B	404	-	5,5,5	0.45	0	5,5,5	0.38	0
5	OXY	D	407	2	1,1,1	0.15	0	-		
3	PER	K	403	2	1,1,1	0.25	0	-		
3	PER	E	405	2	1,1,1	0.36	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	GOL	B	404	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	406	PER	2	0
3	B	403	PER	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	281/322 (87%)	-1.29	0 100 100	17, 28, 43, 69	3 (1%)
1	B	281/322 (87%)	-1.28	0 100 100	16, 28, 40, 79	9 (3%)
1	C	277/322 (86%)	-1.22	0 100 100	14, 31, 47, 76	8 (2%)
1	D	278/322 (86%)	-1.24	0 100 100	19, 29, 43, 81	7 (2%)
1	E	278/322 (86%)	-1.25	0 100 100	18, 29, 45, 99	5 (1%)
1	F	277/322 (86%)	-1.23	0 100 100	15, 29, 44, 59	5 (1%)
1	G	281/322 (87%)	-1.18	0 100 100	20, 34, 52, 70	6 (2%)
1	H	278/322 (86%)	-1.17	0 100 100	22, 35, 51, 83	3 (1%)
1	I	281/322 (87%)	-1.17	0 100 100	15, 35, 53, 84	3 (1%)
1	J	281/322 (87%)	-1.23	0 100 100	16, 31, 47, 72	4 (1%)
1	K	282/322 (87%)	-1.24	0 100 100	19, 30, 49, 73	1 (0%)
1	L	276/322 (85%)	-1.15	0 100 100	16, 37, 52, 60	6 (2%)
All	All	3351/3864 (86%)	-1.22	0 100 100	14, 31, 49, 99	60 (1%)

There are no RSRZ outliers to report.

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 ⓘ

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	CU	A	403	1/1	0.97	0.05	29,29,29,29	1
4	GOL	B	404	6/6	0.98	0.05	37,39,40,44	0
5	OXY	D	407	2/2	0.98	0.07	36,36,36,37	2
2	CU	D	406	1/1	0.99	0.02	33,33,33,33	1
2	CU	E	403	1/1	0.99	0.04	27,27,27,27	1
2	CU	G	403	1/1	0.99	0.04	34,34,34,34	1
2	CU	G	405	1/1	0.99	0.03	33,33,33,33	1
2	CU	H	403	1/1	0.99	0.02	38,38,38,38	1
2	CU	H	404	1/1	0.99	0.02	38,38,38,38	1
2	CU	J	403	1/1	0.99	0.04	34,34,34,34	1
2	CU	J	408	1/1	0.99	0.03	32,32,32,32	1
2	CU	K	405	1/1	0.99	0.03	28,28,28,28	1
3	PER	B	403	2/2	0.99	0.04	16,16,16,23	2
3	PER	D	409	2/2	0.99	0.03	28,28,28,29	2
2	CU	B	406	1/1	0.99	0.05	27,27,27,27	1
2	CU	D	403	1/1	0.99	0.04	46,46,46,46	1
5	OXY	J	405	2/2	0.99	0.05	33,33,33,36	0
2	CU	A	404	1/1	1.00	0.01	31,31,31,31	0
2	CU	D	408	1/1	1.00	0.01	32,32,32,32	0
2	CU	E	401	1/1	1.00	0.01	28,28,28,28	0
2	CU	E	402	1/1	1.00	0.02	33,33,33,33	0
2	CU	A	405	1/1	1.00	0.03	27,27,27,27	1
2	CU	E	404	1/1	1.00	0.01	31,31,31,31	1
2	CU	F	401	1/1	1.00	0.01	25,25,25,25	0
2	CU	G	401	1/1	1.00	0.02	24,24,24,24	0
2	CU	G	402	1/1	1.00	0.01	36,36,36,36	1
2	CU	A	406	1/1	1.00	0.01	35,35,35,35	1
2	CU	G	404	1/1	1.00	0.01	35,35,35,35	0
2	CU	A	407	1/1	1.00	0.01	35,35,35,35	0
2	CU	G	407	1/1	1.00	0.01	40,40,40,40	1
2	CU	G	408	1/1	1.00	0.01	38,38,38,38	0
2	CU	H	401	1/1	1.00	0.01	29,29,29,29	0
2	CU	H	402	1/1	1.00	0.01	42,42,42,42	0
2	CU	B	401	1/1	1.00	0.02	22,22,22,22	0
2	CU	B	402	1/1	1.00	0.01	33,33,33,33	0
2	CU	I	401	1/1	1.00	0.01	30,30,30,30	0
2	CU	J	401	1/1	1.00	0.01	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	J	402	1/1	1.00	0.01	41,41,41,41	1
2	CU	B	405	1/1	1.00	0.02	42,42,42,42	1
2	CU	J	404	1/1	1.00	0.01	29,29,29,29	1
2	CU	J	407	1/1	1.00	0.03	30,30,30,30	1
2	CU	A	402	1/1	1.00	0.01	34,34,34,34	1
2	CU	J	409	1/1	1.00	0.01	41,41,41,41	0
2	CU	K	401	1/1	1.00	0.01	30,30,30,30	0
2	CU	K	402	1/1	1.00	0.01	37,37,37,37	1
2	CU	K	404	1/1	1.00	0.02	38,38,38,38	1
2	CU	C	401	1/1	1.00	0.01	29,29,29,29	0
2	CU	L	401	1/1	1.00	0.01	29,29,29,29	0
2	CU	D	401	1/1	1.00	0.01	26,26,26,26	0
2	CU	D	402	1/1	1.00	0.01	41,41,41,41	1
3	PER	E	405	2/2	1.00	0.03	30,30,30,43	0
3	PER	G	406	2/2	1.00	0.04	23,23,23,31	2
3	PER	J	406	2/2	1.00	0.04	21,21,21,29	2
3	PER	K	403	2/2	1.00	0.02	28,28,28,28	2
2	CU	A	401	1/1	1.00	0.01	22,22,22,22	1
2	CU	D	404	1/1	1.00	0.02	31,31,31,31	0
2	CU	D	405	1/1	1.00	0.01	42,42,42,42	1

6.5 Other polymers

There are no such residues in this entry.