



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:39 am GMT

PDB ID : 4GAM
Title : Complex structure of Methane monooxygenase hydroxylase and regulatory subunit
Authors : Lee, S.J.; Lippard, S.J.; Cho, U.-S.
Deposited on : 2012-07-25
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

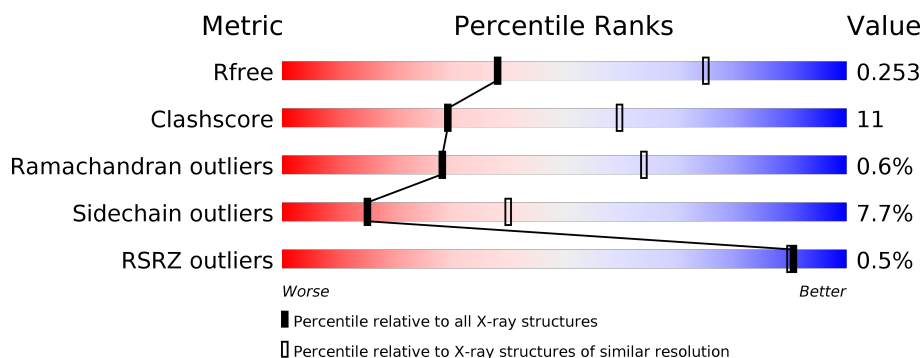
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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. 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	B	389	<div> <div>76%</div> <div>22%</div> <div>•</div> </div>
1	G	389	<div> <div>75%</div> <div>22%</div> <div>•</div> </div>
1	L	389	<div> <div>74%</div> <div>24%</div> <div>•</div> </div>
1	Q	389	<div> <div>70%</div> <div>25%</div> <div>•</div> </div>
2	A	527	<div> <div>69%</div> <div>24%</div> <div>• •</div> </div>
2	F	527	<div> <div>68%</div> <div>25%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	527	 63% 29% 5%
2	P	527	 63% 30% 7%
3	C	170	 77% 20% 3%
3	H	170	 74% 20% 6%
3	M	170	 71% 25% 4%
3	R	170	 68% 27% 5%
4	D	141	 56% 31% 6% 6%
4	I	141	 64% 22% 8% 6%
4	N	141	 57% 31% 5% 6%
4	S	141	 69% 21% 5% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39145 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 Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	388	Total	C	N	O	S	0	0	0
			3190	2051	551	580	8			
1	G	388	Total	C	N	O	S	0	0	0
			3190	2051	551	580	8			
1	L	388	Total	C	N	O	S	0	0	0
			3190	2051	551	580	8			
1	Q	388	Total	C	N	O	S	0	0	0
			3190	2051	551	580	8			

- Molecule 2 is a protein called Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	511	Total	C	N	O	S	0	0	0
			4170	2667	721	764	18			
2	F	511	Total	C	N	O	S	0	0	0
			4170	2667	721	764	18			
2	K	511	Total	C	N	O	S	0	0	0
			4170	2667	721	764	18			
2	P	511	Total	C	N	O	S	0	0	0
			4170	2667	721	764	18			

- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	H	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	M	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	R	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			

- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	132	Total	C	N	O	S	0	0	0
			1045	663	167	212	3			
4	I	132	Total	C	N	O	S	0	0	0
			1045	663	167	212	3			
4	N	132	Total	C	N	O	S	0	0	0
			1045	663	167	212	3			
4	S	132	Total	C	N	O	S	0	0	0
			1045	663	167	212	3			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	2	Total	Fe	0	0
			2	2		
5	A	2	Total	Fe	0	0
			2	2		
5	K	2	Total	Fe	0	0
			2	2		
5	F	2	Total	Fe	0	0
			2	2		

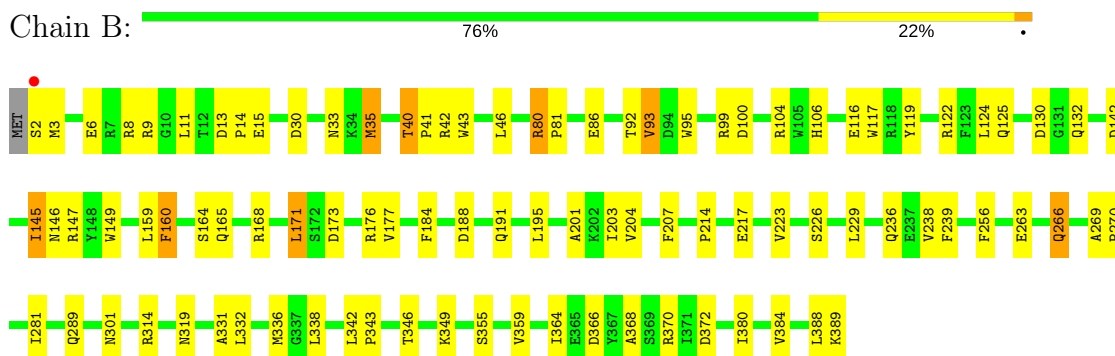
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	10	Total	O	0	0
			10	10		
6	A	11	Total	O	0	0
			11	11		
6	C	3	Total	O	0	0
			3	3		
6	D	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		
6	F	8	Total	O	0	0
			8	8		
6	K	3	Total	O	0	0
			3	3		
6	P	5	Total	O	0	0
			5	5		
6	S	2	Total	O	0	0
			2	2		

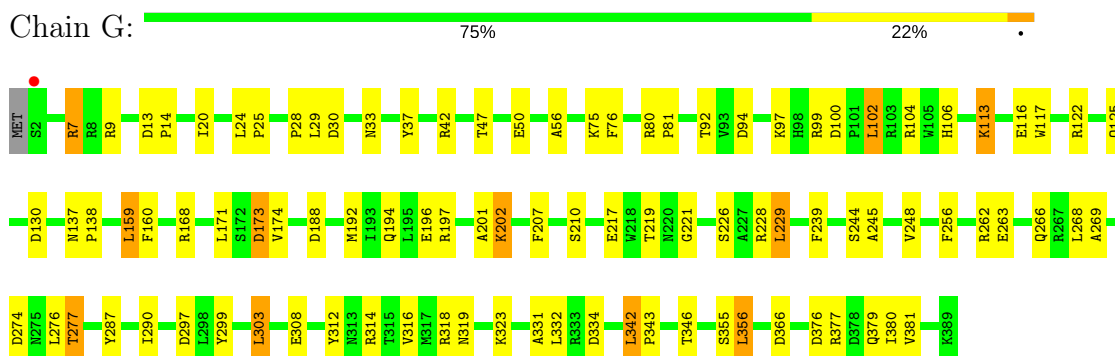
3 Residue-property plots

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

- Molecule 1: Methane monooxygenase component A beta chain



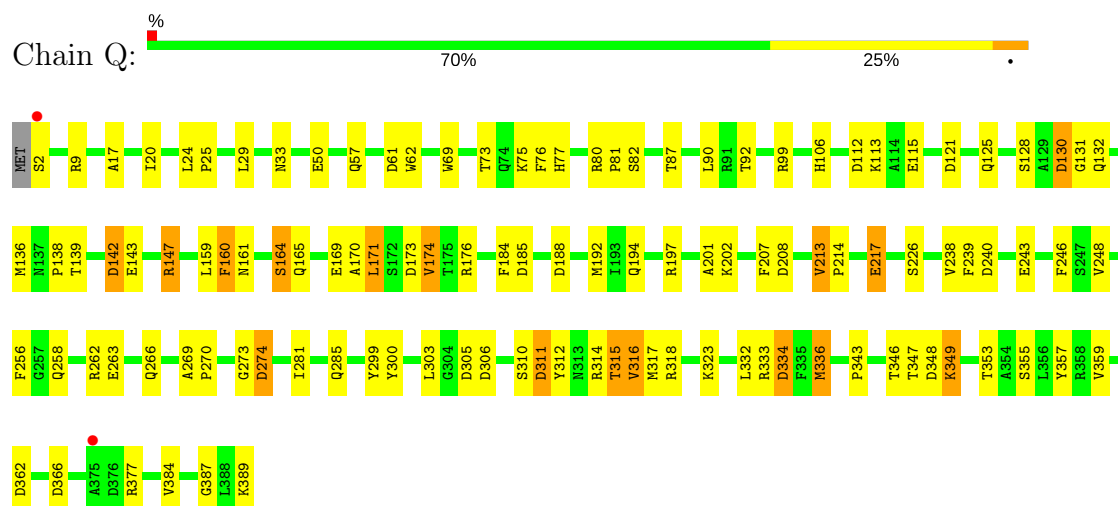
- Molecule 1: Methane monooxygenase component A beta chain



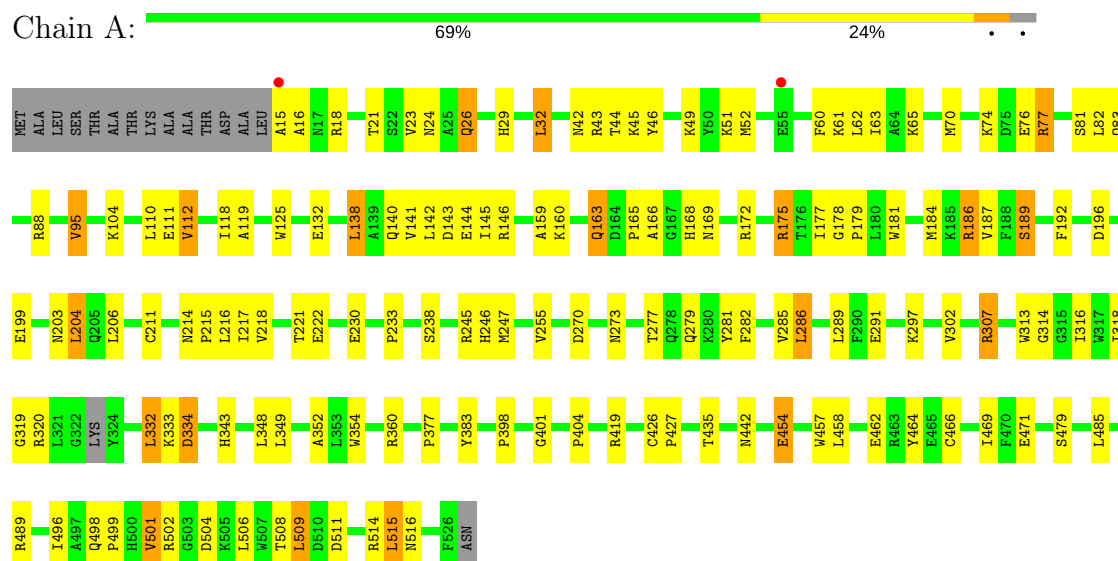
- Molecule 1: Methane monooxygenase component A beta chain



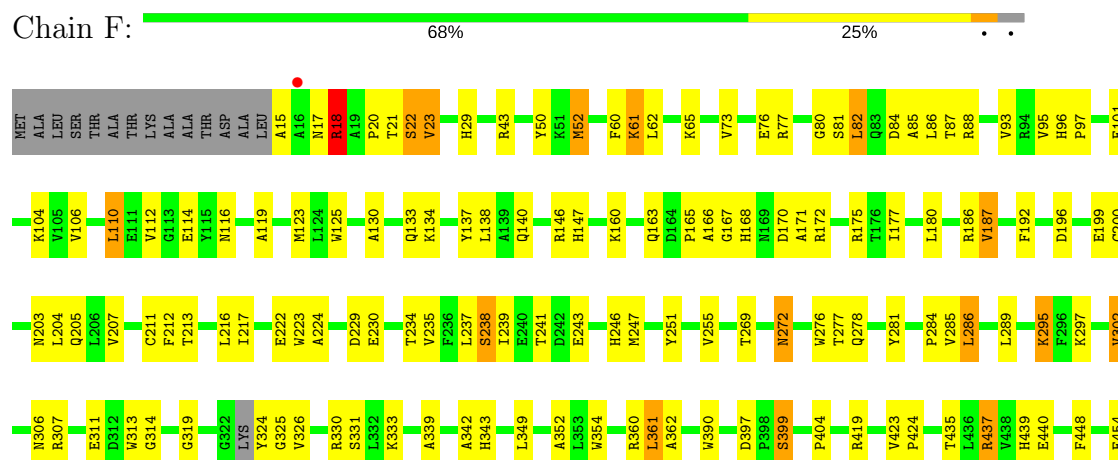
- Molecule 1: Methane monooxygenase component A beta chain



- Molecule 2: Methane monooxygenase component A alpha chain

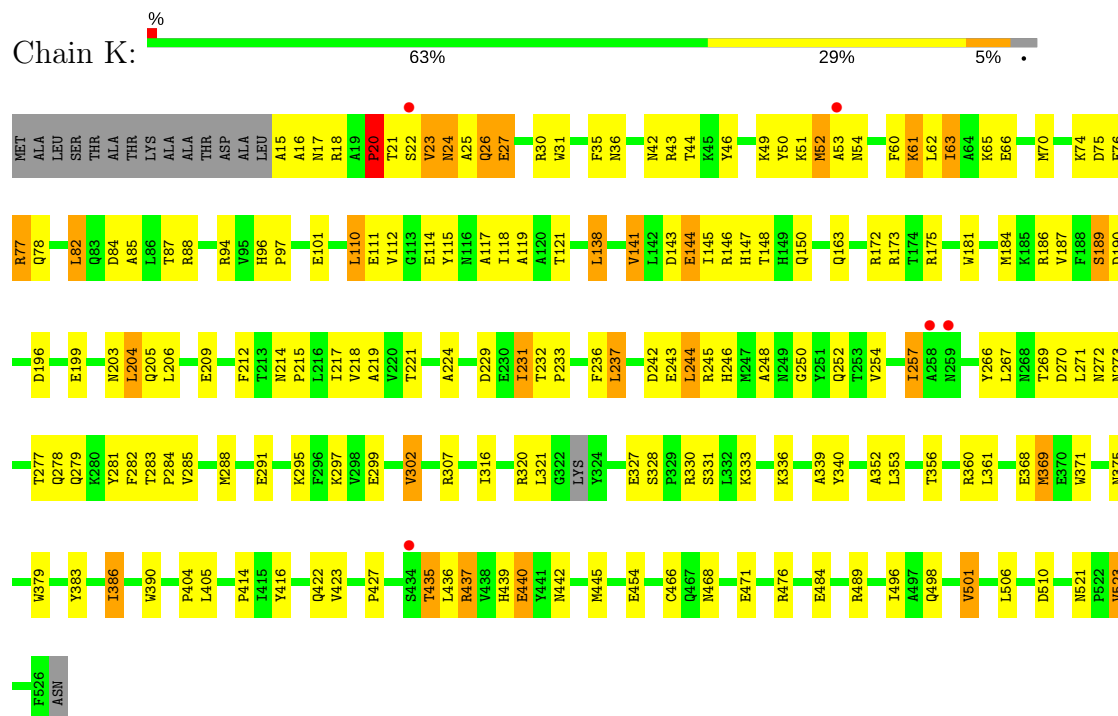


- Molecule 2: Methane monooxygenase component A alpha chain

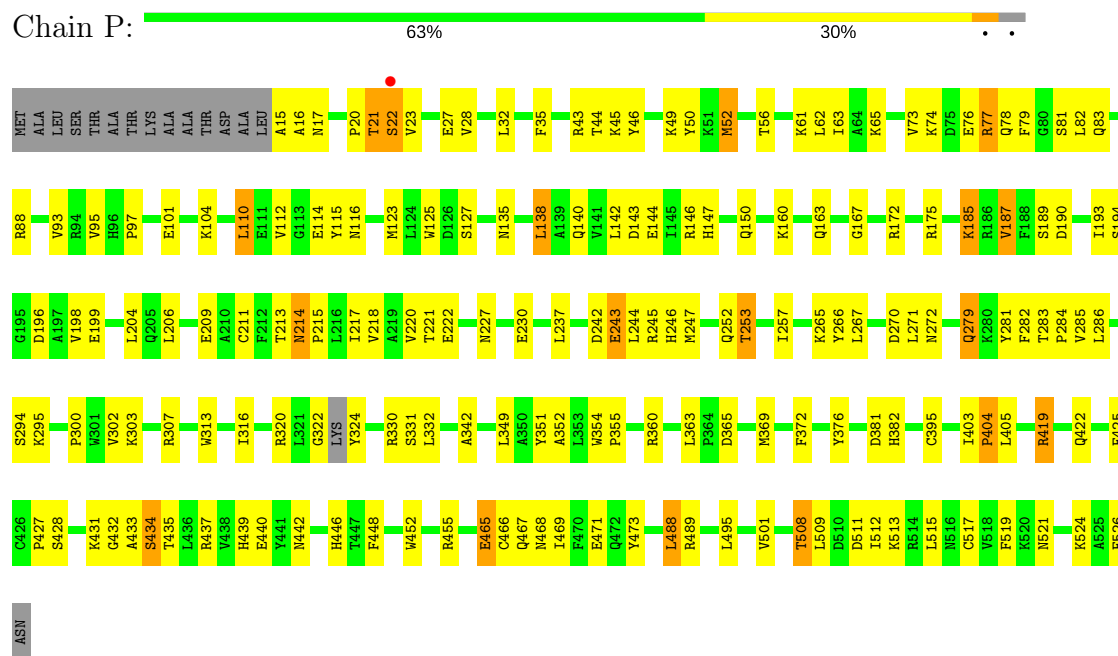




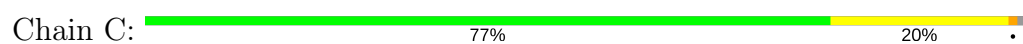
• Molecule 2: Methane monooxygenase component A alpha chain

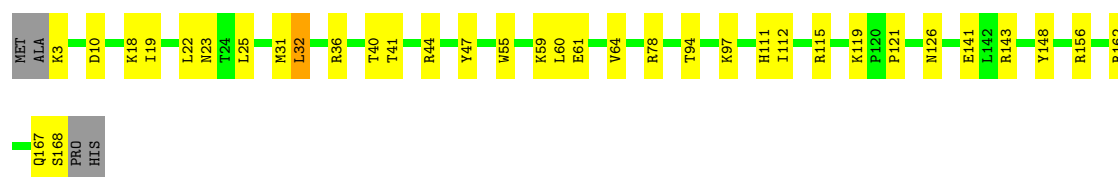


• Molecule 2: Methane monooxygenase component A alpha chain

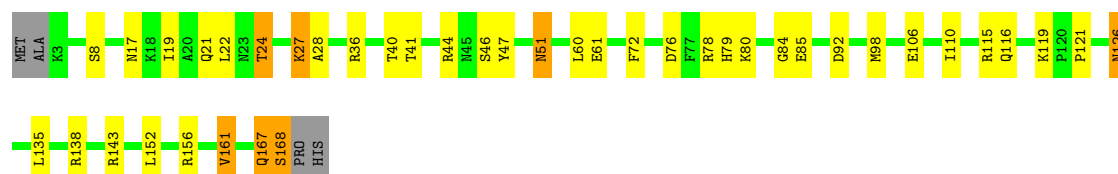


• Molecule 3: Methane monooxygenase component A gamma chain

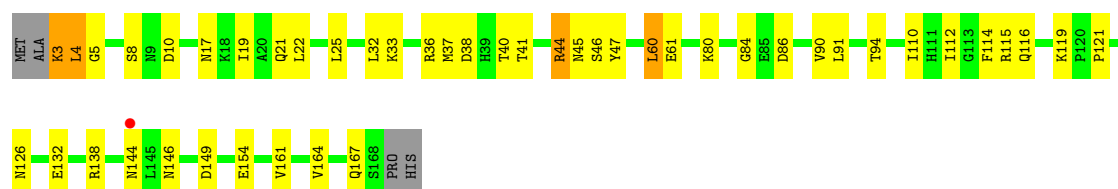
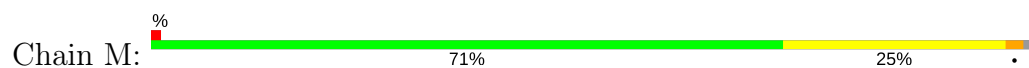




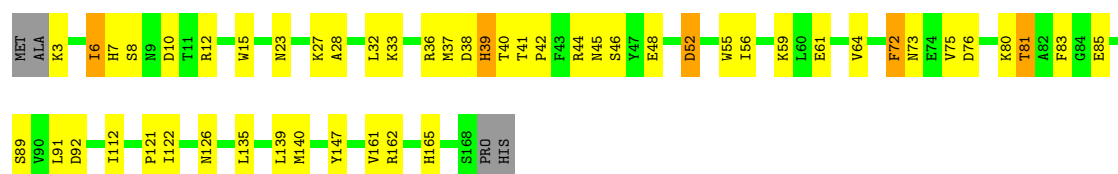
- Molecule 3: Methane monooxygenase component A gamma chain



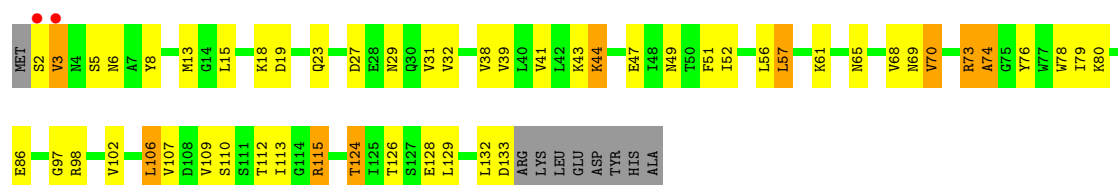
- Molecule 3: Methane monooxygenase component A gamma chain



- Molecule 3: Methane monooxygenase component A gamma chain

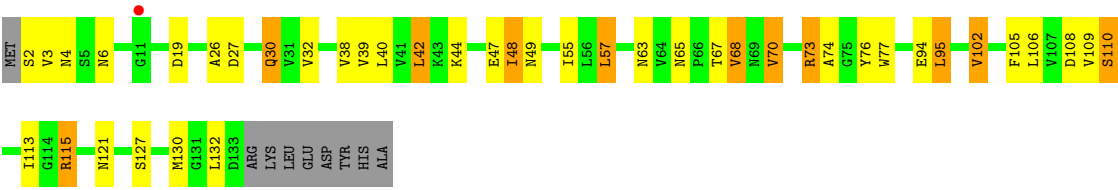


- Molecule 4: Methane monooxygenase regulatory protein B

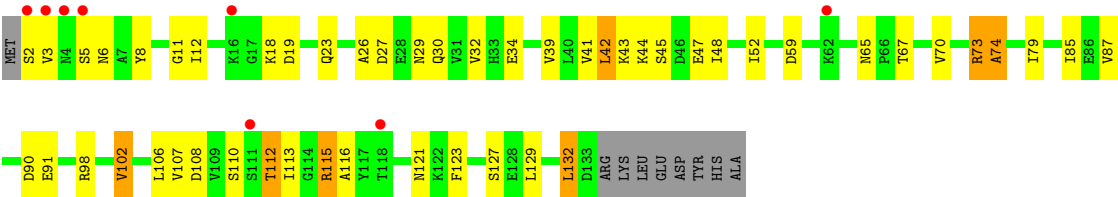


- Molecule 4: Methane monooxygenase regulatory protein B





• Molecule 4: Methane monooxygenase regulatory protein B



• Molecule 4: Methane monooxygenase regulatory protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.59Å 248.97Å 122.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 147.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.90) 90.3 (147.76-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.205 , 0.258 0.198 , 0.253	Depositor DCC
R_{free} test set	5916 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	39145	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: FE

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	B	0.26	0/3286	0.44	0/4460
1	G	0.26	0/3286	0.43	0/4460
1	L	0.25	0/3286	0.43	0/4460
1	Q	0.25	0/3286	0.43	0/4460
2	A	0.26	0/4293	0.45	0/5831
2	F	0.32	1/4293 (0.0%)	0.48	1/5831 (0.0%)
2	K	0.25	0/4293	0.46	0/5831
2	P	0.26	0/4293	0.47	0/5831
3	C	0.24	0/1396	0.43	0/1880
3	H	0.24	0/1396	0.44	0/1880
3	M	0.24	0/1396	0.45	0/1880
3	R	0.25	0/1396	0.46	0/1880
4	D	0.25	0/1062	0.44	0/1438
4	I	0.25	0/1062	0.47	0/1438
4	N	0.26	0/1062	0.48	0/1438
4	S	0.26	0/1062	0.46	0/1438
All	All	0.26	1/40148 (0.0%)	0.45	1/54436 (0.0%)

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
2	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	295	LYS	CE-NZ	10.29	1.74	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	295	LYS	CD-CE-NZ	-8.99	91.03	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	20	PRO	Peptide

5.2 Too-close contacts [i](#)

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	B	3190	0	3033	68	0
1	G	3190	0	3033	70	0
1	L	3190	0	3033	74	0
1	Q	3190	0	3033	83	0
2	A	4170	0	3968	110	0
2	F	4170	0	3968	116	0
2	K	4170	0	3968	142	0
2	P	4170	0	3968	121	0
3	C	1368	0	1363	24	0
3	H	1368	0	1363	26	0
3	M	1368	0	1363	27	0
3	R	1368	0	1363	37	0
4	D	1045	0	1011	36	0
4	I	1045	0	1011	26	0
4	N	1045	0	1011	35	0
4	S	1045	0	1011	27	0
5	A	2	0	0	0	0
5	F	2	0	0	0	0
5	K	2	0	0	0	0
5	P	2	0	0	0	0
6	A	11	0	0	0	0
6	B	10	0	0	4	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	8	0	0	0	0
6	G	2	0	0	0	0
6	K	3	0	0	1	0
6	P	5	0	0	0	0
6	S	2	0	0	0	0
All	All	39145	0	37500	828	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 11.

All (828) 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)
2:F:295:LYS:CE	2:F:295:LYS:NZ	1.74	1.48
1:B:370:ARG:HD3	6:B:409:HOH:O	0.97	1.13
2:P:243:GLU:OE2	2:P:246:HIS:ND1	1.83	1.09
1:B:370:ARG:CD	6:B:409:HOH:O	1.64	0.96
2:F:114:GLU:HG2	2:F:147:HIS:HB2	1.51	0.93
2:F:295:LYS:CD	2:F:295:LYS:NZ	2.34	0.91
4:N:2:SER:N	4:N:5:SER:HG	1.72	0.88
2:F:95:VAL:HG22	2:F:96:HIS:H	1.41	0.86
2:K:114:GLU:HG2	2:K:147:HIS:HB2	1.58	0.85
2:F:21:THR:O	2:F:23:VAL:N	2.12	0.82
2:K:272:ASN:HD21	2:K:330:ARG:H	1.27	0.81
2:F:216:LEU:HD13	2:F:286:LEU:HD11	1.63	0.81
2:K:435:THR:OG1	2:K:437:ARG:NH1	2.13	0.81
2:A:44:THR:HG22	2:A:46:TYR:H	1.45	0.80
2:K:237:LEU:HB3	4:N:43:LYS:HD3	1.63	0.80
2:K:196:ASP:HB3	2:K:199:GLU:HB2	1.63	0.80
1:G:319:ASN:OD1	3:H:78:ARG:NH1	2.13	0.79
2:P:435:THR:OG1	2:P:437:ARG:NH1	2.15	0.79
4:D:2:SER:N	4:D:5:SER:HG	1.80	0.78
1:B:370:ARG:HG3	6:B:409:HOH:O	1.77	0.77
3:H:19:ILE:HD11	3:H:60:LEU:HD13	1.63	0.77
4:N:2:SER:N	4:N:5:SER:OG	2.16	0.77
2:F:137:TYR:HE1	2:F:205:GLN:HE22	1.33	0.77
2:K:244:LEU:HD11	4:N:116:ALA:HB3	1.67	0.77
3:M:146:ASN:ND2	3:M:149:ASP:OD2	2.17	0.76
2:P:49:LYS:HD3	3:R:140:MET:HB3	1.66	0.76
3:R:81:THR:HG23	3:R:83:PHE:H	1.51	0.76
2:P:419:ARG:NH2	2:P:471:GLU:OE2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:147:ARG:HG2	1:Q:217:GLU:HG3	1.67	0.76
1:Q:311:ASP:OD1	1:Q:311:ASP:N	2.16	0.76
2:P:442:ASN:ND2	3:R:42:PRO:O	2.17	0.76
1:L:202:LYS:HD3	2:K:22:SER:HB3	1.69	0.74
1:Q:82:SER:HB3	2:P:193:ILE:HD11	1.70	0.74
2:P:172:ARG:HA	2:P:175:ARG:HD2	1.68	0.73
3:M:80:LYS:HE2	3:M:84:GLY:HA2	1.70	0.73
2:K:44:THR:HG22	2:K:46:TYR:H	1.54	0.73
1:L:132:GLN:NE2	1:Q:266:GLN:OE1	2.20	0.73
2:K:143:ASP:OD2	2:K:245:ARG:NH2	2.21	0.72
2:P:196:ASP:HB3	2:P:199:GLU:HB2	1.71	0.72
3:H:22:LEU:HD23	3:H:28:ALA:HA	1.70	0.72
1:Q:176:ARG:NH1	2:P:115:TYR:OH	2.22	0.72
1:Q:87:THR:HG21	1:Q:169:GLU:HB3	1.70	0.72
1:B:33:ASN:HB2	2:A:160:LYS:HA	1.70	0.72
1:L:201:ALA:HA	1:L:207:PHE:HB3	1.70	0.72
2:F:96:HIS:CD2	2:F:97:PRO:HD2	2.25	0.71
2:P:488:LEU:HD11	2:P:509:LEU:HD11	1.71	0.71
1:G:33:ASN:HB2	2:F:160:LYS:HA	1.72	0.71
1:L:338:LEU:HD12	1:L:341:LYS:HD3	1.70	0.71
2:A:352:ALA:HA	2:A:404:PRO:HB2	1.73	0.70
1:L:160:PHE:HE1	2:K:138:LEU:HD12	1.57	0.70
1:Q:165:GLN:NE2	1:Q:239:PHE:O	2.21	0.70
1:L:267:ARG:HH12	1:L:351:GLU:HB3	1.56	0.69
1:Q:201:ALA:HA	1:Q:207:PHE:HB3	1.74	0.69
1:B:124:LEU:HD11	1:B:195:LEU:HD21	1.75	0.68
1:B:132:GLN:NE2	1:G:266:GLN:OE1	2.28	0.67
3:H:40:THR:HG22	3:H:41:THR:HG23	1.74	0.67
4:D:57:LEU:HD12	4:D:61:LYS:HD2	1.76	0.67
1:Q:188:ASP:OD2	2:P:65:LYS:NZ	2.27	0.67
1:Q:311:ASP:O	1:Q:315:THR:OG1	2.13	0.67
2:K:15:ALA:N	1:Q:366:ASP:OD1	2.28	0.67
1:L:356:LEU:HD23	1:L:381:VAL:HG13	1.75	0.67
2:P:112:VAL:O	2:P:116:ASN:ND2	2.27	0.67
1:L:133:ILE:HD11	1:L:204:VAL:HG22	1.76	0.67
3:M:3:LYS:N	3:M:10:ASP:OD2	2.28	0.66
2:A:83:GLN:HB3	2:F:77:ARG:HH21	1.60	0.66
1:G:20:ILE:HG23	2:F:96:HIS:HB2	1.78	0.66
3:C:3:LYS:N	3:C:10:ASP:OD2	2.29	0.66
1:Q:170:ALA:O	1:Q:176:ARG:NH2	2.29	0.66
1:B:201:ALA:HA	1:B:207:PHE:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:213:VAL:HG13	1:Q:214:PRO:HD3	1.78	0.66
2:F:222:GLU:OE2	4:I:73:ARG:NH1	2.29	0.66
3:M:32:LEU:HD13	3:M:60:LEU:HB3	1.77	0.66
2:K:476:ARG:NH1	2:K:484:GLU:OE1	2.25	0.65
1:L:42:ARG:NH2	1:L:97:LYS:O	2.28	0.65
1:L:160:PHE:CE1	2:K:138:LEU:HD12	2.32	0.65
1:G:42:ARG:NH2	1:G:97:LYS:O	2.26	0.65
3:M:41:THR:HG21	3:M:112:ILE:HG23	1.79	0.65
3:M:40:THR:HG22	3:M:41:THR:HG23	1.77	0.65
2:P:468:ASN:OD1	2:P:471:GLU:N	2.24	0.65
2:K:75:ASP:OD1	2:K:146:ARG:NH1	2.30	0.65
3:H:24:THR:HG23	3:H:27:LYS:HB2	1.79	0.64
2:K:371:TRP:O	2:K:375:ASN:ND2	2.28	0.64
2:P:222:GLU:HA	4:S:74:ALA:HB2	1.79	0.64
1:L:140:TRP:NE1	1:L:145:ILE:HD11	2.12	0.64
2:P:104:LYS:HD3	2:P:167:GLY:HA3	1.80	0.64
4:D:106:LEU:HA	4:D:109:VAL:HG12	1.79	0.63
3:R:40:THR:HG23	3:R:41:THR:HG23	1.80	0.63
1:G:117:TRP:HB2	2:F:65:LYS:HB3	1.79	0.63
2:K:121:THR:HB	2:K:141:VAL:HG23	1.81	0.63
3:M:3:LYS:NZ	3:M:8:SER:OG	2.31	0.63
2:A:51:LYS:NZ	3:C:141:GLU:OE2	2.31	0.63
2:K:74:LYS:HE3	4:N:107:VAL:HA	1.80	0.63
3:M:17:ASN:O	3:M:21:GLN:NE2	2.32	0.63
2:P:21:THR:O	2:P:23:VAL:N	2.32	0.63
1:Q:113:LYS:NZ	1:Q:185:ASP:OD1	2.30	0.63
4:S:39:VAL:HB	4:S:113:ILE:HB	1.81	0.63
2:A:88:ARG:HH22	2:F:234:THR:HG22	1.64	0.62
3:R:81:THR:HG22	3:R:85:GLU:H	1.62	0.62
2:P:77:ARG:NH2	4:S:47:GLU:OE2	2.33	0.62
2:A:318:ILE:HG22	4:D:32:VAL:HG11	1.80	0.62
4:N:43:LYS:NZ	4:N:108:ASP:OD1	2.33	0.62
1:B:366:ASP:OD2	2:F:15:ALA:N	2.33	0.62
3:H:41:THR:O	3:H:44:ARG:HD2	2.00	0.61
1:G:202:LYS:NZ	2:F:22:SER:O	2.31	0.61
1:G:9:ARG:NH2	4:I:74:ALA:O	2.33	0.61
2:K:52:MET:SD	2:K:52:MET:N	2.73	0.61
1:L:76:PHE:HB2	1:L:80:ARG:HB3	1.81	0.61
2:A:112:VAL:HG21	2:A:181:TRP:HH2	1.65	0.61
1:G:226:SER:HB2	1:G:331:ALA:HA	1.82	0.61
3:C:41:THR:HG21	3:C:112:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:LYS:NZ	2:A:334:ASP:OD1	2.33	0.61
4:N:70:VAL:HG22	4:N:79:ILE:HG12	1.82	0.61
2:K:352:ALA:HA	2:K:404:PRO:HB2	1.81	0.61
4:I:39:VAL:HB	4:I:113:ILE:HB	1.83	0.60
1:L:130:ASP:OD2	1:Q:285:GLN:NE2	2.31	0.60
1:L:7:ARG:HH22	4:N:73:ARG:HH12	1.48	0.60
1:Q:77:HIS:HB3	3:R:139:LEU:HD22	1.83	0.60
2:A:32:LEU:HD13	2:A:132:GLU:HA	1.82	0.60
2:K:360:ARG:HG2	2:K:498:GLN:HB2	1.84	0.60
1:L:140:TRP:CE2	1:L:145:ILE:HD11	2.36	0.60
2:P:44:THR:HG22	2:P:46:TYR:H	1.66	0.60
1:B:2:SER:OG	1:B:3:MET:N	2.31	0.60
1:L:289:GLN:NE2	1:Q:130:ASP:OD1	2.35	0.60
2:A:74:LYS:HG2	4:D:107:VAL:HG13	1.83	0.60
2:K:101:GLU:OE2	2:K:360:ARG:NH1	2.35	0.60
1:L:188:ASP:OD2	2:K:65:LYS:NZ	2.35	0.60
2:K:435:THR:HG1	2:K:437:ARG:HH11	1.50	0.60
2:A:398:PRO:O	2:A:514:ARG:NH2	2.34	0.59
4:D:23:GLN:O	4:D:29:ASN:ND2	2.33	0.59
2:P:419:ARG:HD2	2:P:446:HIS:CD2	2.37	0.59
1:Q:90:LEU:HD13	1:Q:303:LEU:HD13	1.84	0.59
2:K:114:GLU:OE2	2:K:147:HIS:ND1	2.35	0.59
4:S:6:ASN:HB3	4:S:80:LYS:HB3	1.84	0.59
2:A:146:ARG:NH2	2:A:238:SER:O	2.35	0.59
1:B:370:ARG:CG	6:B:409:HOH:O	2.07	0.59
2:K:60:PHE:O	2:K:62:LEU:N	2.34	0.59
2:P:74:LYS:NZ	2:P:242:ASP:OD1	2.35	0.59
4:D:61:LYS:NZ	4:D:68:VAL:O	2.35	0.59
4:D:86:GLU:HG2	4:D:124:THR:HB	1.84	0.59
1:B:8:ARG:NH2	1:B:15:GLU:OE1	2.33	0.59
1:Q:138:PRO:O	1:Q:142:ASP:HB2	2.02	0.59
1:G:202:LYS:HG2	2:F:22:SER:HB3	1.85	0.59
2:F:419:ARG:NH2	2:F:471:GLU:OE2	2.35	0.59
1:L:46:LEU:HD12	1:L:47:THR:H	1.67	0.59
1:L:168:ARG:HD2	2:K:119:ALA:HB1	1.85	0.58
2:K:320:ARG:HB3	4:N:129:LEU:HD11	1.85	0.58
2:P:316:ILE:O	4:S:115:ARG:NH2	2.36	0.58
1:B:165:GLN:HE22	1:B:239:PHE:HA	1.68	0.58
4:N:44:LYS:HB2	2:P:88:ARG:HG3	1.84	0.58
4:S:41:VAL:HG12	4:S:110:SER:HB2	1.85	0.58
2:K:61:LYS:HD2	2:K:61:LYS:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLN:HB3	2:A:63:ILE:HD11	1.85	0.58
1:B:336:MET:HB3	1:B:388:LEU:HA	1.84	0.58
2:P:322:GLY:O	2:P:324:TYR:N	2.36	0.58
2:K:272:ASN:HD21	2:K:330:ARG:HG3	1.68	0.58
1:B:145:ILE:HA	1:B:149:TRP:HB3	1.85	0.58
1:G:219:THR:O	1:G:228:ARG:NH1	2.37	0.58
1:L:74:GLN:HB3	2:K:190:ASP:HB3	1.84	0.58
2:F:284:PRO:HB3	2:F:342:ALA:HB1	1.86	0.58
1:Q:299:TYR:HB3	1:Q:317:MET:HE1	1.86	0.58
2:A:60:PHE:O	2:A:62:LEU:N	2.37	0.58
3:M:36:ARG:NH1	3:M:119:LYS:O	2.37	0.57
2:F:295:LYS:HD3	2:F:295:LYS:NZ	2.18	0.57
1:B:130:ASP:O	1:G:262:ARG:NH1	2.37	0.57
1:G:343:PRO:O	1:G:346:THR:OG1	2.19	0.57
4:N:41:VAL:HG12	4:N:110:SER:HB3	1.85	0.57
1:Q:29:LEU:HB3	2:P:489:ARG:HH12	1.69	0.57
4:N:59:ASP:OD1	4:N:59:ASP:N	2.37	0.57
1:Q:269:ALA:HB1	1:Q:274:ASP:HB3	1.86	0.57
2:A:222:GLU:HA	4:D:74:ALA:HB2	1.86	0.57
2:P:143:ASP:OD2	2:P:245:ARG:NH2	2.37	0.57
2:K:489:ARG:NH2	2:K:496:ILE:O	2.37	0.57
3:M:115:ARG:NH1	3:M:132:GLU:OE2	2.32	0.57
2:P:185:LYS:O	2:P:189:SER:HB2	2.05	0.57
2:P:352:ALA:HA	2:P:404:PRO:HB2	1.87	0.57
2:F:276:TRP:CE3	2:F:331:SER:HB2	2.40	0.57
2:A:104:LYS:NZ	2:A:166:ALA:O	2.31	0.56
2:F:238:SER:O	2:F:241:THR:OG1	2.22	0.56
2:A:291:GLU:O	2:A:297:LYS:NZ	2.29	0.56
1:B:80:ARG:NH1	1:B:81:PRO:O	2.37	0.56
2:A:216:LEU:HD13	2:A:286:LEU:HD11	1.87	0.56
2:P:79:PHE:O	2:P:83:GLN:HG2	2.05	0.56
1:Q:238:VAL:O	2:P:45:LYS:NZ	2.30	0.56
2:F:360:ARG:HG2	2:F:498:GLN:HB2	1.87	0.56
1:G:100:ASP:OD2	1:G:104:ARG:NH1	2.32	0.56
2:K:110:LEU:HD11	2:K:217:ILE:HG12	1.87	0.56
2:A:77:ARG:NH2	4:D:47:GLU:OE1	2.39	0.56
1:L:263:GLU:HB3	1:L:355:SER:HB2	1.86	0.56
2:K:244:LEU:HD13	4:N:112:THR:OG1	2.06	0.56
2:K:186:ARG:CZ	2:K:277:THR:HG23	2.36	0.56
2:K:78:GLN:OE1	2:K:150:GLN:NE2	2.38	0.56
1:L:364:ILE:HA	1:L:368:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:GLN:HG3	2:A:246:HIS:CE1	2.40	0.56
4:N:65:ASN:OD1	4:N:67:THR:OG1	2.23	0.55
3:R:61:GLU:HG2	3:R:121:PRO:HD3	1.88	0.55
2:P:282:PHE:CE1	2:P:286:LEU:HD22	2.41	0.55
2:F:114:GLU:HG2	2:F:147:HIS:CB	2.30	0.55
2:A:15:ALA:N	1:G:366:ASP:OD2	2.39	0.55
2:P:50:TYR:OH	2:P:270:ASP:OD2	2.18	0.55
1:L:376:ASP:HB3	1:L:379:GLN:HB3	1.88	0.55
2:F:82:LEU:O	2:F:87:THR:OG1	2.23	0.55
2:K:233:PRO:O	2:K:237:LEU:HB2	2.06	0.55
2:K:369:MET:HG3	2:K:379:TRP:CZ3	2.41	0.55
2:A:273:ASN:OD1	3:C:148:TYR:OH	2.23	0.55
2:K:96:HIS:NE2	2:K:295:LYS:HE3	2.22	0.55
1:Q:73:THR:HA	2:P:466:CYS:HB2	1.88	0.55
1:B:9:ARG:NH2	4:D:74:ALA:O	2.40	0.55
3:M:41:THR:O	3:M:44:ARG:HD2	2.07	0.55
2:A:187:VAL:HG21	2:A:281:TYR:CD1	2.42	0.55
1:G:56:ALA:N	1:G:173:ASP:OD2	2.39	0.55
1:G:50:GLU:OE2	1:G:99:ARG:NH1	2.40	0.55
2:K:333:LYS:HD2	4:N:30:GLN:HG2	1.89	0.55
2:F:110:LEU:HD11	2:F:217:ILE:HG12	1.87	0.54
2:F:251:TYR:O	2:F:255:VAL:HG23	2.07	0.54
4:N:129:LEU:HD13	4:N:132:LEU:HD11	1.89	0.54
4:D:43:LYS:HE2	2:F:88:ARG:NH2	2.22	0.54
1:G:30:ASP:HB3	2:F:165:PRO:HG2	1.88	0.54
2:F:435:THR:OG1	2:F:437:ARG:NH1	2.41	0.54
2:A:159:ALA:O	2:A:165:PRO:HB3	2.08	0.54
2:F:95:VAL:HG22	2:F:96:HIS:N	2.17	0.54
2:A:462:GLU:OE2	3:C:143:ARG:NH1	2.34	0.54
3:H:44:ARG:HD3	3:H:47:TYR:CZ	2.42	0.54
2:K:231:ILE:HG13	2:K:232:THR:N	2.22	0.54
3:M:44:ARG:HD3	3:M:47:TYR:CZ	2.42	0.54
2:K:316:ILE:O	4:N:115:ARG:NH2	2.36	0.54
1:L:266:GLN:HG3	1:L:278:PRO:HB3	1.88	0.54
1:Q:29:LEU:O	2:P:489:ARG:NH1	2.41	0.54
2:F:96:HIS:ND1	2:F:96:HIS:C	2.61	0.54
2:K:476:ARG:HD2	3:M:4:LEU:HD22	1.89	0.54
1:L:137:ASN:HD22	1:L:272:PHE:HD1	1.55	0.54
2:K:118:ILE:HG12	2:K:144:GLU:HB3	1.89	0.54
2:P:281:TYR:CE1	2:P:285:VAL:HG21	2.43	0.54
1:G:80:ARG:NH1	1:G:81:PRO:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:55:ILE:HD11	4:I:95:LEU:HD13	1.89	0.54
1:B:147:ARG:HH11	1:B:217:GLU:HG2	1.74	0.53
1:B:203:ILE:HG13	1:B:204:VAL:HG23	1.90	0.53
2:A:419:ARG:NH2	2:A:471:GLU:OE2	2.35	0.53
2:K:333:LYS:HA	4:N:30:GLN:HG3	1.91	0.53
3:R:15:TRP:CG	3:R:56:ILE:HD13	2.44	0.53
3:R:46:SER:OG	3:R:48:GLU:HG2	2.09	0.53
3:C:19:ILE:HG12	3:C:60:LEU:HD13	1.89	0.53
2:K:369:MET:HG3	2:K:379:TRP:HZ3	1.73	0.53
4:I:63:ASN:OD1	1:L:40:THR:OG1	2.21	0.53
2:K:217:ILE:HG23	2:K:236:PHE:HB3	1.89	0.53
2:K:269:THR:O	2:K:273:ASN:ND2	2.24	0.53
4:D:70:VAL:HB	4:D:79:ILE:HG13	1.90	0.53
2:P:95:VAL:O	2:P:163:GLN:NE2	2.39	0.53
1:Q:314:ARG:O	1:Q:318:ARG:HB2	2.08	0.53
2:K:187:VAL:HG23	2:K:278:GLN:HA	1.90	0.53
2:P:360:ARG:NH2	2:P:501:VAL:O	2.42	0.53
1:B:160:PHE:CE1	2:A:138:LEU:HD12	2.44	0.53
1:G:201:ALA:HA	1:G:207:PHE:HB3	1.91	0.53
1:B:238:VAL:O	2:A:45:LYS:NZ	2.35	0.52
1:B:319:ASN:OD1	3:C:78:ARG:NE	2.37	0.52
1:B:239:PHE:HB2	3:C:126:ASN:HA	1.91	0.52
2:F:237:LEU:O	4:I:110:SER:OG	2.27	0.52
2:F:255:VAL:HG13	4:I:132:LEU:HG	1.91	0.52
2:P:101:GLU:HG3	2:P:360:ARG:HB2	1.91	0.52
2:A:29:HIS:CD2	2:A:32:LEU:HD12	2.44	0.52
2:F:104:LYS:NZ	2:F:166:ALA:O	2.28	0.52
2:F:86:LEU:HD11	2:F:234:THR:HG21	1.90	0.52
2:K:206:LEU:HD22	2:K:254:VAL:HG21	1.91	0.52
2:K:291:GLU:O	2:K:297:LYS:NZ	2.39	0.52
1:B:42:ARG:HB2	1:B:99:ARG:HG3	1.91	0.52
2:K:112:VAL:HG21	2:K:181:TRP:HH2	1.75	0.52
3:R:3:LYS:N	3:R:10:ASP:OD2	2.43	0.52
1:L:173:ASP:O	1:L:177:VAL:HG23	2.10	0.52
1:L:45:ARG:HH21	4:S:95:LEU:HD22	1.75	0.52
2:F:343:HIS:CD2	2:F:343:HIS:H	2.27	0.52
1:G:125:GLN:HG3	2:F:21:THR:HB	1.92	0.52
1:L:76:PHE:CD1	1:L:80:ARG:HD3	2.44	0.52
2:K:77:ARG:NH2	4:N:47:GLU:OE1	2.42	0.52
2:A:140:GLN:O	2:A:144:GLU:HG2	2.10	0.52
1:L:118:ARG:NH2	1:Q:112:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:498:GLN:HG3	2:A:506:LEU:HD22	1.92	0.52
1:B:314:ARG:NH1	1:B:372:ASP:OD1	2.42	0.52
4:N:39:VAL:HB	4:N:113:ILE:HB	1.91	0.52
2:A:76:GLU:HG3	2:F:76:GLU:HG3	1.91	0.52
2:P:265:LYS:HG3	2:P:266:TYR:CD2	2.45	0.52
2:K:76:GLU:HG3	2:P:76:GLU:HG3	1.92	0.52
2:P:455:ARG:NH1	3:R:147:TYR:O	2.43	0.52
2:A:215:PRO:HB2	2:A:282:PHE:HZ	1.75	0.52
3:C:32:LEU:HD12	3:C:64:VAL:HG21	1.90	0.52
1:G:197:ARG:NH2	1:G:210:SER:O	2.39	0.52
2:P:74:LYS:HG2	4:S:107:VAL:HG13	1.92	0.52
2:P:222:GLU:OE2	4:S:73:ARG:NH1	2.43	0.52
1:L:336:MET:HB3	1:L:388:LEU:HA	1.92	0.51
2:K:435:THR:HA	3:M:167:GLN:NE2	2.25	0.51
4:S:41:VAL:HB	4:S:111:SER:HB3	1.92	0.51
2:K:184:MET:O	2:K:189:SER:OG	2.28	0.51
1:L:8:ARG:NH2	1:L:15:GLU:OE2	2.42	0.51
2:A:118:ILE:HG12	2:A:144:GLU:HB2	1.93	0.51
1:G:269:ALA:HB1	1:G:274:ASP:HB3	1.92	0.51
2:K:427:PRO:HG2	2:K:436:LEU:HB2	1.93	0.51
1:L:184:PHE:HD1	2:K:138:LEU:HD13	1.75	0.51
3:M:146:ASN:HB3	3:M:149:ASP:HB2	1.93	0.51
1:Q:266:GLN:HB2	1:Q:281:ILE:HG21	1.92	0.51
3:R:36:ARG:O	3:R:40:THR:HG22	2.10	0.51
3:R:55:TRP:CZ2	3:R:59:LYS:HE3	2.45	0.51
4:I:2:SER:HB3	4:I:67:THR:HG22	1.93	0.51
2:F:125:TRP:CZ3	2:F:138:LEU:HD13	2.45	0.51
2:F:60:PHE:O	2:F:62:LEU:N	2.43	0.51
2:P:295:LYS:NZ	2:P:365:ASP:OD2	2.43	0.51
1:Q:33:ASN:HB2	2:P:160:LYS:HA	1.92	0.51
2:F:352:ALA:HA	2:F:404:PRO:HB2	1.93	0.51
1:G:263:GLU:HB3	1:G:355:SER:HB2	1.93	0.51
2:P:209:GLU:O	2:P:213:THR:OG1	2.28	0.51
4:S:19:ASP:OD1	4:S:19:ASP:N	2.43	0.51
2:F:272:ASN:OD1	2:F:330:ARG:N	2.38	0.51
2:K:302:VAL:HG11	2:K:340:TYR:CD2	2.46	0.51
2:A:479:SER:HB2	2:A:509:LEU:HD22	1.93	0.51
2:F:187:VAL:HG13	2:F:281:TYR:HB3	1.93	0.51
2:K:281:TYR:HD1	2:K:423:VAL:HG22	1.76	0.51
2:K:299:GLU:OE2	4:N:8:TYR:OH	2.21	0.51
2:P:365:ASP:O	2:P:369:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:GLN:OE1	2:P:150:GLN:NE2	2.44	0.51
2:A:218:VAL:O	2:A:221:THR:OG1	2.28	0.50
1:G:194:GLN:OE1	1:G:197:ARG:NH1	2.44	0.50
1:L:82:SER:OG	2:K:190:ASP:OD1	2.20	0.50
4:D:15:LEU:HD22	4:D:19:ASP:HB3	1.94	0.50
1:L:117:TRP:HB2	2:K:65:LYS:HB3	1.93	0.50
2:P:495:LEU:HD11	2:P:512:ILE:HG13	1.92	0.50
4:D:6:ASN:HB3	4:D:80:LYS:HG2	1.93	0.50
2:K:221:THR:HG21	2:K:237:LEU:HD13	1.93	0.50
1:Q:50:GLU:OE2	1:Q:99:ARG:NH1	2.45	0.50
2:A:175:ARG:HD3	2:A:181:TRP:CE2	2.47	0.50
4:I:47:GLU:OE1	4:I:47:GLU:N	2.37	0.50
2:K:111:GLU:OE2	2:K:172:ARG:NH2	2.31	0.50
1:L:73:THR:HG22	2:K:422:GLN:HG3	1.94	0.50
1:Q:62:TRP:HB3	3:R:55:TRP:HA	1.93	0.50
1:B:119:TYR:CD1	1:G:116:GLU:HG2	2.47	0.50
1:G:168:ARG:O	1:G:168:ARG:NH1	2.40	0.50
1:G:94:ASP:HB3	1:G:97:LYS:HG3	1.94	0.50
2:P:425:PHE:CE2	2:P:427:PRO:HG3	2.46	0.50
1:B:364:ILE:HA	1:B:368:ALA:HB3	1.92	0.50
1:G:202:LYS:NZ	2:F:22:SER:OG	2.40	0.49
1:L:348:ASP:N	1:L:348:ASP:OD1	2.44	0.49
2:P:127:SER:HB3	2:P:198:VAL:HG22	1.93	0.49
1:Q:160:PHE:CE1	2:P:138:LEU:HD12	2.47	0.49
2:A:143:ASP:OD2	2:A:245:ARG:NH2	2.44	0.49
2:F:439:HIS:HB3	3:H:161:VAL:HG21	1.93	0.49
2:F:95:VAL:HG13	2:F:96:HIS:N	2.27	0.49
2:K:114:GLU:OE1	6:K:702:HOH:O	2.19	0.49
1:G:239:PHE:HB2	3:H:126:ASN:HA	1.95	0.49
2:K:52:MET:HG2	2:K:257:ILE:HA	1.93	0.49
2:K:281:TYR:CZ	2:K:285:VAL:HG11	2.47	0.49
2:P:214:ASN:N	2:P:214:ASN:OD1	2.44	0.49
2:P:140:GLN:HG3	2:P:246:HIS:CE1	2.48	0.49
3:R:39:HIS:HA	3:R:44:ARG:HB2	1.94	0.49
2:F:186:ARG:CZ	2:F:277:THR:HG23	2.42	0.49
2:K:203:ASN:O	2:K:278:GLN:NE2	2.44	0.49
2:K:82:LEU:O	2:K:87:THR:OG1	2.31	0.49
2:K:320:ARG:NH1	4:N:34:GLU:OE2	2.42	0.49
4:N:42:LEU:HD23	4:N:52:ILE:HD11	1.94	0.49
1:B:146:ASN:O	1:B:214:PRO:HG3	2.13	0.49
2:F:104:LYS:HG2	2:F:168:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:ARG:NH2	2:F:222:GLU:OE2	2.46	0.49
2:K:360:ARG:NH2	2:K:501:VAL:O	2.44	0.49
2:P:508:THR:OG1	2:P:509:LEU:N	2.45	0.49
2:A:118:ILE:HG23	2:A:141:VAL:HG13	1.95	0.49
4:D:39:VAL:HB	4:D:113:ILE:HB	1.93	0.49
2:K:15:ALA:HA	1:Q:362:ASP:HA	1.93	0.49
1:B:168:ARG:HD2	2:A:119:ALA:HB1	1.93	0.49
2:A:70:MET:HG2	2:A:74:LYS:HE2	1.94	0.49
2:F:196:ASP:HB3	2:F:199:GLU:HB3	1.95	0.49
1:G:312:TYR:O	1:G:316:VAL:HG23	2.12	0.49
2:K:21:THR:C	2:K:23:VAL:H	2.14	0.49
2:F:222:GLU:CD	4:I:73:ARG:HH11	2.17	0.49
3:M:4:LEU:HD23	3:M:5:GLY:H	1.78	0.49
1:Q:69:TRP:CG	3:R:6:ILE:HD11	2.48	0.49
2:A:398:PRO:HB3	2:A:511:ASP:OD2	2.13	0.49
2:A:419:ARG:NH1	2:A:466:CYS:O	2.46	0.49
2:F:77:ARG:NH1	4:I:108:ASP:OD2	2.46	0.49
3:H:80:LYS:HD3	3:H:84:GLY:HA2	1.94	0.49
2:K:218:VAL:HG11	4:N:41:VAL:HG11	1.95	0.49
2:P:110:LEU:HD11	2:P:217:ILE:HG12	1.94	0.49
3:R:23:ASN:OD1	3:R:23:ASN:N	2.46	0.49
1:B:160:PHE:HE1	2:A:138:LEU:HD12	1.78	0.48
2:K:272:ASN:ND2	2:K:330:ARG:H	2.05	0.48
3:M:19:ILE:HD11	3:M:60:LEU:HD22	1.95	0.48
3:R:12:ARG:HE	3:R:52:ASP:HB3	1.78	0.48
2:A:457:TRP:HD1	2:A:464:TYR:HB2	1.77	0.48
4:D:52:ILE:HA	4:D:56:LEU:HB3	1.95	0.48
2:K:112:VAL:HG11	2:K:181:TRP:CZ3	2.47	0.48
1:Q:173:ASP:OD1	1:Q:174:VAL:N	2.45	0.48
3:R:76:ASP:O	3:R:80:LYS:HB3	2.13	0.48
2:A:32:LEU:HB3	2:A:132:GLU:HG2	1.95	0.48
3:C:55:TRP:CZ2	3:C:59:LYS:HE3	2.48	0.48
2:P:526:PHE:HE2	3:R:165:HIS:HB2	1.78	0.48
2:P:187:VAL:HG13	2:P:281:TYR:HB3	1.93	0.48
2:F:222:GLU:OE1	4:I:76:TYR:OH	2.13	0.48
1:G:42:ARG:NH1	1:G:297:ASP:OD2	2.32	0.48
4:I:26:ALA:HA	4:I:27:ASP:HA	1.70	0.48
1:Q:9:ARG:NH1	2:P:230:GLU:OE2	2.45	0.48
4:S:115:ARG:NH1	4:S:127:SER:O	2.46	0.48
2:P:52:MET:SD	2:P:257:ILE:HD13	2.54	0.48
1:Q:194:GLN:OE1	1:Q:197:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:87:VAL:HB	4:N:123:PHE:HB3	1.96	0.48
2:P:144:GLU:OE1	2:P:246:HIS:HE1	1.97	0.48
1:L:262:ARG:HG3	1:Q:132:GLN:HE21	1.77	0.48
1:Q:75:LYS:HB3	1:Q:80:ARG:O	2.14	0.48
3:C:23:ASN:ND2	4:S:28:GLU:OE2	2.37	0.48
3:C:44:ARG:HD3	3:C:47:TYR:CZ	2.49	0.48
2:P:363:LEU:HD11	2:P:395:CYS:SG	2.54	0.48
2:A:360:ARG:HD2	2:A:489:ARG:HH22	1.78	0.48
1:B:188:ASP:OD2	2:A:65:LYS:NZ	2.46	0.48
2:F:224:ALA:HB1	2:F:229:ASP:HB3	1.95	0.48
2:K:414:PRO:HB2	2:K:416:TYR:CE1	2.49	0.48
2:P:112:VAL:HG22	2:P:116:ASN:HD21	1.79	0.48
2:P:469:ILE:HG13	2:P:473:TYR:CD2	2.49	0.48
1:Q:263:GLU:HB3	1:Q:355:SER:HB2	1.95	0.48
4:D:44:LYS:NZ	4:D:49:ASN:HD21	2.11	0.48
2:F:462:GLU:OE2	3:H:143:ARG:NH1	2.32	0.48
3:H:152:LEU:O	3:H:156:ARG:HG3	2.14	0.48
1:Q:184:PHE:HD1	2:P:138:LEU:HD13	1.79	0.48
1:G:256:PHE:HA	1:G:332:LEU:HD21	1.95	0.47
1:Q:239:PHE:HB2	3:R:126:ASN:HA	1.96	0.47
2:A:214:ASN:HB2	2:A:215:PRO:HD3	1.96	0.47
2:A:307:ARG:NH1	4:D:8:TYR:O	2.46	0.47
2:A:88:ARG:HG3	4:I:44:LYS:HB2	1.95	0.47
2:K:204:LEU:HD22	2:K:209:GLU:HG3	1.95	0.47
2:K:49:LYS:HE3	3:M:144:ASN:HD22	1.80	0.47
1:L:161:ASN:HB3	1:L:235:TRP:CE2	2.50	0.47
2:K:435:THR:HA	3:M:167:GLN:HE21	1.80	0.47
1:Q:343:PRO:O	1:Q:346:THR:OG1	2.25	0.47
2:A:255:VAL:HG22	4:D:132:LEU:HD23	1.96	0.47
2:P:272:ASN:OD1	2:P:330:ARG:N	2.47	0.47
2:P:73:VAL:O	2:P:77:ARG:HG3	2.14	0.47
4:S:78:TRP:HH2	4:S:80:LYS:HD2	1.80	0.47
3:C:41:THR:O	3:C:44:ARG:HD2	2.14	0.47
1:Q:160:PHE:HE1	2:P:138:LEU:HD12	1.79	0.47
2:A:316:ILE:HG21	4:D:113:ILE:HG22	1.96	0.47
1:G:20:ILE:CG2	2:F:96:HIS:HB2	2.42	0.47
2:K:297:LYS:NZ	2:K:368:GLU:OE1	2.45	0.47
1:Q:349:LYS:O	1:Q:353:THR:OG1	2.27	0.47
1:B:164:SER:HA	2:A:125:TRP:CE3	2.48	0.47
4:D:65:ASN:O	4:D:68:VAL:HG12	2.15	0.47
2:K:77:ARG:HH22	4:N:45:SER:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:38:ASP:OD1	3:M:45:ASN:ND2	2.38	0.47
2:P:147:HIS:NE2	2:P:242:ASP:OD2	2.44	0.47
2:P:97:PRO:HB2	2:P:501:VAL:HG22	1.97	0.47
1:B:117:TRP:CG	2:A:65:LYS:HB3	2.49	0.47
4:I:115:ARG:NH1	4:I:127:SER:O	2.48	0.47
1:L:243:GLU:OE2	1:L:323:LYS:NZ	2.34	0.47
4:D:41:VAL:HG12	4:D:110:SER:HB2	1.97	0.47
2:F:140:GLN:HG3	2:F:246:HIS:CE1	2.50	0.47
2:F:50:TYR:HB3	2:F:52:MET:HE2	1.97	0.47
2:F:93:VAL:C	2:F:95:VAL:H	2.17	0.47
1:G:159:LEU:HG	1:G:248:VAL:HG13	1.97	0.47
4:I:40:LEU:HG	4:I:42:LEU:HD22	1.97	0.47
1:Q:128:SER:HB2	2:P:20:PRO:HD2	1.97	0.47
4:D:78:TRP:CH2	4:D:80:LYS:HD3	2.49	0.47
2:K:445:MET:HB3	2:K:523:VAL:HG11	1.96	0.47
1:L:21:LEU:HD21	2:K:94:ARG:NH2	2.30	0.47
1:L:239:PHE:HB2	3:M:126:ASN:HA	1.97	0.47
2:F:314:GLY:O	2:F:319:GLY:N	2.45	0.47
2:K:284:PRO:O	2:K:288:MET:HG2	2.15	0.47
1:L:57:GLN:OE1	1:L:176:ARG:NH1	2.48	0.47
3:M:61:GLU:O	3:M:121:PRO:HG3	2.15	0.47
1:B:236:GLN:HE21	2:A:42:ASN:HA	1.80	0.47
2:F:18:ARG:HG3	2:F:20:PRO:HD3	1.97	0.47
2:P:372:PHE:O	2:P:376:TYR:N	2.41	0.47
1:L:115:GLU:HG2	1:Q:115:GLU:HG2	1.95	0.47
1:B:343:PRO:O	1:B:346:THR:OG1	2.22	0.46
2:K:50:TYR:OH	2:K:270:ASP:OD2	2.27	0.46
2:P:281:TYR:CZ	2:P:285:VAL:HG11	2.50	0.46
2:P:331:SER:HB3	2:P:452:TRP:CE2	2.50	0.46
3:C:44:ARG:HD3	3:C:47:TYR:CE1	2.50	0.46
1:G:75:LYS:HG2	1:G:81:PRO:HA	1.97	0.46
2:F:333:LYS:HG3	4:I:30:GLN:HG2	1.96	0.46
1:L:46:LEU:HD12	1:L:47:THR:N	2.29	0.46
2:P:244:LEU:HB2	4:S:112:THR:CG2	2.44	0.46
3:R:80:LYS:HE3	3:R:80:LYS:HB2	1.79	0.46
4:S:78:TRP:CH2	4:S:80:LYS:HD2	2.51	0.46
2:A:435:THR:HG23	3:C:167:GLN:HG2	1.98	0.46
2:K:353:LEU:O	2:K:356:THR:OG1	2.33	0.46
4:S:47:GLU:CD	4:S:47:GLU:H	2.18	0.46
2:A:74:LYS:NZ	4:D:106:LEU:O	2.49	0.46
3:C:36:ARG:O	3:C:40:THR:HB	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:CYS:O	2:F:204:LEU:HB3	2.15	0.46
2:F:354:TRP:CH2	2:F:499:PRO:HD3	2.50	0.46
4:D:43:LYS:HE2	2:F:88:ARG:HH21	1.81	0.46
2:F:390:TRP:CE2	2:F:404:PRO:HB3	2.50	0.46
2:K:224:ALA:HB1	2:K:229:ASP:HB3	1.98	0.46
1:L:197:ARG:NH2	1:L:210:SER:O	2.32	0.46
2:P:432:GLY:O	2:P:434:SER:N	2.49	0.46
2:A:49:LYS:NZ	2:A:270:ASP:OD2	2.49	0.46
2:A:281:TYR:CZ	2:A:285:VAL:HG21	2.51	0.46
1:B:165:GLN:HE22	1:B:239:PHE:CA	2.28	0.46
2:F:130:ALA:O	2:F:134:LYS:HG3	2.16	0.46
4:N:11:GLY:HA2	4:N:12:ILE:C	2.37	0.46
2:A:177:ILE:HG23	2:A:485:LEU:HD12	1.98	0.46
2:A:196:ASP:HB3	2:A:199:GLU:HB2	1.97	0.46
1:B:164:SER:HA	2:A:125:TRP:CZ3	2.51	0.46
2:P:227:ASN:ND2	2:P:294:SER:HB2	2.31	0.46
2:P:382:HIS:ND1	2:P:431:LYS:HE2	2.31	0.46
1:Q:159:LEU:HG	1:Q:248:VAL:HG13	1.98	0.46
1:Q:171:LEU:HD12	1:Q:171:LEU:HA	1.82	0.46
1:G:76:PHE:HB2	1:G:80:ARG:HB3	1.98	0.46
2:K:84:ASP:OD1	2:K:85:ALA:N	2.48	0.46
2:P:419:ARG:HD2	2:P:446:HIS:HD2	1.79	0.46
1:Q:61:ASP:HB3	3:R:55:TRP:CD1	2.51	0.46
4:N:2:SER:O	4:N:6:ASN:ND2	2.49	0.45
2:P:140:GLN:O	2:P:144:GLU:HG2	2.15	0.45
2:P:218:VAL:HG21	4:S:111:SER:HB2	1.97	0.45
3:H:36:ARG:O	3:H:116:GLN:NE2	2.46	0.45
2:K:27:GLU:HG3	2:K:30:ARG:HH21	1.81	0.45
1:Q:143:GLU:OE2	1:Q:147:ARG:NE	2.44	0.45
2:K:215:PRO:HA	2:K:219:ALA:HB3	1.97	0.45
2:K:63:ILE:HG22	2:K:66:GLU:H	1.82	0.45
2:K:163:GLN:HA	1:Q:2:SER:OG	2.17	0.45
4:S:58:THR:O	4:S:62:LYS:NZ	2.35	0.45
2:A:110:LEU:HD11	2:A:217:ILE:HD11	1.99	0.45
2:A:360:ARG:NH2	2:A:501:VAL:O	2.49	0.45
3:C:111:HIS:O	3:C:115:ARG:HG3	2.17	0.45
2:F:281:TYR:CZ	2:F:285:VAL:HG21	2.52	0.45
2:F:84:ASP:OD1	2:F:88:ARG:NH2	2.48	0.45
1:B:116:GLU:HG3	1:G:122:ARG:HH21	1.81	0.45
1:B:176:ARG:HD3	2:A:118:ILE:HG21	1.98	0.45
4:I:57:LEU:HD11	4:I:70:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:THR:HA	2:K:466:CYS:HB2	1.99	0.45
2:P:419:ARG:O	2:P:422:GLN:NE2	2.50	0.45
2:A:186:ARG:CZ	2:A:277:THR:HG23	2.47	0.45
2:F:101:GLU:OE2	2:F:360:ARG:NH1	2.50	0.45
1:Q:82:SER:OG	2:P:190:ASP:OD1	2.29	0.45
2:P:214:ASN:HB2	2:P:215:PRO:HD3	1.98	0.45
2:A:88:ARG:NH2	2:F:234:THR:HG22	2.32	0.45
2:F:80:GLY:O	2:F:84:ASP:N	2.37	0.45
1:G:268:LEU:HD13	1:G:342:LEU:HD21	1.99	0.45
1:B:263:GLU:HB3	1:B:355:SER:HB2	1.99	0.45
1:Q:263:GLU:HG3	1:Q:359:VAL:HG23	1.98	0.45
1:Q:61:ASP:HB3	3:R:55:TRP:HD1	1.82	0.45
4:S:93:SER:HB2	4:S:100:PHE:HB3	1.97	0.45
1:B:106:HIS:CE1	2:A:146:ARG:HD3	2.51	0.45
1:G:102:LEU:HD23	1:G:290:ILE:HG23	1.99	0.45
4:I:65:ASN:O	4:I:68:VAL:HG12	2.17	0.45
1:L:54:VAL:O	2:K:172:ARG:NH1	2.50	0.45
1:L:117:TRP:CG	2:K:65:LYS:HB3	2.52	0.45
1:L:184:PHE:CD1	2:K:138:LEU:HD13	2.52	0.45
2:A:192:PHE:HA	2:A:203:ASN:ND2	2.31	0.44
1:B:35:MET:HA	2:A:169:ASN:HA	1.98	0.44
1:L:57:GLN:OE1	2:K:115:TYR:OH	2.22	0.44
2:A:184:MET:O	2:A:189:SER:OG	2.35	0.44
1:B:41:PRO:HB2	1:B:43:TRP:O	2.17	0.44
3:H:17:ASN:O	3:H:21:GLN:NE2	2.46	0.44
2:K:437:ARG:NE	2:K:454:GLU:OE1	2.24	0.44
2:K:336:LYS:NZ	4:N:29:ASN:O	2.41	0.44
2:A:118:ILE:HD13	2:A:145:ILE:HG12	1.99	0.44
2:F:192:PHE:HA	2:F:203:ASN:ND2	2.33	0.44
3:H:126:ASN:N	3:H:126:ASN:OD1	2.49	0.44
1:L:366:ASP:OD2	2:P:15:ALA:N	2.51	0.44
4:N:23:GLN:O	4:N:29:ASN:ND2	2.39	0.44
1:Q:17:ALA:HA	1:Q:20:ILE:HB	1.99	0.44
2:A:95:VAL:O	2:A:163:GLN:NE2	2.50	0.44
1:B:40:THR:HA	1:B:41:PRO:HD3	1.89	0.44
2:K:521:ASN:OD1	2:K:523:VAL:HG23	2.18	0.44
1:Q:246:PHE:HB2	1:Q:299:TYR:CE1	2.52	0.44
1:Q:61:ASP:CG	3:R:7:HIS:HD1	2.21	0.44
2:P:300:PRO:HD2	2:P:303:LYS:HD2	1.98	0.44
2:A:454:GLU:OE1	3:C:156:ARG:NH2	2.45	0.44
3:H:115:ARG:O	3:H:119:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:36:ARG:O	3:H:40:THR:HB	2.18	0.44
4:I:48:ILE:HA	4:I:48:ILE:HD13	1.68	0.44
2:A:104:LYS:HG2	2:A:168:HIS:CE1	2.52	0.44
2:A:222:GLU:OE1	4:D:76:TYR:OH	2.31	0.44
2:F:73:VAL:O	2:F:77:ARG:HG3	2.18	0.44
2:A:211:CYS:HB2	2:A:313:TRP:CD1	2.53	0.44
1:B:184:PHE:HD1	2:A:138:LEU:HD13	1.83	0.44
1:B:92:THR:OG1	1:B:93:VAL:N	2.51	0.44
1:G:376:ASP:O	1:G:380:ILE:HG13	2.18	0.44
2:K:184:MET:HA	2:K:187:VAL:HG12	1.99	0.44
2:K:61:LYS:HD2	2:K:61:LYS:N	2.33	0.44
2:A:178:GLY:HA2	2:A:179:PRO:HD3	1.79	0.44
2:A:247:MET:HE1	4:D:112:THR:O	2.18	0.44
2:A:348:LEU:HD11	2:A:383:TYR:CD1	2.53	0.44
2:F:302:VAL:HG13	2:F:339:ALA:O	2.17	0.44
1:G:137:ASN:HA	1:G:138:PRO:HD3	1.87	0.44
2:K:468:ASN:OD1	2:K:471:GLU:N	2.25	0.44
1:B:256:PHE:HA	1:B:332:LEU:HD21	1.99	0.43
1:B:349:LYS:HG2	1:B:388:LEU:HD21	1.98	0.43
1:B:2:SER:HB2	1:G:28:PRO:HG3	1.99	0.43
2:P:473:TYR:O	2:P:519:PHE:HB2	2.17	0.43
1:Q:240:ASP:HB3	1:Q:243:GLU:HB3	1.99	0.43
3:R:32:LEU:HD23	3:R:122:ILE:HD11	1.99	0.43
3:R:33:LYS:O	3:R:37:MET:HG2	2.18	0.43
2:F:362:ALA:HB2	2:F:501:VAL:HB	2.00	0.43
2:K:25:ALA:HB1	2:K:63:ILE:HB	1.99	0.43
1:L:268:LEU:HD23	1:L:342:LEU:HD21	2.00	0.43
4:N:102:VAL:HG22	4:N:121:ASN:HA	1.99	0.43
2:P:62:LEU:O	2:P:135:ASN:ND2	2.50	0.43
1:Q:121:ASP:O	1:Q:125:GLN:HG3	2.17	0.43
2:F:235:VAL:O	2:F:239:ILE:HG13	2.18	0.43
2:F:243:GLU:O	2:F:247:MET:HG3	2.18	0.43
2:F:397:ASP:OD1	2:F:399:SER:OG	2.36	0.43
2:K:186:ARG:HA	2:K:190:ASP:HB2	2.00	0.43
2:K:390:TRP:CD2	2:K:404:PRO:HB3	2.54	0.43
1:B:226:SER:HB2	1:B:331:ALA:HA	2.00	0.43
1:L:128:SER:HB2	2:K:20:PRO:HD2	2.00	0.43
2:K:147:HIS:NE2	2:K:242:ASP:OD2	2.34	0.43
1:L:42:ARG:HB2	1:L:99:ARG:HG3	2.00	0.43
1:Q:136:MET:HG3	1:Q:273:GLY:O	2.18	0.43
2:A:442:ASN:ND2	3:C:44:ARG:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:26:GLN:CD	2:K:26:GLN:H	2.21	0.43
1:L:282:ASN:O	1:L:286:THR:OG1	2.27	0.43
1:L:9:ARG:NH2	4:N:74:ALA:O	2.51	0.43
2:F:187:VAL:CG1	2:F:281:TYR:HB3	2.49	0.43
2:F:77:ARG:O	2:F:81:SER:OG	2.30	0.43
4:I:49:ASN:OD1	4:I:77:TRP:NE1	2.44	0.43
3:M:36:ARG:O	3:M:40:THR:HB	2.19	0.43
4:N:18:LYS:HE2	4:N:18:LYS:HB3	1.77	0.43
2:A:314:GLY:O	2:A:319:GLY:N	2.50	0.43
1:B:266:GLN:HB2	1:B:281:ILE:HG21	2.00	0.43
2:F:172:ARG:HA	2:F:175:ARG:HD2	2.01	0.43
2:P:28:VAL:HB	2:P:63:ILE:HG21	2.01	0.43
4:S:129:LEU:O	4:S:133:ASP:HB2	2.19	0.43
2:A:489:ARG:NH2	2:A:496:ILE:O	2.52	0.43
2:F:180:LEU:O	2:F:281:TYR:OH	2.32	0.43
1:G:106:HIS:CE1	2:F:146:ARG:HD2	2.54	0.43
4:N:48:ILE:O	4:N:52:ILE:HG12	2.18	0.43
2:P:437:ARG:HB2	2:P:448:PHE:HB2	1.99	0.43
3:R:28:ALA:HB1	3:R:64:VAL:HG22	2.00	0.43
3:C:36:ARG:CZ	3:C:119:LYS:HB3	2.48	0.43
3:C:94:THR:HA	3:C:97:LYS:HD3	2.00	0.43
1:L:337:GLY:O	1:L:341:LYS:NZ	2.35	0.43
4:S:52:ILE:O	4:S:57:LEU:HB2	2.18	0.43
1:B:13:ASP:HA	1:B:14:PRO:HD2	1.75	0.43
4:D:129:LEU:HD13	4:D:132:LEU:HD11	2.01	0.43
2:F:112:VAL:O	2:F:116:ASN:ND2	2.40	0.43
1:G:168:ARG:HD3	2:F:123:MET:HG3	2.00	0.43
3:H:98:MET:HG3	3:H:138:ARG:HG2	2.01	0.43
2:K:248:ALA:O	2:K:252:GLN:HG2	2.19	0.43
1:Q:92:THR:HB	1:Q:303:LEU:HD23	2.00	0.43
1:G:323:LYS:HE2	3:H:78:ARG:HD2	2.00	0.42
2:P:114:GLU:OE1	2:P:147:HIS:ND1	2.52	0.42
2:P:50:TYR:CD1	2:P:257:ILE:HD12	2.53	0.42
1:Q:75:LYS:HZ1	2:P:465:GLU:HG3	1.84	0.42
2:A:196:ASP:HB3	2:A:199:GLU:CB	2.49	0.42
2:A:426:CYS:HA	2:A:427:PRO:HD3	1.85	0.42
1:G:29:LEU:HD23	2:F:506:LEU:HD11	2.00	0.42
1:G:116:GLU:OE1	1:G:287:TYR:OH	2.23	0.42
1:G:196:GLU:OE2	1:G:277:THR:HG22	2.19	0.42
3:H:78:ARG:HG2	3:H:79:HIS:CE1	2.54	0.42
1:Q:226:SER:OG	1:Q:334:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:357:TYR:HD1	1:Q:377:ARG:HH21	1.66	0.42
4:S:129:LEU:HB3	4:S:132:LEU:HD12	2.01	0.42
1:B:95:TRP:NE1	1:B:171:LEU:HD23	2.33	0.42
4:D:47:GLU:OE2	4:D:98:ARG:NH2	2.53	0.42
2:F:472:GLN:HA	3:H:51:ASN:OD1	2.19	0.42
2:K:96:HIS:CG	2:K:97:PRO:HD2	2.54	0.42
2:P:125:TRP:CH2	2:P:138:LEU:HG	2.55	0.42
2:P:279:GLN:O	2:P:283:THR:OG1	2.38	0.42
2:P:508:THR:HG23	2:P:511:ASP:OD2	2.19	0.42
1:Q:161:ASN:O	1:Q:164:SER:OG	2.29	0.42
3:R:91:LEU:HD12	3:R:92:ASP:N	2.34	0.42
1:B:30:ASP:HB3	2:A:165:PRO:HG2	2.01	0.42
2:A:360:ARG:HG2	2:A:498:GLN:HB2	2.01	0.42
2:K:24:ASN:OD1	2:K:26:GLN:HG2	2.18	0.42
1:Q:164:SER:HA	2:P:125:TRP:CE3	2.54	0.42
1:Q:258:GLN:O	1:Q:262:ARG:HB3	2.20	0.42
4:S:26:ALA:HA	4:S:27:ASP:HA	1.74	0.42
1:B:100:ASP:OD2	1:B:104:ARG:HD3	2.18	0.42
1:B:125:GLN:HB2	2:A:21:THR:HB	2.01	0.42
1:L:140:TRP:HZ2	1:L:269:ALA:HB2	1.85	0.42
2:P:211:CYS:HB2	2:P:313:TRP:CD1	2.55	0.42
4:S:115:ARG:HG2	4:S:115:ARG:H	1.66	0.42
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.86	0.42
2:F:133:GLN:O	2:F:137:TYR:N	2.45	0.42
3:H:72:PHE:CD2	3:H:76:ASP:HB3	2.54	0.42
4:I:105:PHE:O	4:I:109:VAL:HG23	2.19	0.42
1:L:125:GLN:HG3	2:K:21:THR:H	1.84	0.42
1:L:240:ASP:HB3	1:L:243:GLU:HB3	2.01	0.42
3:R:41:THR:HG21	3:R:112:ILE:HG23	2.02	0.42
2:A:343:HIS:CD2	2:A:343:HIS:H	2.37	0.42
2:K:242:ASP:O	2:K:244:LEU:N	2.53	0.42
2:P:221:THR:HG21	2:P:237:LEU:HG	2.02	0.42
1:Q:164:SER:HA	2:P:125:TRP:CZ3	2.55	0.42
1:Q:76:PHE:HB2	1:Q:80:ARG:HB3	2.02	0.42
3:C:22:LEU:HD11	3:C:31:MET:SD	2.60	0.42
2:A:377:PRO:HG2	4:D:18:LYS:CD	2.49	0.42
2:F:106:VAL:O	2:F:110:LEU:HB2	2.19	0.42
1:G:113:LYS:HE3	1:G:188:ASP:OD2	2.19	0.42
1:L:153:LEU:HD21	2:K:35:PHE:CD1	2.55	0.42
1:L:24:LEU:HA	1:L:25:PRO:HD3	1.90	0.42
4:D:3:VAL:O	4:D:69:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ASP:OD2	1:G:104:ARG:HD3	2.19	0.42
1:B:122:ARG:HH21	1:G:116:GLU:HG3	1.84	0.42
1:L:15:GLU:O	1:L:19:VAL:HG13	2.19	0.42
3:M:86:ASP:O	3:M:90:VAL:HG23	2.19	0.42
3:R:38:ASP:O	3:R:45:ASN:N	2.53	0.42
2:F:324:TYR:O	2:F:326:VAL:N	2.52	0.42
2:K:214:ASN:HB2	2:K:215:PRO:HD3	2.02	0.42
1:L:64:ALA:HB3	1:L:95:TRP:CD1	2.55	0.42
2:P:23:VAL:HA	2:P:27:GLU:OE1	2.20	0.42
2:P:187:VAL:HG21	2:P:281:TYR:CD1	2.54	0.42
1:Q:300:TYR:O	1:Q:305:ASP:N	2.52	0.42
2:A:111:GLU:CD	2:A:172:ARG:HH21	2.23	0.41
3:C:61:GLU:O	3:C:121:PRO:HG3	2.20	0.41
1:G:168:ARG:HD2	2:F:119:ALA:HB1	2.02	0.41
2:A:81:SER:HB3	2:F:85:ALA:HB2	2.01	0.41
3:H:167:GLN:HG3	3:H:168:SER:N	2.35	0.41
3:R:27:LYS:HD2	3:R:27:LYS:N	2.35	0.41
2:A:354:TRP:CH2	2:A:499:PRO:HD3	2.55	0.41
2:A:508:THR:HG22	2:A:509:LEU:N	2.35	0.41
2:F:187:VAL:HG12	2:F:278:GLN:HA	2.01	0.41
4:I:44:LYS:HG2	4:I:77:TRP:NE1	2.34	0.41
2:K:205:GLN:HB3	2:K:250:GLY:HA3	2.01	0.41
2:P:284:PRO:HB3	2:P:342:ALA:HB1	2.02	0.41
2:P:403:ILE:O	2:P:405:LEU:N	2.53	0.41
1:L:270:PRO:HB3	1:Q:270:PRO:HB3	2.02	0.41
1:B:380:ILE:O	1:B:384:VAL:HG23	2.20	0.41
1:B:86:GLU:OE1	3:C:115:ARG:NH2	2.53	0.41
2:F:230:GLU:O	2:F:234:THR:HG23	2.20	0.41
2:F:423:VAL:HA	2:F:424:PRO:HD3	1.95	0.41
1:G:117:TRP:CG	2:F:65:LYS:HB3	2.56	0.41
1:G:303:LEU:HD12	1:G:303:LEU:HA	1.95	0.41
4:I:115:ARG:H	4:I:115:ARG:HG2	1.58	0.41
1:L:165:GLN:HG3	2:K:46:TYR:OH	2.21	0.41
1:L:355:SER:O	1:L:359:VAL:HG23	2.20	0.41
3:R:72:PHE:HD1	3:R:72:PHE:HA	1.73	0.41
2:A:24:ASN:OD1	2:A:26:GLN:HG2	2.20	0.41
2:A:509:LEU:HD23	2:A:509:LEU:HA	1.86	0.41
4:D:97:GLY:HA3	1:G:47:THR:HA	2.03	0.41
2:F:207:VAL:O	2:F:211:CYS:HB3	2.20	0.41
2:F:29:HIS:ND1	2:F:61:LYS:HB3	2.34	0.41
1:Q:336:MET:SD	1:Q:384:VAL:HG12	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ALA:N	1:B:270:PRO:HD2	2.34	0.41
2:F:212:PHE:O	2:F:216:LEU:HB3	2.20	0.41
1:L:141:ARG:HD2	1:L:204:VAL:HG21	2.02	0.41
1:Q:24:LEU:HA	1:Q:25:PRO:HD3	1.86	0.41
1:G:20:ILE:HA	2:F:96:HIS:HD2	1.86	0.41
1:G:228:ARG:HE	1:G:228:ARG:HB3	1.71	0.41
1:G:229:LEU:HD12	1:G:229:LEU:HA	1.85	0.41
1:G:24:LEU:HA	1:G:25:PRO:HD3	1.90	0.41
2:P:253:THR:O	2:P:253:THR:OG1	2.37	0.41
1:Q:131:GLY:CA	2:P:16:ALA:HB2	2.50	0.41
1:Q:312:TYR:O	1:Q:316:VAL:HG12	2.20	0.41
1:B:263:GLU:HG3	1:B:359:VAL:HG23	2.03	0.41
1:G:37:TYR:CE1	2:F:170:ASP:HB3	2.56	0.41
2:F:223:TRP:CZ3	2:F:297:LYS:HA	2.54	0.41
2:F:437:ARG:HB2	2:F:448:PHE:HB2	2.02	0.41
1:G:13:ASP:HA	1:G:14:PRO:HD2	1.84	0.41
4:I:2:SER:O	4:I:6:ASN:ND2	2.54	0.41
2:K:244:LEU:O	2:K:244:LEU:HD12	2.19	0.41
2:K:390:TRP:CE2	2:K:404:PRO:HB3	2.55	0.41
1:Q:76:PHE:CE1	2:P:194:SER:HA	2.56	0.41
3:R:61:GLU:O	3:R:121:PRO:HG3	2.21	0.41
3:R:73:ASN:OD1	3:R:76:ASP:HB2	2.21	0.41
1:G:217:GLU:O	1:G:221:GLY:HA3	2.20	0.41
2:K:18:ARG:C	2:K:20:PRO:HD3	2.40	0.41
2:K:187:VAL:HG11	2:K:281:TYR:CD2	2.56	0.41
2:K:272:ASN:ND2	2:K:330:ARG:HG3	2.33	0.41
1:L:113:LYS:NZ	1:L:185:ASP:OD1	2.50	0.41
2:P:439:HIS:HB3	3:R:161:VAL:HG21	2.03	0.41
2:A:221:THR:HG22	2:A:233:PRO:HA	2.02	0.41
2:A:360:ARG:NH2	2:A:502:ARG:O	2.53	0.41
1:B:11:LEU:HD22	2:A:230:GLU:HG3	2.02	0.41
1:B:289:GLN:NE2	1:G:130:ASP:OD1	2.54	0.41
2:F:361:LEU:HA	2:F:361:LEU:HD12	1.87	0.41
2:K:281:TYR:O	2:K:284:PRO:HD2	2.20	0.41
3:M:94:THR:HG21	3:M:114:PHE:CD1	2.55	0.41
1:Q:333:ARG:HG3	1:Q:387:GLY:HA3	2.03	0.41
3:H:44:ARG:HG3	3:H:46:SER:O	2.21	0.41
2:K:118:ILE:HD13	2:K:145:ILE:HG12	2.03	0.41
2:K:257:ILE:HD11	2:K:267:LEU:HD12	2.03	0.41
2:K:283:THR:HG21	2:K:339:ALA:HA	2.02	0.41
1:L:46:LEU:CD1	1:L:50:GLU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:187:VAL:CG1	2:P:281:TYR:HB3	2.51	0.41
1:Q:256:PHE:HA	1:Q:332:LEU:HD21	2.03	0.41
2:A:88:ARG:HH12	2:F:234:THR:HG22	1.86	0.41
1:B:117:TRP:HB2	2:A:65:LYS:HB3	2.03	0.41
2:A:222:GLU:CD	4:D:73:ARG:HD3	2.42	0.41
1:G:314:ARG:O	1:G:318:ARG:HG3	2.21	0.41
1:Q:106:HIS:CE1	2:P:146:ARG:HD3	2.55	0.41
1:Q:202:LYS:NZ	1:Q:202:LYS:O	2.36	0.41
1:Q:306:ASP:O	1:Q:310:SER:HB2	2.21	0.41
1:G:9:ARG:NH1	2:F:230:GLU:OE2	2.50	0.40
2:F:478:LEU:O	2:F:482:ILE:HG13	2.21	0.40
1:G:356:LEU:HA	1:G:356:LEU:HD12	1.88	0.40
2:K:327:GLU:HB3	2:K:328:SER:H	1.68	0.40
2:K:383:TYR:O	2:K:386:ILE:HG22	2.20	0.40
1:L:203:ILE:HG13	1:L:204:VAL:HG23	2.02	0.40
1:L:256:PHE:HA	1:L:332:LEU:HD13	2.03	0.40
3:M:37:MET:HA	3:M:116:GLN:NE2	2.36	0.40
4:N:26:ALA:HA	4:N:27:ASP:HA	1.79	0.40
2:P:123:MET:O	2:P:127:SER:OG	2.23	0.40
2:P:243:GLU:OE2	2:P:246:HIS:CG	2.69	0.40
2:A:192:PHE:CE2	2:A:204:LEU:HD23	2.56	0.40
2:A:316:ILE:O	4:D:115:ARG:NH2	2.54	0.40
2:F:101:GLU:HG3	2:F:360:ARG:HB2	2.02	0.40
2:F:211:CYS:HB2	2:F:313:TRP:CD1	2.56	0.40
2:F:97:PRO:HD3	2:F:163:GLN:HE22	1.86	0.40
3:H:106:GLU:O	3:H:110:ILE:HG13	2.21	0.40
4:I:102:VAL:HG22	4:I:121:ASN:HA	2.03	0.40
2:K:283:THR:HB	2:K:284:PRO:HD3	2.03	0.40
2:K:70:MET:HG2	2:K:74:LYS:NZ	2.35	0.40
3:M:44:ARG:HG3	3:M:46:SER:O	2.21	0.40
2:P:222:GLU:OE1	4:S:76:TYR:OH	2.32	0.40
2:P:56:THR:HG21	2:P:252:GLN:O	2.21	0.40
2:P:32:LEU:HD12	2:P:35:PHE:CE2	2.56	0.40
1:Q:57:GLN:OE1	1:Q:176:ARG:NH1	2.49	0.40
2:A:332:LEU:HA	2:A:332:LEU:HD22	1.84	0.40
1:B:342:LEU:HA	1:B:343:PRO:HD2	1.86	0.40
2:F:167:GLY:O	2:F:171:ALA:HB2	2.22	0.40
2:F:196:ASP:HB3	2:F:199:GLU:CB	2.51	0.40
2:F:177:ILE:HG12	2:F:485:LEU:HD12	2.03	0.40
2:K:214:ASN:HA	2:K:218:VAL:HG23	2.02	0.40
1:L:124:LEU:HD12	2:K:21:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:ARG:HG3	2:K:31:TRP:CD1	2.57	0.40
2:K:88:ARG:NH2	4:S:43:LYS:HE2	2.36	0.40
2:A:401:GLY:HA2	2:A:515:LEU:HD23	2.02	0.40
1:G:377:ARG:O	1:G:381:VAL:HG23	2.22	0.40
2:K:117:ALA:O	2:K:121:THR:OG1	2.26	0.40
2:K:212:PHE:HD2	2:K:282:PHE:CD2	2.40	0.40
2:K:209:GLU:OE1	2:K:246:HIS:HB3	2.21	0.40
2:P:351:TYR:O	2:P:354:TRP:HD1	2.03	0.40
2:P:521:ASN:O	2:P:524:LYS:HG2	2.21	0.40
2:P:52:MET:H	2:P:52:MET:HG3	1.41	0.40
2:P:97:PRO:HB2	2:P:501:VAL:CG2	2.52	0.40
2:A:320:ARG:HH21	4:D:128:GLU:HA	1.86	0.40
1:B:388:LEU:O	1:B:389:LYS:HG2	2.21	0.40
2:F:302:VAL:O	2:F:306:ASN:N	2.51	0.40
1:G:245:ALA:HB3	1:G:299:TYR:OH	2.21	0.40
3:H:61:GLU:O	3:H:121:PRO:HG2	2.21	0.40
2:K:144:GLU:O	2:K:148:THR:OG1	2.32	0.40
2:K:440:GLU:HG2	2:K:445:MET:HG3	2.02	0.40
2:P:243:GLU:O	2:P:247:MET:HG3	2.22	0.40
2:P:354:TRP:CG	2:P:355:PRO:HD3	2.56	0.40
2:P:440:GLU:HB3	3:R:162:ARG:HB3	2.01	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	B	386/389 (99%)	363 (94%)	23 (6%)	0	100	100
1	G	386/389 (99%)	369 (96%)	17 (4%)	0	100	100
1	L	386/389 (99%)	355 (92%)	29 (8%)	2 (0%)	32	68
1	Q	386/389 (99%)	362 (94%)	23 (6%)	1 (0%)	44	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	507/527 (96%)	462 (91%)	42 (8%)	3 (1%)	28	64
2	F	507/527 (96%)	472 (93%)	31 (6%)	4 (1%)	22	57
2	K	507/527 (96%)	458 (90%)	41 (8%)	8 (2%)	11	37
2	P	507/527 (96%)	466 (92%)	35 (7%)	6 (1%)	15	46
3	C	164/170 (96%)	158 (96%)	6 (4%)	0	100	100
3	H	164/170 (96%)	154 (94%)	10 (6%)	0	100	100
3	M	164/170 (96%)	158 (96%)	6 (4%)	0	100	100
3	R	164/170 (96%)	156 (95%)	8 (5%)	0	100	100
4	D	130/141 (92%)	118 (91%)	11 (8%)	1 (1%)	22	57
4	I	130/141 (92%)	124 (95%)	6 (5%)	0	100	100
4	N	130/141 (92%)	115 (88%)	14 (11%)	1 (1%)	22	57
4	S	130/141 (92%)	112 (86%)	17 (13%)	1 (1%)	22	57
All	All	4748/4908 (97%)	4402 (93%)	319 (7%)	27 (1%)	28	64

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	23	VAL
2	F	22	SER
2	F	61	LYS
1	L	143	GLU
2	K	61	LYS
2	P	22	SER
2	A	16	ALA
2	A	61	LYS
4	D	74	ALA
2	F	325	GLY
1	L	141	ARG
2	P	17	ASN
2	P	61	LYS
2	P	433	ALA
4	S	74	ALA
2	K	17	ASN
2	K	243	GLU
2	K	244	LEU
2	K	321	LEU
4	N	74	ALA
2	F	18	ARG

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Mol	Chain	Res	Type
2	K	16	ALA
2	P	404	PRO
2	K	20	PRO
2	K	53	ALA
1	Q	81	PRO
2	P	467	GLN

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	B	321/323 (99%)	304 (95%)	17 (5%)	26	60
1	G	321/323 (99%)	300 (94%)	21 (6%)	20	49
1	L	321/323 (99%)	306 (95%)	15 (5%)	30	65
1	Q	321/323 (99%)	298 (93%)	23 (7%)	17	43
2	A	430/442 (97%)	397 (92%)	33 (8%)	15	40
2	F	430/442 (97%)	403 (94%)	27 (6%)	21	51
2	K	430/442 (97%)	387 (90%)	43 (10%)	9	27
2	P	430/442 (97%)	393 (91%)	37 (9%)	12	35
3	C	144/147 (98%)	139 (96%)	5 (4%)	41	75
3	H	144/147 (98%)	133 (92%)	11 (8%)	15	41
3	M	144/147 (98%)	131 (91%)	13 (9%)	11	33
3	R	144/147 (98%)	135 (94%)	9 (6%)	21	51
4	D	116/124 (94%)	100 (86%)	16 (14%)	4	12
4	I	116/124 (94%)	97 (84%)	19 (16%)	2	8
4	N	116/124 (94%)	101 (87%)	15 (13%)	5	15
4	S	116/124 (94%)	107 (92%)	9 (8%)	15	39
All	All	4044/4144 (98%)	3731 (92%)	313 (8%)	15	40

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	GLU
1	B	35	MET
1	B	40	THR
1	B	46	LEU
1	B	80	ARG
1	B	93	VAL
1	B	142	ASP
1	B	145	ILE
1	B	159	LEU
1	B	160	PHE
1	B	171	LEU
1	B	173	ASP
1	B	177	VAL
1	B	223	VAL
1	B	229	LEU
1	B	266	GLN
1	B	301	ASN
2	A	18	ARG
2	A	26	GLN
2	A	32	LEU
2	A	43	ARG
2	A	52	MET
2	A	77	ARG
2	A	82	LEU
2	A	95	VAL
2	A	112	VAL
2	A	138	LEU
2	A	142	LEU
2	A	163	GLN
2	A	175	ARG
2	A	186	ARG
2	A	189	SER
2	A	204	LEU
2	A	206	LEU
2	A	279	GLN
2	A	286	LEU
2	A	289	LEU
2	A	302	VAL
2	A	307	ARG
2	A	332	LEU
2	A	334	ASP
2	A	349	LEU
2	A	454	GLU

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Mol	Chain	Res	Type
2	A	458	LEU
2	A	469	ILE
2	A	501	VAL
2	A	504	ASP
2	A	509	LEU
2	A	515	LEU
2	A	516	ASN
3	C	18	LYS
3	C	25	LEU
3	C	32	LEU
3	C	162	ARG
3	C	168	SER
4	D	3	VAL
4	D	13	MET
4	D	27	ASP
4	D	31	VAL
4	D	38	VAL
4	D	44	LYS
4	D	51	PHE
4	D	57	LEU
4	D	70	VAL
4	D	73	ARG
4	D	102	VAL
4	D	106	LEU
4	D	115	ARG
4	D	124	THR
4	D	126	THR
4	D	133	ASP
1	G	7	ARG
1	G	92	THR
1	G	102	LEU
1	G	113	LYS
1	G	159	LEU
1	G	160	PHE
1	G	171	LEU
1	G	173	ASP
1	G	174	VAL
1	G	192	MET
1	G	202	LYS
1	G	229	LEU
1	G	244	SER
1	G	276	LEU

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Mol	Chain	Res	Type
1	G	277	THR
1	G	303	LEU
1	G	308	GLU
1	G	334	ASP
1	G	342	LEU
1	G	356	LEU
1	G	379	GLN
2	F	17	ASN
2	F	18	ARG
2	F	23	VAL
2	F	43	ARG
2	F	52	MET
2	F	82	LEU
2	F	110	LEU
2	F	187	VAL
2	F	213	THR
2	F	238	SER
2	F	269	THR
2	F	272	ASN
2	F	286	LEU
2	F	289	LEU
2	F	302	VAL
2	F	307	ARG
2	F	311	GLU
2	F	349	LEU
2	F	361	LEU
2	F	399	SER
2	F	437	ARG
2	F	440	GLU
2	F	454	GLU
2	F	458	LEU
2	F	501	VAL
2	F	515	LEU
2	F	523	VAL
3	H	8	SER
3	H	24	THR
3	H	27	LYS
3	H	51	ASN
3	H	85	GLU
3	H	92	ASP
3	H	126	ASN
3	H	135	LEU

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Mol	Chain	Res	Type
3	H	161	VAL
3	H	167	GLN
3	H	168	SER
4	I	3	VAL
4	I	4	ASN
4	I	19	ASP
4	I	30	GLN
4	I	32	VAL
4	I	38	VAL
4	I	42	LEU
4	I	48	ILE
4	I	57	LEU
4	I	68	VAL
4	I	70	VAL
4	I	73	ARG
4	I	94	GLU
4	I	95	LEU
4	I	102	VAL
4	I	106	LEU
4	I	110	SER
4	I	115	ARG
4	I	130	MET
1	L	19	VAL
1	L	35	MET
1	L	40	THR
1	L	133	ILE
1	L	142	ASP
1	L	160	PHE
1	L	164	SER
1	L	173	ASP
1	L	174	VAL
1	L	202	LYS
1	L	229	LEU
1	L	276	LEU
1	L	301	ASN
1	L	303	LEU
1	L	336	MET
2	K	23	VAL
2	K	24	ASN
2	K	26	GLN
2	K	27	GLU
2	K	36	ASN

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Mol	Chain	Res	Type
2	K	42	ASN
2	K	43	ARG
2	K	51	LYS
2	K	52	MET
2	K	54	ASN
2	K	63	ILE
2	K	77	ARG
2	K	82	LEU
2	K	110	LEU
2	K	138	LEU
2	K	141	VAL
2	K	144	GLU
2	K	173	ARG
2	K	175	ARG
2	K	189	SER
2	K	204	LEU
2	K	231	ILE
2	K	237	LEU
2	K	257	ILE
2	K	266	TYR
2	K	271	LEU
2	K	279	GLN
2	K	302	VAL
2	K	307	ARG
2	K	331	SER
2	K	361	LEU
2	K	369	MET
2	K	386	ILE
2	K	405	LEU
2	K	435	THR
2	K	437	ARG
2	K	439	HIS
2	K	440	GLU
2	K	442	ASN
2	K	501	VAL
2	K	506	LEU
2	K	510	ASP
2	K	523	VAL
3	M	3	LYS
3	M	4	LEU
3	M	22	LEU
3	M	25	LEU

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Mol	Chain	Res	Type
3	M	33	LYS
3	M	44	ARG
3	M	60	LEU
3	M	91	LEU
3	M	110	ILE
3	M	138	ARG
3	M	154	GLU
3	M	161	VAL
3	M	164	VAL
4	N	3	VAL
4	N	19	ASP
4	N	32	VAL
4	N	42	LEU
4	N	73	ARG
4	N	85	ILE
4	N	90	ASP
4	N	91	GLU
4	N	98	ARG
4	N	102	VAL
4	N	106	LEU
4	N	112	THR
4	N	115	ARG
4	N	127	SER
4	N	132	LEU
1	Q	130	ASP
1	Q	139	THR
1	Q	142	ASP
1	Q	147	ARG
1	Q	160	PHE
1	Q	164	SER
1	Q	171	LEU
1	Q	174	VAL
1	Q	192	MET
1	Q	208	ASP
1	Q	213	VAL
1	Q	217	GLU
1	Q	274	ASP
1	Q	311	ASP
1	Q	315	THR
1	Q	316	VAL
1	Q	323	LYS
1	Q	334	ASP

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Mol	Chain	Res	Type
1	Q	336	MET
1	Q	347	THR
1	Q	348	ASP
1	Q	349	LYS
1	Q	389	LYS
2	P	21	THR
2	P	22	SER
2	P	43	ARG
2	P	52	MET
2	P	77	ARG
2	P	81	SER
2	P	82	LEU
2	P	93	VAL
2	P	110	LEU
2	P	138	LEU
2	P	142	LEU
2	P	185	LYS
2	P	187	VAL
2	P	204	LEU
2	P	206	LEU
2	P	214	ASN
2	P	220	VAL
2	P	243	GLU
2	P	253	THR
2	P	267	LEU
2	P	271	LEU
2	P	279	GLN
2	P	302	VAL
2	P	307	ARG
2	P	320	ARG
2	P	332	LEU
2	P	349	LEU
2	P	381	ASP
2	P	419	ARG
2	P	428	SER
2	P	434	SER
2	P	465	GLU
2	P	488	LEU
2	P	508	THR
2	P	513	LYS
2	P	515	LEU
2	P	517	CYS

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Mol	Chain	Res	Type
3	R	6	ILE
3	R	8	SER
3	R	39	HIS
3	R	52	ASP
3	R	72	PHE
3	R	75	VAL
3	R	81	THR
3	R	89	SER
3	R	135	LEU
4	S	3	VAL
4	S	19	ASP
4	S	57	LEU
4	S	73	ARG
4	S	94	GLU
4	S	102	VAL
4	S	115	ARG
4	S	124	THR
4	S	133	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	GLN
1	B	165	GLN
2	A	29	HIS
2	A	90	ASN
2	A	203	ASN
2	A	306	ASN
4	D	49	ASN
2	F	140	GLN
2	F	155	ASN
2	F	163	GLN
2	F	168	HIS
2	F	205	GLN
3	H	79	HIS
2	K	78	GLN
2	K	150	GLN
2	K	272	ASN
3	M	21	GLN
3	M	144	ASN
1	Q	106	HIS
1	Q	379	GLN

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Mol	Chain	Res	Type
2	P	446	HIS
2	P	500	HIS
3	R	116	GLN
3	R	144	ASN
4	S	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	B	388/389 (99%)	-0.45	1 (0%) 93 93	14, 30, 47, 72	0
1	G	388/389 (99%)	-0.35	1 (0%) 93 93	23, 35, 55, 87	0
1	L	388/389 (99%)	-0.21	1 (0%) 93 93	25, 44, 68, 92	0
1	Q	388/389 (99%)	-0.07	2 (0%) 90 90	31, 54, 77, 99	0
2	A	511/527 (96%)	-0.29	2 (0%) 92 92	18, 36, 57, 88	0
2	F	511/527 (96%)	-0.34	1 (0%) 94 95	17, 33, 54, 104	0
2	K	511/527 (96%)	0.02	5 (0%) 82 81	29, 56, 79, 111	0
2	P	511/527 (96%)	-0.07	1 (0%) 94 95	24, 48, 75, 107	0
3	C	166/170 (97%)	-0.35	0 100 100	15, 34, 55, 70	0
3	H	166/170 (97%)	-0.24	0 100 100	26, 46, 67, 91	0
3	M	166/170 (97%)	-0.13	1 (0%) 89 88	31, 50, 81, 98	0
3	R	166/170 (97%)	0.06	0 100 100	45, 65, 87, 101	0
4	D	132/141 (93%)	0.23	2 (1%) 74 72	35, 49, 76, 90	0
4	I	132/141 (93%)	-0.17	1 (0%) 86 85	16, 38, 60, 72	0
4	N	132/141 (93%)	0.69	8 (6%) 22 17	49, 74, 92, 124	0
4	S	132/141 (93%)	-0.07	0 100 100	21, 42, 63, 76	0
All	All	4788/4908 (97%)	-0.16	26 (0%) 90 90	14, 43, 75, 124	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	2	SER	6.8
4	D	2	SER	4.5
1	Q	2	SER	4.2
2	K	22	SER	4.1
2	F	16	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	2	SER	3.6
4	D	3	VAL	3.2
4	N	4	ASN	3.1
2	K	434	SER	2.9
2	K	53	ALA	2.8
4	N	3	VAL	2.6
4	I	11	GLY	2.6
1	Q	375	ALA	2.5
4	N	5	SER	2.4
2	A	15	ALA	2.4
2	A	55	GLU	2.4
2	P	22	SER	2.3
4	N	16	LYS	2.3
1	B	2	SER	2.3
1	L	2	SER	2.2
4	N	118	THR	2.2
4	N	111	SER	2.2
4	N	62	LYS	2.1
2	K	258	ALA	2.1
2	K	259	ASN	2.1
3	M	144	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
5	FE	F	602	1/1	0.95	0.13	-1.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	FE	K	601	1/1	0.93	0.12	-1.53	75,75,75,75	0
5	FE	P	602	1/1	0.98	0.08	-2.62	51,51,51,51	0
5	FE	A	601	1/1	0.95	0.07	-3.04	46,46,46,46	0
5	FE	F	601	1/1	0.96	0.08	-3.16	40,40,40,40	0
5	FE	A	602	1/1	0.98	0.04	-3.35	36,36,36,36	0
5	FE	P	601	1/1	0.95	0.09	-3.38	55,55,55,55	0
5	FE	K	602	1/1	0.85	0.06	-9.24	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.