



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:15 AM GMT

PDB ID : 3HPV
Title : Crystal Structure Analysis of the 2,3-dioxygenase LapB from Pseudomonas sp. KL28
Authors : Cho, J.-H.; Rhee, S.
Deposited on : 2009-06-05
Resolution : 2.30 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

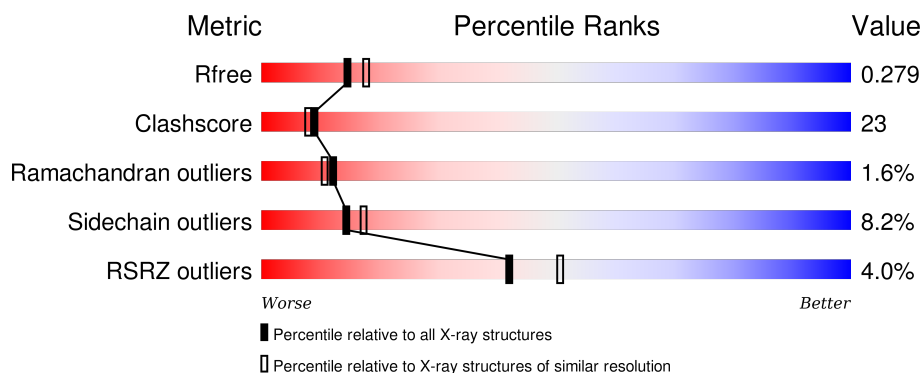
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	A	309	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>• •</div> </div> </div>
1	B	309	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>30%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	309	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>34%</div> <div>6%</div> <div>7%</div> </div> </div>
1	D	309	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>6%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9606 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 Catechol 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2373	1509	406	445	13			
1	B	288	Total	C	N	O	S	0	0	0
			2300	1464	392	431	13			
1	C	288	Total	C	N	O	S	0	0	0
			2300	1464	392	431	13			
1	D	288	Total	C	N	O	S	0	0	0
			2300	1464	392	431	13			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

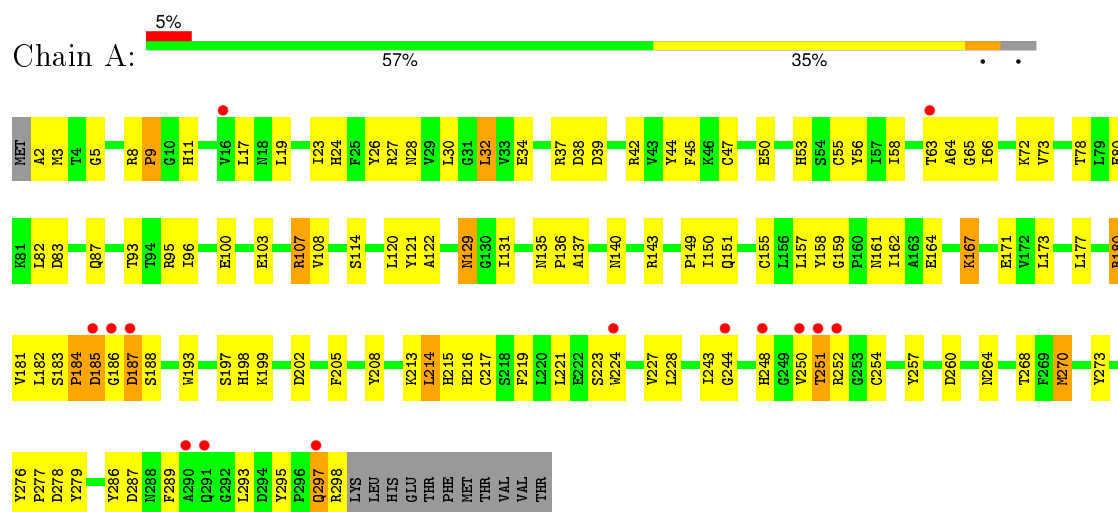
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	74	Total	O	0	0
			74	74		
3	C	74	Total	O	0	0
			74	74		
3	D	102	Total	O	0	0
			102	102		

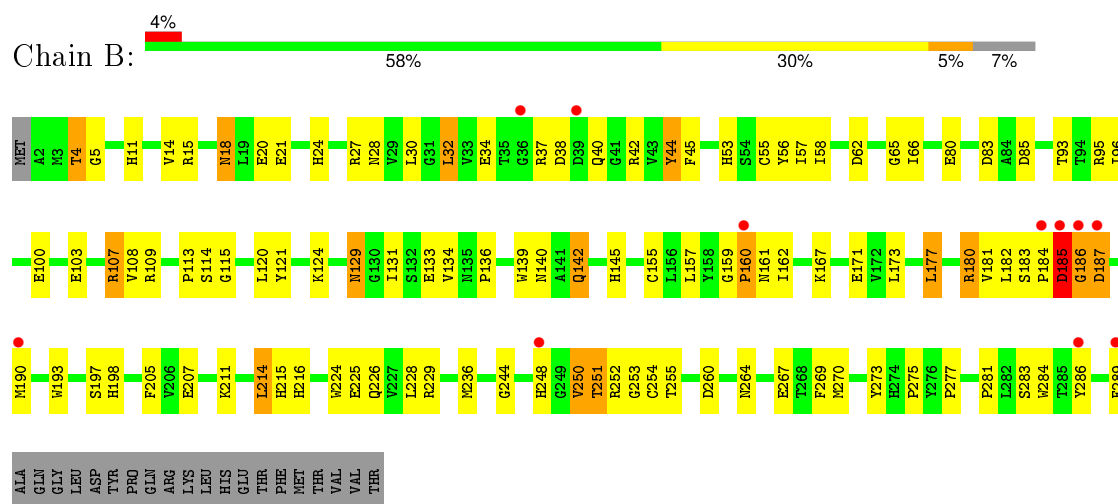
3 Residue-property plots

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

• Molecule 1: Catechol 2,3-dioxygenase

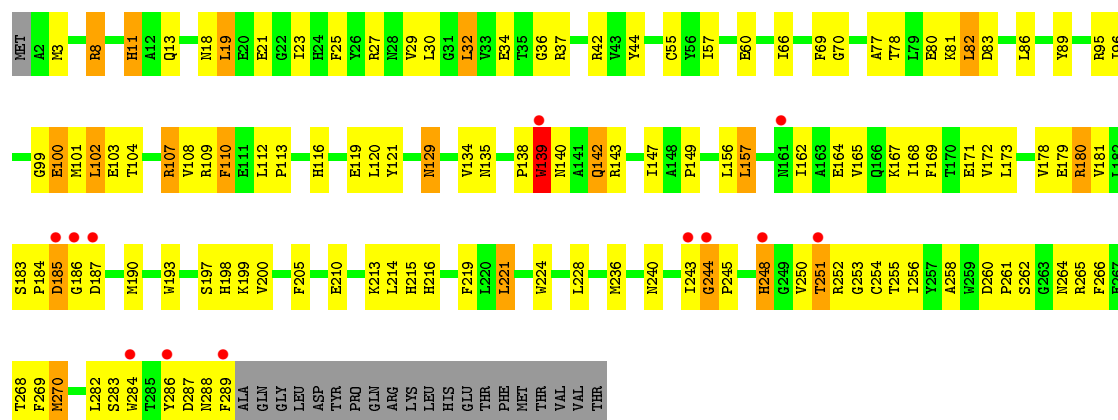


• Molecule 1: Catechol 2,3-dioxygenase

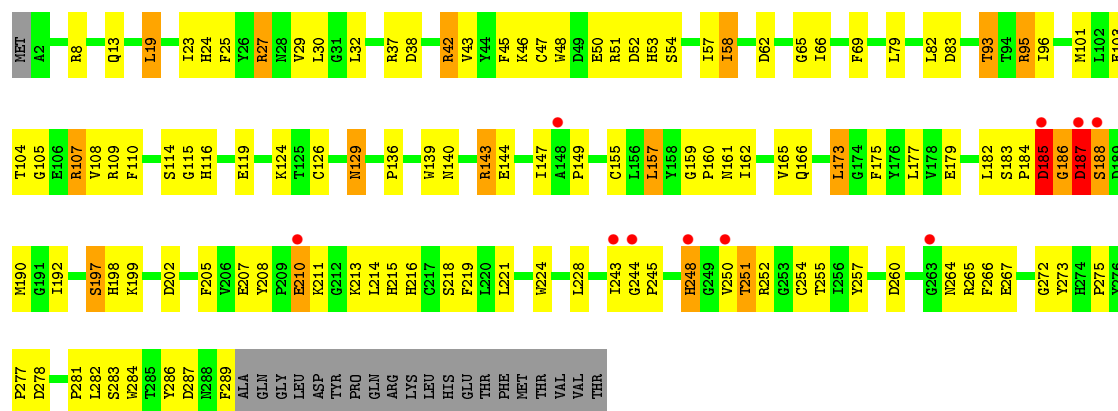


• Molecule 1: Catechol 2,3-dioxygenase





• Molecule 1: Catechol 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.90 Å 97.00 Å 133.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.71 – 2.30 44.71 – 2.29	Depositor EDS
% Data completeness (in resolution range)	75.9 (44.71-2.30) 92.9 (44.71-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.269 0.217 , 0.279	Depositor DCC
R_{free} test set	5618 reflections (12.12%)	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.2	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55593 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9606	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.24 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2669e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FE2

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	0.50	0/2438	0.77	1/3312 (0.0%)
1	B	0.47	0/2363	0.75	2/3210 (0.1%)
1	C	0.45	0/2363	0.75	2/3210 (0.1%)
1	D	0.50	0/2363	0.82	4/3210 (0.1%)
All	All	0.48	0/9527	0.77	9/12942 (0.1%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	GLY	C-N-CA	-11.60	92.69	121.70
1	D	187	ASP	C-N-CA	-10.68	95.00	121.70
1	C	139	TRP	CA-CB-CG	7.80	128.52	113.70
1	C	186	GLY	N-CA-C	-6.64	96.49	113.10
1	D	186	GLY	CA-C-N	5.86	130.10	117.20
1	A	186	GLY	N-CA-C	-5.38	99.65	113.10
1	D	185	ASP	CA-C-N	-5.38	105.44	116.20
1	B	187	ASP	N-CA-C	5.11	124.80	111.00
1	B	160	PRO	N-CA-C	5.08	125.31	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2373	0	2261	111	0
1	B	2300	0	2193	110	0
1	C	2300	0	2193	128	0
1	D	2300	0	2193	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	79	0	0	4	0
3	B	74	0	0	4	0
3	C	74	0	0	7	0
3	D	102	0	0	10	0
All	All	9606	0	8840	420	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 23.

All (420) 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:D:187:ASP:OD1	3:D:389:HOH:O	1.58	1.18
1:C:250:VAL:O	1:C:251:THR:HG22	1.60	1.02
1:B:215:HIS:HD2	1:B:216:HIS:HD1	1.08	0.98
1:C:102:LEU:HD22	1:C:103:GLU:HG2	1.47	0.96
1:D:65:GLY:H	1:D:264:ASN:HD21	1.15	0.94
1:C:215:HIS:CD2	1:C:216:HIS:HD1	1.87	0.93
1:D:95:ARG:HH11	1:D:95:ARG:HB2	1.35	0.90
1:B:215:HIS:CD2	1:B:216:HIS:HD1	1.91	0.89
1:A:224:TRP:NE1	1:B:228:LEU:HB2	1.88	0.88
1:B:83:ASP:OD1	1:B:93:THR:HG21	1.73	0.88
1:A:183:SER:HB3	1:A:187:ASP:HA	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:THR:HG23	1:C:253:GLY:H	1.37	0.86
1:A:224:TRP:HE1	1:B:228:LEU:HB2	1.41	0.86
1:D:186:GLY:O	1:D:187:ASP:CB	2.04	0.84
1:C:164:GLU:O	1:C:168:ILE:HD12	1.79	0.82
1:D:115:GLY:HA3	1:D:211:LYS:HG3	1.62	0.81
1:A:297:GLN:O	1:A:298:ARG:HG2	1.81	0.81
1:D:186:GLY:O	1:D:187:ASP:HB3	1.82	0.79
1:D:83:ASP:OD2	1:D:93:THR:HG21	1.83	0.79
1:D:250:VAL:O	1:D:251:THR:HB	1.81	0.78
1:A:114:SER:HB2	1:A:159:GLY:HA3	1.65	0.78
1:D:27:ARG:HG2	1:D:45:PHE:HE2	1.49	0.77
1:A:198:HIS:HE1	1:D:198:HIS:H	1.31	0.77
1:C:215:HIS:HD2	1:C:216:HIS:HD1	1.34	0.75
1:A:215:HIS:HD2	1:A:216:HIS:ND1	1.87	0.73
1:C:86:LEU:HD23	1:C:172:VAL:HG11	1.71	0.73
1:A:252:ARG:HD2	1:A:273:TYR:HD2	1.54	0.72
1:A:47:CYS:HB2	1:A:50:GLU:HG3	1.70	0.72
1:C:102:LEU:CD2	1:C:103:GLU:HG2	2.20	0.72
1:D:208:TYR:CE2	1:D:210:GLU:HB2	2.25	0.71
1:C:251:THR:OG1	3:C:329:HOH:O	2.09	0.71
1:C:251:THR:O	1:C:252:ARG:HB2	1.91	0.71
1:A:198:HIS:H	1:D:198:HIS:HE1	1.36	0.71
1:C:180:ARG:HD3	1:C:283:SER:OG	1.91	0.71
1:A:65:GLY:H	1:A:264:ASN:HD21	1.38	0.70
1:B:215:HIS:HD2	1:B:216:HIS:ND1	1.86	0.70
1:A:100:GLU:OE2	1:A:107:ARG:NH2	2.25	0.70
1:A:19:LEU:O	1:A:23:ILE:HG13	1.93	0.69
1:A:161:ASN:HB3	1:A:164:GLU:OE1	1.92	0.69
1:A:162:ILE:HD12	1:A:205:PHE:HB3	1.74	0.69
1:A:260:ASP:HB2	1:A:264:ASN:O	1.92	0.68
1:D:107:ARG:HD2	1:D:119:GLU:OE1	1.93	0.68
1:A:197:SER:HB2	1:D:198:HIS:CE1	2.29	0.68
1:C:139:TRP:HE3	1:C:139:TRP:C	1.96	0.67
1:A:224:TRP:CZ3	1:A:254:CYS:HB3	2.30	0.67
1:B:27:ARG:HD2	1:B:32:LEU:O	1.95	0.66
1:C:167:LYS:O	1:C:171:GLU:HB2	1.94	0.66
1:D:43:VAL:HG12	1:D:58:ILE:HG22	1.75	0.66
1:B:65:GLY:H	1:B:264:ASN:HD21	1.41	0.66
1:A:53:HIS:CD2	1:A:103:GLU:HG3	2.29	0.66
1:B:198:HIS:HE1	1:C:198:HIS:H	1.41	0.66
1:D:162:ILE:HD12	1:D:205:PHE:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HB2	1:D:252:ARG:HH22	1.60	0.66
1:B:38:ASP:OD2	1:B:42:ARG:HD3	1.96	0.66
1:C:180:ARG:HB3	1:C:180:ARG:HH11	1.61	0.65
1:B:183:SER:HA	1:B:190:MET:HG2	1.79	0.65
1:B:53:HIS:CD2	1:B:103:GLU:HG3	2.32	0.65
1:C:180:ARG:HH11	1:C:180:ARG:CB	2.10	0.65
1:A:224:TRP:CZ2	1:B:228:LEU:HD13	2.32	0.64
1:A:158:TYR:HB2	1:A:213:LYS:HB2	1.79	0.64
1:C:250:VAL:HG12	1:C:284:TRP:CD1	2.32	0.64
1:A:278:ASP:OD1	1:D:8:ARG:NH2	2.30	0.64
1:D:243:ILE:HD11	3:D:372:HOH:O	1.96	0.64
1:D:252:ARG:HG3	1:D:252:ARG:HH11	1.62	0.64
1:D:224:TRP:CZ3	1:D:254:CYS:HB3	2.32	0.64
1:C:156:LEU:C	1:C:156:LEU:HD23	2.17	0.64
1:D:101:MET:HG3	1:D:107:ARG:NH2	2.13	0.64
1:D:248:HIS:HE1	1:D:257:TYR:OH	1.80	0.64
1:C:101:MET:HB2	1:C:107:ARG:NH2	2.13	0.64
1:C:224:TRP:CZ3	1:C:254:CYS:HB3	2.33	0.64
1:A:187:ASP:HB2	3:A:356:HOH:O	1.97	0.63
1:C:30:LEU:HG	1:C:32:LEU:HD13	1.80	0.63
1:A:93:THR:HG23	1:A:108:VAL:HG13	1.81	0.63
1:D:23:ILE:O	1:D:27:ARG:HB2	1.98	0.63
1:C:167:LYS:NZ	1:C:167:LYS:HB3	2.14	0.63
1:D:48:TRP:CZ2	1:D:143:ARG:HG2	2.34	0.62
1:C:245:PRO:HB3	1:C:256:ILE:HD11	1.81	0.62
1:A:185:ASP:O	1:A:187:ASP:N	2.32	0.61
1:A:72:LYS:HE3	1:A:122:ALA:O	2.00	0.61
1:B:260:ASP:HB2	1:B:264:ASN:O	2.00	0.61
1:B:4:THR:HG23	1:B:5:GLY:N	2.16	0.61
1:D:46:LYS:HD2	1:D:52:ASP:O	2.01	0.61
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.66	0.60
1:B:181:VAL:HG11	1:B:289:PHE:CG	2.36	0.60
1:C:181:VAL:HG23	1:C:193:TRP:CZ3	2.36	0.60
1:A:198:HIS:CE1	1:D:197:SER:HB2	2.37	0.60
1:D:183:SER:HA	1:D:190:MET:HG2	1.83	0.60
1:D:66:ILE:HG22	1:D:214:LEU:HB2	1.84	0.60
1:B:197:SER:HB2	1:C:198:HIS:CE1	2.37	0.60
1:C:179:GLU:HG2	1:C:282:LEU:HB2	1.83	0.60
1:D:215:HIS:HD2	1:D:216:HIS:HD1	1.48	0.60
1:B:180:ARG:HE	1:B:283:SER:HB3	1.67	0.60
1:C:57:ILE:HD12	1:C:57:ILE:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HD12	1:C:205:PHE:HB3	1.84	0.60
1:B:100:GLU:OE2	1:B:107:ARG:NH2	2.35	0.60
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.67	0.60
1:A:8:ARG:HG3	1:A:9:PRO:O	2.01	0.59
1:C:143:ARG:HD2	3:C:318:HOH:O	2.00	0.59
1:C:250:VAL:O	1:C:250:VAL:HG23	2.02	0.59
1:A:198:HIS:H	1:D:198:HIS:CE1	2.18	0.59
1:C:240:ASN:HA	3:C:327:HOH:O	2.02	0.59
1:A:24:HIS:O	1:A:28:ASN:HB2	2.02	0.59
1:B:183:SER:HA	1:B:190:MET:CG	2.33	0.59
1:A:155:CYS:SG	1:A:157:LEU:HD21	2.43	0.59
1:B:20:GLU:CD	1:B:20:GLU:H	2.04	0.58
1:B:27:ARG:HH12	1:B:145:HIS:CD2	2.20	0.58
1:B:225:GLU:HG2	3:B:318:HOH:O	2.03	0.58
1:D:95:ARG:HB2	1:D:95:ARG:NH1	2.12	0.58
1:D:162:ILE:O	1:D:165:VAL:HB	2.03	0.58
1:B:273:TYR:CD1	1:B:275:PRO:HD3	2.37	0.58
1:A:129:ASN:HD21	1:A:131:ILE:HB	1.68	0.58
1:A:30:LEU:HG	1:A:32:LEU:HD13	1.85	0.58
1:B:30:LEU:HG	1:B:32:LEU:CD1	2.34	0.57
1:D:114:SER:HB2	1:D:159:GLY:HA3	1.86	0.57
1:A:260:ASP:HB3	1:A:264:ASN:H	1.69	0.57
1:B:224:TRP:CZ3	1:B:254:CYS:HB3	2.39	0.57
1:C:139:TRP:CE3	1:C:139:TRP:C	2.76	0.57
1:A:184:PRO:HG3	1:A:286:TYR:CG	2.39	0.57
1:C:13:GLN:HA	1:C:57:ILE:O	2.03	0.57
1:C:80:GLU:CD	1:C:95:ARG:HH22	2.07	0.57
1:C:228:LEU:HB2	1:D:224:TRP:NE1	2.20	0.57
1:D:29:VAL:O	1:D:147:ILE:HG13	2.04	0.57
1:B:136:PRO:HG3	1:C:282:LEU:HD13	1.86	0.57
1:C:66:ILE:HD11	1:C:69:PHE:HB2	1.87	0.57
1:A:129:ASN:ND2	1:A:131:ILE:H	2.02	0.57
1:B:18:ASN:HD22	1:B:18:ASN:C	2.07	0.57
1:C:215:HIS:CD2	1:C:216:HIS:ND1	2.67	0.56
1:B:198:HIS:CE1	1:C:197:SER:HB2	2.40	0.56
1:A:2:ALA:HB2	3:D:314:HOH:O	2.05	0.56
1:B:184:PRO:O	1:B:186:GLY:N	2.38	0.56
1:B:45:PHE:CE1	1:B:58:ILE:HD13	2.41	0.56
1:B:34:GLU:OE2	1:B:37:ARG:HD2	2.05	0.56
1:B:183:SER:HB2	1:B:184:PRO:HD2	1.87	0.56
1:C:240:ASN:HD22	1:C:240:ASN:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:MET:SD	1:D:139:TRP:HE3	2.28	0.56
1:A:63:THR:HG22	1:A:64:ALA:O	2.05	0.55
1:A:297:GLN:HG2	1:A:298:ARG:H	1.70	0.55
1:D:250:VAL:O	1:D:251:THR:CB	2.53	0.55
1:C:34:GLU:OE2	1:C:37:ARG:HD2	2.05	0.55
1:D:57:ILE:HD12	1:D:57:ILE:N	2.20	0.55
1:D:185:ASP:C	1:D:187:ASP:OD2	2.43	0.55
1:A:56:TYR:CD2	1:A:58:ILE:HD11	2.41	0.55
1:B:96:ILE:HD11	1:B:109:ARG:CZ	2.36	0.55
1:C:149:PRO:CB	1:C:219:PHE:HB3	2.37	0.55
1:D:208:TYR:HE2	1:D:210:GLU:HB2	1.71	0.55
1:A:279:TYR:HB3	1:D:51:ARG:NH1	2.22	0.55
1:C:215:HIS:HD2	1:C:216:HIS:ND1	2.02	0.55
1:C:36:GLY:O	1:C:44:TYR:N	2.31	0.55
1:C:11:HIS:HD2	1:C:70:GLY:H	1.53	0.55
1:C:29:VAL:O	1:C:147:ILE:HG13	2.07	0.55
1:A:223:SER:C	1:A:270:MET:HG2	2.27	0.55
1:D:65:GLY:N	1:D:264:ASN:HD21	1.95	0.55
1:D:115:GLY:HA3	1:D:211:LYS:CG	2.35	0.55
1:A:66:ILE:HG22	1:A:214:LEU:HB2	1.87	0.55
1:C:250:VAL:O	1:C:251:THR:CG2	2.45	0.54
1:A:297:GLN:O	1:A:298:ARG:CG	2.53	0.54
1:B:113:PRO:HB2	1:B:161:ASN:HB2	1.87	0.54
1:A:224:TRP:CE2	1:B:228:LEU:HD13	2.42	0.54
1:D:188:SER:O	3:D:381:HOH:O	2.18	0.54
1:C:100:GLU:C	1:C:100:GLU:OE1	2.46	0.54
1:D:182:LEU:CD1	1:D:283:SER:HB3	2.38	0.54
1:B:255:THR:OG1	1:B:267:GLU:HG3	2.07	0.54
1:C:96:ILE:HD12	1:C:96:ILE:N	2.23	0.54
1:C:169:PHE:HA	1:C:173:LEU:HD23	1.90	0.54
1:C:156:LEU:HD23	1:C:157:LEU:N	2.23	0.54
1:B:229:ARG:HD2	1:D:144:GLU:OE1	2.08	0.54
1:B:121:TYR:CZ	1:B:124:LYS:HE2	2.43	0.53
1:B:66:ILE:HB	1:B:214:LEU:HG	1.89	0.53
1:B:56:TYR:CD2	1:B:58:ILE:HD11	2.43	0.53
1:B:96:ILE:HD11	1:B:109:ARG:NE	2.22	0.53
1:D:182:LEU:HD13	1:D:283:SER:HB3	1.90	0.53
1:A:65:GLY:N	1:A:264:ASN:HD21	2.06	0.53
1:A:37:ARG:HG3	3:A:377:HOH:O	2.07	0.53
1:A:83:ASP:O	1:A:87:GLN:HG2	2.09	0.53
1:C:116:HIS:CD2	1:C:157:LEU:HG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD23	1:B:32:LEU:CD2	2.39	0.53
1:D:215:HIS:O	1:D:265:ARG:HB3	2.09	0.53
1:D:281:PRO:HD3	3:D:394:HOH:O	2.09	0.52
1:B:162:ILE:HD12	1:B:205:PHE:HB3	1.90	0.52
1:C:260:ASP:HB2	1:C:264:ASN:O	2.08	0.52
1:C:181:VAL:HG11	1:C:289:PHE:CG	2.44	0.52
1:D:289:PHE:CG	1:D:289:PHE:O	2.62	0.52
1:B:4:THR:CG2	1:B:5:GLY:N	2.72	0.52
1:B:18:ASN:ND2	1:B:21:GLU:H	2.07	0.52
1:D:19:LEU:HD22	1:D:23:ILE:HG13	1.92	0.52
1:A:221:LEU:HD11	1:A:268:THR:HB	1.90	0.52
1:B:198:HIS:H	1:C:198:HIS:HE1	1.56	0.52
1:C:36:GLY:O	1:C:37:ARG:HG3	2.10	0.52
1:C:83:ASP:HB2	1:C:108:VAL:HG21	1.92	0.52
1:B:45:PHE:HE1	1:B:58:ILE:HD13	1.75	0.52
1:B:155:CYS:SG	1:B:157:LEU:HD13	2.50	0.52
1:C:243:ILE:O	1:C:243:ILE:HG23	2.10	0.52
1:D:65:GLY:H	1:D:264:ASN:ND2	1.97	0.52
1:A:140:ASN:HA	1:C:236:MET:HE1	1.92	0.52
1:A:295:TYR:CE2	1:A:297:GLN:HB3	2.45	0.51
1:D:27:ARG:HG3	1:D:27:ARG:NH1	2.25	0.51
1:B:44:TYR:CD1	1:B:44:TYR:N	2.77	0.51
1:C:251:THR:HG23	1:C:253:GLY:N	2.16	0.51
1:D:54:SER:O	1:D:124:LYS:HE2	2.10	0.51
1:A:56:TYR:CE2	1:A:58:ILE:HD11	2.46	0.51
1:A:197:SER:HB2	1:D:198:HIS:HE1	1.70	0.51
1:A:224:TRP:CD1	1:B:228:LEU:HD22	2.45	0.51
1:C:221:LEU:CD2	1:C:268:THR:HB	2.41	0.51
1:C:77:ALA:O	1:C:81:LYS:HB2	2.11	0.51
1:B:198:HIS:CE1	1:C:198:HIS:H	2.27	0.51
1:C:224:TRP:CE3	1:C:254:CYS:HB3	2.46	0.51
1:C:8:ARG:NH1	3:C:317:HOH:O	2.44	0.51
1:A:243:ILE:HG22	1:A:257:TYR:HB2	1.94	0.50
1:B:250:VAL:O	1:B:250:VAL:HG23	2.11	0.50
1:B:30:LEU:HG	1:B:32:LEU:HD13	1.92	0.50
1:A:214:LEU:HD22	1:A:216:HIS:N	2.27	0.50
1:B:11:HIS:HA	1:B:55:CYS:O	2.11	0.50
1:D:27:ARG:HH11	1:D:27:ARG:HG3	1.75	0.50
1:D:30:LEU:HG	1:D:32:LEU:HD13	1.94	0.50
1:D:47:CYS:HB2	1:D:50:GLU:HG3	1.93	0.50
1:A:167:LYS:HD3	1:A:171:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:SER:HB2	1:C:184:PRO:HD2	1.94	0.50
1:D:38:ASP:OD2	1:D:42:ARG:HD3	2.12	0.50
1:D:251:THR:O	1:D:252:ARG:HB2	2.11	0.50
1:B:115:GLY:HA3	1:B:211:LYS:HB3	1.94	0.50
1:B:27:ARG:HH11	1:B:27:ARG:HG3	1.77	0.50
1:C:162:ILE:CD1	1:C:205:PHE:HB3	2.42	0.50
1:C:80:GLU:OE2	1:C:95:ARG:NH2	2.44	0.49
1:A:11:HIS:HA	1:A:55:CYS:O	2.12	0.49
1:A:96:ILE:N	1:A:96:ILE:HD12	2.27	0.49
1:A:224:TRP:HZ3	1:A:227:VAL:HG11	1.78	0.49
1:B:27:ARG:HG2	3:B:315:HOH:O	2.10	0.49
1:D:214:LEU:HD13	1:D:214:LEU:C	2.32	0.49
1:B:80:GLU:OE1	1:B:95:ARG:NH2	2.42	0.49
1:D:210:GLU:HG2	1:D:213:LYS:HE3	1.94	0.49
1:B:40:GLN:HB3	3:B:328:HOH:O	2.13	0.49
1:A:224:TRP:CD1	1:B:224:TRP:CD1	3.00	0.49
1:A:83:ASP:OD2	1:A:93:THR:HG21	2.12	0.49
1:A:135:ASN:HA	1:D:284:TRP:CE3	2.47	0.49
1:B:286:TYR:O	1:B:289:PHE:HB3	2.13	0.49
1:C:245:PRO:HA	1:C:256:ILE:HG12	1.94	0.49
1:C:149:PRO:HB2	1:C:219:PHE:HB3	1.95	0.49
1:C:190:MET:HG3	1:C:286:TYR:CE1	2.47	0.49
1:D:179:GLU:HG2	1:D:282:LEU:HB2	1.95	0.48
1:C:157:LEU:HD23	1:C:205:PHE:CE2	2.48	0.48
1:B:250:VAL:O	1:B:251:THR:HB	2.13	0.48
1:A:277:PRO:HG3	3:D:387:HOH:O	2.13	0.48
1:A:5:GLY:HA2	1:A:78:THR:HG21	1.95	0.48
1:D:161:ASN:O	1:D:165:VAL:HG23	2.14	0.48
1:B:181:VAL:HG21	1:B:289:PHE:CD1	2.49	0.48
1:D:224:TRP:CE3	1:D:254:CYS:HB3	2.49	0.48
1:C:215:HIS:O	1:C:265:ARG:HB3	2.13	0.48
1:C:245:PRO:CA	1:C:256:ILE:HG12	2.44	0.48
1:D:260:ASP:HB2	1:D:264:ASN:O	2.14	0.48
1:B:58:ILE:N	1:B:58:ILE:HD12	2.28	0.48
1:C:36:GLY:C	1:C:37:ARG:HG3	2.34	0.48
1:A:228:LEU:HD13	1:B:224:TRP:CE2	2.49	0.48
1:B:30:LEU:HD23	1:B:32:LEU:HD21	1.94	0.48
1:A:149:PRO:HB2	1:A:219:PHE:HB3	1.96	0.48
1:D:255:THR:OG1	1:D:267:GLU:HG3	2.14	0.47
1:D:116:HIS:CD2	1:D:157:LEU:HG	2.50	0.47
1:A:208:TYR:CE2	1:A:213:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:HIS:CE1	1:D:257:TYR:OH	2.65	0.47
1:D:215:HIS:CD2	1:D:216:HIS:HD1	2.31	0.47
1:B:167:LYS:HE3	1:B:171:GLU:OE1	2.14	0.47
1:C:185:ASP:HA	1:C:187:ASP:OD2	2.13	0.47
1:D:199:LYS:HE2	1:D:202:ASP:OD1	2.14	0.47
1:A:297:GLN:O	1:A:298:ARG:CB	2.61	0.47
1:C:110:PHE:CD2	1:C:110:PHE:N	2.82	0.47
1:D:160:PRO:O	1:D:207:GLU:OE2	2.33	0.47
1:A:224:TRP:CE2	1:B:224:TRP:NE1	2.82	0.47
1:A:228:LEU:HD13	1:B:224:TRP:CZ2	2.50	0.47
1:C:139:TRP:HE3	1:C:139:TRP:O	1.97	0.47
1:B:4:THR:HG23	1:B:5:GLY:H	1.79	0.47
1:A:184:PRO:HG3	1:A:286:TYR:CD2	2.50	0.47
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.30	0.47
1:C:99:GLY:O	1:C:100:GLU:C	2.54	0.47
1:B:177:LEU:O	1:B:281:PRO:HB3	2.15	0.47
1:D:184:PRO:HG3	1:D:286:TYR:CD2	2.50	0.47
1:D:13:GLN:HG3	1:D:57:ILE:HB	1.96	0.46
1:B:114:SER:HB2	1:B:159:GLY:HA3	1.96	0.46
1:C:248:HIS:CE1	1:C:255:THR:HG21	2.50	0.46
1:D:69:PHE:CE2	1:D:155:CYS:HB3	2.51	0.46
1:D:272:GLY:HA3	3:D:386:HOH:O	2.16	0.46
1:C:78:THR:HG22	1:C:82:LEU:HD22	1.97	0.46
1:B:183:SER:CA	1:B:190:MET:HG2	2.44	0.46
1:A:276:TYR:CB	1:D:8:ARG:HH21	2.29	0.46
1:B:56:TYR:C	1:B:57:ILE:HD12	2.35	0.46
1:B:250:VAL:HG12	1:B:284:TRP:CD1	2.51	0.46
1:B:24:HIS:O	1:B:28:ASN:HB2	2.16	0.46
1:B:181:VAL:HG23	1:B:193:TRP:CZ3	2.51	0.46
1:C:134:VAL:HG13	1:C:134:VAL:O	2.15	0.46
1:D:23:ILE:HD13	1:D:37:ARG:NH2	2.31	0.45
1:C:224:TRP:CE2	1:D:228:LEU:HB2	2.52	0.45
1:A:80:GLU:OE2	1:A:95:ARG:NH2	2.49	0.45
1:A:137:ALA:O	1:D:252:ARG:NH2	2.49	0.45
1:B:27:ARG:NH1	1:B:145:HIS:CD2	2.85	0.45
1:B:140:ASN:ND2	1:B:142:GLN:H	2.15	0.45
1:B:27:ARG:HG3	1:B:27:ARG:NH1	2.32	0.45
1:D:143:ARG:HG3	1:D:143:ARG:NH1	2.30	0.45
1:D:96:ILE:N	1:D:96:ILE:HD12	2.31	0.45
1:A:217:CYS:HB2	3:A:378:HOH:O	2.16	0.45
1:D:79:LEU:HD11	1:D:108:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HB3	1:C:164:GLU:OE2	2.17	0.45
1:C:224:TRP:NE1	1:D:228:LEU:HB2	2.32	0.45
1:A:223:SER:HA	1:A:270:MET:HE3	1.98	0.45
1:D:53:HIS:CD2	1:D:103:GLU:HG3	2.51	0.45
1:C:18:ASN:HA	1:C:60:GLU:OE1	2.15	0.45
1:D:183:SER:HA	1:D:190:MET:CG	2.46	0.45
1:C:19:LEU:O	1:C:23:ILE:HG13	2.17	0.45
1:B:226:GLN:NE2	3:B:371:HOH:O	2.50	0.45
1:C:288:ASN:HD22	1:C:288:ASN:N	2.15	0.44
1:A:143:ARG:HG3	3:A:318:HOH:O	2.16	0.44
1:B:255:THR:HB	1:B:269:PHE:CB	2.47	0.44
1:D:273:TYR:CD1	1:D:275:PRO:HD3	2.52	0.44
1:C:109:ARG:HD2	3:C:323:HOH:O	2.16	0.44
1:C:23:ILE:O	1:C:27:ARG:HB3	2.17	0.44
1:C:221:LEU:HD22	1:C:268:THR:HB	1.99	0.44
1:D:129:ASN:H	1:D:129:ASN:HD22	1.64	0.44
1:D:24:HIS:HB2	3:D:380:HOH:O	2.16	0.44
1:B:14:VAL:HG12	1:B:15:ARG:N	2.32	0.44
1:A:129:ASN:ND2	1:A:131:ILE:HB	2.32	0.44
1:C:244:GLY:N	3:C:386:HOH:O	2.48	0.44
1:B:131:ILE:HD11	1:B:139:TRP:HA	1.99	0.44
1:A:184:PRO:O	1:A:185:ASP:HB2	2.17	0.44
1:B:184:PRO:O	1:B:185:ASP:C	2.56	0.44
1:A:181:VAL:HG11	1:A:289:PHE:CD2	2.53	0.44
1:C:129:ASN:HD22	1:C:129:ASN:H	1.65	0.44
1:A:47:CYS:SG	1:A:151:GLN:HA	2.58	0.44
1:A:260:ASP:OD1	1:A:264:ASN:HB2	2.18	0.44
1:B:181:VAL:HG11	1:B:289:PHE:CD2	2.53	0.44
1:B:185:ASP:O	1:B:187:ASP:N	2.51	0.43
1:B:57:ILE:N	1:B:57:ILE:HD12	2.33	0.43
1:D:218:SER:HB2	1:D:267:GLU:OE1	2.18	0.43
1:A:252:ARG:HD2	1:A:273:TYR:CD2	2.42	0.43
1:B:14:VAL:HG13	1:B:65:GLY:O	2.18	0.43
1:C:25:PHE:HB2	1:C:261:PRO:HG2	2.01	0.43
1:B:129:ASN:ND2	1:B:131:ILE:H	2.17	0.43
1:B:250:VAL:HG12	1:B:284:TRP:CE2	2.54	0.43
1:B:134:VAL:HA	1:C:283:SER:O	2.18	0.43
1:C:139:TRP:CE3	1:C:140:ASN:N	2.87	0.43
1:C:140:ASN:ND2	1:C:142:GLN:CB	2.81	0.43
1:A:129:ASN:HD22	1:A:131:ILE:H	1.66	0.43
1:B:251:THR:HG23	1:B:253:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HG3	3:C:355:HOH:O	2.19	0.43
1:A:293:LEU:N	1:A:293:LEU:HD12	2.33	0.43
1:B:18:ASN:HD21	1:B:20:GLU:HG2	1.82	0.43
1:C:86:LEU:O	1:C:89:TYR:HB3	2.18	0.43
1:C:30:LEU:CG	1:C:32:LEU:HD13	2.48	0.43
1:C:178:VAL:HG21	1:C:200:VAL:O	2.19	0.43
1:B:180:ARG:HD3	1:B:283:SER:HA	2.00	0.43
1:A:199:LYS:HE2	1:A:202:ASP:OD1	2.18	0.43
1:D:185:ASP:O	1:D:187:ASP:OD2	2.37	0.43
1:C:251:THR:O	1:C:252:ARG:CB	2.64	0.43
1:D:43:VAL:HG12	1:D:58:ILE:CG2	2.44	0.43
1:B:251:THR:O	1:B:252:ARG:HB2	2.18	0.43
1:A:8:ARG:NH2	1:D:278:ASP:OD1	2.52	0.43
1:C:25:PHE:HZ	1:C:266:PHE:CZ	2.36	0.43
1:B:277:PRO:HG2	1:C:3:MET:HB2	2.00	0.42
1:C:258:ALA:HB3	1:C:266:PHE:CZ	2.54	0.42
1:B:93:THR:HG23	1:B:108:VAL:HG13	2.00	0.42
1:A:136:PRO:HG3	1:D:282:LEU:HD13	2.01	0.42
1:C:255:THR:HB	1:C:269:PHE:CB	2.50	0.42
1:A:129:ASN:C	1:A:129:ASN:ND2	2.72	0.42
1:D:166:GLN:HB2	1:D:192:ILE:HD13	2.01	0.42
1:A:224:TRP:CZ3	1:A:227:VAL:HG11	2.54	0.42
1:C:162:ILE:HD12	1:C:205:PHE:CB	2.48	0.42
1:C:243:ILE:O	1:C:243:ILE:CG2	2.67	0.42
1:D:104:THR:HG22	1:D:105:GLY:O	2.19	0.42
1:C:101:MET:HB3	1:C:104:THR:HB	2.02	0.42
1:D:25:PHE:HZ	1:D:266:PHE:CE2	2.38	0.42
1:B:184:PRO:HD3	1:B:286:TYR:CD1	2.55	0.42
1:C:116:HIS:CE1	1:C:157:LEU:HB3	2.55	0.42
1:C:255:THR:OG1	1:C:256:ILE:N	2.53	0.42
1:D:149:PRO:HB2	1:D:219:PHE:HB3	2.01	0.42
1:D:109:ARG:HG2	1:D:110:PHE:N	2.34	0.42
1:C:30:LEU:HD23	1:C:32:LEU:HD22	2.00	0.42
1:B:248:HIS:NE2	1:B:250:VAL:HG22	2.35	0.42
1:A:80:GLU:CD	1:A:95:ARG:HH22	2.22	0.42
1:A:278:ASP:CG	1:D:8:ARG:HH22	2.24	0.42
1:C:119:GLU:O	1:C:120:LEU:HD12	2.20	0.42
1:A:252:ARG:HH22	1:D:136:PRO:HB2	1.85	0.41
1:B:270:MET:C	1:B:270:MET:SD	2.97	0.41
1:C:138:PRO:O	1:C:139:TRP:HB3	2.19	0.41
1:A:129:ASN:C	1:A:129:ASN:HD22	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:HD22	1:C:21:GLU:HB3	1.85	0.41
1:A:180:ARG:HH11	1:A:180:ARG:HG2	1.85	0.41
1:C:245:PRO:HG2	1:D:245:PRO:O	2.20	0.41
1:A:66:ILE:CG2	1:A:214:LEU:HB2	2.50	0.41
1:C:199:LYS:O	1:C:200:VAL:C	2.59	0.41
1:B:180:ARG:NE	1:B:283:SER:HB3	2.33	0.41
1:B:160:PRO:O	1:B:207:GLU:OE2	2.39	0.41
1:A:224:TRP:CZ2	1:B:224:TRP:CZ2	3.08	0.41
1:C:82:LEU:O	1:C:86:LEU:HG	2.20	0.41
1:C:100:GLU:HB3	1:C:107:ARG:HH21	1.85	0.41
1:A:93:THR:CG2	1:A:108:VAL:HG13	2.48	0.41
1:D:183:SER:HB3	1:D:188:SER:O	2.21	0.41
1:A:34:GLU:OE2	1:A:37:ARG:HD2	2.20	0.41
1:B:185:ASP:O	1:B:187:ASP:OD1	2.38	0.41
1:C:107:ARG:HB3	1:C:121:TYR:HB3	2.01	0.41
1:B:273:TYR:HD1	1:B:275:PRO:HD3	1.81	0.41
1:C:11:HIS:HA	1:C:55:CYS:O	2.20	0.41
1:C:270:MET:HB2	1:C:270:MET:HE3	1.96	0.41
1:D:42:ARG:NH2	3:D:400:HOH:O	2.54	0.41
1:C:213:LYS:HD3	1:C:213:LYS:HA	1.88	0.41
1:D:126:CYS:SG	1:D:126:CYS:O	2.79	0.41
1:A:297:GLN:CG	1:A:298:ARG:N	2.84	0.41
1:B:250:VAL:HG12	1:B:284:TRP:CG	2.56	0.41
1:C:112:LEU:HB3	1:C:165:VAL:HG22	2.03	0.41
1:A:73:VAL:HG22	1:A:121:TYR:O	2.20	0.41
1:D:173:LEU:HB3	1:D:175:PHE:CE1	2.55	0.41
1:A:30:LEU:HD23	1:A:32:LEU:HD22	2.03	0.40
1:A:32:LEU:HB3	1:A:45:PHE:HB3	2.02	0.40
1:C:260:ASP:C	1:C:262:SER:H	2.23	0.40
1:C:102:LEU:HD23	1:C:103:GLU:N	2.35	0.40
1:D:161:ASN:HB3	3:D:360:HOH:O	2.19	0.40
1:C:66:ILE:HG22	1:C:214:LEU:HB2	2.02	0.40
1:D:252:ARG:HG3	1:D:252:ARG:NH1	2.34	0.40
1:D:101:MET:HG3	1:D:107:ARG:HH22	1.86	0.40
1:A:181:VAL:HG23	1:A:193:TRP:CZ3	2.57	0.40
1:A:131:ILE:HG13	1:A:140:ASN:ND2	2.37	0.40
1:A:38:ASP:OD2	1:A:42:ARG:HD3	2.22	0.40
1:D:66:ILE:CG2	1:D:214:LEU:HB2	2.51	0.40
1:B:284:TRP:CE3	1:C:135:ASN:HA	2.57	0.40
1:A:3:MET:HB2	1:D:277:PRO:HG2	2.03	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	295/309 (96%)	272 (92%)	15 (5%)	8 (3%)	6	4
1	B	286/309 (93%)	267 (93%)	14 (5%)	5 (2%)	11	10
1	C	286/309 (93%)	262 (92%)	22 (8%)	2 (1%)	26	31
1	D	286/309 (93%)	265 (93%)	17 (6%)	4 (1%)	14	13
All	All	1153/1236 (93%)	1066 (92%)	68 (6%)	19 (2%)	12	11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	THR
1	B	185	ASP
1	B	251	THR
1	A	185	ASP
1	A	188	SER
1	A	244	GLY
1	A	250	VAL
1	B	186	GLY
1	B	250	VAL
1	C	244	GLY
1	C	251	THR
1	D	187	ASP
1	A	187	ASP
1	A	248	HIS
1	B	244	GLY
1	D	251	THR
1	D	197	SER
1	D	244	GLY
1	A	184	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/264 (96%)	231 (92%)	21 (8%)	14	17
1	B	245/264 (93%)	228 (93%)	17 (7%)	19	24
1	C	245/264 (93%)	224 (91%)	21 (9%)	13	15
1	D	245/264 (93%)	223 (91%)	22 (9%)	12	14
All	All	987/1056 (94%)	906 (92%)	81 (8%)	14	17

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	17	LEU
1	A	27	ARG
1	A	32	LEU
1	A	39	ASP
1	A	44	TYR
1	A	82	LEU
1	A	107	ARG
1	A	120	LEU
1	A	129	ASN
1	A	150	ILE
1	A	167	LYS
1	A	173	LEU
1	A	177	LEU
1	A	180	ARG
1	A	182	LEU
1	A	214	LEU
1	A	251	THR
1	A	270	MET
1	A	287	ASP
1	A	297	GLN
1	B	4	THR
1	B	18	ASN
1	B	32	LEU

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Mol	Chain	Res	Type
1	B	44	TYR
1	B	62	ASP
1	B	85	ASP
1	B	107	ARG
1	B	120	LEU
1	B	129	ASN
1	B	133	GLU
1	B	142	GLN
1	B	173	LEU
1	B	177	LEU
1	B	180	ARG
1	B	182	LEU
1	B	185	ASP
1	B	214	LEU
1	C	8	ARG
1	C	11	HIS
1	C	19	LEU
1	C	32	LEU
1	C	42	ARG
1	C	82	LEU
1	C	100	GLU
1	C	102	LEU
1	C	107	ARG
1	C	110	PHE
1	C	129	ASN
1	C	139	TRP
1	C	142	GLN
1	C	157	LEU
1	C	180	ARG
1	C	185	ASP
1	C	210	GLU
1	C	221	LEU
1	C	248	HIS
1	C	270	MET
1	C	287	ASP
1	D	19	LEU
1	D	27	ARG
1	D	42	ARG
1	D	58	ILE
1	D	62	ASP
1	D	82	LEU
1	D	93	THR

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Mol	Chain	Res	Type
1	D	95	ARG
1	D	107	ARG
1	D	129	ASN
1	D	140	ASN
1	D	143	ARG
1	D	157	LEU
1	D	173	LEU
1	D	177	LEU
1	D	185	ASP
1	D	187	ASP
1	D	188	SER
1	D	210	GLU
1	D	221	LEU
1	D	248	HIS
1	D	287	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	198	HIS
1	A	215	HIS
1	A	237	ASN
1	A	264	ASN
1	B	18	ASN
1	B	24	HIS
1	B	28	ASN
1	B	129	ASN
1	B	140	ASN
1	B	166	GLN
1	B	198	HIS
1	B	215	HIS
1	B	226	GLN
1	B	240	ASN
1	B	264	ASN
1	B	288	ASN
1	C	18	ASN
1	C	28	ASN
1	C	129	ASN
1	C	140	ASN
1	C	166	GLN
1	C	198	HIS

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Mol	Chain	Res	Type
1	C	215	HIS
1	C	226	GLN
1	C	237	ASN
1	C	240	ASN
1	C	248	HIS
1	C	288	ASN
1	D	24	HIS
1	D	28	ASN
1	D	129	ASN
1	D	198	HIS
1	D	226	GLN
1	D	237	ASN
1	D	240	ASN
1	D	248	HIS
1	D	264	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	297/309 (96%)	0.20	14 (4%)	35 44	12, 27, 49, 74	0
1	B	288/309 (93%)	0.17	11 (3%)	44 53	13, 27, 46, 73	0
1	C	288/309 (93%)	0.32	12 (4%)	40 49	17, 33, 51, 75	0
1	D	288/309 (93%)	0.26	10 (3%)	48 56	13, 30, 45, 59	0
All	All	1161/1236 (93%)	0.24	47 (4%)	42 51	12, 29, 48, 75	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TRP	5.8
1	C	139	TRP	5.4
1	A	185	ASP	5.4
1	D	187	ASP	4.6
1	A	297	GLN	4.4
1	B	185	ASP	4.2
1	C	185	ASP	4.2
1	D	244	GLY	4.0
1	C	244	GLY	3.9
1	B	184	PRO	3.8
1	B	186	GLY	3.7
1	A	186	GLY	3.6
1	C	186	GLY	3.5
1	D	185	ASP	3.5
1	D	188	SER	3.4
1	A	248	HIS	3.2
1	D	248	HIS	3.1
1	C	289	PHE	3.1
1	B	248	HIS	3.0
1	B	190	MET	2.9
1	A	187	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	2.6
1	C	251	THR	2.5
1	B	289	PHE	2.5
1	B	187	ASP	2.5
1	C	161	ASN	2.4
1	C	243	ILE	2.4
1	D	263	GLY	2.4
1	C	248	HIS	2.4
1	D	210	GLU	2.3
1	A	252	ARG	2.3
1	C	187	ASP	2.3
1	B	286	TYR	2.2
1	B	39	ASP	2.2
1	A	290	ALA	2.2
1	A	63	THR	2.1
1	A	251	THR	2.1
1	A	291	GLN	2.1
1	A	244	GLY	2.1
1	D	148	ALA	2.1
1	B	160	PRO	2.1
1	B	36	GLY	2.1
1	C	286	TYR	2.1
1	D	243	ILE	2.0
1	C	284	TRP	2.0
1	A	16	VAL	2.0
1	D	250	VAL	2.0

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(\AA^2)	Q<0.9
2	FE2	A	310	1/1	0.97	0.17	0.31	27,27,27,27	0
2	FE2	C	310	1/1	0.99	0.12	-0.50	29,29,29,29	0
2	FE2	D	310	1/1	0.98	0.13	-0.54	33,33,33,33	0
2	FE2	B	310	1/1	0.98	0.09	-1.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.