Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 02:00 PM EST

PDB ID	:	3HQ0
Title	:	Crystal Structure Analysis of the 2,3-dioxygenase LapB from Pseudomonas in complex with a product
Authors	:	Cho, J.-H.; Rhee, S.
Deposited on	:	2009-06-05
Resolution	:	2.00 Å(reported)

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

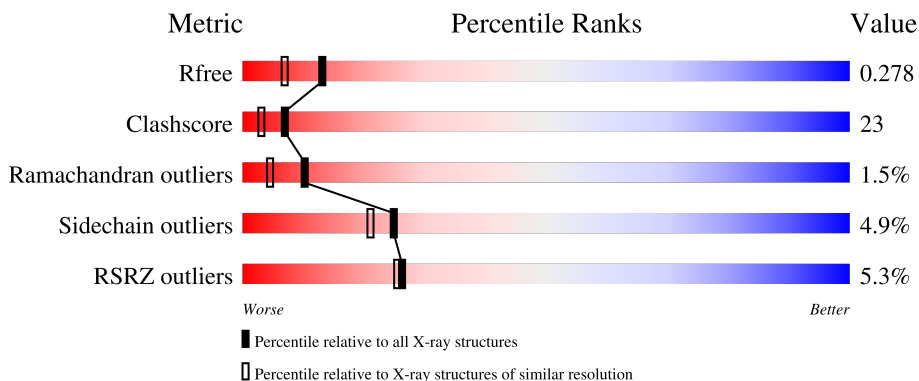|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.278
Clashscore		23
Ramachandran outliers		1.5%
Sidechain outliers		4.9%
RSRZ outliers		5.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% · 59% · 32% · 5% · ·
1	B	309	5% · 58% · 31% · · · 7%
1	C	309	5% · 55% · 38% · · ·
1	D	309	4% · 61% · 30% · · 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	M3P	C	311	-	X	X	-
3	M3P	D	311	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9781 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	296	Total	C	N	O	S	0	0	0
			2362	1503	402	444	13			
1	D	288	Total	C	N	O	S	0	0	0
			2300	1464	392	431	13			

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

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

- Molecule 3 is (2E,4E)-2-hydroxy-6-oxohepta-2,4-dienoic acid (three-letter code: M3P) (formula: $C_7H_8O_4$).

M3P
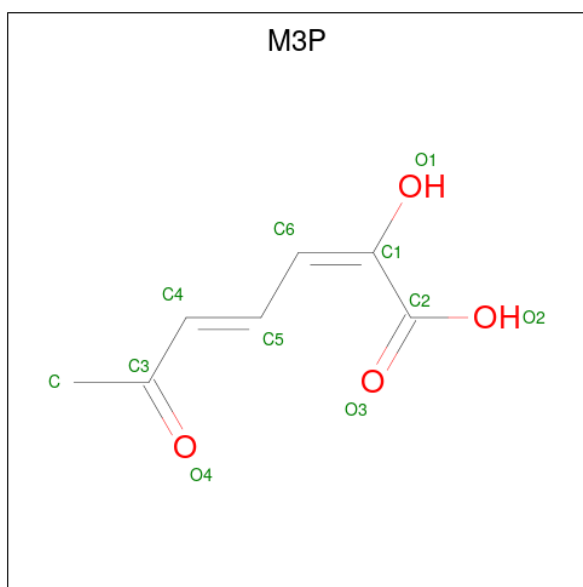
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 11	C 7	O 4	0	0
3	C	1	Total 11	C 7	O 4	0	0
3	D	1	Total 11	C 7	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total 115	O 115	0	0
4	B	102	Total 102	O 102	0	0
4	C	92	Total 92	O 92	0	0
4	D	100	Total 100	O 100	0	0

3 Residue-property plots ⓘ

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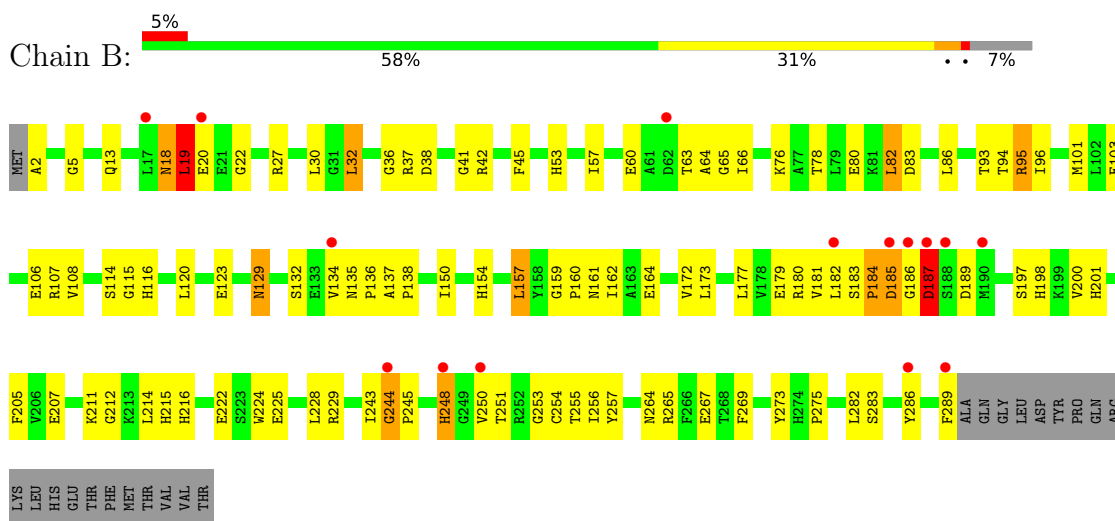shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit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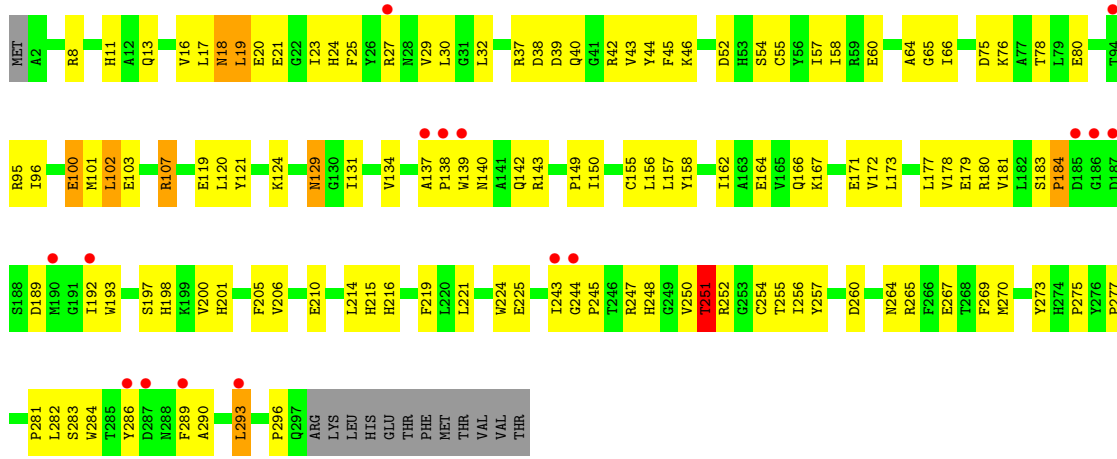
- Molecule 1: Catechol 2,3-dioxygenase
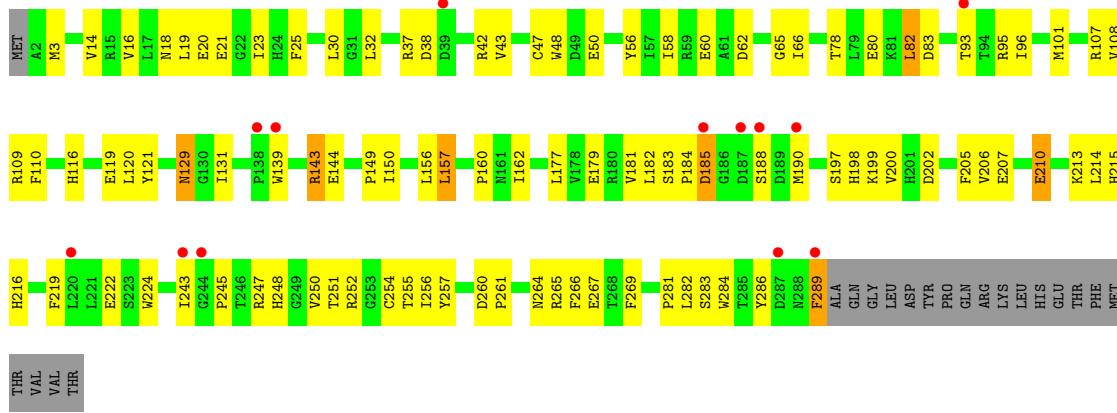

- Molecule 1: Catechol 2,3-dioxygenase

- Molecule 1: Catechol 2,3-dioxygenase

MET A2 R8 H11 A12 Q13 V16 L17 N18 L19 E20 E21 G22 I23 H24 F25 Y26 R27 N28 V29 L30 G31 L32 R37 D38 D39 Q40 G41 R42 V43 Y44 F45 K46 D52 H53 S54 C55 Y56 I57 I58 R59 E60 A64 G65 I66 D75 K76 A77 T78 L79 E80 T94

R95 I96 E100 M101 L102 E103 R107 E119 L120 Y121 K124 N129 G130 I131 V134 A137 P138 W139 N140 A141 Q142 R143 P149 I150 C155 L156 L157 Y158 I162 A163 E164 V165 Q166 K167 E171 V172 L173 L177 V178 E179 R180 V181 L182 S183 P184 D185 G186 D187

S188 D189 M190 G191 I192 W193 S197 H198 K199 V200 H201 F205 V206 E210 L214 H215 H216 F219 L220 L221 W224 E225 I243 G244 P245 T246 R247 H248 G249 V250 T251 R252 G253 C254 T255 I256 Y257 D260 N264 R265 F266 E267 T268 F269 M270 Y273 H274 P275 Y276 P277

P281 L282 S283 W284 T285 Y286 D287 N288 F289 A290 L293 P296 Q297 ARG LYS LEU HIS GLU THR PHE MET THR VAL VAL THR

• Molecule 1: Catechol 2,3-dioxygenase

Chain D:

4%

61% 30% · 7%

MET A2 M3 V14 R15 V16 L17 N18 L19 E20 E21 G22 I23 H24 F25 L30 G31 L32 R37 D38 D39 R42 V43 C47 W48 D49 E50 Y56 I57 I58 R59 E60 A61 D62 G65 I66 T78 L79 E80 K81 L82 D83 T93 T94 R95 I96 M101 R107 V108

R109 F110 H116 E119 L120 Y121 N129 G130 I131 P138 W139 R143 E144 P149 I150 L156 L157 P160 M161 I162 L177 V178 E179 R180 V181 L182 S183 P184 D185 G186 D187 S188 D189 M190 S197 H198 K199 V200 H201 D202 F205 V206 E207 E210 K213 L214 H215

H216 F219 L220 L221 E222 S223 W224 I243 G244 P245 T246 R247 H248 G249 V250 T251 R252 G253 C254 T255 I256 Y257 D260 P261 N264 R265 F266 E267 T268 F269 P281 L282 S283 W284 T285 Y286 D287 N288 F289 ALA GLN GLY LEU ASP TYR PRO GLN ARG LYS LEU HIS GLU THR PHE MET

THR VAL VAL THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.90Å 97.40Å 133.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 45.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.3 (50.00-2.00) 92.9 (45.13-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.269 0.233 , 0.278	Depositor DCC
R_{free} test set	8543 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9781	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 32.35 % 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 9.5395e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, M3P

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	0.36	0/2438	0.67	0/3312
1	B	0.35	0/2363	0.65	0/3210
1	C	0.34	0/2427	0.65	0/3298
1	D	0.35	0/2363	0.64	0/3210
All	All	0.35	0/9591	0.65	0/13030

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2373	0	2261	117	0
1	B	2300	0	2193	96	0
1	C	2362	0	2247	140	0
1	D	2300	0	2193	88	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	B	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	11	0	7	11	0
3	D	11	0	7	7	0
4	A	115	0	0	3	0
4	B	102	0	0	4	0
4	C	92	0	0	3	0
4	D	100	0	0	4	0
All	All	9781	0	8916	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)
3:D:311:M3P:C4	3:D:311:M3P:C3	1.75	1.58
3:D:311:M3P:C6	3:D:311:M3P:C5	1.74	1.57
1:B:215:HIS:HD2	1:B:216:HIS:HD1	1.03	1.02
1:C:200:VAL:HG11	1:C:251:THR:CG2	1.92	0.99
1:C:215:HIS:HD2	1:C:216:HIS:HD1	1.13	0.96
1:C:179:GLU:HG2	1:C:282:LEU:HB2	1.50	0.94
1:A:215:HIS:HD2	1:A:216:HIS:HD1	1.08	0.93
1:D:139:TRP:HB2	1:D:143:ARG:HG3	1.54	0.90
1:B:250:VAL:HG22	1:B:251:THR:HG23	1.53	0.89
1:A:297:GLN:O	1:A:298:ARG:HB2	1.71	0.88
1:C:200:VAL:HG11	1:C:251:THR:HG22	1.55	0.87
1:A:215:HIS:CD2	1:A:216:HIS:HD1	1.94	0.85
1:A:224:TRP:HE1	1:B:228:LEU:HB2	1.39	0.85
1:D:215:HIS:HD2	1:D:216:HIS:HD1	1.21	0.84
1:A:224:TRP:NE1	1:B:228:LEU:HB2	1.93	0.84
1:B:215:HIS:CD2	1:B:216:HIS:HD1	1.94	0.83
1:D:162:ILE:HD12	1:D:205:PHE:HB3	1.61	0.83
1:D:38:ASP:OD2	1:D:42:ARG:HD3	1.79	0.82
1:D:18:ASN:ND2	1:D:21:GLU:H	1.78	0.81
1:D:65:GLY:H	1:D:264:ASN:HD21	1.25	0.81
1:B:150:ILE:HD11	1:B:222:GLU:HG2	1.61	0.80
1:D:210:GLU:HG2	1:D:213:LYS:HE3	1.63	0.80
1:B:161:ASN:HB3	1:B:164:GLU:CD	2.02	0.80
1:C:200:VAL:HG11	1:C:251:THR:HG23	1.62	0.79
1:D:18:ASN:HD22	1:D:21:GLU:H	1.29	0.79
1:C:102:LEU:HD22	1:C:103:GLU:HG2	1.65	0.79
1:D:243:ILE:HG22	1:D:257:TYR:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:HE1	1:D:198:HIS:H	1.28	0.78
1:C:293:LEU:HB2	3:C:311:M3P:HA	1.66	0.78
1:C:215:HIS:CD2	1:C:216:HIS:HD1	2.03	0.75
1:C:164:GLU:HA	1:C:167:LYS:NZ	2.02	0.74
1:A:19:LEU:O	1:A:23:ILE:HG13	1.87	0.74
1:A:185:ASP:C	1:A:187:ASP:H	1.91	0.73
1:C:200:VAL:CG1	1:C:251:THR:HG23	2.19	0.73
1:C:293:LEU:HB2	3:C:311:M3P:C	2.19	0.73
1:D:156:LEU:HD21	1:D:206:VAL:HG23	1.70	0.72
1:C:200:VAL:CG1	1:C:251:THR:CG2	2.67	0.72
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.55	0.72
1:B:162:ILE:HD12	1:B:205:PHE:HB3	1.71	0.71
1:B:182:LEU:HD11	1:B:283:SER:HB2	1.72	0.71
1:B:18:ASN:C	1:B:18:ASN:HD22	1.93	0.70
1:B:225:GLU:HG3	4:D:314:HOH:O	1.92	0.70
1:C:293:LEU:HD23	3:C:311:M3P:HA	1.74	0.70
1:A:155:CYS:SG	1:A:157:LEU:HD21	2.32	0.70
1:A:162:ILE:HD12	1:A:205:PHE:HB3	1.73	0.69
1:A:215:HIS:HD2	1:A:216:HIS:ND1	1.89	0.69
1:C:293:LEU:CB	3:C:311:M3P:HA	2.21	0.69
1:A:224:TRP:CZ3	1:A:254:CYS:HB3	2.28	0.69
1:B:38:ASP:OD2	1:B:42:ARG:HD3	1.94	0.68
1:B:198:HIS:H	1:C:198:HIS:HE1	1.42	0.68
1:B:150:ILE:HD11	1:B:222:GLU:CG	2.23	0.67
1:A:251:THR:HG23	1:A:253:GLY:H	1.58	0.67
1:C:260:ASP:OD2	1:C:264:ASN:HB2	1.95	0.67
1:B:185:ASP:C	1:B:187:ASP:H	1.98	0.66
1:C:131:ILE:HG12	1:C:140:ASN:HD22	1.60	0.66
1:B:179:GLU:OE1	1:B:250:VAL:HG23	1.95	0.66
1:A:80:GLU:OE2	1:A:95:ARG:NH2	2.28	0.66
1:C:38:ASP:OD2	1:C:42:ARG:HD3	1.96	0.66
1:C:27:ARG:HH11	1:C:27:ARG:HG2	1.60	0.66
1:C:76:LYS:NZ	1:C:76:LYS:HB3	2.10	0.65
1:C:46:LYS:HD2	1:C:52:ASP:O	1.97	0.65
1:A:198:HIS:CE1	1:D:197:SER:HB2	2.32	0.65
1:A:295:TYR:CE2	1:A:297:GLN:HB3	2.31	0.65
1:A:107:ARG:HG2	1:A:121:TYR:HB3	1.80	0.64
1:A:248:HIS:HD2	1:A:293:LEU:HD13	1.63	0.63
1:C:293:LEU:CG	3:C:311:M3P:HA	2.28	0.63
1:A:248:HIS:HB2	1:A:253:GLY:O	1.99	0.63
1:C:24:HIS:HB2	4:C:396:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:HIS:HD2	1:B:216:HIS:ND1	1.86	0.63
1:B:114:SER:HB2	1:B:159:GLY:HA3	1.82	0.62
1:C:162:ILE:HG22	1:C:192:ILE:HD12	1.81	0.62
1:D:215:HIS:CD2	1:D:216:HIS:HD1	2.11	0.62
1:B:161:ASN:O	1:B:164:GLU:HG2	2.00	0.62
1:C:173:LEU:N	1:C:173:LEU:HD22	2.14	0.62
1:C:245:PRO:HA	1:C:256:ILE:HG12	1.82	0.62
1:B:65:GLY:H	1:B:264:ASN:HD21	1.49	0.61
1:B:197:SER:HB2	1:C:198:HIS:CE1	2.36	0.61
1:B:255:THR:OG1	1:B:267:GLU:HG3	1.99	0.61
1:B:161:ASN:HB3	1:B:164:GLU:CG	2.31	0.61
1:C:257:TYR:CE1	1:C:267:GLU:HB2	2.35	0.61
1:C:247:ARG:HB3	1:C:296:PRO:HD3	1.83	0.61
1:C:162:ILE:HD12	1:C:205:PHE:HB3	1.83	0.61
1:D:116:HIS:CD2	1:D:157:LEU:HG	2.36	0.60
1:D:182:LEU:HD11	1:D:283:SER:HB3	1.83	0.60
1:B:93:THR:CG2	1:B:108:VAL:HG13	2.31	0.60
1:D:47:CYS:HB2	1:D:50:GLU:HG3	1.84	0.60
1:C:193:TRP:HZ2	3:C:311:M3P:H4	1.67	0.60
1:A:197:SER:HB2	1:D:198:HIS:CE1	2.36	0.60
1:A:157:LEU:N	1:A:157:LEU:HD22	2.17	0.59
1:A:185:ASP:C	1:A:187:ASP:N	2.56	0.59
1:B:19:LEU:O	1:B:22:GLY:N	2.36	0.59
1:D:184:PRO:HG3	1:D:286:TYR:CD2	2.37	0.59
1:A:19:LEU:HB2	1:A:60:GLU:HB2	1.84	0.59
1:C:164:GLU:HA	1:C:167:LYS:HZ3	1.68	0.59
1:A:198:HIS:H	1:D:198:HIS:HE1	1.49	0.59
1:C:177:LEU:HD22	1:C:281:PRO:HB3	1.84	0.59
1:D:250:VAL:O	1:D:251:THR:HB	2.03	0.59
1:A:76:LYS:HD2	1:A:123:GLU:OE1	2.02	0.59
1:C:177:LEU:HD22	1:C:281:PRO:CB	2.33	0.59
1:A:243:ILE:HG22	1:A:257:TYR:HB2	1.85	0.58
1:A:96:ILE:HG21	1:A:107:ARG:NH2	2.18	0.58
1:A:30:LEU:HG	1:A:32:LEU:HD13	1.85	0.58
1:C:200:VAL:CG1	1:C:251:THR:HG22	2.31	0.58
1:A:72:LYS:HE3	1:A:122:ALA:O	2.04	0.58
1:C:129:ASN:HD22	1:C:129:ASN:H	1.52	0.58
1:A:184:PRO:HG3	1:A:286:TYR:CD2	2.38	0.57
1:A:38:ASP:OD1	1:A:42:ARG:HD3	2.04	0.57
1:A:182:LEU:HD21	1:A:283:SER:HB3	1.85	0.57
1:C:96:ILE:HD12	1:C:96:ILE:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLY:H	1:A:264:ASN:HD21	1.50	0.57
1:C:293:LEU:CD2	3:C:311:M3P:HA	2.35	0.57
1:D:80:GLU:OE2	1:D:95:ARG:NH2	2.38	0.57
1:D:156:LEU:HD11	3:D:311:M3P:HB	1.87	0.57
1:C:32:LEU:HB3	1:C:45:PHE:HB3	1.86	0.57
1:B:184:PRO:HG3	1:B:286:TYR:CD2	2.39	0.56
1:D:251:THR:O	1:D:252:ARG:HB2	2.05	0.56
1:A:183:SER:OG	1:A:187:ASP:HA	2.06	0.56
1:C:27:ARG:HG2	1:C:27:ARG:NH1	2.19	0.56
1:A:57:ILE:N	1:A:57:ILE:HD12	2.21	0.56
1:C:177:LEU:HD23	1:C:178:VAL:N	2.21	0.56
1:B:198:HIS:HE1	1:C:198:HIS:H	1.52	0.56
1:A:36:GLY:C	1:A:37:ARG:HG3	2.27	0.56
1:C:180:ARG:HD2	1:C:189:ASP:OD1	2.06	0.56
3:D:311:M3P:C4	3:D:311:M3P:C6	2.68	0.56
1:A:180:ARG:HD3	1:A:283:SER:OG	2.06	0.56
1:C:80:GLU:CD	1:C:95:ARG:HH22	2.08	0.56
1:C:245:PRO:HG2	1:D:245:PRO:O	2.06	0.56
1:D:48:TRP:CZ2	1:D:143:ARG:HG2	2.41	0.56
1:C:40:GLN:HB2	1:C:42:ARG:HD2	1.87	0.55
1:C:215:HIS:O	1:C:265:ARG:HB3	2.06	0.55
1:D:107:ARG:HG2	1:D:121:TYR:HB3	1.87	0.55
1:B:150:ILE:HD11	1:B:222:GLU:CD	2.26	0.55
1:D:150:ILE:N	1:D:150:ILE:HD12	2.22	0.55
1:B:255:THR:OG1	1:B:256:ILE:N	2.39	0.55
1:C:18:ASN:HD22	1:C:18:ASN:C	2.10	0.55
1:C:215:HIS:HD2	1:C:216:HIS:ND1	1.95	0.55
1:A:198:HIS:CE1	1:D:198:HIS:H	2.18	0.55
1:B:160:PRO:O	1:B:207:GLU:OE2	2.25	0.55
1:C:121:TYR:HE2	1:C:124:LYS:HB2	1.72	0.55
1:B:198:HIS:CE1	1:C:197:SER:HB2	2.43	0.55
1:C:251:THR:O	1:C:252:ARG:HB2	2.07	0.54
1:D:215:HIS:O	1:D:265:ARG:HB3	2.07	0.54
1:A:228:LEU:HD21	1:B:254:CYS:SG	2.48	0.54
1:B:53:HIS:CD2	1:B:103:GLU:HG3	2.42	0.54
1:C:65:GLY:H	1:C:264:ASN:HD21	1.54	0.54
1:C:164:GLU:HA	1:C:167:LYS:HZ1	1.71	0.54
1:D:101:MET:HG3	1:D:107:ARG:NH2	2.22	0.54
3:D:311:M3P:C3	3:D:311:M3P:C5	2.70	0.54
1:B:93:THR:HG21	1:B:108:VAL:HG13	1.89	0.54
1:B:179:GLU:HG2	1:B:282:LEU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:THR:OG1	1:C:267:GLU:HG3	2.08	0.54
1:A:242:ASP:CG	1:A:298:ARG:HH22	2.11	0.54
1:B:96:ILE:N	1:B:96:ILE:HD12	2.22	0.54
1:A:129:ASN:HD21	1:A:131:ILE:HB	1.73	0.54
1:B:115:GLY:HA3	1:B:211:LYS:HB2	1.89	0.53
1:A:255:THR:HB	1:A:269:PHE:CB	2.38	0.53
1:D:56:TYR:CE2	1:D:58:ILE:HD11	2.44	0.53
1:A:250:VAL:O	1:A:251:THR:HB	2.09	0.53
1:C:156:LEU:C	1:C:156:LEU:HD23	2.29	0.53
1:A:295:TYR:CD1	1:A:296:PRO:HD2	2.43	0.53
1:A:78:THR:HG22	1:A:82:LEU:HD22	1.90	0.53
1:D:255:THR:OG1	1:D:256:ILE:N	2.42	0.53
1:A:255:THR:OG1	1:A:267:GLU:HG3	2.08	0.52
1:D:65:GLY:N	1:D:264:ASN:HD21	2.02	0.52
1:A:185:ASP:O	1:A:187:ASP:N	2.39	0.52
1:C:289:PHE:CZ	3:C:311:M3P:C	2.93	0.52
1:A:63:THR:HG22	1:A:64:ALA:O	2.10	0.52
1:B:13:GLN:HA	1:B:57:ILE:O	2.09	0.52
1:A:252:ARG:HG3	1:A:252:ARG:NH1	2.22	0.52
1:C:30:LEU:HG	1:C:32:LEU:CD1	2.39	0.52
1:C:107:ARG:HD3	1:C:119:GLU:OE1	2.09	0.52
1:C:101:MET:HG3	1:C:107:ARG:NH2	2.24	0.52
1:C:172:VAL:HB	1:C:173:LEU:HD22	1.91	0.52
1:D:43:VAL:CG2	1:D:58:ILE:HB	2.40	0.51
1:C:129:ASN:HD22	1:C:129:ASN:N	2.07	0.51
1:C:257:TYR:CD1	1:C:267:GLU:HB2	2.45	0.51
1:A:30:LEU:HD23	1:A:32:LEU:HD22	1.91	0.51
1:D:224:TRP:CZ3	1:D:254:CYS:HB3	2.46	0.51
1:B:180:ARG:HD2	1:B:189:ASP:OD1	2.09	0.51
1:C:76:LYS:HB3	1:C:76:LYS:HZ3	1.73	0.51
1:C:248:HIS:CE1	1:C:255:THR:HG21	2.45	0.51
1:C:18:ASN:HB3	1:C:21:GLU:HG2	1.92	0.51
1:A:42:ARG:NH2	4:A:404:HOH:O	2.43	0.51
1:B:76:LYS:HG3	4:B:404:HOH:O	2.11	0.51
1:B:224:TRP:CZ3	1:B:254:CYS:HB3	2.45	0.51
1:B:273:TYR:CD1	1:B:275:PRO:HD3	2.45	0.51
1:B:182:LEU:N	1:B:182:LEU:HD12	2.26	0.51
1:B:243:ILE:HG22	1:B:257:TYR:HB2	1.92	0.50
4:B:391:HOH:O	1:C:277:PRO:HG3	2.11	0.50
1:C:167:LYS:O	1:C:171:GLU:HB2	2.12	0.50
1:B:184:PRO:C	1:B:186:GLY:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:VAL:HG13	1:D:65:GLY:O	2.11	0.50
1:A:34:GLU:OE2	1:A:37:ARG:HD2	2.11	0.50
1:A:242:ASP:OD1	1:A:298:ARG:NH2	2.43	0.50
1:A:210:GLU:OE1	1:A:213:LYS:HD2	2.12	0.50
1:B:184:PRO:O	1:B:186:GLY:N	2.44	0.50
1:B:185:ASP:C	1:B:187:ASP:N	2.64	0.50
1:C:139:TRP:CB	1:C:143:ARG:HD3	2.42	0.50
1:C:166:GLN:OE1	1:C:192:ILE:HD13	2.12	0.50
1:C:149:PRO:HB2	1:C:219:PHE:HB3	1.94	0.50
1:D:150:ILE:HD11	1:D:222:GLU:HG2	1.94	0.50
1:D:200:VAL:HG11	1:D:251:THR:HA	1.94	0.50
1:B:86:LEU:HD23	1:B:172:VAL:HG11	1.93	0.49
1:C:149:PRO:CB	1:C:219:PHE:HB3	2.42	0.49
1:C:193:TRP:CZ2	3:C:311:M3P:H4	2.46	0.49
1:A:46:LYS:HD2	1:A:52:ASP:O	2.13	0.49
1:B:19:LEU:HG	1:B:60:GLU:HB2	1.94	0.49
1:C:131:ILE:HG12	1:C:140:ASN:ND2	2.26	0.49
1:A:135:ASN:HA	1:D:284:TRP:CE3	2.48	0.49
1:A:245:PRO:HG2	1:B:245:PRO:O	2.13	0.49
1:B:18:ASN:C	1:B:18:ASN:ND2	2.63	0.49
1:C:243:ILE:HG23	1:C:243:ILE:O	2.12	0.49
1:D:210:GLU:HG2	1:D:213:LYS:CE	2.39	0.49
1:D:181:VAL:HG11	1:D:289:PHE:CE2	2.48	0.49
1:A:293:LEU:N	1:A:293:LEU:HD12	2.28	0.49
1:A:107:ARG:HD2	1:A:119:GLU:OE1	2.13	0.49
1:B:215:HIS:O	1:B:265:ARG:HB3	2.13	0.49
1:D:93:THR:CG2	1:D:108:VAL:HG13	2.42	0.49
1:A:224:TRP:CZ2	1:B:228:LEU:HD13	2.47	0.49
1:D:199:LYS:HE2	1:D:202:ASP:OD1	2.13	0.49
1:A:143:ARG:HG3	4:A:364:HOH:O	2.13	0.48
1:C:293:LEU:O	1:C:293:LEU:HD22	2.13	0.48
1:C:13:GLN:HA	1:C:57:ILE:O	2.13	0.48
1:D:255:THR:OG1	1:D:267:GLU:HG3	2.13	0.48
1:D:20:GLU:CD	1:D:20:GLU:H	2.15	0.48
1:D:66:ILE:HG22	1:D:214:LEU:HB2	1.95	0.48
1:D:183:SER:HB3	1:D:188:SER:O	2.13	0.48
1:A:18:ASN:HB3	1:A:21:GLU:HG2	1.95	0.48
1:C:245:PRO:CA	1:C:256:ILE:HG12	2.43	0.48
1:B:2:ALA:HB2	4:B:319:HOH:O	2.14	0.48
1:C:23:ILE:CD1	1:C:37:ARG:HH22	2.26	0.48
1:C:27:ARG:HG3	1:C:45:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TRP:CD1	1:D:224:TRP:CD1	3.02	0.48
1:A:17:LEU:HD23	1:A:262:SER:HB3	1.94	0.48
1:D:38:ASP:HB2	4:D:353:HOH:O	2.14	0.48
1:C:64:ALA:HB1	1:C:264:ASN:ND2	2.28	0.48
1:A:297:GLN:HG2	1:A:298:ARG:N	2.28	0.48
1:D:200:VAL:HG11	1:D:251:THR:HG23	1.95	0.48
1:A:248:HIS:CD2	1:A:293:LEU:HD13	2.46	0.47
1:C:100:GLU:OE2	1:C:107:ARG:NH2	2.47	0.47
1:C:290:ALA:HB3	4:C:395:HOH:O	2.12	0.47
1:D:109:ARG:HG2	1:D:110:PHE:N	2.30	0.47
1:A:255:THR:HB	1:A:269:PHE:HB3	1.97	0.47
1:B:129:ASN:H	1:B:129:ASN:HD22	1.63	0.47
1:C:18:ASN:C	1:C:18:ASN:ND2	2.68	0.47
1:B:132:SER:O	1:B:136:PRO:HB3	2.15	0.47
1:B:181:VAL:HG11	1:B:289:PHE:CG	2.50	0.47
1:B:229:ARG:HD2	1:D:144:GLU:OE1	2.15	0.47
1:C:80:GLU:OE2	1:C:95:ARG:NH2	2.47	0.47
1:C:134:VAL:HG13	4:C:359:HOH:O	2.13	0.47
1:C:221:LEU:O	1:C:270:MET:HB3	2.14	0.47
1:C:255:THR:OG1	1:C:256:ILE:N	2.47	0.47
1:C:273:TYR:CD1	1:C:275:PRO:HD3	2.50	0.47
1:C:183:SER:O	1:C:184:PRO:O	2.33	0.47
1:A:230:ALA:O	1:A:234:MET:HG3	2.15	0.47
1:A:295:TYR:O	1:A:297:GLN:O	2.32	0.47
1:C:11:HIS:HA	1:C:55:CYS:O	2.15	0.47
1:D:248:HIS:CE1	1:D:255:THR:HG21	2.49	0.47
1:A:252:ARG:NH1	4:A:341:HOH:O	2.48	0.46
1:A:260:ASP:HB2	1:A:264:ASN:O	2.15	0.46
1:B:93:THR:HG23	1:B:108:VAL:HG13	1.97	0.46
1:B:183:SER:O	1:B:185:ASP:N	2.48	0.46
1:C:129:ASN:H	1:C:129:ASN:ND2	2.14	0.46
1:C:289:PHE:CZ	3:C:311:M3P:H	2.50	0.46
1:A:255:THR:HB	1:A:269:PHE:HB2	1.97	0.46
1:A:297:GLN:O	1:A:298:ARG:CB	2.53	0.46
1:D:30:LEU:HG	1:D:32:LEU:HD13	1.97	0.46
1:B:93:THR:HG22	1:B:94:THR:N	2.30	0.46
1:A:66:ILE:HG22	1:A:214:LEU:HB2	1.97	0.46
1:A:178:VAL:HG21	1:A:200:VAL:O	2.16	0.46
1:A:293:LEU:HD12	1:A:293:LEU:H	1.80	0.46
1:C:140:ASN:OD1	1:C:142:GLN:HB2	2.16	0.46
1:A:38:ASP:HB3	1:A:102:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:NZ	1:A:167:LYS:HB3	2.30	0.46
1:A:134:VAL:HG13	1:A:134:VAL:O	2.16	0.46
1:B:95:ARG:NE	1:B:106:GLU:OE1	2.48	0.46
1:D:37:ARG:HA	1:D:42:ARG:O	2.15	0.46
1:D:179:GLU:OE1	1:D:250:VAL:HG13	2.16	0.46
1:C:250:VAL:HG22	1:C:284:TRP:CD1	2.51	0.46
1:D:184:PRO:O	1:D:185:ASP:C	2.53	0.46
1:B:80:GLU:OE1	1:B:95:ARG:NH2	2.49	0.46
1:A:182:LEU:N	1:A:182:LEU:HD22	2.31	0.46
1:A:213:LYS:HE3	1:A:213:LYS:HA	1.98	0.46
1:C:18:ASN:HD22	1:C:19:LEU:N	2.14	0.46
1:C:64:ALA:HB1	1:C:264:ASN:HD21	1.81	0.46
1:A:260:ASP:HB2	1:A:264:ASN:HB2	1.99	0.45
1:B:5:GLY:HA2	1:B:78:THR:HG21	1.97	0.45
1:C:193:TRP:HD1	1:C:201:HIS:CD2	2.34	0.45
1:C:19:LEU:O	1:C:23:ILE:HG13	2.16	0.45
1:C:66:ILE:HG22	1:C:214:LEU:HB2	1.98	0.45
1:D:179:GLU:HG2	1:D:282:LEU:HB2	1.98	0.45
1:A:17:LEU:CD2	1:A:262:SER:HB3	2.47	0.45
1:B:63:THR:HG22	1:B:64:ALA:O	2.17	0.45
1:D:83:ASP:OD2	1:D:93:THR:HG21	2.17	0.45
1:A:198:HIS:HE1	1:D:197:SER:HB2	1.79	0.45
1:A:224:TRP:CD1	1:B:228:LEU:HD22	2.51	0.45
1:B:150:ILE:CD1	1:B:222:GLU:HG2	2.39	0.45
1:D:160:PRO:HA	1:D:207:GLU:OE2	2.16	0.45
1:C:137:ALA:HB1	1:C:138:PRO:HD2	1.99	0.45
1:C:254:CYS:O	1:C:269:PHE:HB2	2.16	0.45
1:C:16:VAL:O	1:C:60:GLU:HA	2.17	0.45
1:A:183:SER:HA	1:A:190:MET:HG2	1.99	0.45
1:A:129:ASN:ND2	1:A:131:ILE:H	2.14	0.45
1:D:19:LEU:O	1:D:23:ILE:HG13	2.16	0.45
1:A:224:TRP:HZ3	1:A:227:VAL:HG11	1.82	0.44
1:C:177:LEU:HD23	1:C:177:LEU:C	2.37	0.44
1:C:23:ILE:HD13	1:C:37:ARG:HH22	1.82	0.44
1:C:224:TRP:CZ3	1:C:254:CYS:HB3	2.52	0.44
1:A:66:ILE:HB	1:A:214:LEU:HG	1.99	0.44
1:D:224:TRP:CE3	1:D:254:CYS:HB3	2.51	0.44
1:D:182:LEU:N	1:D:182:LEU:HD12	2.33	0.44
1:A:224:TRP:HA	1:A:224:TRP:CE3	2.53	0.44
1:C:155:CYS:SG	1:C:157:LEU:HD21	2.58	0.44
1:D:190:MET:HG3	1:D:286:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:C	1:A:156:LEU:HD23	2.38	0.44
1:A:197:SER:HB2	1:D:198:HIS:HE1	1.82	0.44
1:A:24:HIS:O	1:A:28:ASN:HB2	2.18	0.44
1:B:36:GLY:C	1:B:37:ARG:HG3	2.38	0.44
1:B:83:ASP:OD2	1:B:93:THR:HG21	2.18	0.44
1:C:39:ASP:OD1	1:C:40:GLN:HG3	2.18	0.44
1:C:139:TRP:HB2	1:C:143:ARG:HD3	2.00	0.44
1:D:129:ASN:ND2	1:D:131:ILE:H	2.15	0.44
1:A:37:ARG:HA	1:A:42:ARG:O	2.18	0.43
1:A:116:HIS:CD2	1:A:212:GLY:HA2	2.53	0.43
1:A:149:PRO:CB	1:A:219:PHE:HB3	2.47	0.43
1:A:37:ARG:HG2	1:A:43:VAL:HG22	2.00	0.43
1:B:19:LEU:HD11	1:B:41:GLY:O	2.18	0.43
1:B:78:THR:HG22	1:B:82:LEU:HD22	2.00	0.43
1:D:78:THR:HG22	1:D:82:LEU:HD22	1.99	0.43
1:D:182:LEU:CD1	1:D:283:SER:HB3	2.47	0.43
1:A:91:LEU:HD11	1:A:168:ILE:HD13	2.00	0.43
1:C:156:LEU:HD23	1:C:157:LEU:N	2.33	0.43
1:B:32:LEU:HB3	1:B:45:PHE:HB3	2.00	0.43
1:C:19:LEU:O	1:C:19:LEU:HD13	2.19	0.43
1:C:289:PHE:CZ	3:C:311:M3P:HB	2.53	0.43
1:A:260:ASP:HB3	1:A:264:ASN:H	1.84	0.43
1:A:198:HIS:H	1:D:198:HIS:CE1	2.34	0.43
1:A:223:SER:C	1:A:270:MET:HG2	2.39	0.43
1:A:224:TRP:HA	1:A:224:TRP:HE3	1.83	0.43
1:B:66:ILE:CG2	1:B:214:LEU:HB2	2.49	0.43
1:B:101:MET:HB2	1:B:107:ARG:NH2	2.33	0.43
1:B:134:VAL:HA	1:C:283:SER:O	2.18	0.43
1:C:158:TYR:CE1	1:C:206:VAL:HB	2.54	0.43
1:D:25:PHE:HZ	1:D:266:PHE:CE2	2.36	0.43
1:D:177:LEU:HD22	1:D:281:PRO:CB	2.48	0.43
1:B:248:HIS:N	1:B:253:GLY:O	2.45	0.43
1:C:19:LEU:HD23	1:C:60:GLU:N	2.33	0.43
1:C:164:GLU:HG2	1:C:167:LYS:HZ1	1.84	0.43
1:C:179:GLU:OE1	1:C:284:TRP:NE1	2.50	0.43
1:A:255:THR:OG1	1:A:256:ILE:N	2.52	0.43
1:B:30:LEU:HD23	1:B:32:LEU:HD22	2.00	0.43
1:C:96:ILE:N	1:C:96:ILE:CD1	2.82	0.43
1:C:257:TYR:HE1	1:C:267:GLU:HB2	1.82	0.43
1:D:25:PHE:CD2	1:D:261:PRO:HD3	2.54	0.43
1:D:16:VAL:O	1:D:60:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HB3	1:A:45:PHE:HB3	2.01	0.42
1:B:27:ARG:NH1	4:B:410:HOH:O	2.51	0.42
1:C:181:VAL:HG11	1:C:289:PHE:CD1	2.54	0.42
1:C:225:GLU:HG3	4:D:334:HOH:O	2.20	0.42
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.93	0.42
1:A:3:MET:SD	1:D:3:MET:SD	3.17	0.42
1:A:113:PRO:HD2	1:A:165:VAL:HG22	2.00	0.42
1:A:160:PRO:HA	1:A:207:GLU:OE2	2.20	0.42
1:B:93:THR:CG2	1:B:94:THR:N	2.82	0.42
1:C:177:LEU:HD22	1:C:281:PRO:HB2	2.00	0.42
1:C:177:LEU:HD23	1:C:179:GLU:N	2.34	0.42
1:B:18:ASN:HD22	1:B:19:LEU:N	2.17	0.42
1:D:149:PRO:CB	1:D:219:PHE:HB3	2.49	0.42
1:D:93:THR:HG23	1:D:108:VAL:HG13	2.01	0.42
1:A:210:GLU:CD	1:A:213:LYS:HD2	2.40	0.42
1:B:66:ILE:HG22	1:B:214:LEU:HB2	2.01	0.42
1:B:198:HIS:H	1:C:198:HIS:CE1	2.30	0.42
1:C:150:ILE:HD12	1:C:150:ILE:N	2.35	0.42
1:D:107:ARG:HD2	1:D:119:GLU:OE1	2.20	0.42
1:C:18:ASN:ND2	1:C:20:GLU:H	2.17	0.42
1:A:44:TYR:CD1	1:A:44:TYR:N	2.88	0.41
1:C:25:PHE:O	1:C:29:VAL:HB	2.20	0.41
1:C:177:LEU:HG	1:C:192:ILE:HG23	2.01	0.41
1:A:182:LEU:CD2	1:A:283:SER:HB3	2.49	0.41
1:A:273:TYR:CD1	1:A:275:PRO:HD3	2.55	0.41
1:C:173:LEU:N	1:C:173:LEU:CD2	2.82	0.41
1:A:251:THR:O	1:A:252:ARG:HB2	2.20	0.41
1:C:44:TYR:CD1	1:C:44:TYR:N	2.89	0.41
1:D:254:CYS:O	1:D:269:PHE:HB2	2.20	0.41
1:D:260:ASP:OD2	1:D:264:ASN:HB2	2.21	0.41
1:B:185:ASP:O	1:B:187:ASP:N	2.53	0.41
1:C:178:VAL:HG21	1:C:200:VAL:O	2.20	0.41
1:A:72:LYS:HD3	1:A:73:VAL:O	2.21	0.41
1:A:224:TRP:CH2	1:A:254:CYS:HB3	2.56	0.41
1:B:65:GLY:N	1:B:264:ASN:HD21	2.16	0.41
1:B:129:ASN:HD22	1:B:129:ASN:N	2.18	0.41
1:B:245:PRO:HA	1:B:255:THR:O	2.21	0.41
1:B:255:THR:HB	1:B:269:PHE:CB	2.51	0.41
1:C:157:LEU:N	1:C:157:LEU:HD22	2.34	0.41
1:D:214:LEU:HD13	1:D:214:LEU:C	2.40	0.41
1:D:255:THR:HG1	1:D:267:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLY:HA3	1:A:211:LYS:HB3	2.02	0.41
1:C:286:TYR:O	1:C:289:PHE:HB2	2.20	0.41
1:B:76:LYS:HE2	1:B:123:GLU:OE2	2.20	0.41
1:B:135:ASN:N	1:B:136:PRO:CD	2.83	0.41
1:B:198:HIS:CE1	1:C:198:HIS:H	2.36	0.41
1:B:200:VAL:HG23	1:B:201:HIS:ND1	2.36	0.41
1:C:255:THR:HB	1:C:269:PHE:CB	2.51	0.41
1:D:96:ILE:HD11	1:D:109:ARG:CZ	2.50	0.41
1:A:250:VAL:O	1:A:250:VAL:HG23	2.21	0.41
1:B:116:HIS:CD2	1:B:212:GLY:HA2	2.56	0.41
1:C:75:ASP:O	1:C:78:THR:HB	2.21	0.41
1:C:164:GLU:CG	1:C:167:LYS:HZ1	2.34	0.41
1:D:109:ARG:HD2	4:D:382:HOH:O	2.21	0.41
1:B:255:THR:HB	1:B:269:PHE:HB3	2.02	0.40
1:D:66:ILE:CG2	1:D:214:LEU:HB2	2.51	0.40
1:B:116:HIS:CD2	1:B:157:LEU:HG	2.57	0.40
1:B:137:ALA:HB1	1:B:138:PRO:HD2	2.02	0.40
1:C:46:LYS:HB3	1:C:54:SER:HA	2.03	0.40
3:D:311:M3P:C5	3:D:311:M3P:C1	2.74	0.40
1:A:80:GLU:CD	1:A:95:ARG:HH22	2.24	0.40
1:B:243:ILE:O	1:B:244:GLY:O	2.40	0.40
1:C:43:VAL:HG12	1:C:58:ILE:HG13	2.02	0.40
1:D:18:ASN:HD21	1:D:20:GLU:HB2	1.87	0.40
1:D:206:VAL:HG21	3:D:311:M3P:C	2.52	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%)	277 (94%)	12 (4%)	6 (2%)	7	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	286/309 (93%)	267 (93%)	12 (4%)	7 (2%)	6 2
1	C	294/309 (95%)	278 (95%)	13 (4%)	3 (1%)	15 9
1	D	286/309 (93%)	269 (94%)	16 (6%)	1 (0%)	41 37
All	All	1161/1236 (94%)	1091 (94%)	53 (5%)	17 (2%)	10 4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ASP
1	A	248	HIS
1	A	251	THR
1	A	185	ASP
1	B	19	LEU
1	B	187	ASP
1	B	244	GLY
1	C	184	PRO
1	C	244	GLY
1	A	250	VAL
1	C	251	THR
1	B	154	HIS
1	D	185	ASP
1	A	188	SER
1	B	185	ASP
1	B	20	GLU
1	B	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%)	236 (94%)	16 (6%)	18 13
1	B	245/264 (93%)	233 (95%)	12 (5%)	25 21
1	C	251/264 (95%)	239 (95%)	12 (5%)	25 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	245/264 (93%)	236 (96%)	9 (4%)	34	32
All	All	993/1056 (94%)	944 (95%)	49 (5%)	25	21

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	44	TYR
1	A	72	LYS
1	A	82	LEU
1	A	95	ARG
1	A	120	LEU
1	A	129	ASN
1	A	157	LEU
1	A	173	LEU
1	A	180	ARG
1	A	187	ASP
1	A	213	LYS
1	A	214	LEU
1	A	224	TRP
1	A	248	HIS
1	A	287	ASP
1	B	18	ASN
1	B	19	LEU
1	B	32	LEU
1	B	82	LEU
1	B	95	ARG
1	B	120	LEU
1	B	129	ASN
1	B	157	LEU
1	B	173	LEU
1	B	177	LEU
1	B	187	ASP
1	B	248	HIS
1	C	8	ARG
1	C	17	LEU
1	C	18	ASN
1	C	19	LEU
1	C	100	GLU
1	C	102	LEU
1	C	107	ARG
1	C	120	LEU

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Mol	Chain	Res	Type
1	C	129	ASN
1	C	210	GLU
1	C	251	THR
1	C	293	LEU
1	D	62	ASP
1	D	82	LEU
1	D	120	LEU
1	D	129	ASN
1	D	143	ARG
1	D	157	LEU
1	D	210	GLU
1	D	247	ARG
1	D	289	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	28	ASN
1	A	129	ASN
1	A	198	HIS
1	A	215	HIS
1	A	226	GLN
1	A	237	ASN
1	A	264	ASN
1	B	18	ASN
1	B	28	ASN
1	B	129	ASN
1	B	145	HIS
1	B	198	HIS
1	B	215	HIS
1	B	237	ASN
1	B	240	ASN
1	B	264	ASN
1	B	288	ASN
1	C	18	ASN
1	C	28	ASN
1	C	87	GLN
1	C	129	ASN
1	C	198	HIS
1	C	215	HIS
1	C	237	ASN

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Mol	Chain	Res	Type
1	C	240	ASN
1	C	248	HIS
1	C	264	ASN
1	C	288	ASN
1	C	297	GLN
1	D	18	ASN
1	D	129	ASN
1	D	198	HIS
1	D	215	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	M3P	D	311	2	10,10,10	7.50	6 (60%)	11,12,12	1.60	3 (27%)
3	M3P	B	311	2	10,10,10	7.41	7 (70%)	11,12,12	1.45	2 (18%)
3	M3P	C	311	2	10,10,10	7.36	8 (80%)	11,12,12	3.10	5 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M3P	D	311	2	-	3/9/10/10	-
3	M3P	B	311	2	-	3/9/10/10	-
3	M3P	C	311	2	-	4/9/10/10	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	311	M3P	C1-C2	17.72	1.70	1.48
3	C	311	M3P	C1-C2	17.52	1.70	1.48
3	D	311	M3P	C1-C2	17.10	1.69	1.48
3	D	311	M3P	C4-C3	11.40	1.75	1.47
3	B	311	M3P	C4-C3	10.31	1.73	1.47
3	D	311	M3P	C5-C6	10.09	1.74	1.43
3	C	311	M3P	C4-C3	9.81	1.72	1.47
3	B	311	M3P	C5-C6	9.41	1.72	1.43
3	C	311	M3P	C5-C6	9.31	1.72	1.43
3	B	311	M3P	O2-C2	4.41	1.43	1.30
3	D	311	M3P	O2-C2	4.28	1.43	1.30
3	C	311	M3P	C6-C1	-4.08	1.30	1.39
3	C	311	M3P	O2-C2	4.04	1.42	1.30
3	D	311	M3P	O1-C1	3.28	1.42	1.34
3	B	311	M3P	C6-C1	-2.71	1.33	1.39
3	C	311	M3P	O1-C1	2.69	1.40	1.34
3	B	311	M3P	O1-C1	2.66	1.40	1.34
3	C	311	M3P	C5-C4	-2.37	1.28	1.34
3	B	311	M3P	C-C3	2.28	1.55	1.50
3	C	311	M3P	C-C3	2.15	1.54	1.50
3	D	311	M3P	C6-C1	-2.15	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	311	M3P	C6-C1-C2	7.17	131.31	122.69
3	C	311	M3P	O1-C1-C2	-5.44	110.72	114.01
3	D	311	M3P	O1-C1-C2	-3.04	112.17	114.01
3	B	311	M3P	C6-C1-C2	2.89	126.17	122.69
3	D	311	M3P	C6-C1-C2	2.88	126.16	122.69
3	C	311	M3P	O1-C1-C6	-2.85	117.96	122.92
3	C	311	M3P	C6-C5-C4	-2.74	114.68	123.22
3	D	311	M3P	O3-C2-C1	2.69	123.17	120.08
3	B	311	M3P	O3-C2-C1	2.37	122.80	120.08
3	C	311	M3P	O3-C2-C1	2.16	122.56	120.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	311	M3P	O1-C1-C6-C5
3	C	311	M3P	O1-C1-C6-C5
3	C	311	M3P	C-C3-C4-C5
3	C	311	M3P	O4-C3-C4-C5
3	C	311	M3P	C4-C5-C6-C1
3	D	311	M3P	O1-C1-C6-C5
3	D	311	M3P	C-C3-C4-C5
3	D	311	M3P	O4-C3-C4-C5
3	B	311	M3P	C-C3-C4-C5
3	B	311	M3P	O4-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	311	M3P	7	0
3	C	311	M3P	11	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	297/309 (96%)	0.29	18 (6%)	21	20	11, 22, 40, 61	0
1	B	288/309 (93%)	0.38	15 (5%)	27	26	12, 23, 41, 58	0
1	C	296/309 (95%)	0.47	16 (5%)	25	24	14, 26, 42, 59	0
1	D	288/309 (93%)	0.34	13 (4%)	33	32	12, 22, 38, 55	0
All	All	1169/1236 (94%)	0.37	62 (5%)	26	25	11, 23, 41, 61	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	TRP	8.2
1	D	185	ASP	6.5
1	C	244	GLY	6.3
1	C	139	TRP	6.2
1	D	187	ASP	6.0
1	C	185	ASP	6.0
1	A	224	TRP	5.7
1	B	248	HIS	4.9
1	B	244	GLY	4.7
1	A	250	VAL	4.6
1	C	243	ILE	4.4
1	B	186	GLY	4.3
1	B	185	ASP	4.3
1	D	138	PRO	4.1
1	A	297	GLN	3.9
1	C	186	GLY	3.8
1	A	244	GLY	3.6
1	B	188	SER	3.5
1	D	244	GLY	3.5
1	A	187	ASP	3.4
1	A	185	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	293	LEU	3.3
1	B	190	MET	3.3
1	C	289	PHE	3.3
1	C	138	PRO	3.2
1	A	249	GLY	3.0
1	B	250	VAL	2.9
1	B	17	LEU	2.9
1	A	293	LEU	2.9
1	B	289	PHE	2.8
1	A	295	TYR	2.8
1	A	19	LEU	2.7
1	C	137	ALA	2.7
1	A	17	LEU	2.6
1	A	254	CYS	2.6
1	D	243	ILE	2.5
1	B	187	ASP	2.5
1	C	190	MET	2.5
1	A	243	ILE	2.5
1	D	190	MET	2.4
1	A	251	THR	2.4
1	A	248	HIS	2.3
1	A	186	GLY	2.3
1	B	182	LEU	2.3
1	C	192	ILE	2.3
1	C	287	ASP	2.2
1	C	94	THR	2.2
1	A	289	PHE	2.2
1	A	184	PRO	2.2
1	D	287	ASP	2.2
1	D	289	PHE	2.2
1	C	187	ASP	2.2
1	C	27	ARG	2.2
1	B	134	VAL	2.2
1	D	220	LEU	2.1
1	C	286	TYR	2.1
1	B	20	GLU	2.1
1	D	93	THR	2.1
1	B	62	ASP	2.1
1	D	39	ASP	2.1
1	B	286	TYR	2.1
1	D	188	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	M3P	D	311	11/11	0.62	0.38	45,46,48,49	0
3	M3P	B	311	11/11	0.74	0.34	40,44,47,47	0
3	M3P	C	311	11/11	0.77	0.35	46,47,49,49	0
2	FE	D	310	1/1	0.99	0.07	21,21,21,21	0
2	FE	A	310	1/1	0.99	0.08	23,23,23,23	0
2	FE	B	310	1/1	0.99	0.08	23,23,23,23	0
2	FE	C	310	1/1	0.99	0.09	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.