



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:53 AM UTC

PDB ID : 3HQ0 / pdb_00003hq0
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

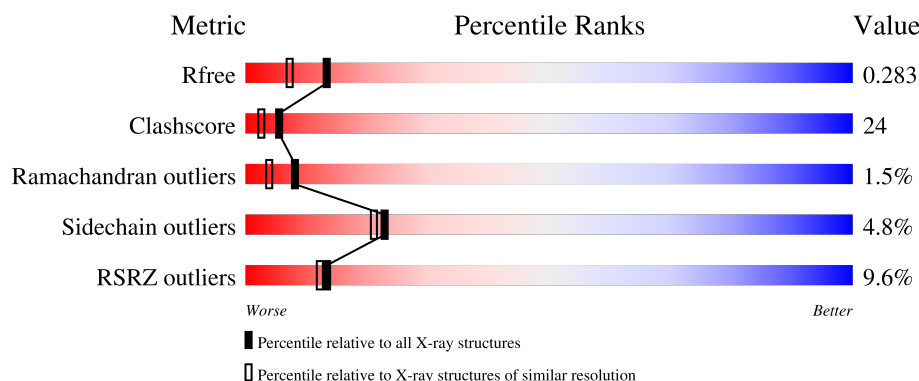
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	9% 56% 34% 6% • •
1	B	309	9% 57% 30% 6% • 7%
1	C	309	11% 54% 39% • •
1	D	309	6% 58% 31% • 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	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.

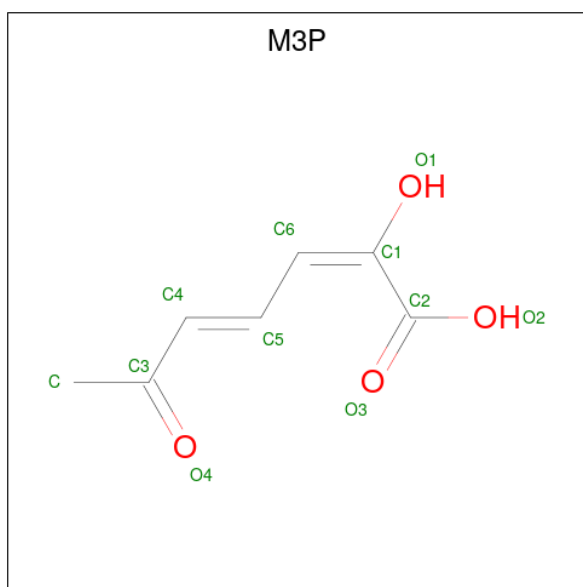
- Molecule 1 is a protein called Catechol 2,3-dioxygenase.

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 (CCD ID: 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 (CCD ID: M3P) (formula: C₇H₈O₄).



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

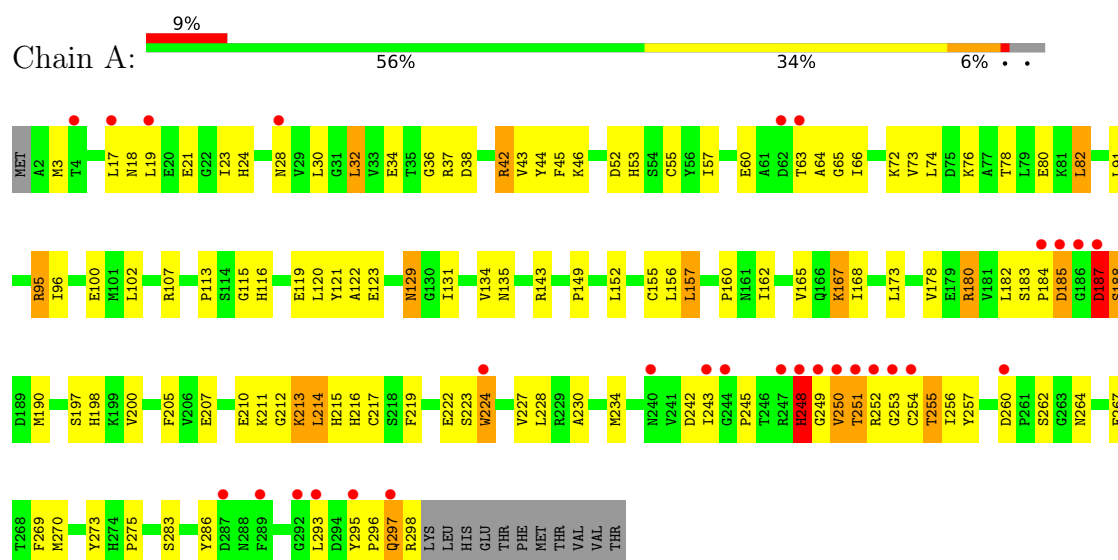
- Molecule 4 is water.

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

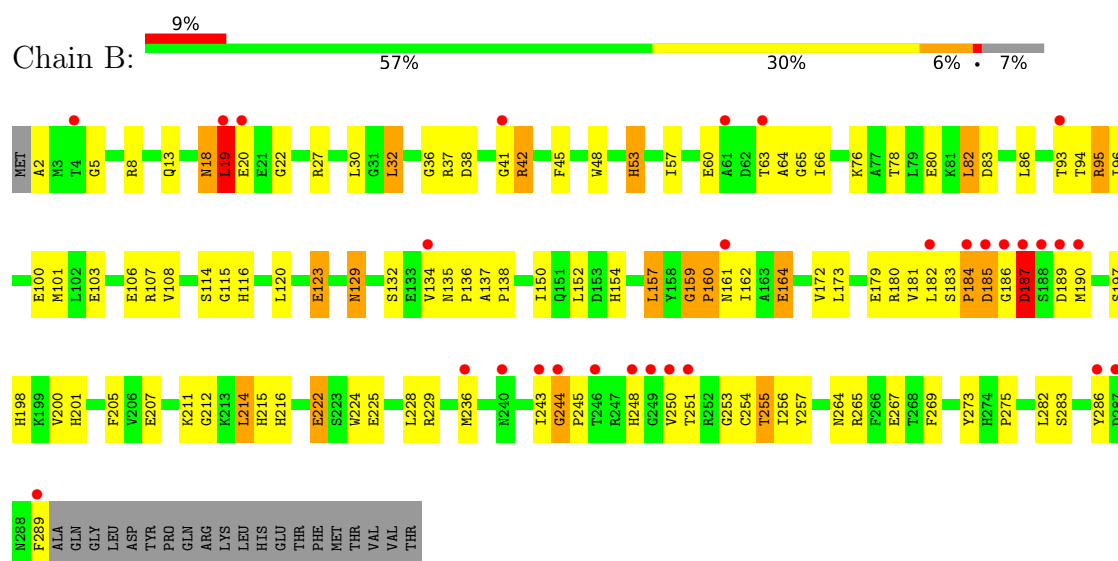
3 Residue-property plots [i](#)

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.

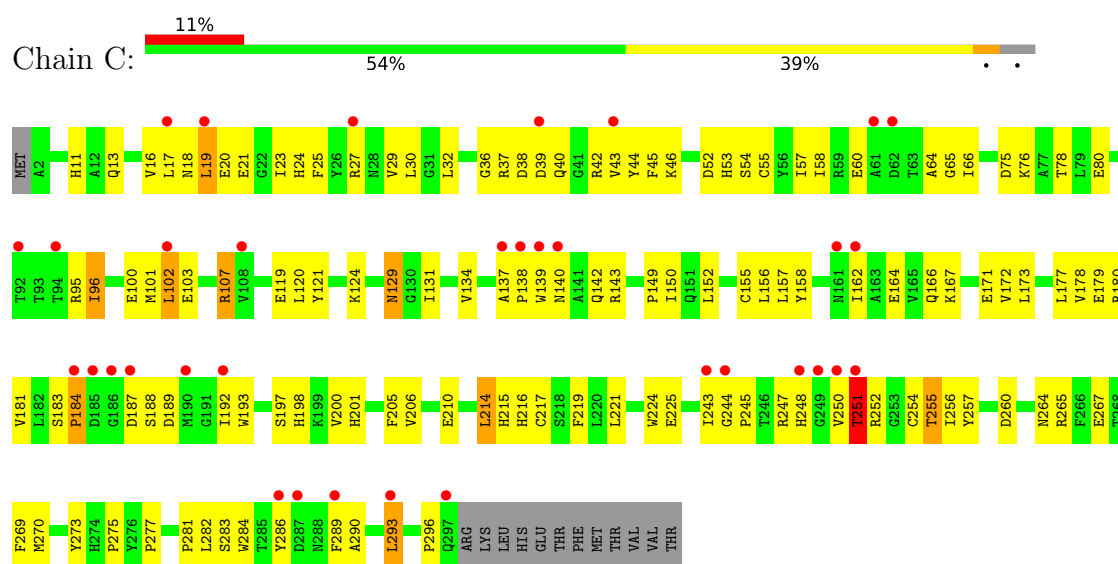
• Molecule 1: Catechol 2,3-dioxygenase



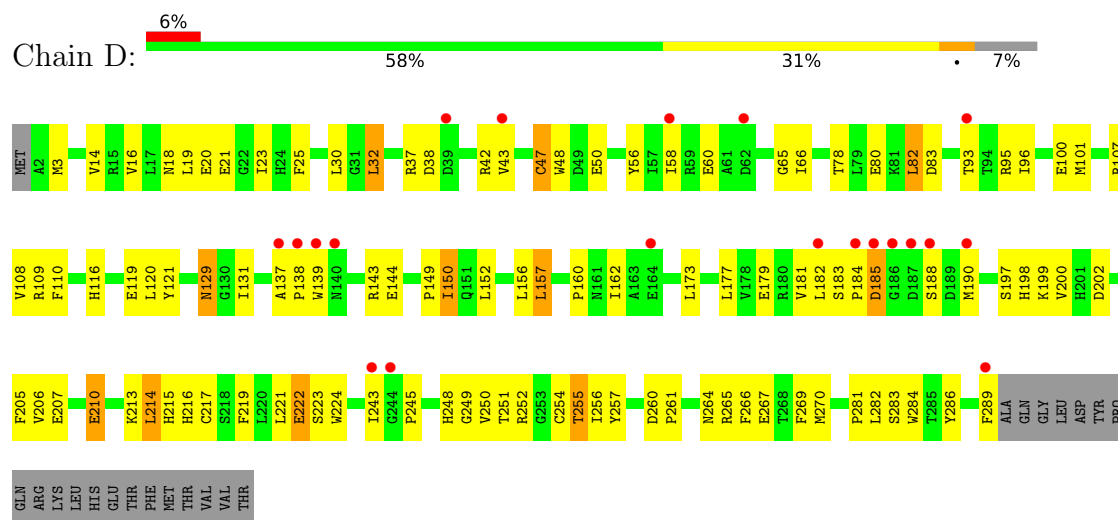
• Molecule 1: Catechol 2,3-dioxygenase



• Molecule 1: Catechol 2,3-dioxygenase



• 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	95.90Å 97.40Å 133.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.3 (50.00-2.00) 92.9 (50.00-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.269 0.239 , 0.283	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)	0.37 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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, 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	0.39	0/2438	0.98	10/3312 (0.3%)
1	B	0.39	0/2363	0.98	10/3210 (0.3%)
1	C	0.38	0/2427	0.95	6/3298 (0.2%)
1	D	0.38	0/2363	0.93	8/3210 (0.2%)
All	All	0.39	0/9591	0.96	34/13030 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASP	N-CA-C	8.07	121.33	110.35
1	D	152	LEU	N-CA-C	-7.99	97.85	109.59
1	B	255	THR	N-CA-C	7.33	119.59	109.18
1	B	152	LEU	N-CA-C	-7.32	98.60	109.15
1	D	255	THR	N-CA-C	7.05	118.80	108.86
1	D	100	GLU	N-CA-C	-7.01	103.65	111.71
1	C	152	LEU	N-CA-C	-6.83	98.08	108.67
1	A	53	HIS	N-CA-C	6.79	119.54	111.33
1	B	160	PRO	N-CA-C	6.71	122.39	113.40
1	B	8	ARG	N-CA-C	6.61	114.08	108.13
1	A	297	GLN	N-CA-C	-6.53	99.94	110.32
1	C	255	THR	N-CA-C	6.50	117.72	108.74
1	A	222	GLU	N-CA-C	6.41	118.35	111.36
1	B	222	GLU	N-CA-C	6.39	118.32	111.36
1	C	188	SER	N-CA-C	-6.16	98.78	108.14
1	A	188	SER	N-CA-C	-6.15	97.71	110.80
1	A	152	LEU	N-CA-C	-6.13	99.17	108.67
1	C	217	CYS	N-CA-C	-6.00	100.40	109.95
1	B	53	HIS	N-CA-C	5.84	119.22	111.75
1	A	255	THR	N-CA-C	5.81	117.79	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	LEU	N-CA-C	5.80	118.08	111.11
1	D	217	CYS	N-CA-C	-5.78	100.28	109.59
1	D	173	LEU	N-CA-C	5.71	120.25	113.28
1	D	249	GLY	N-CA-C	-5.69	105.90	112.50
1	B	48	TRP	N-CA-C	5.66	117.90	111.11
1	A	55	CYS	N-CA-C	-5.58	107.72	114.75
1	B	159	GLY	CA-C-N	5.56	124.91	118.85
1	B	159	GLY	C-N-CA	5.56	124.91	118.85
1	C	53	HIS	N-CA-C	5.40	117.86	111.33
1	A	217	CYS	N-CA-C	-5.38	101.40	109.95
1	A	100	GLU	N-CA-C	-5.19	105.74	111.71
1	D	47	CYS	N-CA-C	-5.11	102.92	110.48
1	B	123	GLU	N-CA-C	5.11	117.77	109.24
1	D	150	ILE	N-CA-C	5.11	116.57	111.00

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	118	0
1	B	2300	0	2193	103	0
1	C	2362	0	2247	142	0
1	D	2300	0	2193	92	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9781	0	8916	433	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 24.

All (433) 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:C:164:GLU:HA	1:C:167:LYS:HZ3	1.42	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:161:ASN:HB3	1:B:164:GLU:CD	2.02	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: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
1:A:185:ASP:C	1:A:187:ASP:H	1.91	0.78
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:B:18:ASN:C	1:B:18:ASN:HD22	1.93	0.77
1:C:215:HIS:CD2	1:C:216:HIS:HD1	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:O	1:A:23:ILE:HG13	1.87	0.74
1:C:164:GLU:HA	1:C:167:LYS:NZ	2.02	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:B:185:ASP:C	1:B:187:ASP:H	1.98	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: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:223:SER:HA	1:A:270:MET:HE3	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: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:B:190:MET:HE2	1:B:286:TYR:HE1	1.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:80:GLU:CD	1:C:95:ARG:HH22	2.08	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:A:36:GLY:C	1:A:37:ARG:HG3	2.27	0.60
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:B:150:ILE:HD11	1:B:222:GLU:CD	2.26	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:C:18:ASN:HD22	1:C:18:ASN:C	2.10	0.59
1:A:242:ASP:CG	1:A:298:ARG:HH22	2.11	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: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:B:190:MET:HE2	1:B:286:TYR:CE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HD12	1:C:96:ILE:N	2.18	0.57
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:156:LEU:C	1:C:156:LEU:HD23	2.29	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: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: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:184:PRO:C	1:B:186:GLY:H	2.14	0.55
1:D:150:ILE:N	1:D:150:ILE:HD12	2.22	0.55
1:A:185:ASP:C	1:A:187:ASP:N	2.56	0.55
1:B:255:THR:OG1	1:B:256:ILE:N	2.39	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: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
1:C:255:THR:OG1	1:C:267:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:185:ASP:C	1:B:187:ASP:N	2.64	0.53
1:D:20:GLU:CD	1:D:20:GLU:H	2.15	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:D:184:PRO:O	1:D:185:ASP:C	2.53	0.50
1:D:14:VAL:HG13	1:D:65:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:18:ASN:C	1:B:18:ASN:ND2	2.63	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:C:18:ASN:C	1:C:18:ASN:ND2	2.68	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: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:C:177:LEU:HD23	1:C:177:LEU:C	2.37	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:A:156:LEU:C	1:A:156:LEU:HD23	2.38	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:C:11:HIS:ND1	1:C:101:MET:HE1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:HG3	1:C:45:PHE:HE2	1.78	0.48
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:223:SER:HA	1:D:270:MET:HE3	1.96	0.47
1:B:36:GLY:C	1:B:37:ARG:HG3	2.38	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:B:132:SER:O	1:B:136:PRO:HB3	2.15	0.47
1:A:223:SER:C	1:A:270:MET:HG2	2.39	0.47
1:B:57:ILE:HD11	1:B:101:MET:HE3	1.97	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: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:210:GLU:CD	1:A:213:LYS:HD2	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:167:LYS:NZ	1:A:167:LYS:HB3	2.30	0.46
1:D:214:LEU:HD13	1:D:214:LEU:C	2.40	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: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:B:93:THR:HG22	1:B:94:THR:N	2.30	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:A:80:GLU:CD	1:A:95:ARG:HH22	2.24	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:255:THR:OG1	1:C:256:ILE:N	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ILE:CD1	1:B:101:MET:HE3	2.48	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
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:D:260:ASP:OD1	1:D:260:ASP:C	2.60	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:C:260:ASP:OD1	1:C:260:ASP:C	2.61	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:18:ASN:HB3	1:C:21:GLU:CD	2.44	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:249:GLY:C	1:A:251:THR:H	2.26	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: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:C:177:LEU:HD21	1:C:179:GLU:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:236:MET:HE2	1:D:139:TRP:O	2.20	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:D:137:ALA:O	1:D:138:PRO:C	2.62	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:D:129:ASN:C	1:D:129:ASN:HD22	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:GLY:C	1:C:37:ARG:HG3	2.44	0.41
1:C:157:LEU:N	1:C:157:LEU:HD22	2.34	0.41
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:95:ARG:HE	1:B:106:GLU:CD	2.29	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: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: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:100:GLU:C	1:B:100:GLU:OE2	2.64	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: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%)	6	2
1	B	286/309 (93%)	267 (93%)	12 (4%)	7 (2%)	4	2
1	C	294/309 (95%)	278 (95%)	13 (4%)	3 (1%)	12	8
1	D	286/309 (93%)	269 (94%)	16 (6%)	1 (0%)	36	35
All	All	1161/1236 (94%)	1091 (94%)	53 (5%)	17 (2%)	8	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%)	237 (94%)	15 (6%)	17	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	245/264 (93%)	232 (95%)	13 (5%)	20	18
1	C	251/264 (95%)	240 (96%)	11 (4%)	25	24
1	D	245/264 (93%)	236 (96%)	9 (4%)	30	30
All	All	993/1056 (94%)	945 (95%)	48 (5%)	23	21

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	42	ARG
1	A	82	LEU
1	A	95	ARG
1	A	120	LEU
1	A	129	ASN
1	A	157	LEU
1	A	167	LYS
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	B	18	ASN
1	B	19	LEU
1	B	32	LEU
1	B	42	ARG
1	B	82	LEU
1	B	95	ARG
1	B	120	LEU
1	B	129	ASN
1	B	157	LEU
1	B	164	GLU
1	B	173	LEU
1	B	187	ASP
1	B	214	LEU
1	C	17	LEU
1	C	19	LEU
1	C	96	ILE
1	C	102	LEU
1	C	107	ARG

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Mol	Chain	Res	Type
1	C	120	LEU
1	C	129	ASN
1	C	210	GLU
1	C	214	LEU
1	C	251	THR
1	C	293	LEU
1	D	32	LEU
1	D	82	LEU
1	D	120	LEU
1	D	129	ASN
1	D	157	LEU
1	D	210	GLU
1	D	214	LEU
1	D	221	LEU
1	D	222	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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	264	ASN
1	A	288	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	240	ASN
1	B	248	HIS
1	B	264	ASN
1	C	18	ASN
1	C	87	GLN
1	C	129	ASN
1	C	145	HIS
1	C	198	HIS
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	240	ASN
1	C	248	HIS
1	C	264	ASN
1	C	291	GLN
1	C	297	GLN
1	D	18	ASN
1	D	28	ASN
1	D	129	ASN
1	D	198	HIS
1	D	215	HIS
1	D	226	GLN
1	D	240	ASN
1	D	248	HIS
1	D	264	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	B	311	2	10,10,10	7.02	7 (70%)	11,12,12	1.35	2 (18%)
3	M3P	C	311	2	10,10,10	6.97	8 (80%)	11,12,12	2.62	5 (45%)
3	M3P	D	311	2	10,10,10	7.17	7 (70%)	11,12,12	1.40	3 (27%)

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	B	311	2	-	3/10/10/10	-
3	M3P	C	311	2	-	4/10/10/10	-
3	M3P	D	311	2	-	3/10/10/10	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	311	M3P	C1-C2	15.20	1.70	1.48
3	C	311	M3P	C1-C2	15.03	1.70	1.48
3	D	311	M3P	C1-C2	14.66	1.69	1.48
3	D	311	M3P	C4-C3	12.32	1.75	1.47
3	B	311	M3P	C4-C3	11.15	1.73	1.47
3	C	311	M3P	C4-C3	10.62	1.72	1.47
3	D	311	M3P	C5-C6	10.17	1.74	1.43
3	B	311	M3P	C5-C6	9.49	1.72	1.43
3	C	311	M3P	C5-C6	9.39	1.72	1.43
3	B	311	M3P	O2-C2	4.73	1.43	1.30
3	D	311	M3P	O2-C2	4.60	1.43	1.30
3	C	311	M3P	O2-C2	4.34	1.42	1.30
3	C	311	M3P	C6-C1	-4.17	1.30	1.39
3	D	311	M3P	O1-C1	3.30	1.42	1.33
3	B	311	M3P	C-C3	2.84	1.55	1.50
3	B	311	M3P	C6-C1	-2.78	1.33	1.39
3	C	311	M3P	O1-C1	2.72	1.40	1.33
3	B	311	M3P	O1-C1	2.68	1.40	1.33
3	C	311	M3P	C-C3	2.68	1.54	1.50
3	C	311	M3P	C5-C4	-2.38	1.28	1.34
3	D	311	M3P	C-C3	2.36	1.54	1.50
3	D	311	M3P	C6-C1	-2.21	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	M3P	C6-C1-C2	6.03	131.31	122.51
3	C	311	M3P	O1-C1-C2	-3.63	110.72	114.17
3	C	311	M3P	C6-C5-C4	-2.94	114.68	123.20
3	D	311	M3P	O3-C2-C1	2.66	123.17	120.12
3	C	311	M3P	O1-C1-C6	-2.51	117.96	122.72
3	B	311	M3P	C6-C1-C2	2.51	126.17	122.51
3	D	311	M3P	C6-C1-C2	2.50	126.16	122.51
3	B	311	M3P	O3-C2-C1	2.33	122.80	120.12
3	C	311	M3P	O3-C2-C1	2.12	122.56	120.12
3	D	311	M3P	O1-C1-C2	-2.10	112.17	114.17

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	C4-C5-C6-C1
3	D	311	M3P	O1-C1-C6-C5
3	B	311	M3P	C-C3-C4-C5
3	B	311	M3P	O4-C3-C4-C5
3	C	311	M3P	C-C3-C4-C5
3	C	311	M3P	O4-C3-C4-C5
3	D	311	M3P	O4-C3-C4-C5
3	D	311	M3P	C-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 18 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.52	29 (9%) 13 12	11, 22, 40, 61	0
1	B	288/309 (93%)	0.67	29 (10%) 12 11	12, 23, 41, 58	0
1	C	296/309 (95%)	0.85	34 (11%) 9 8	14, 26, 42, 59	0
1	D	288/309 (93%)	0.54	20 (6%) 23 21	12, 22, 38, 55	0
All	All	1169/1236 (94%)	0.65	112 (9%) 13 12	11, 23, 41, 61	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	TRP	9.0
1	C	139	TRP	7.4
1	A	224	TRP	6.9
1	C	244	GLY	6.6
1	A	250	VAL	6.4
1	D	244	GLY	6.3
1	D	187	ASP	6.0
1	D	185	ASP	5.6
1	D	138	PRO	5.6
1	B	244	GLY	5.4
1	A	244	GLY	5.4
1	B	186	GLY	5.3
1	C	138	PRO	5.3
1	C	185	ASP	5.2
1	C	137	ALA	4.9
1	B	248	HIS	4.8
1	B	188	SER	4.4
1	A	251	THR	4.3
1	B	250	VAL	4.1
1	B	289	PHE	4.0
1	C	243	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	289	PHE	4.0
1	C	186	GLY	3.8
1	D	289	PHE	3.8
1	C	293	LEU	3.8
1	B	187	ASP	3.7
1	A	185	ASP	3.6
1	C	184	PRO	3.6
1	A	249	GLY	3.6
1	A	254	CYS	3.6
1	D	186	GLY	3.6
1	D	188	SER	3.6
1	A	297	GLN	3.5
1	A	248	HIS	3.5
1	A	186	GLY	3.2
1	A	243	ILE	3.2
1	C	39	ASP	3.2
1	B	185	ASP	3.2
1	C	187	ASP	3.2
1	C	249	GLY	3.2
1	C	192	ILE	3.1
1	D	243	ILE	3.1
1	B	20	GLU	3.0
1	A	17	LEU	3.0
1	A	293	LEU	3.0
1	C	27	ARG	3.0
1	D	184	PRO	3.0
1	B	19	LEU	2.9
1	B	243	ILE	2.9
1	C	297	GLN	2.9
1	B	4	THR	2.9
1	B	190	MET	2.9
1	C	92	THR	2.9
1	C	94	THR	2.9
1	A	252	ARG	2.8
1	C	251	THR	2.8
1	B	61	ALA	2.7
1	A	247	ARG	2.7
1	C	190	MET	2.7
1	B	161	ASN	2.7
1	D	190	MET	2.6
1	D	43	VAL	2.6
1	B	251	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	19	LEU	2.5
1	B	182	LEU	2.5
1	D	93	THR	2.5
1	B	184	PRO	2.5
1	A	187	ASP	2.4
1	A	287	ASP	2.4
1	D	182	LEU	2.4
1	B	134	VAL	2.4
1	D	58	ILE	2.4
1	B	286	TYR	2.4
1	C	19	LEU	2.4
1	B	246	THR	2.4
1	A	240	ASN	2.4
1	C	140	ASN	2.4
1	D	39	ASP	2.3
1	D	140	ASN	2.3
1	A	253	GLY	2.3
1	C	108	VAL	2.3
1	A	28	ASN	2.3
1	A	260	ASP	2.3
1	C	17	LEU	2.3
1	C	162	ILE	2.3
1	C	161	ASN	2.3
1	D	62	ASP	2.3
1	C	248	HIS	2.2
1	C	250	VAL	2.2
1	C	61	ALA	2.2
1	A	295	TYR	2.2
1	B	287	ASP	2.2
1	D	164	GLU	2.2
1	C	286	TYR	2.2
1	B	93	THR	2.2
1	B	236	MET	2.1
1	A	62	ASP	2.1
1	A	63	THR	2.1
1	B	249	GLY	2.1
1	B	189	ASP	2.1
1	A	4	THR	2.1
1	D	137	ALA	2.1
1	C	102	LEU	2.1
1	C	62	ASP	2.1
1	A	184	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	THR	2.0
1	A	292	GLY	2.0
1	A	289	PHE	2.0
1	C	43	VAL	2.0
1	B	240	ASN	2.0
1	C	287	ASP	2.0
1	B	41	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M3P	C	311	11/11	0.67	0.23	46,47,49,49	0
3	M3P	D	311	11/11	0.70	0.26	45,46,48,49	0
3	M3P	B	311	11/11	0.74	0.20	40,44,47,47	0
2	FE	A	310	1/1	0.99	0.02	23,23,23,23	0
2	FE	B	310	1/1	0.99	0.02	23,23,23,23	0
2	FE	D	310	1/1	0.99	0.02	21,21,21,21	0
2	FE	C	310	1/1	1.00	0.02	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.