



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:40 PM UTC

PDB ID : 2G5F / pdb_00002g5f
Title : The structure of MbtI from Mycobacterium Tuberculosis, the first enzyme in the synthesis of Mycobactin, reveals it to be a salicylate synthase
Authors : Harrison, A.J.; Lott, J.S.; Yu, M.; Ramsay, R.; Baker, E.N.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2006-02-22
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

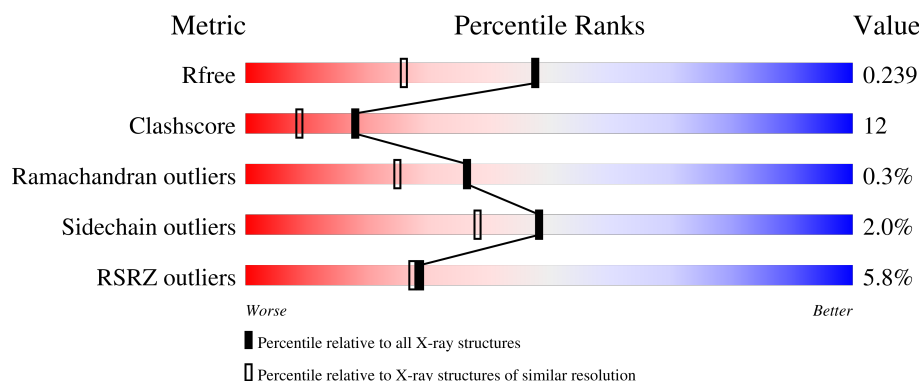
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	450	7% 73% 21% ..
1	B	450	5% 72% 22% ..
1	C	450	6% 73% 23% ..
1	D	450	4% 75% 21% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PYR	A	2001	-	X	-	-
2	PYR	B	2002	-	X	-	-
4	GOL	A	4003	-	X	-	-
4	GOL	B	4004	-	X	-	-
4	GOL	C	4001	-	X	-	-
4	GOL	C	4005	-	X	-	-
4	GOL	D	4002	-	X	-	-
4	GOL	D	4006	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14171 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.

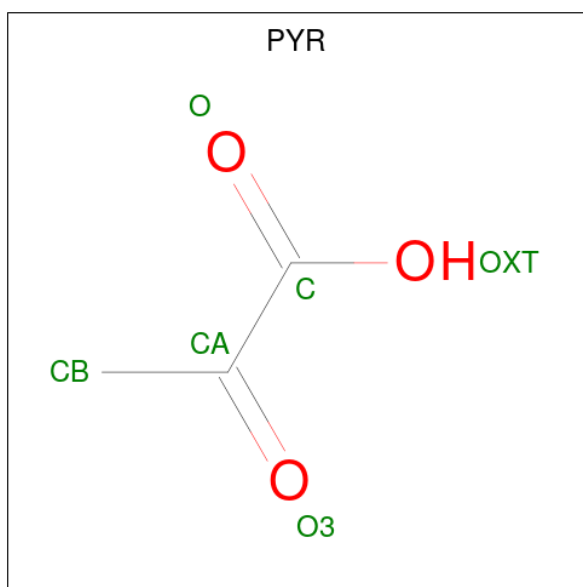
- Molecule 1 is a protein called COG0147: Anthranilate/para-aminobenzoate synthases component I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3275	2053	599	613	10			
1	B	430	Total	C	N	O	S	0	0	0
			3252	2040	591	611	10			
1	C	435	Total	C	N	O	S	0	0	0
			3285	2057	600	618	10			
1	D	435	Total	C	N	O	S	0	0	0
			3298	2063	601	624	10			

There are 4 discrepancies between the modelled and reference sequences:

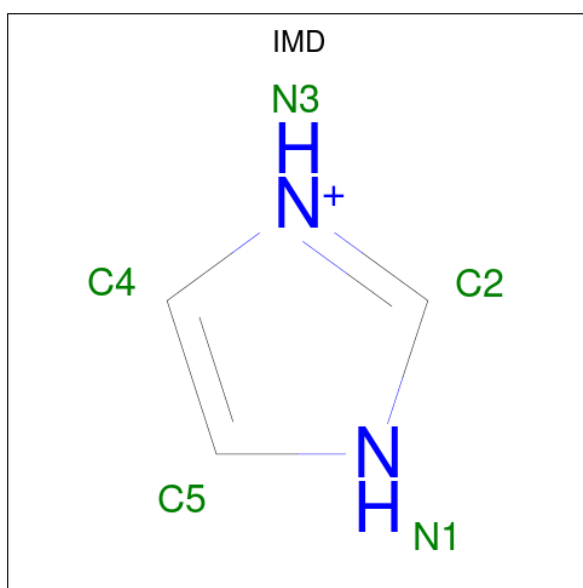
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	cloning artifact	UNP Q7D785
B	1	VAL	-	cloning artifact	UNP Q7D785
C	1	VAL	-	cloning artifact	UNP Q7D785
D	1	VAL	-	cloning artifact	UNP Q7D785

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



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

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



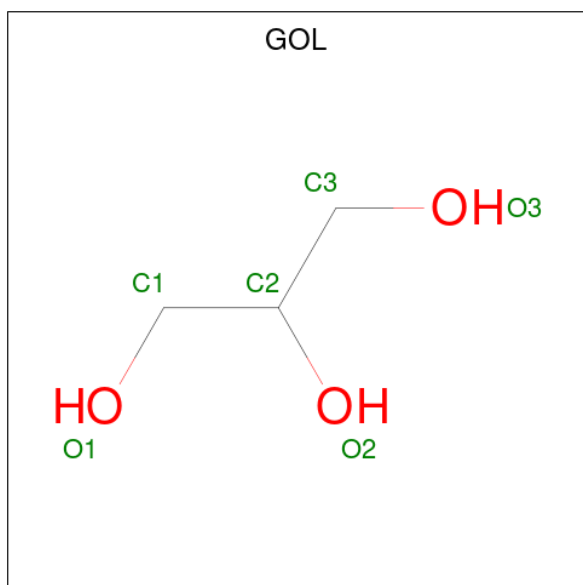
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	222	Total	O	0	0
			222	222		

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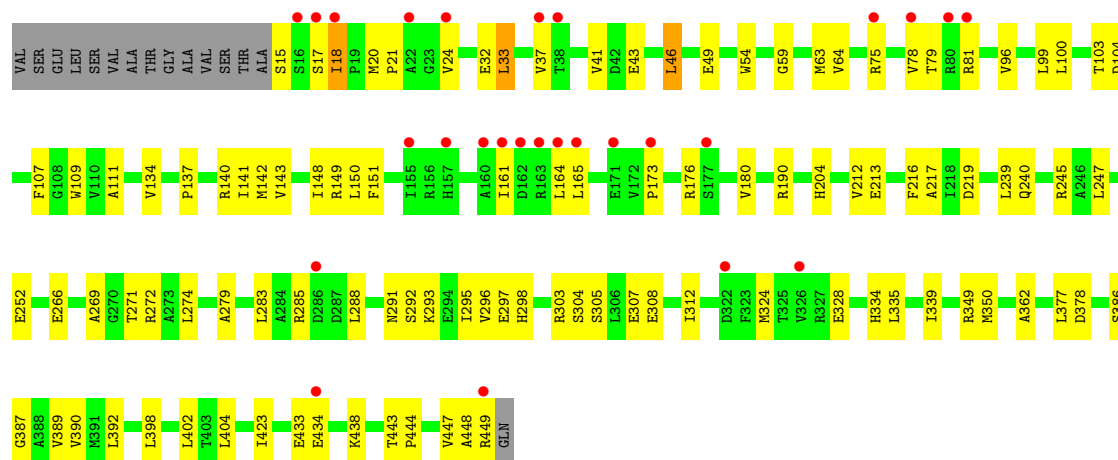
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	231	Total 231	O 231	0	0
5	C	273	Total 273	O 273	0	0
5	D	267	Total 267	O 267	0	0

- Molecule 1: COG0147: Anthranilate/para-aminobenzoate synthases component I

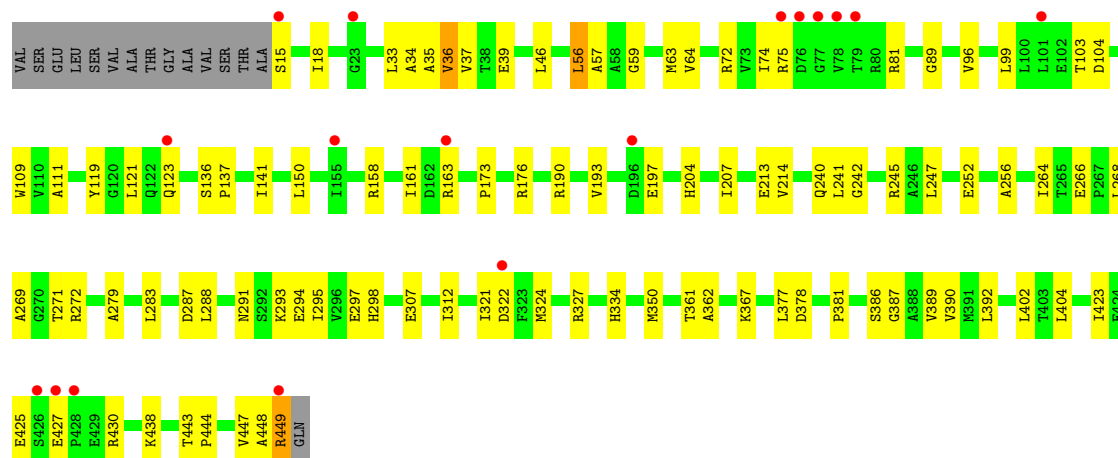


Chain C:  6% 73% 23% ..



• Molecule 1: COG0147: Anthranilate/para-aminobenzoate synthases component I

Chain D:  4% 75% 21% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.82Å 163.37Å 194.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-1.80) 99.4 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.240 0.205 , 0.239	Depositor DCC
R_{free} test set	15321 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14171	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PYR, IMD

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	0.35	0/3333	0.89	12/4531 (0.3%)
1	B	0.36	0/3308	0.87	8/4494 (0.2%)
1	C	0.37	0/3343	0.88	4/4544 (0.1%)
1	D	0.36	0/3356	0.89	7/4559 (0.2%)
All	All	0.36	0/13340	0.89	31/18128 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	ILE	N-CA-C	8.38	120.47	111.58
1	A	42	ASP	N-CA-C	-8.10	100.44	110.65
1	A	20	MET	CA-C-N	7.93	128.40	119.92
1	A	20	MET	C-N-CA	7.93	128.40	119.92
1	D	36	VAL	N-CA-C	6.61	117.36	110.62
1	B	387	GLY	N-CA-C	-6.60	103.16	112.60
1	B	136	SER	N-CA-C	-6.54	100.14	109.62
1	A	387	GLY	N-CA-C	-6.46	103.37	112.60
1	D	214	VAL	N-CA-C	-6.29	101.32	107.55
1	A	389	VAL	N-CA-C	-6.18	99.50	108.71
1	C	104	ASP	N-CA-C	6.08	119.89	112.23
1	A	136	SER	N-CA-C	-6.06	100.83	109.62
1	A	147	GLU	N-CA-C	5.92	117.14	108.14
1	D	136	SER	N-CA-C	-5.84	101.15	109.62
1	A	41	VAL	N-CA-C	5.79	121.39	109.34
1	A	101	LEU	N-CA-C	-5.64	105.89	112.89
1	C	387	GLY	N-CA-C	-5.64	104.57	112.13
1	B	147	GLU	N-CA-C	5.64	116.83	108.60
1	B	390	VAL	N-CA-C	5.63	118.03	108.86
1	D	390	VAL	N-CA-C	5.61	118.00	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	387	GLY	N-CA-C	-5.58	104.52	112.55
1	B	232	THR	CA-C-N	5.50	125.47	120.03
1	B	232	THR	C-N-CA	5.50	125.47	120.03
1	C	389	VAL	N-CA-C	-5.45	100.56	108.36
1	D	389	VAL	N-CA-C	-5.39	100.65	108.36
1	C	390	VAL	N-CA-C	5.37	117.61	108.86
1	B	389	VAL	N-CA-C	-5.36	100.70	108.36
1	A	448	ALA	N-CA-C	5.32	117.55	110.53
1	A	390	VAL	N-CA-C	5.11	117.38	108.95
1	A	172	VAL	N-CA-C	5.05	112.55	107.55
1	B	415	TRP	N-CA-C	5.04	115.96	108.60

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	3275	0	3258	91	0
1	B	3252	0	3236	82	0
1	C	3285	0	3268	76	0
1	D	3298	0	3282	72	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
3	A	5	0	5	0	0
3	C	10	0	10	0	0
3	D	5	0	5	1	0
4	A	6	0	4	0	0
4	B	6	0	4	1	0
4	C	12	0	8	0	0
4	D	12	0	8	1	0
5	A	222	0	0	4	0
5	B	231	0	0	4	0
5	C	273	0	0	1	0
5	D	267	0	0	7	0
All	All	14171	0	13088	320	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 12.

All (320) 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:A:268:LEU:HD11	1:A:334:HIS:HB3	1.39	1.01
1:D:121:LEU:HA	1:D:123:GLN:HE22	1.30	0.97
1:A:163:ARG:HH11	1:A:163:ARG:HB2	1.34	0.91
1:A:41:VAL:HG12	1:A:42:ASP:H	1.34	0.89
1:B:120:GLY:HA2	1:B:122:GLN:HE22	1.40	0.85
1:B:120:GLY:CA	1:B:122:GLN:HE22	1.91	0.84
1:C:292:SER:O	1:C:296:VAL:HG23	1.84	0.78
1:A:20:MET:HE1	1:A:29:LEU:HD23	1.67	0.77
1:B:268:LEU:HD11	1:B:334:HIS:HB3	1.68	0.76
1:C:293:LYS:HE3	1:C:423:ILE:HD11	1.68	0.76
1:C:18:ILE:HG23	1:C:148:ILE:HB	1.68	0.75
1:C:448:ALA:O	1:C:449:ARG:HG2	1.86	0.75
1:C:362:ALA:HB1	1:C:386:SER:HB2	1.69	0.74
1:C:33:LEU:HD13	1:C:164:LEU:HD23	1.69	0.74
1:A:94:GLU:HG3	1:A:98:ARG:NH1	2.04	0.73
1:D:121:LEU:HA	1:D:123:GLN:NE2	2.04	0.73
1:A:303:ARG:O	1:A:307:GLU:HG3	1.89	0.73
1:B:117:HIS:HA	1:B:122:GLN:HE21	1.54	0.73
1:A:323:PHE:CE2	1:A:324:MET:HE2	2.24	0.72
1:A:305:SER:HB2	1:A:339:ILE:HD12	1.72	0.72
1:A:140:ARG:HD3	5:A:4078:HOH:O	1.90	0.71
1:D:448:ALA:O	1:D:449:ARG:HB2	1.91	0.71
1:A:96:VAL:HG11	1:A:392:LEU:HD22	1.71	0.71
1:C:20:MET:HE1	1:C:143:VAL:HG13	1.74	0.70
1:D:96:VAL:HG11	1:D:392:LEU:HD22	1.73	0.69
1:D:362:ALA:HB1	1:D:386:SER:HB2	1.75	0.67
1:D:150:LEU:HD11	1:D:161:ILE:HD11	1.77	0.67
1:A:92:LEU:HD23	1:A:350:MET:HE1	1.77	0.67
1:C:303:ARG:O	1:C:307:GLU:HG3	1.97	0.65
1:B:303:ARG:O	1:B:307:GLU:HG3	1.96	0.65
1:D:213:GLU:HG2	5:D:4208:HOH:O	1.98	0.64
1:B:122:GLN:CD	1:B:122:GLN:H	2.05	0.64
1:D:293:LYS:HE3	1:D:423:ILE:HD11	1.80	0.64
1:C:176:ARG:HD2	1:C:216:PHE:CE2	2.31	0.64
1:D:72:ARG:HG2	1:D:81:ARG:HG2	1.79	0.63
1:A:25:ASN:HB3	1:A:28:ASP:OD2	1.99	0.63
1:A:38:THR:HG23	1:A:43:GLU:CB	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:CG2	1:B:402:LEU:HB2	2.28	0.63
1:D:438:LYS:HB3	4:D:4002:GOL:H12	1.79	0.63
1:C:140:ARG:HB3	1:C:151:PHE:HB2	1.80	0.63
1:B:117:HIS:HA	1:B:122:GLN:NE2	2.14	0.63
1:B:258:ARG:HB2	1:B:262:VAL:HG12	1.80	0.63
1:C:449:ARG:HG3	1:C:449:ARG:O	1.98	0.63
1:A:100:LEU:HD12	1:A:349:ARG:HH22	1.63	0.62
1:B:63:MET:HE3	1:B:134:VAL:O	1.99	0.62
1:A:38:THR:HG23	1:A:43:GLU:HB3	1.80	0.62
1:C:252:GLU:HG3	1:C:266:GLU:O	2.00	0.62
1:D:123:GLN:CD	1:D:123:GLN:H	2.06	0.62
1:D:35:ALA:O	1:D:39:GLU:HG3	1.98	0.62
1:C:32:GLU:HG2	1:C:164:LEU:HD11	1.82	0.62
1:A:41:VAL:CG1	1:A:42:ASP:H	1.99	0.62
1:B:398:LEU:HD23	1:B:399:ASP:N	2.15	0.61
1:A:305:SER:HB2	1:A:339:ILE:CD1	2.30	0.61
1:D:241:LEU:HD22	5:D:4023:HOH:O	2.00	0.61
1:D:361:THR:HG23	5:D:4038:HOH:O	1.99	0.61
1:A:163:ARG:HB2	1:A:163:ARG:NH1	2.12	0.61
1:A:25:ASN:ND2	1:A:27:ALA:HB3	2.15	0.61
1:A:263:VAL:C	1:A:264:ILE:HD12	2.26	0.61
1:D:427:GLU:HG3	1:D:430:ARG:HB3	1.83	0.61
1:C:150:LEU:HD21	1:C:161:ILE:CD1	2.30	0.61
1:A:269:ALA:HB2	1:A:298:HIS:CG	2.36	0.60
1:A:298:HIS:HE1	1:A:337:SER:OG	1.83	0.60
1:D:448:ALA:O	1:D:449:ARG:CB	2.48	0.60
1:D:74:ILE:HD12	1:D:74:ILE:N	2.16	0.60
1:B:94:GLU:HG2	1:B:98:ARG:HH12	1.65	0.60
1:A:262:VAL:HG12	1:A:264:ILE:HD11	1.82	0.60
1:B:244:ILE:HG22	1:B:410:VAL:HG22	1.84	0.60
1:D:293:LYS:HE3	1:D:423:ILE:CD1	2.32	0.60
1:D:150:LEU:HD11	1:D:161:ILE:CD1	2.32	0.59
1:B:269:ALA:HB2	1:B:298:HIS:CG	2.37	0.59
1:D:272:ARG:HG2	1:D:288:LEU:HD13	1.83	0.59
1:C:279:ALA:O	1:C:283:LEU:HD13	2.00	0.59
1:C:204:HIS:HE1	1:C:297:GLU:OE2	1.86	0.59
1:D:63:MET:HE1	1:D:241:LEU:HD21	1.84	0.59
1:A:305:SER:CB	1:A:339:ILE:HD12	2.33	0.59
1:B:122:GLN:H	1:B:122:GLN:NE2	2.01	0.59
1:D:279:ALA:O	1:D:283:LEU:HD13	2.02	0.59
1:B:271:THR:OG1	1:B:334:HIS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ILE:HD11	1:D:158:ARG:NH1	2.18	0.58
1:A:72:ARG:HG2	1:A:81:ARG:HG2	1.86	0.58
1:C:173:PRO:HG2	1:C:447:VAL:HG13	1.86	0.58
1:A:99:LEU:O	1:A:102:GLU:HG2	2.04	0.58
1:C:75:ARG:O	1:C:78:VAL:HG12	2.03	0.58
1:C:269:ALA:HB2	1:C:298:HIS:CG	2.38	0.58
1:D:269:ALA:HB2	1:D:298:HIS:CG	2.39	0.58
1:B:398:LEU:HD23	1:B:398:LEU:C	2.28	0.57
1:C:20:MET:HE1	1:C:143:VAL:CG1	2.33	0.57
1:A:41:VAL:HG12	1:A:42:ASP:N	2.13	0.57
1:C:271:THR:OG1	1:C:334:HIS:HD2	1.87	0.57
1:B:312:ILE:C	1:B:312:ILE:HD12	2.30	0.57
1:A:94:GLU:HG3	1:A:98:ARG:HH12	1.69	0.57
1:A:29:LEU:HD21	1:A:148:ILE:HD11	1.86	0.56
1:C:109:TRP:HZ3	1:C:111:ALA:HB2	1.70	0.56
1:A:92:LEU:HD23	1:A:350:MET:CE	2.34	0.56
1:A:100:LEU:CD1	1:A:349:ARG:HH22	2.19	0.55
1:B:342:ARG:HG2	1:B:342:ARG:HH11	1.71	0.55
1:A:392:LEU:HG	1:A:398:LEU:HD23	1.88	0.55
1:A:312:ILE:C	1:A:312:ILE:HD12	2.32	0.54
1:A:18:ILE:HD11	1:A:158:ARG:HD2	1.88	0.54
1:A:239:LEU:C	1:A:239:LEU:HD12	2.32	0.54
1:C:142:MET:HE3	1:C:151:PHE:CE2	2.42	0.54
1:A:262:VAL:HG12	1:A:264:ILE:CD1	2.38	0.54
1:C:350:MET:HE3	1:C:392:LEU:HD21	1.89	0.53
1:B:241:LEU:O	1:B:244:ILE:HG12	2.08	0.53
1:A:268:LEU:CD1	1:A:334:HIS:HB3	2.27	0.53
1:D:33:LEU:O	1:D:37:VAL:HG22	2.09	0.53
1:B:260:ASP:OD1	1:B:262:VAL:HG12	2.08	0.53
1:C:272:ARG:NH1	1:C:288:LEU:HD13	2.23	0.53
1:A:269:ALA:HB2	1:A:298:HIS:CD2	2.43	0.53
1:C:161:ILE:O	1:C:165:LEU:HD13	2.08	0.53
1:A:25:ASN:HD21	1:A:27:ALA:HB3	1.72	0.52
1:A:29:LEU:HD21	1:A:148:ILE:CD1	2.40	0.52
1:A:53:GLN:OE1	1:A:144:SER:HB3	2.09	0.52
1:D:64:VAL:HG23	1:D:99:LEU:HD11	1.91	0.52
1:D:449:ARG:HB3	5:D:4064:HOH:O	2.08	0.52
1:D:109:TRP:HZ3	1:D:111:ALA:HB2	1.74	0.52
1:C:41:VAL:HG12	1:C:43:GLU:HG3	1.91	0.52
1:A:260:ASP:OD1	1:A:262:VAL:HG23	2.10	0.52
1:C:63:MET:HE3	1:C:134:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HD12	1:A:335:LEU:O	2.10	0.52
1:B:197:GLU:HG2	1:B:202:ARG:HD3	1.92	0.52
1:D:173:PRO:HG2	1:D:447:VAL:HG13	1.92	0.51
1:D:271:THR:OG1	1:D:334:HIS:HD2	1.92	0.51
1:A:220:PHE:HE1	1:A:409:GLN:HE21	1.58	0.51
1:D:63:MET:CE	1:D:241:LEU:HD21	2.40	0.51
1:D:252:GLU:HG3	1:D:266:GLU:O	2.11	0.51
1:D:150:LEU:N	1:D:150:LEU:HD22	2.26	0.51
1:A:245:ARG:HB2	1:A:409:GLN:HB3	1.92	0.51
1:A:40:SER:C	1:A:41:VAL:HG23	2.36	0.51
1:A:100:LEU:HD12	1:A:349:ARG:NH2	2.26	0.51
1:B:448:ALA:O	1:B:449:ARG:HB2	2.10	0.51
1:D:241:LEU:HD23	1:D:242:GLY:N	2.26	0.51
1:A:92:LEU:HB3	1:A:350:MET:HE2	1.91	0.50
1:C:41:VAL:HG12	1:C:41:VAL:O	2.11	0.50
1:C:434:GLU:OE1	1:C:438:LYS:HE3	2.11	0.50
1:B:254:VAL:HG22	1:B:402:LEU:HB2	1.93	0.50
1:A:18:ILE:HD11	1:A:158:ARG:CD	2.42	0.50
1:A:23:GLY:O	1:A:24:VAL:C	2.53	0.50
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.77	0.50
1:B:434:GLU:OE1	1:B:438:LYS:HE3	2.12	0.50
1:C:269:ALA:HB2	1:C:298:HIS:ND1	2.27	0.50
1:D:427:GLU:HG3	1:D:430:ARG:CB	2.40	0.50
1:C:63:MET:HE1	1:C:134:VAL:N	2.26	0.50
1:B:334:HIS:HE1	5:B:4059:HOH:O	1.95	0.50
1:D:268:LEU:HD11	1:D:334:HIS:CD2	2.46	0.50
1:A:38:THR:O	1:A:38:THR:HG22	2.11	0.49
1:B:26:PRO:HB2	1:B:54:TRP:CZ3	2.47	0.49
1:C:20:MET:CE	1:C:143:VAL:HG13	2.42	0.49
1:C:291:ASN:O	1:C:295:ILE:HG13	2.12	0.49
1:C:46:LEU:HG	1:C:107:PHE:HB3	1.95	0.49
1:D:119:TYR:OH	1:D:367:LYS:HD2	2.12	0.49
1:A:298:HIS:CE1	1:A:337:SER:OG	2.65	0.49
1:D:121:LEU:CA	1:D:123:GLN:HE22	2.15	0.49
1:B:448:ALA:O	1:B:449:ARG:CB	2.61	0.49
1:C:33:LEU:O	1:C:37:VAL:HG23	2.13	0.49
1:D:381:PRO:HG3	5:D:4178:HOH:O	2.13	0.49
1:A:150:LEU:HD21	1:A:161:ILE:CD1	2.42	0.49
1:A:392:LEU:N	1:A:392:LEU:HD12	2.27	0.49
1:B:433:GLU:O	1:B:437:GLU:HG3	2.13	0.49
1:A:29:LEU:HG	1:A:33:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLN:HE22	1:A:245:ARG:NH2	2.11	0.49
1:A:156:ARG:HD3	1:B:342:ARG:HH12	1.78	0.48
1:C:21:PRO:O	1:C:24:VAL:HG12	2.13	0.48
1:A:93:GLY:CA	1:A:350:MET:HG3	2.42	0.48
1:B:94:GLU:HG2	1:B:98:ARG:NH1	2.28	0.48
1:C:190:ARG:HD2	1:C:377:LEU:O	2.14	0.48
1:D:307:GLU:OE2	3:D:3004:IMD:H5	2.13	0.48
1:D:312:ILE:C	1:D:312:ILE:HD12	2.37	0.48
1:B:204:HIS:HE1	1:B:297:GLU:OE2	1.96	0.48
1:C:398:LEU:HD23	1:C:398:LEU:C	2.39	0.48
1:B:218:ILE:C	1:B:449:ARG:O	2.57	0.48
1:B:360:VAL:CG2	1:B:365:ILE:HD11	2.44	0.48
1:C:298:HIS:HD2	1:C:324:MET:HG2	1.79	0.48
1:B:33:LEU:O	1:B:37:VAL:HG22	2.14	0.48
1:C:304:SER:O	1:C:308:GLU:HG2	2.14	0.47
1:A:63:MET:HE1	1:A:241:LEU:HD11	1.97	0.47
1:A:398:LEU:HD22	1:A:399:ASP:N	2.29	0.47
1:B:150:LEU:N	1:B:150:LEU:HD12	2.29	0.47
1:B:256:ALA:HB3	1:B:264:ILE:CG1	2.44	0.47
1:B:256:ALA:HB3	1:B:264:ILE:HG12	1.97	0.47
1:D:15:SER:N	1:D:150:LEU:O	2.47	0.47
1:D:89:GLY:O	1:D:350:MET:HG2	2.13	0.47
1:A:247:LEU:HD12	1:A:247:LEU:C	2.39	0.47
1:C:443:THR:OG1	1:C:444:PRO:HD3	2.15	0.47
1:A:20:MET:HE3	1:A:26:PRO:HA	1.95	0.47
1:C:312:ILE:HD12	1:C:312:ILE:C	2.40	0.47
1:D:190:ARG:HD2	1:D:377:LEU:O	2.15	0.47
1:C:293:LYS:HE3	1:C:423:ILE:CD1	2.40	0.47
1:D:293:LYS:HD2	1:D:425:GLU:OE2	2.15	0.47
1:B:306:LEU:HD11	1:B:320:VAL:CG2	2.45	0.46
1:C:402:LEU:HG	1:C:404:LEU:HG	1.97	0.46
1:D:443:THR:N	1:D:444:PRO:CD	2.79	0.46
1:C:239:LEU:HD12	1:C:239:LEU:C	2.40	0.46
1:A:298:HIS:HD2	5:A:4014:HOH:O	1.97	0.46
1:A:398:LEU:C	1:A:398:LEU:HD13	2.41	0.46
1:C:32:GLU:HB3	1:C:164:LEU:HD21	1.96	0.46
1:C:285:ARG:HD2	5:C:4067:HOH:O	2.14	0.46
1:B:173:PRO:HG2	1:B:447:VAL:HG13	1.96	0.46
1:D:15:SER:N	5:D:4045:HOH:O	2.48	0.46
1:D:18:ILE:CG1	1:D:158:ARG:HH12	2.28	0.46
1:B:64:VAL:HG23	1:B:99:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:SER:HB2	1:C:150:LEU:O	2.14	0.46
1:D:204:HIS:HE1	1:D:297:GLU:OE2	1.98	0.46
1:B:353:LEU:O	1:B:357:PHE:HB2	2.15	0.46
1:B:57:ALA:HB1	1:B:137:PRO:HB3	1.98	0.46
1:B:247:LEU:C	1:B:247:LEU:HD12	2.41	0.46
1:B:118:ARG:HD2	5:B:4116:HOH:O	2.15	0.46
1:B:138:ARG:HD2	5:B:4234:HOH:O	2.15	0.46
1:B:439:LEU:O	1:B:443:THR:HG23	2.15	0.45
1:C:180:VAL:HG12	1:C:212:VAL:HG11	1.98	0.45
1:D:295:ILE:HG23	1:D:324:MET:HE1	1.97	0.45
1:A:38:THR:HG23	1:A:43:GLU:HB2	1.97	0.45
1:A:360:VAL:CG2	1:A:365:ILE:HD11	2.46	0.45
1:B:117:HIS:HA	1:B:122:GLN:HG3	1.99	0.45
1:B:321:ILE:HG13	1:B:338:THR:HB	1.98	0.45
1:B:292:SER:O	1:B:296:VAL:HG23	2.16	0.45
1:D:247:LEU:C	1:D:247:LEU:HD12	2.42	0.45
1:C:59:GLY:O	1:C:137:PRO:HA	2.16	0.45
1:B:405:ARG:HA	1:B:405:ARG:NE	2.31	0.45
1:C:247:LEU:HD12	1:C:247:LEU:C	2.42	0.45
1:A:29:LEU:CD2	1:A:148:ILE:HD11	2.47	0.45
1:A:425:GLU:CD	1:A:425:GLU:H	2.25	0.45
1:B:443:THR:N	1:B:444:PRO:CD	2.80	0.45
1:C:362:ALA:CB	1:C:386:SER:HB2	2.42	0.45
1:D:295:ILE:HG12	1:D:324:MET:HE1	1.98	0.45
1:B:443:THR:N	1:B:444:PRO:HD3	2.32	0.45
1:A:57:ALA:HB1	1:A:137:PRO:HB3	2.00	0.44
1:B:120:GLY:C	1:B:122:GLN:HE22	2.24	0.44
1:B:121:LEU:N	1:B:122:GLN:NE2	2.65	0.44
1:B:180:VAL:HG11	1:B:443:THR:HG21	1.99	0.44
1:D:46:LEU:HD23	1:D:46:LEU:C	2.43	0.44
1:A:193:VAL:O	1:A:197:GLU:HG3	2.18	0.44
1:C:217:ALA:O	1:C:449:ARG:N	2.40	0.44
1:A:304:SER:O	1:A:308:GLU:HG3	2.17	0.44
1:B:109:TRP:HZ3	1:B:111:ALA:HB2	1.82	0.44
1:B:244:ILE:CG2	1:B:410:VAL:HG22	2.47	0.44
1:D:241:LEU:HD23	1:D:241:LEU:C	2.42	0.44
1:C:99:LEU:O	1:C:103:THR:HG22	2.18	0.44
1:D:57:ALA:HB1	1:D:137:PRO:HB3	2.00	0.44
1:C:305:SER:CB	1:C:339:ILE:HD12	2.48	0.44
1:D:327:ARG:NH1	5:D:4129:HOH:O	2.51	0.44
1:B:149:ARG:NH1	1:B:150:LEU:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ILE:N	1:B:207:ILE:HD12	2.33	0.44
1:D:256:ALA:HB3	1:D:264:ILE:HG12	1.99	0.44
1:D:240:GLN:HE22	1:D:245:ARG:NH2	2.15	0.43
1:C:33:LEU:HD13	1:C:164:LEU:CD2	2.43	0.43
1:A:292:SER:O	1:A:296:VAL:HG23	2.18	0.43
1:B:32:GLU:O	1:B:36:VAL:HG23	2.18	0.43
1:B:71:LEU:C	1:B:71:LEU:HD23	2.43	0.43
1:A:160:ALA:HA	1:A:163:ARG:NH1	2.33	0.43
1:A:287:ASP:O	1:A:291:ASN:HB2	2.19	0.43
1:B:425:GLU:HG3	5:B:4093:HOH:O	2.18	0.43
1:C:350:MET:HE2	1:C:398:LEU:HD12	1.99	0.43
1:D:141:ILE:HG12	1:D:150:LEU:CD1	2.49	0.43
1:A:424:GLU:HB3	1:A:425:GLU:OE2	2.17	0.43
1:B:360:VAL:HB	1:B:367:LYS:HE3	2.00	0.43
1:A:171:GLU:HG2	5:A:4009:HOH:O	2.19	0.43
1:B:63:MET:HE2	1:B:64:VAL:O	2.19	0.43
1:C:149:ARG:HG2	1:C:149:ARG:HH11	1.84	0.43
1:C:305:SER:HB2	1:C:339:ILE:HD12	2.01	0.43
1:A:448:ALA:C	1:A:449:ARG:HG3	2.44	0.42
1:B:154:GLY:O	1:B:158:ARG:HG2	2.19	0.42
1:A:307:GLU:HB2	5:A:4134:HOH:O	2.18	0.42
1:C:49:GLU:HG3	1:C:54:TRP:CE2	2.54	0.42
1:D:33:LEU:HA	1:D:36:VAL:HG22	2.00	0.42
1:B:154:GLY:H	1:B:157:HIS:HD2	1.65	0.42
1:D:163:ARG:HG2	1:D:163:ARG:HH11	1.84	0.42
1:A:444:PRO:HG2	1:A:445:TYR:CE2	2.54	0.42
1:B:342:ARG:HG2	1:B:342:ARG:NH1	2.34	0.42
1:D:287:ASP:O	1:D:291:ASN:HB2	2.20	0.42
1:D:402:LEU:HG	1:D:404:LEU:HG	2.01	0.42
1:A:108:GLY:HA3	1:A:133:ARG:O	2.19	0.42
1:A:405:ARG:HA	1:A:405:ARG:NE	2.33	0.42
1:C:17:SER:HB3	1:C:149:ARG:NH1	2.34	0.42
1:D:103:THR:HG22	1:D:104:ASP:N	2.35	0.42
1:D:158:ARG:HG3	1:D:158:ARG:HH11	1.84	0.42
1:B:259:ALA:HB2	1:B:395:ASP:OD2	2.20	0.42
1:C:219:ASP:HB2	1:C:449:ARG:O	2.19	0.42
1:B:81:ARG:HG2	1:B:81:ARG:HH11	1.85	0.42
1:C:288:LEU:O	1:C:335:LEU:HD22	2.18	0.42
1:D:240:GLN:NE2	1:D:245:ARG:NH2	2.67	0.42
1:A:109:TRP:HZ3	1:A:111:ALA:HB2	1.86	0.41
1:A:425:GLU:CD	1:A:425:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLY:O	1:B:350:MET:HG2	2.20	0.41
1:B:306:LEU:O	1:B:309:ILE:HG22	2.20	0.41
1:C:141:ILE:HG12	1:C:150:LEU:HD22	2.02	0.41
1:C:288:LEU:HG	1:C:335:LEU:HB2	2.01	0.41
1:B:28:ASP:O	1:B:32:GLU:HB2	2.21	0.41
1:B:268:LEU:HD11	1:B:334:HIS:CB	2.46	0.41
1:B:393:SER:OG	1:B:395:ASP:OD1	2.26	0.41
1:B:398:LEU:C	1:B:398:LEU:CD2	2.93	0.41
1:C:63:MET:HE3	1:C:64:VAL:H	1.84	0.41
1:D:268:LEU:HD23	1:D:268:LEU:C	2.46	0.41
1:B:113:GLU:O	1:B:116:VAL:HG22	2.20	0.41
1:C:96:VAL:HG11	1:C:392:LEU:HD22	2.03	0.41
1:C:100:LEU:HD12	1:C:349:ARG:HH22	1.86	0.41
1:D:34:ALA:HA	1:D:56:LEU:HD11	2.01	0.41
1:D:193:VAL:O	1:D:197:GLU:HG3	2.21	0.41
1:C:79:THR:HG21	1:C:81:ARG:NH1	2.36	0.41
1:C:392:LEU:N	1:C:392:LEU:HD12	2.36	0.41
1:A:64:VAL:HG23	1:A:99:LEU:HD11	2.02	0.41
1:B:258:ARG:HB2	1:B:262:VAL:CG1	2.49	0.41
1:A:94:GLU:CG	1:A:98:ARG:HH12	2.33	0.41
1:D:59:GLY:O	1:D:137:PRO:HA	2.21	0.41
1:D:158:ARG:NH1	1:D:158:ARG:HG3	2.36	0.41
1:A:240:GLN:NE2	1:A:245:ARG:NH2	2.69	0.41
1:A:264:ILE:HG22	1:A:265:THR:N	2.36	0.41
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.88	0.41
1:C:141:ILE:HG12	1:C:150:LEU:CD2	2.50	0.41
1:C:150:LEU:HD21	1:C:161:ILE:HD13	2.00	0.41
1:C:240:GLN:HE21	1:C:245:ARG:NE	2.19	0.41
1:B:108:GLY:HA3	1:B:133:ARG:O	2.20	0.40
1:A:93:GLY:HA2	1:A:350:MET:HG3	2.03	0.40
1:B:327:ARG:HG3	4:B:4004:GOL:H12	2.03	0.40
1:A:55:VAL:HG13	1:A:55:VAL:O	2.21	0.40
1:A:240:GLN:NE2	1:A:245:ARG:CZ	2.84	0.40
1:C:274:LEU:CD2	1:C:328:GLU:HB3	2.52	0.40
1:D:207:ILE:HD12	1:D:207:ILE:N	2.37	0.40
1:B:157:HIS:O	1:B:161:ILE:HG13	2.21	0.40
1:B:55:VAL:O	1:B:55:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/450 (96%)	416 (96%)	12 (3%)	5 (1%)	10	3
1	B	424/450 (94%)	413 (97%)	11 (3%)	0	100	100
1	C	433/450 (96%)	430 (99%)	3 (1%)	0	100	100
1	D	433/450 (96%)	428 (99%)	5 (1%)	0	100	100
All	All	1723/1800 (96%)	1687 (98%)	31 (2%)	5 (0%)	36	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	22	ALA
1	A	41	VAL
1	A	40	SER
1	A	278	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	333/358 (93%)	324 (97%)	9 (3%)	39	27
1	B	332/358 (93%)	327 (98%)	5 (2%)	57	49
1	C	336/358 (94%)	330 (98%)	6 (2%)	51	43
1	D	339/358 (95%)	332 (98%)	7 (2%)	47	36
All	All	1340/1432 (94%)	1313 (98%)	27 (2%)	48	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	41	VAL
1	A	42	ASP
1	A	163	ARG
1	A	283	LEU
1	A	286	ASP
1	A	357	PHE
1	A	378	ASP
1	A	398	LEU
1	B	357	PHE
1	B	378	ASP
1	B	398	LEU
1	B	434	GLU
1	B	449	ARG
1	C	18	ILE
1	C	33	LEU
1	C	46	LEU
1	C	213	GLU
1	C	378	ASP
1	C	433	GLU
1	D	56	LEU
1	D	75	ARG
1	D	176	ARG
1	D	294	GLU
1	D	322	ASP
1	D	378	ASP
1	D	449	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	231	ASN
1	A	240	GLN
1	A	298	HIS
1	A	409	GLN
1	B	25	ASN
1	B	53	GLN
1	B	122	GLN
1	B	128	HIS
1	B	157	HIS

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Mol	Chain	Res	Type
1	B	204	HIS
1	B	334	HIS
1	B	409	GLN
1	C	128	HIS
1	C	204	HIS
1	C	334	HIS
1	D	53	GLN
1	D	123	GLN
1	D	128	HIS
1	D	240	GLN
1	D	334	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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	$\# Z > 2$
4	GOL	B	4004	-	5,5,5	4.77	5 (100%)	5,5,5	6.23	3 (60%)
4	GOL	D	4002	-	5,5,5	4.75	5 (100%)	5,5,5	6.15	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PYR	A	2001	-	5,5,5	7.25	2 (40%)	3,6,6	1.77	1 (33%)
3	IMD	A	3001	-	5,5,5	0.64	0	5,5,5	0.90	0
3	IMD	C	3002	-	5,5,5	0.65	0	5,5,5	0.88	0
2	PYR	B	2002	-	5,5,5	6.78	1 (20%)	3,6,6	2.10	1 (33%)
4	GOL	A	4003	-	5,5,5	4.79	5 (100%)	5,5,5	6.11	3 (60%)
3	IMD	D	3004	-	5,5,5	0.65	0	5,5,5	0.91	0
4	GOL	D	4006	-	5,5,5	4.81	5 (100%)	5,5,5	6.12	3 (60%)
4	GOL	C	4001	-	5,5,5	4.77	5 (100%)	5,5,5	6.13	3 (60%)
4	GOL	C	4005	-	5,5,5	4.82	5 (100%)	5,5,5	6.13	3 (60%)
3	IMD	C	3003	-	5,5,5	0.64	0	5,5,5	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	4004	-	-	2/4/4/4	-
4	GOL	D	4002	-	-	2/4/4/4	-
2	PYR	A	2001	-	-	3/4/4/4	-
3	IMD	A	3001	-	-	-	0/1/1/1
2	PYR	B	2002	-	-	4/4/4/4	-
3	IMD	C	3002	-	-	-	0/1/1/1
4	GOL	A	4003	-	-	2/4/4/4	-
4	GOL	D	4006	-	-	2/4/4/4	-
3	IMD	D	3004	-	-	-	0/1/1/1
4	GOL	C	4001	-	-	2/4/4/4	-
4	GOL	C	4005	-	-	2/4/4/4	-
3	IMD	C	3003	-	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	PYR	O-C	15.97	1.61	1.22
2	B	2002	PYR	O-C	14.98	1.59	1.22
4	B	4004	GOL	C3-C2	-8.19	1.20	1.51
4	C	4005	GOL	C3-C2	-8.15	1.20	1.51
4	D	4006	GOL	C3-C2	-8.08	1.21	1.51
4	A	4003	GOL	C3-C2	-8.03	1.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4001	GOL	C3-C2	-8.01	1.21	1.51
4	D	4002	GOL	C3-C2	-7.95	1.21	1.51
4	C	4005	GOL	O1-C1	4.54	1.61	1.42
4	A	4003	GOL	O1-C1	4.54	1.61	1.42
4	D	4006	GOL	O1-C1	4.53	1.61	1.42
4	D	4002	GOL	O1-C1	4.49	1.61	1.42
4	C	4001	GOL	O1-C1	4.46	1.61	1.42
4	B	4004	GOL	O1-C1	4.44	1.61	1.42
4	D	4002	GOL	O3-C3	3.51	1.57	1.42
4	C	4001	GOL	O3-C3	3.42	1.56	1.42
4	A	4003	GOL	O3-C3	3.40	1.56	1.42
4	D	4006	GOL	O3-C3	3.34	1.56	1.42
4	B	4004	GOL	O3-C3	3.32	1.56	1.42
4	C	4005	GOL	O3-C3	3.28	1.56	1.42
4	B	4004	GOL	C1-C2	-3.14	1.39	1.51
4	D	4006	GOL	C1-C2	-3.12	1.39	1.51
4	C	4005	GOL	C1-C2	-3.12	1.39	1.51
4	C	4001	GOL	C1-C2	-3.10	1.40	1.51
4	A	4003	GOL	C1-C2	-3.09	1.40	1.51
4	D	4002	GOL	C1-C2	-3.02	1.40	1.51
4	D	4006	GOL	O2-C2	-2.96	1.34	1.43
4	A	4003	GOL	O2-C2	-2.95	1.34	1.43
4	C	4005	GOL	O2-C2	-2.95	1.34	1.43
4	C	4001	GOL	O2-C2	-2.89	1.35	1.43
4	D	4002	GOL	O2-C2	-2.84	1.35	1.43
4	B	4004	GOL	O2-C2	-2.48	1.36	1.43
2	A	2001	PYR	OXT-C	-2.00	1.25	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4004	GOL	O3-C3-C2	11.43	161.82	110.38
4	D	4002	GOL	O3-C3-C2	11.22	160.89	110.38
4	C	4001	GOL	O3-C3-C2	11.16	160.62	110.38
4	D	4006	GOL	O3-C3-C2	11.11	160.41	110.38
4	C	4005	GOL	O3-C3-C2	11.11	160.41	110.38
4	A	4003	GOL	O3-C3-C2	11.10	160.35	110.38
4	D	4006	GOL	O2-C2-C3	7.20	139.00	109.18
4	C	4005	GOL	O2-C2-C3	7.20	139.00	109.18
4	C	4001	GOL	O2-C2-C3	7.19	138.95	109.18
4	A	4003	GOL	O2-C2-C3	7.17	138.87	109.18
4	D	4002	GOL	O2-C2-C3	7.16	138.82	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4004	GOL	O2-C2-C3	7.16	138.82	109.18
4	C	4005	GOL	O1-C1-C2	3.46	125.95	110.38
4	D	4002	GOL	O1-C1-C2	3.44	125.88	110.38
2	B	2002	PYR	OXT-C-CA	3.39	122.99	113.59
4	B	4004	GOL	O1-C1-C2	3.36	125.51	110.38
4	A	4003	GOL	O1-C1-C2	3.36	125.50	110.38
4	D	4006	GOL	O1-C1-C2	3.36	125.49	110.38
4	C	4001	GOL	O1-C1-C2	3.33	125.35	110.38
2	A	2001	PYR	OXT-C-CA	2.72	121.14	113.59

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	PYR	O-C-CA-CB
2	A	2001	PYR	OXT-C-CA-CB
2	B	2002	PYR	O-C-CA-O3
2	B	2002	PYR	OXT-C-CA-O3
2	B	2002	PYR	OXT-C-CA-CB
4	A	4003	GOL	C1-C2-C3-O3
4	B	4004	GOL	C1-C2-C3-O3
4	C	4001	GOL	O1-C1-C2-C3
4	C	4001	GOL	C1-C2-C3-O3
4	C	4005	GOL	C1-C2-C3-O3
4	D	4002	GOL	C1-C2-C3-O3
4	D	4006	GOL	C1-C2-C3-O3
4	A	4003	GOL	O1-C1-C2-O2
4	B	4004	GOL	O1-C1-C2-O2
4	D	4002	GOL	O1-C1-C2-O2
4	D	4006	GOL	O1-C1-C2-O2
4	C	4005	GOL	O1-C1-C2-O2
2	B	2002	PYR	O-C-CA-CB
2	A	2001	PYR	O-C-CA-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4004	GOL	1	0
4	D	4002	GOL	1	0
3	D	3004	IMD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	435/450 (96%)	0.47	33 (7%) 20 18	11, 23, 43, 55	0
1	B	430/450 (95%)	0.39	23 (5%) 32 31	11, 22, 37, 50	0
1	C	435/450 (96%)	0.34	27 (6%) 26 25	10, 20, 40, 51	0
1	D	435/450 (96%)	0.20	17 (3%) 43 43	9, 20, 33, 47	0
All	All	1735/1800 (96%)	0.35	100 (5%) 29 27	9, 21, 39, 55	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	78	VAL	5.6
1	A	155	ILE	5.1
1	A	23	GLY	4.9
1	C	18	ILE	4.9
1	C	155	ILE	4.9
1	B	37	VAL	4.7
1	D	322	ASP	4.4
1	D	449	ARG	4.3
1	A	41	VAL	4.3
1	D	123	GLN	4.3
1	D	15	SER	4.2
1	A	449	ARG	4.1
1	B	78	VAL	3.9
1	B	449	ARG	3.8
1	A	22	ALA	3.8
1	C	449	ARG	3.7
1	B	77	GLY	3.6
1	A	42	ASP	3.6
1	C	165	LEU	3.5
1	A	40	SER	3.5
1	C	16	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	17	SER	3.3
1	B	38	THR	3.2
1	A	25	ASN	3.2
1	D	76	ASP	3.2
1	A	21	PRO	3.1
1	A	37	VAL	3.1
1	A	15	SER	3.1
1	D	427	GLU	3.1
1	A	39	GLU	3.0
1	B	244	ILE	2.9
1	C	161	ILE	2.9
1	C	163	ARG	2.9
1	A	17	SER	2.9
1	A	279	ALA	2.8
1	C	37	VAL	2.8
1	C	160	ALA	2.8
1	C	177	SER	2.7
1	A	18	ILE	2.6
1	A	348	ASP	2.6
1	B	166	ALA	2.6
1	A	152	ASP	2.6
1	A	38	THR	2.6
1	B	161	ILE	2.5
1	B	165	LEU	2.5
1	B	442	LEU	2.5
1	D	155	ILE	2.5
1	A	43	GLU	2.5
1	C	164	LEU	2.4
1	A	278	PRO	2.4
1	C	78	VAL	2.4
1	D	75	ARG	2.4
1	D	23	GLY	2.4
1	D	163	ARG	2.4
1	B	345	PRO	2.4
1	B	36	VAL	2.4
1	D	426	SER	2.4
1	A	286	ASP	2.4
1	C	80	ARG	2.4
1	A	16	SER	2.4
1	C	75	ARG	2.3
1	D	79	THR	2.3
1	A	80	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	2.3
1	D	428	PRO	2.3
1	B	430	ARG	2.3
1	C	286	ASP	2.3
1	B	242	GLY	2.2
1	C	173	PRO	2.2
1	B	177	SER	2.2
1	B	51	ASP	2.2
1	B	182	ASP	2.2
1	A	153	ALA	2.2
1	A	81	ARG	2.2
1	A	36	VAL	2.2
1	C	17	SER	2.2
1	D	77	GLY	2.2
1	D	196	ASP	2.2
1	C	24	VAL	2.2
1	A	120	GLY	2.2
1	A	442	LEU	2.2
1	D	101	LEU	2.2
1	B	342	ARG	2.2
1	C	81	ARG	2.2
1	C	157	HIS	2.1
1	C	322	ASP	2.1
1	A	156	ARG	2.1
1	C	171	GLU	2.1
1	C	162	ASP	2.1
1	A	151	PHE	2.1
1	B	260	ASP	2.1
1	B	344	ASP	2.1
1	A	166	ALA	2.1
1	B	180	VAL	2.0
1	A	163	ARG	2.0
1	A	344	ASP	2.0
1	C	434	GLU	2.0
1	C	38	THR	2.0
1	B	158	ARG	2.0
1	C	326	VAL	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 [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($\text{\AA}^2$)	Q<0.9
4	GOL	C	4005	6/6	0.72	0.28	53,54,55,56	0
4	GOL	D	4002	6/6	0.72	0.24	45,47,48,50	0
4	GOL	D	4006	6/6	0.72	0.20	47,47,47,48	0
4	GOL	C	4001	6/6	0.74	0.27	59,60,60,61	0
4	GOL	A	4003	6/6	0.76	0.25	53,54,55,55	0
3	IMD	A	3001	5/5	0.77	0.17	50,50,51,51	0
2	PYR	A	2001	6/6	0.79	0.18	30,34,38,39	0
4	GOL	B	4004	6/6	0.80	0.15	39,40,41,42	0
3	IMD	D	3004	5/5	0.81	0.13	40,40,41,41	0
2	PYR	B	2002	6/6	0.85	0.14	19,24,28,29	0
3	IMD	C	3003	5/5	0.90	0.12	36,36,37,37	0
3	IMD	C	3002	5/5	0.92	0.12	44,44,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.