



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:30 AM UTC

PDB ID : 3HYL / pdb_00003hyl
Title : Crystal Structure of Transketolase from Bacillus anthracis
Authors : Maltseva, N.; Kim, Y.; Kwon, K.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-06-22
Resolution : 2.16 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

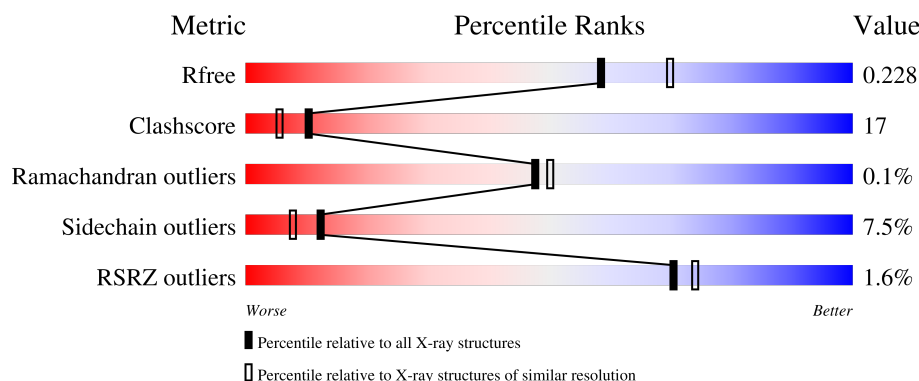
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	690	% 73% 20% . .
1	B	690	2% 66% 26% . .

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	FMT	A	669	-	-	X	-
3	FMT	A	673	-	-	X	-
3	FMT	B	668	-	-	X	-
3	FMT	B	674	-	-	X	-
4	PEG	A	677	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10868 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 Transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	Se	0	2	0
			5087	3198	862	1005	1	21			
1	B	663	Total	C	N	O	S	Se	0	3	0
			5096	3205	863	1006	1	21			

There are 48 discrepancies between the modelled and reference sequences:

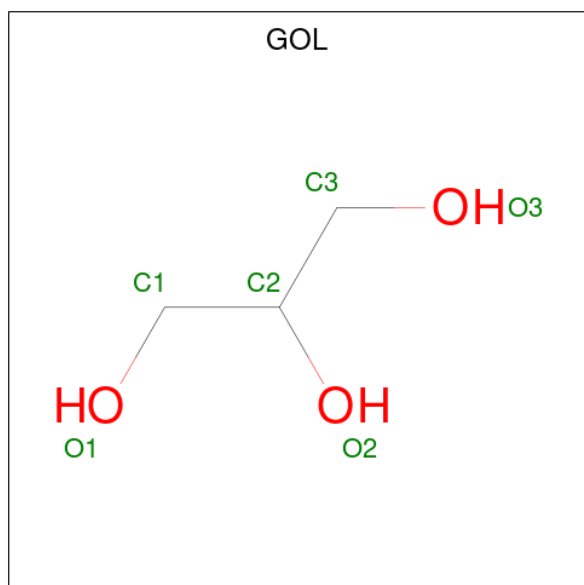
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	expression tag	UNP C3P4P9
A	-22	HIS	-	expression tag	UNP C3P4P9
A	-21	HIS	-	expression tag	UNP C3P4P9
A	-20	HIS	-	expression tag	UNP C3P4P9
A	-19	HIS	-	expression tag	UNP C3P4P9
A	-18	HIS	-	expression tag	UNP C3P4P9
A	-17	HIS	-	expression tag	UNP C3P4P9
A	-16	SER	-	expression tag	UNP C3P4P9
A	-15	SER	-	expression tag	UNP C3P4P9
A	-14	GLY	-	expression tag	UNP C3P4P9
A	-13	VAL	-	expression tag	UNP C3P4P9
A	-12	ASP	-	expression tag	UNP C3P4P9
A	-11	LEU	-	expression tag	UNP C3P4P9
A	-10	GLY	-	expression tag	UNP C3P4P9
A	-9	THR	-	expression tag	UNP C3P4P9
A	-8	GLU	-	expression tag	UNP C3P4P9
A	-7	ASN	-	expression tag	UNP C3P4P9
A	-6	LEU	-	expression tag	UNP C3P4P9
A	-5	TYR	-	expression tag	UNP C3P4P9
A	-4	PHE	-	expression tag	UNP C3P4P9
A	-3	GLN	-	expression tag	UNP C3P4P9
A	-2	SER	-	expression tag	UNP C3P4P9
A	-1	ASN	-	expression tag	UNP C3P4P9
A	0	ALA	-	expression tag	UNP C3P4P9
B	-23	MSE	-	expression tag	UNP C3P4P9

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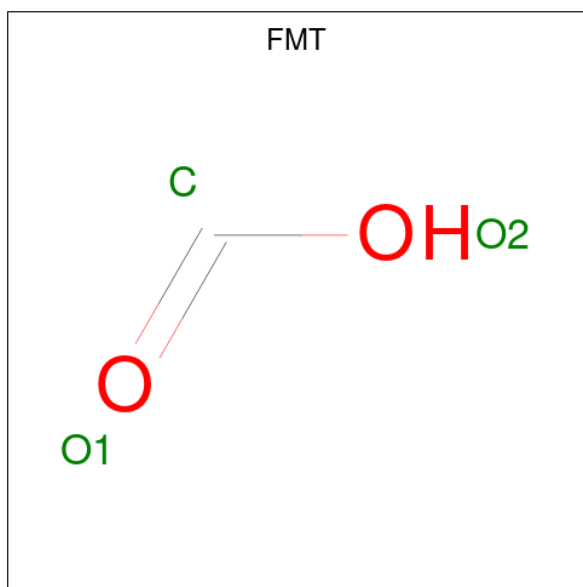
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP C3P4P9
B	-21	HIS	-	expression tag	UNP C3P4P9
B	-20	HIS	-	expression tag	UNP C3P4P9
B	-19	HIS	-	expression tag	UNP C3P4P9
B	-18	HIS	-	expression tag	UNP C3P4P9
B	-17	HIS	-	expression tag	UNP C3P4P9
B	-16	SER	-	expression tag	UNP C3P4P9
B	-15	SER	-	expression tag	UNP C3P4P9
B	-14	GLY	-	expression tag	UNP C3P4P9
B	-13	VAL	-	expression tag	UNP C3P4P9
B	-12	ASP	-	expression tag	UNP C3P4P9
B	-11	LEU	-	expression tag	UNP C3P4P9
B	-10	GLY	-	expression tag	UNP C3P4P9
B	-9	THR	-	expression tag	UNP C3P4P9
B	-8	GLU	-	expression tag	UNP C3P4P9
B	-7	ASN	-	expression tag	UNP C3P4P9
B	-6	LEU	-	expression tag	UNP C3P4P9
B	-5	TYR	-	expression tag	UNP C3P4P9
B	-4	PHE	-	expression tag	UNP C3P4P9
B	-3	GLN	-	expression tag	UNP C3P4P9
B	-2	SER	-	expression tag	UNP C3P4P9
B	-1	ASN	-	expression tag	UNP C3P4P9
B	0	ALA	-	expression tag	UNP C3P4P9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

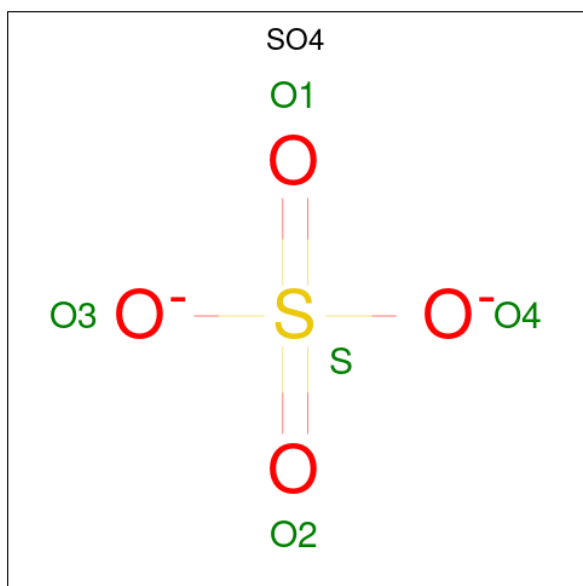
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



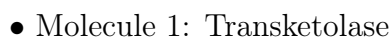
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

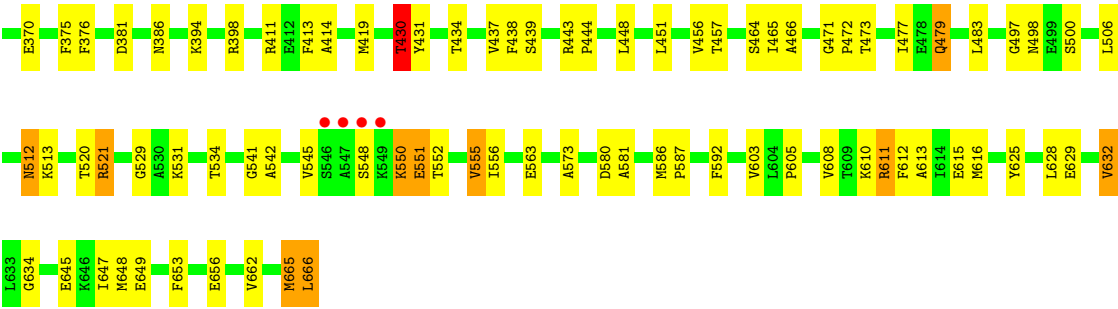
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	343	Total	O	0	0
			343	343		
8	B	261	Total	O	0	0
			261	261		

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- Molecule 1: Transketolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.80Å 70.97Å 145.79Å 90.00° 117.35° 90.00°	Depositor
Resolution (Å)	36.35 – 2.16 36.35 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.35-2.16) 99.6 (36.35-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.176 , 0.230 0.173 , 0.228	Depositor DCC
R_{free} test set	3423 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10868	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: CL, MG, GOL, FMT, SO4, PEG

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	0.84	0/5174	1.03	11/6988 (0.2%)
1	B	0.77	0/5187	1.04	11/7005 (0.2%)
All	All	0.81	0/10361	1.04	22/13993 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	531	LYS	N-CA-C	6.94	118.50	111.07
1	A	430	THR	CB-CA-C	-6.82	97.44	109.71
1	B	430	THR	CB-CA-C	-6.52	97.98	109.71
1	B	471	GLY	CA-C-N	6.51	126.44	119.28
1	B	471	GLY	C-N-CA	6.51	126.44	119.28
1	B	28	HIS	CA-C-N	6.33	127.75	119.84
1	B	28	HIS	C-N-CA	6.33	127.75	119.84
1	A	665	MSE	CG-SE-CE	-6.17	85.36	98.92
1	B	269	VAL	N-CA-C	6.08	116.82	110.62
1	B	31	MSE	CG-SE-CE	-5.66	86.46	98.92
1	A	280	ALA	N-CA-C	-5.54	105.15	112.24
1	A	319	TYR	N-CA-C	-5.51	105.17	111.07
1	A	464	SER	N-CA-C	5.51	116.35	108.74
1	A	551	GLU	N-CA-C	-5.38	105.98	112.54
1	A	312	TRP	N-CA-C	-5.37	105.34	111.14
1	B	439	SER	N-CA-C	-5.37	105.54	111.71
1	A	604	LEU	CA-C-N	5.37	126.55	119.84
1	A	604	LEU	C-N-CA	5.37	126.55	119.84
1	B	555	VAL	CB-CA-C	-5.32	104.40	111.80
1	B	647	ILE	CB-CA-C	-5.25	105.25	111.97
1	A	345	ASN	N-CA-C	5.15	118.34	111.75
1	A	226	ILE	N-CA-C	-5.13	105.39	110.62

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	5087	0	4921	139	0
1	B	5096	0	4930	207	0
2	A	12	0	16	2	0
3	A	15	0	5	7	0
3	B	18	0	6	7	0
4	A	21	0	30	7	0
4	B	7	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	B	5	0	0	0	0
8	A	343	0	0	5	0
8	B	261	0	0	12	0
All	All	10868	0	9918	343	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 17.

All (343) 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:B:142:ASP:HB2	8:B:866:HOH:O	1.26	1.30
1:B:616:MSE:SE	8:B:741:HOH:O	2.12	1.16
1:B:465:ILE:HD11	1:B:616:MSE:HE2	1.26	1.12
1:B:616:MSE:HE3	1:B:653:PHE:CD2	1.85	1.12
1:A:130:MSE:SE	8:A:927:HOH:O	2.21	1.09
1:B:18:ILE:HG12	1:B:33:MSE:HE2	1.35	1.08
1:A:57:PHE:CD2	1:A:334:MSE:HE2	1.89	1.07
1:A:42:LEU:HG	1:A:47:MSE:HE2	1.37	1.06
1:B:465:ILE:HD11	1:B:616:MSE:CE	1.86	1.06
1:B:332:ALA:HA	1:B:337:LEU:HD12	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:677:PEG:H21	1:B:205:ASP:HB3	1.41	0.98
1:A:43:TRP:HA	1:A:47:MSE:HE3	1.44	0.98
1:A:397:THR:HG23	1:A:399:ASP:H	1.30	0.97
1:B:126:VAL:HG12	1:B:130:MSE:CE	1.95	0.95
1:A:249:ILE:HD12	1:A:249:ILE:H	1.30	0.95
1:A:29:PRO:HB2	1:A:33:MSE:HE3	1.47	0.94
1:A:31:MSE:HG3	1:A:32:PRO:HD3	1.47	0.94
1:B:44:THR:HG22	1:B:45:GLN:HG3	1.49	0.94
2:A:667:GOL:H31	3:A:669:FMT:O2	1.69	0.91
1:B:38:MSE:HE1	1:B:183:LEU:HB3	1.54	0.90
1:B:129:ALA:HA	1:B:132[B]:GLU:OE2	1.71	0.89
1:B:145:ASN:OD1	1:B:315:MSE:SE	2.40	0.89
1:B:126:VAL:HG12	1:B:130:MSE:HE2	1.54	0.87
1:A:33:MSE:HE1	1:A:267:LEU:HD13	1.58	0.85
1:B:136:ALA:O	1:B:140:ASN:HB2	1.76	0.85
1:B:18:ILE:CG1	1:B:33:MSE:HE2	2.07	0.84
1:A:349:TYR:H	1:A:498:ASN:HD21	1.23	0.84
1:B:616:MSE:HE3	1:B:653:PHE:CG	2.13	0.84
1:A:161:MSE:HE2	1:B:411:ARG:CZ	2.08	0.83
1:B:268:GLY:O	1:B:272:THR:HG23	1.78	0.83
1:A:126:VAL:CG1	1:A:130:MSE:HE3	2.09	0.83
1:A:29:PRO:HB2	1:A:33:MSE:CE	2.10	0.82
1:B:78:HIS:HE1	1:B:294:TYR:OH	1.61	0.82
1:A:57:PHE:CG	1:A:334:MSE:HE2	2.14	0.82
1:A:126:VAL:HG12	1:A:130:MSE:HE3	1.61	0.81
1:A:451:LEU:HD21	1:B:472:PRO:HB2	1.63	0.81
1:B:57:PHE:CD2	1:B:334:MSE:HE2	2.16	0.80
1:A:249:ILE:HD12	1:A:249:ILE:N	1.96	0.80
1:B:551:GLU:CD	1:B:551:GLU:H	1.88	0.80
1:A:249:ILE:H	1:A:249:ILE:CD1	1.91	0.79
1:B:199:PHE:CZ	1:B:201:GLU:HG2	2.17	0.79
1:A:205:ASP:HB3	4:A:677:PEG:O1	1.82	0.79
1:B:18:ILE:HG12	1:B:33:MSE:CE	2.12	0.79
1:A:239:ARG:HH21	1:A:239:ARG:HG3	1.49	0.78
1:B:92:PHE:CZ	1:B:93:ARG:HD2	2.20	0.77
1:B:479:GLN:H	1:B:479:GLN:HE21	1.30	0.76
1:A:42:LEU:CG	1:A:47:MSE:HE2	2.15	0.75
1:A:43:TRP:CA	1:A:47:MSE:HE3	2.15	0.75
1:A:267:LEU:H	1:A:267:LEU:CD2	2.00	0.75
1:B:254:PRO:HD2	1:B:271:GLU:OE1	1.87	0.74
1:A:479:GLN:H	1:A:479:GLN:HE21	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MSE:HE2	1:B:411:ARG:NH1	2.03	0.73
1:B:126:VAL:HG12	1:B:130:MSE:HE3	1.70	0.73
1:A:42:LEU:HG	1:A:47:MSE:CE	2.18	0.73
1:B:497:GLY:O	1:B:500:SER:HB3	1.89	0.72
1:A:479:GLN:H	1:A:479:GLN:NE2	1.87	0.72
1:B:97:SER:O	1:B:107[A]:HIS:HE1	1.71	0.72
1:B:249:ILE:HD13	1:B:249:ILE:N	2.05	0.72
1:A:97:SER:HB3	1:A:99:THR:H	1.54	0.71
1:A:18:ILE:HG23	1:A:267:LEU:HD21	1.71	0.71
1:B:332:ALA:CA	1:B:337:LEU:HD12	2.19	0.71
1:A:267:LEU:H	1:A:267:LEU:HD23	1.56	0.71
1:A:161:MSE:HE1	1:A:198:SER:HB2	1.72	0.70
1:A:239:ARG:HG3	1:A:239:ARG:NH2	2.06	0.69
1:B:38:MSE:HE3	1:B:183:LEU:HD23	1.72	0.69
1:A:15:THR:HG21	1:A:281:TRP:CZ2	2.27	0.69
1:B:140:ASN:O	1:B:141:ARG:HG2	1.92	0.69
1:A:92:PHE:CZ	1:A:93:ARG:HD2	2.28	0.69
1:A:397:THR:HG23	1:A:399:ASP:N	2.06	0.68
1:A:236:ASP:OD2	1:A:239:ARG:NH2	2.26	0.68
2:A:667:GOL:H31	3:A:669:FMT:C	2.24	0.68
1:B:249:ILE:HD13	1:B:249:ILE:H	1.59	0.68
1:A:57:PHE:CD2	1:A:334:MSE:CE	2.74	0.67
1:B:332:ALA:HA	1:B:337:LEU:CD1	2.22	0.67
1:A:224:GLU:O	1:A:228:LYS:HG3	1.95	0.67
1:B:134:HIS:NE2	1:B:138:LYS:HD2	2.10	0.67
1:B:40:TYR:O	1:B:44:THR:HB	1.94	0.66
1:B:133:ARG:NE	1:B:133:ARG:HA	2.10	0.66
1:B:18:ILE:CD1	1:B:33:MSE:HE2	2.25	0.66
1:B:325[A]:GLU:CD	1:B:325[A]:GLU:H	2.03	0.66
1:B:140:ASN:C	1:B:141:ARG:HG2	2.21	0.65
1:B:222:ASP:O	1:B:226:ILE:HG13	1.96	0.65
1:A:142:ASP:O	1:A:143:ALA:HB3	1.96	0.65
1:A:161:MSE:HE1	1:A:198:SER:CB	2.27	0.65
1:B:550:LYS:HD2	1:B:580:ASP:OD2	1.96	0.65
1:B:465:ILE:CD1	1:B:616:MSE:HE2	2.16	0.64
1:B:59:ARG:HG3	1:B:60:ASP:O	1.98	0.64
1:A:208:LYS:O	4:A:677:PEG:H42	1.99	0.63
1:B:204:GLU:HG3	1:B:214:VAL:HG11	1.81	0.63
1:B:343:GLU:HB2	1:B:346:LEU:HD22	1.80	0.63
1:B:187:ASN:ND2	1:B:249:ILE:HG23	2.13	0.62
1:B:325[B]:GLU:CD	1:B:325[B]:GLU:H	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MSE:HE1	1:A:89:LEU:HG	1.80	0.62
1:A:267:LEU:HD23	1:A:267:LEU:N	2.13	0.62
1:A:126:VAL:HG12	1:A:130:MSE:CE	2.30	0.61
1:B:357:THR:HA	1:B:360:SER:HB2	1.83	0.61
1:B:616:MSE:CE	1:B:653:PHE:CD2	2.75	0.61
1:A:29:PRO:O	1:A:33:MSE:HG3	2.00	0.61
1:B:92:PHE:CE2	1:B:93:ARG:CD	2.84	0.61
1:B:92:PHE:CE2	1:B:93:ARG:HD2	2.36	0.61
1:A:43:TRP:HE3	1:A:47:MSE:HE1	1.66	0.61
1:A:199:PHE:CZ	1:A:201:GLU:HG2	2.36	0.60
1:B:157:ASP:N	3:B:668:FMT:H	2.16	0.60
1:B:148:ASP:OD1	1:B:179:ARG:NH2	2.34	0.60
3:A:672:FMT:H	8:B:712:HOH:O	2.01	0.60
1:B:157:ASP:H	3:B:668:FMT:H	1.67	0.60
1:A:5:ILE:CD1	1:A:296:ASN:HB2	2.31	0.60
1:B:307:THR:O	1:B:311:GLU:HG3	1.99	0.60
1:A:325:GLU:H	1:A:325:GLU:CD	2.09	0.60
1:B:498:ASN:C	1:B:534:THR:HG21	2.27	0.60
1:B:512:ASN:C	1:B:512:ASN:HD22	2.10	0.59
1:A:275:THR:HG22	1:A:279:TYR:CE2	2.37	0.59
1:B:86:MSE:HE1	1:B:287:PHE:CD1	2.38	0.59
1:A:577:ASP:HB3	1:A:663:LYS:HZ3	1.67	0.59
1:A:663:LYS:HA	1:A:666:LEU:HD11	1.84	0.59
1:A:97:SER:HB2	3:A:673:FMT:C	2.32	0.58
1:A:161:MSE:HE2	1:B:411:ARG:NH2	2.18	0.58
1:A:345:ASN:ND2	1:A:367:ALA:O	2.36	0.58
1:B:542:ALA:HB2	1:B:586:MSE:HG2	1.85	0.58
1:B:130:MSE:SE	8:B:935:HOH:O	2.71	0.58
1:B:249:ILE:H	1:B:249:ILE:CD1	2.15	0.58
1:B:573:ALA:HB2	8:B:877:HOH:O	2.03	0.58
1:A:477:ILE:H	1:A:479:GLN:HE22	1.52	0.58
1:B:479:GLN:HE21	1:B:479:GLN:N	1.98	0.57
1:B:268:GLY:O	1:B:272:THR:CG2	2.51	0.57
1:B:645:GLU:O	1:B:649:GLU:HG3	2.05	0.57
1:A:161:MSE:HE3	1:A:199:PHE:HD2	1.69	0.57
1:B:276:LYS:HD3	1:B:281:TRP:CD1	2.40	0.57
1:A:126:VAL:CG1	1:A:130:MSE:CE	2.83	0.56
1:A:195:LEU:HG	1:A:199:PHE:HB3	1.87	0.56
1:B:520:THR:HG23	3:B:674:FMT:C	2.35	0.56
1:A:616:MSE:SE	1:A:648:MSE:HG2	2.56	0.56
1:B:78:HIS:CE1	1:B:294:TYR:OH	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:MSE:HG3	1:A:32:PRO:CD	2.28	0.56
1:B:14:ARG:O	1:B:18:ILE:HG13	2.06	0.56
1:B:196:ASN:C	1:B:196:ASN:HD22	2.12	0.56
1:B:256:LYS:HA	1:B:259:LYS:HD2	1.88	0.56
1:B:541:GLY:O	1:B:587:PRO:HD2	2.06	0.55
1:A:43:TRP:CE3	1:A:47:MSE:HE1	2.42	0.55
1:A:619:THR:HG22	1:A:632:VAL:HG22	1.89	0.55
4:A:677:PEG:H31	1:B:205:ASP:OD2	2.05	0.55
1:B:586:MSE:HE1	1:B:625:TYR:CE1	2.41	0.55
1:B:179:ARG:HD2	1:B:237:GLU:OE1	2.06	0.55
1:A:78:HIS:HE1	1:A:294:TYR:OH	1.89	0.55
1:B:358:ARG:HD3	1:B:521:ARG:HA	1.88	0.55
1:A:199:PHE:CZ	1:A:201:GLU:CG	2.91	0.54
1:B:44:THR:HG22	1:B:45:GLN:CG	2.33	0.54
1:B:139:TYR:CD2	1:B:330:LEU:HD13	2.41	0.54
1:B:187:ASN:ND2	1:B:249:ILE:CG2	2.69	0.54
1:B:236:ASP:OD2	1:B:239:ARG:NH2	2.41	0.54
1:A:206:ARG:HG3	1:B:206:ARG:HG3	1.90	0.54
1:B:376:PHE:O	1:B:430:THR:HG22	2.07	0.54
1:B:349:TYR:H	1:B:498:ASN:HD21	1.54	0.54
1:A:91:ASN:O	1:A:97:SER:OG	2.24	0.54
1:A:161:MSE:HE3	1:A:199:PHE:CD2	2.43	0.54
1:B:126:VAL:CG1	1:B:130:MSE:HE2	2.34	0.54
1:B:140:ASN:O	1:B:141:ARG:CG	2.55	0.54
1:B:176:GLN:NE2	1:B:398:ARG:HD2	2.23	0.54
1:A:376:PHE:O	1:A:430:THR:HG22	2.08	0.54
1:A:255:ASN:HB2	1:A:271:GLU:OE1	2.08	0.53
1:A:196[B]:ASN:OD1	1:A:199:PHE:O	2.27	0.53
1:B:33:MSE:HE1	1:B:267:LEU:HD22	1.89	0.53
1:B:92:PHE:CE2	1:B:93:ARG:HD3	2.43	0.53
1:B:71:MSE:HE1	1:B:89:LEU:HG	1.91	0.53
1:A:33:MSE:CE	1:A:267:LEU:HD13	2.35	0.53
1:A:126:VAL:HG13	1:A:130:MSE:HE3	1.89	0.53
1:B:249:ILE:N	1:B:249:ILE:CD1	2.71	0.53
1:B:29:PRO:HB3	1:B:33:MSE:CE	2.39	0.52
1:B:437:VAL:HG13	1:B:438:PHE:CD1	2.44	0.52
1:B:204:GLU:OE2	3:B:672:FMT:C	2.57	0.52
1:B:612:PHE:HD2	1:B:665:MSE:HE3	1.74	0.52
1:A:282:THR:O	1:A:283:ALA:C	2.53	0.52
1:B:49:HIS:N	1:B:49:HIS:CD2	2.77	0.52
1:B:479:GLN:H	1:B:479:GLN:NE2	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:MSE:HE3	1:B:90:LYS:HG3	1.92	0.52
1:B:133:ARG:HA	1:B:133:ARG:HE	1.74	0.52
1:A:369:ALA:HB2	1:A:390:MSE:SE	2.60	0.51
8:A:909:HOH:O	1:B:197:ARG:HD2	2.09	0.51
1:A:408:TYR:CE2	1:A:415:MSE:HG3	2.46	0.51
1:B:520:THR:CG2	3:B:674:FMT:C	2.89	0.51
1:A:199:PHE:CE2	1:A:201:GLU:HG2	2.46	0.51
1:A:512:ASN:C	1:A:512:ASN:HD22	2.17	0.51
1:B:285:GLN:OE1	1:B:285:GLN:HA	2.11	0.51
1:B:86:MSE:CE	1:B:90:LYS:HG3	2.40	0.51
1:B:314:THR:O	1:B:318:GLU:HG2	2.10	0.51
1:B:465:ILE:HD11	1:B:616:MSE:HE1	1.85	0.51
1:B:199:PHE:CZ	1:B:201:GLU:CG	2.94	0.50
1:B:529:GLY:HA3	1:B:545:VAL:O	2.12	0.50
1:A:529:GLY:HA3	1:A:545:VAL:O	2.11	0.50
1:B:555:VAL:O	1:B:581:ALA:HA	2.12	0.50
1:A:117:PRO:HD3	1:B:473:THR:HB	1.93	0.50
1:A:239:ARG:HH21	1:A:239:ARG:CG	2.21	0.50
1:A:267:LEU:CD2	1:A:267:LEU:N	2.68	0.50
1:A:92:PHE:CE2	1:A:93:ARG:HD3	2.47	0.50
1:B:134:HIS:NE2	1:B:138:LYS:CD	2.75	0.50
1:A:33:MSE:SE	1:A:250:GLY:HA2	2.61	0.50
1:A:41:THR:OG1	1:A:223:ILE:HG13	2.13	0.49
1:A:479:GLN:NE2	1:A:479:GLN:N	2.60	0.49
1:B:563:GLU:CD	1:B:616:MSE:HG3	2.37	0.49
1:A:78:HIS:CE1	1:A:294:TYR:OH	2.66	0.49
1:A:130:MSE:HE2	1:A:175:LEU:HD12	1.94	0.49
1:B:142:ASP:C	1:B:144:TYR:H	2.21	0.49
1:A:473:THR:HB	1:B:117:PRO:HD3	1.95	0.48
1:A:149:HIS:HE1	8:A:800:HOH:O	1.96	0.48
1:A:142:ASP:O	1:A:143:ALA:CB	2.61	0.48
1:A:167:GLU:HB2	1:A:414:ALA:HB2	1.95	0.48
1:A:64:LEU:O	1:A:115:THR:HG21	2.14	0.48
1:B:219:ASP:OD2	1:B:219:ASP:C	2.56	0.48
1:A:87[B]:ASP:O	1:A:88:ASP:C	2.57	0.48
1:A:274:LEU:O	1:A:277:GLU:HB2	2.14	0.47
1:A:38:MSE:HG3	1:A:39:ALA:N	2.28	0.47
1:B:29:PRO:HB3	1:B:33:MSE:HE3	1.96	0.47
1:B:29:PRO:HG2	1:B:265:SER:O	2.14	0.47
1:B:31:MSE:HB3	1:B:32:PRO:HD3	1.96	0.47
1:B:57:PHE:CG	1:B:334:MSE:HE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASN:O	1:B:141:ARG:HD3	2.14	0.47
1:A:92:PHE:CE2	1:A:93:ARG:CD	2.97	0.47
1:B:351:LEU:H	1:B:351:LEU:HD22	1.79	0.47
1:A:236:ASP:OD2	1:A:239:ARG:HG3	2.14	0.47
1:B:223:ILE:HB	8:B:754:HOH:O	2.14	0.47
1:B:613:ALA:HB3	1:B:632:VAL:HB	1.96	0.47
1:B:4:SER:N	8:B:851:HOH:O	2.47	0.47
1:B:132[B]:GLU:OE2	1:B:151:THR:OG1	2.32	0.47
1:A:255:ASN:O	1:A:259:LYS:HE3	2.15	0.47
1:A:286:ASP:O	1:A:287:PHE:HB2	2.15	0.47
1:B:142:ASP:O	1:B:143:ALA:HB3	2.14	0.47
1:B:512:ASN:C	1:B:512:ASN:ND2	2.72	0.47
1:A:161:MSE:HE3	1:A:199:PHE:HB2	1.96	0.46
1:B:234:LYS:HB3	1:B:234:LYS:HE3	1.53	0.46
1:A:97:SER:HB2	3:A:673:FMT:O2	2.15	0.46
1:B:22:GLU:CD	1:B:272:THR:HG21	2.40	0.46
1:B:542:ALA:CB	1:B:586:MSE:HG2	2.45	0.46
1:A:97:SER:CB	3:A:673:FMT:H	2.46	0.46
1:A:437:VAL:HG13	1:A:438:PHE:CD1	2.51	0.46
1:B:196:ASN:HA	1:B:199:PHE:O	2.16	0.46
1:B:38:MSE:CE	1:B:183:LEU:HB3	2.37	0.46
1:B:662:VAL:O	1:B:665:MSE:HG3	2.15	0.46
1:A:555:VAL:HG23	1:A:610:LYS:O	2.16	0.45
1:B:104:GLU:HB3	1:B:107[B]:HIS:HD2	1.82	0.45
1:B:608:VAL:O	1:B:611:ARG:HD2	2.17	0.45
1:B:431:TYR:HA	1:B:457:THR:O	2.16	0.45
1:A:239:ARG:HE	4:A:678:PEG:H41	1.80	0.45
1:A:212:TRP:CE3	1:A:240:PRO:HB2	2.51	0.45
1:B:253:SER:O	1:B:257:SER:HB3	2.16	0.45
1:B:479:GLN:N	1:B:479:GLN:NE2	2.62	0.45
1:A:586:MSE:SE	1:A:589:MSE:HG2	2.67	0.45
1:B:33:MSE:HE1	1:B:267:LEU:CD2	2.46	0.45
1:B:176:GLN:HB3	1:B:238:LYS:O	2.17	0.45
1:B:615:GLU:O	1:B:634:GLY:HA2	2.17	0.45
1:A:5:ILE:HD11	1:A:296:ASN:HB2	1.99	0.45
1:B:556:ILE:HD11	1:B:605:PRO:HD2	1.98	0.45
1:B:148:ASP:HA	1:B:179:ARG:NH2	2.31	0.45
1:B:158:GLY:H	3:B:668:FMT:C	2.30	0.45
1:A:128:MSE:HE2	1:A:424:LEU:HD13	1.99	0.44
1:A:38:MSE:HE1	1:A:185:ASP:HA	1.98	0.44
1:A:133:ARG:HA	1:A:133:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:HA	1:B:179:ARG:HH22	1.82	0.44
1:B:239:ARG:HB2	1:B:240:PRO:CD	2.47	0.44
1:A:239:ARG:HE	4:A:678:PEG:C4	2.30	0.44
1:A:408:TYR:CD2	1:A:415:MSE:HG3	2.52	0.44
1:B:4:SER:N	8:B:849:HOH:O	2.50	0.44
1:B:134:HIS:CE1	1:B:138:LYS:HD2	2.52	0.44
1:B:164:VAL:HB	1:B:413:PHE:CD2	2.52	0.44
1:B:267:LEU:HB3	1:B:272:THR:HG22	1.99	0.44
1:A:477:ILE:H	1:A:479:GLN:NE2	2.14	0.44
1:B:204:GLU:HG3	1:B:214:VAL:CG1	2.46	0.44
1:B:464:SER:C	1:B:466:ALA:N	2.75	0.44
1:B:573:ALA:N	8:B:877:HOH:O	2.50	0.44
1:B:612:PHE:CD2	1:B:665:MSE:HE3	2.53	0.44
1:A:107:HIS:HB3	8:A:844:HOH:O	2.17	0.44
1:A:218:GLU:OE2	1:A:218:GLU:HA	2.16	0.43
1:A:113:ALA:HB2	1:A:128:MSE:HE1	2.00	0.43
1:A:212:TRP:CD2	1:A:240:PRO:HB2	2.53	0.43
1:B:175:LEU:O	1:B:176:GLN:C	2.61	0.43
1:B:419:MSE:HE2	1:B:456:VAL:HB	2.00	0.43
1:B:189:ILE:HG13	1:B:249:ILE:HD11	1.99	0.43
1:B:224:GLU:OE2	1:B:224:GLU:HA	2.18	0.43
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.71	0.43
1:B:616:MSE:HE1	1:B:648:MSE:HA	1.98	0.43
1:A:157:ASP:O	1:A:158:GLY:C	2.61	0.43
1:B:443:ARG:HB3	1:B:444:PRO:HD3	2.00	0.43
1:A:279:TYR:O	1:A:280:ALA:HB3	2.18	0.43
1:B:196:ASN:HD22	1:B:197:ARG:N	2.16	0.43
1:B:612:PHE:HB2	1:B:665:MSE:HE3	2.00	0.43
1:A:87[B]:ASP:O	1:A:90:LYS:N	2.50	0.43
1:B:196:ASN:C	1:B:196:ASN:ND2	2.77	0.43
1:B:477:ILE:H	1:B:479:GLN:HE22	1.66	0.43
1:B:506:LEU:HD23	1:B:506:LEU:HA	1.89	0.43
1:B:611:ARG:O	1:B:665:MSE:HE1	2.18	0.43
1:A:146:ILE:HD12	1:A:316:LEU:HD23	2.00	0.43
1:B:78:HIS:HD2	1:B:84:VAL:O	2.02	0.43
1:A:293:VAL:O	1:A:294:TYR:C	2.61	0.42
1:B:38:MSE:HG2	8:B:752:HOH:O	2.18	0.42
1:B:140:ASN:C	1:B:141:ARG:CG	2.91	0.42
1:B:603:VAL:HG22	8:B:729:HOH:O	2.18	0.42
1:A:211:GLY:HA2	4:A:678:PEG:H22	2.00	0.42
1:A:257:SER:O	1:A:259:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:MSE:CE	1:A:456:VAL:HB	2.48	0.42
1:B:216:ARG:NH2	3:B:675:FMT:O1	2.52	0.42
1:B:227:ALA:O	1:B:231:GLU:HG3	2.19	0.42
1:B:542:ALA:HB3	1:B:592:PHE:CD1	2.55	0.42
1:A:42:LEU:CD2	1:A:47:MSE:HE2	2.49	0.42
1:B:555:VAL:HG12	1:B:666:LEU:HD11	2.02	0.42
1:A:154:ILE:HA	1:A:183:LEU:O	2.19	0.42
1:A:569:GLU:O	1:A:570:ALA:C	2.61	0.42
1:B:10:ILE:CD1	1:B:223:ILE:HD11	2.50	0.42
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.92	0.42
1:B:610:LYS:NZ	1:B:629:GLU:HG2	2.34	0.42
1:A:137:ALA:HB1	1:A:402:SER:HB3	2.02	0.42
1:B:140:ASN:O	1:B:141:ARG:CD	2.68	0.42
1:B:145:ASN:H	1:B:315:MSE:SE	2.53	0.42
1:B:53:ASN:ND2	1:B:309:GLN:HE22	2.18	0.42
1:B:53:ASN:HD22	1:B:309:GLN:HE22	1.67	0.42
1:B:187:ASN:CG	1:B:249:ILE:HG23	2.44	0.42
1:B:230:ILE:O	1:B:234:LYS:HG3	2.20	0.42
1:B:350:GLU:O	1:B:351:LEU:C	2.60	0.41
1:A:249:ILE:N	1:A:249:ILE:CD1	2.61	0.41
1:B:29:PRO:CB	1:B:33:MSE:HE3	2.50	0.41
1:B:38:MSE:HA	1:B:226:ILE:HD13	2.01	0.41
1:A:189:ILE:HG13	1:A:249:ILE:HG12	2.01	0.41
1:A:603:VAL:C	1:A:605:PRO:HD3	2.45	0.41
1:B:22:GLU:CG	1:B:272:THR:HG21	2.50	0.41
1:B:318:GLU:HG2	1:B:318:GLU:H	1.64	0.41
1:B:145:ASN:ND2	8:B:902:HOH:O	2.53	0.41
1:B:167:GLU:HB2	1:B:414:ALA:HB2	2.02	0.41
1:B:253:SER:HA	1:B:254:PRO:HD3	1.74	0.41
1:A:91:ASN:O	1:A:92:PHE:C	2.64	0.41
1:A:220:GLY:HA3	1:A:247:THR:HG22	2.03	0.41
1:A:364:VAL:HG11	1:A:504:TRP:CG	2.55	0.41
1:B:80:SER:HA	1:B:297:PHE:HB3	2.02	0.41
1:B:386:ASN:HD21	1:B:434:THR:HA	1.86	0.41
1:B:611:ARG:C	1:B:665:MSE:HE1	2.45	0.41
3:A:669:FMT:C	8:A:871:HOH:O	2.69	0.41
1:B:38:MSE:HE3	1:B:38:MSE:HB2	1.93	0.40
1:B:350:GLU:O	1:B:353:SER:OG	2.37	0.40
1:B:29:PRO:CB	1:B:33:MSE:CE	2.98	0.40
1:A:376:PHE:O	1:A:430:THR:HA	2.22	0.40
1:A:560:THR:O	1:A:561:GLY:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:HB3	1:B:37:PRO:HD3	2.03	0.40
1:B:236:ASP:OD1	1:B:238:LYS:HB2	2.21	0.40
1:B:464:SER:C	1:B:466:ALA:H	2.28	0.40
1:B:38:MSE:HE1	1:B:183:LEU:CB	2.38	0.40
1:B:189:ILE:HG13	1:B:249:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/690 (96%)	637 (96%)	25 (4%)	1 (0%)	43	44
1	B	664/690 (96%)	634 (96%)	30 (4%)	0	100	100
All	All	1327/1380 (96%)	1271 (96%)	55 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	528/527 (100%)	495 (94%)	33 (6%)	16	11
1	B	529/527 (100%)	482 (91%)	47 (9%)	9	5
All	All	1057/1054 (100%)	977 (92%)	80 (8%)	12	8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	15	THR
1	A	16	LEU
1	A	31	MSE
1	A	49	HIS
1	A	55	THR
1	A	64	LEU
1	A	89	LEU
1	A	97	SER
1	A	197	ARG
1	A	239	ARG
1	A	248	THR
1	A	249	ILE
1	A	267	LEU
1	A	285	GLN
1	A	309	GLN
1	A	316	LEU
1	A	328	ASN
1	A	346	LEU
1	A	398	ARG
1	A	430	THR
1	A	451	LEU
1	A	479	GLN
1	A	483	LEU
1	A	512	ASN
1	A	513	LYS
1	A	549	LYS
1	A	572	LYS
1	A	609	THR
1	A	632	VAL
1	A	660	ARG
1	A	665	MSE

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Mol	Chain	Res	Type
1	A	666	LEU
1	B	10	ILE
1	B	44	THR
1	B	49	HIS
1	B	55	THR
1	B	59	ARG
1	B	64	LEU
1	B	89	LEU
1	B	196	ASN
1	B	224	GLU
1	B	228	LYS
1	B	234	LYS
1	B	239	ARG
1	B	249	ILE
1	B	265	SER
1	B	267	LEU
1	B	272	THR
1	B	285	GLN
1	B	306	GLU
1	B	314	THR
1	B	316	LEU
1	B	318	GLU
1	B	325[A]	GLU
1	B	325[B]	GLU
1	B	337	LEU
1	B	346	LEU
1	B	360	SER
1	B	370	GLU
1	B	375	PHE
1	B	381	ASP
1	B	394	LYS
1	B	430	THR
1	B	451	LEU
1	B	479	GLN
1	B	483	LEU
1	B	512	ASN
1	B	513	LYS
1	B	521	ARG
1	B	548	SER
1	B	550	LYS
1	B	551	GLU
1	B	552	THR

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Mol	Chain	Res	Type
1	B	611	ARG
1	B	628	LEU
1	B	632	VAL
1	B	656	GLU
1	B	665	MSE
1	B	666	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	91	ASN
1	A	285	GLN
1	A	302	GLN
1	A	386	ASN
1	A	479	GLN
1	A	488	ASN
1	A	498	ASN
1	A	512	ASN
1	B	53	ASN
1	B	78	HIS
1	B	91	ASN
1	B	176	GLN
1	B	196	ASN
1	B	213	GLN
1	B	313	ASN
1	B	386	ASN
1	B	479	GLN
1	B	488	ASN
1	B	498	ASN
1	B	512	ASN
1	B	623	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	FMT	B	675	-	2,2,2	0.64	0	1,1,1	0.13	0
4	PEG	B	669	-	6,6,6	0.59	0	5,5,5	2.30	3 (60%)
3	FMT	B	672	-	2,2,2	0.57	0	1,1,1	0.09	0
4	PEG	A	674	-	6,6,6	0.53	0	5,5,5	1.65	1 (20%)
3	FMT	B	667	-	2,2,2	0.66	0	1,1,1	0.23	0
3	FMT	A	673	-	2,2,2	0.67	0	1,1,1	0.56	0
4	PEG	A	677	-	6,6,6	0.53	0	5,5,5	1.48	1 (20%)
3	FMT	A	672	-	2,2,2	0.61	0	1,1,1	0.05	0
2	GOL	A	668	-	5,5,5	0.39	0	5,5,5	0.56	0
4	PEG	A	678	-	6,6,6	0.51	0	5,5,5	1.86	2 (40%)
3	FMT	B	674	-	2,2,2	0.74	0	1,1,1	0.42	0
3	FMT	B	668	5	2,2,2	0.69	0	1,1,1	0.21	0
3	FMT	B	673	-	2,2,2	0.61	0	1,1,1	0.03	0
2	GOL	A	667	-	5,5,5	0.40	0	5,5,5	0.57	0
3	FMT	A	671	-	2,2,2	0.62	0	1,1,1	0.04	0
3	FMT	A	669	-	2,2,2	0.57	0	1,1,1	0.40	0
7	SO4	B	671	-	4,4,4	0.26	0	6,6,6	0.18	0
3	FMT	A	670	-	2,2,2	0.62	0	1,1,1	0.02	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	PEG	B	669	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	677	-	-	2/4/4/4	-
2	GOL	A	668	-	-	3/4/4/4	-
4	PEG	A	678	-	-	1/4/4/4	-
4	PEG	A	674	-	-	3/4/4/4	-
2	GOL	A	667	-	-	0/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	669	PEG	O2-C3-C4	3.19	124.18	110.11
4	A	677	PEG	O2-C3-C4	2.43	120.84	110.11
4	B	669	PEG	C3-O2-C2	2.35	123.56	113.26
4	B	669	PEG	O2-C2-C1	2.28	120.14	110.11
4	A	678	PEG	O2-C2-C1	2.26	120.07	110.11
4	A	678	PEG	O2-C3-C4	2.19	119.77	110.11
4	A	674	PEG	O2-C2-C1	2.16	119.62	110.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	669	PEG	C4-C3-O2-C2
2	A	668	GOL	O1-C1-C2-C3
4	A	677	PEG	O1-C1-C2-O2
4	B	669	PEG	O2-C3-C4-O4
2	A	668	GOL	O1-C1-C2-O2
4	A	677	PEG	O2-C3-C4-O4
4	A	674	PEG	O1-C1-C2-O2
4	A	674	PEG	O2-C3-C4-O4
4	A	678	PEG	O1-C1-C2-O2
4	A	674	PEG	C4-C3-O2-C2
2	A	668	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	675	FMT	1	0
3	B	672	FMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	673	FMT	3	0
4	A	677	PEG	4	0
3	A	672	FMT	1	0
4	A	678	PEG	3	0
3	B	674	FMT	2	0
3	B	668	FMT	3	0
2	A	667	GOL	2	0
3	A	669	FMT	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	642/690 (93%)	-0.13	8 (1%) 76 79	17, 42, 77, 120	2 (0%)
1	B	642/690 (93%)	0.12	13 (2%) 65 69	19, 53, 91, 126	3 (0%)
All	All	1284/1380 (93%)	-0.00	21 (1%) 70 74	17, 47, 87, 126	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	548	SER	4.7
1	B	142	ASP	3.3
1	B	145	ASN	3.2
1	B	351	LEU	3.1
1	B	144	TYR	3.1
1	B	139	TYR	3.0
1	B	143	ALA	2.9
1	B	249	ILE	2.8
1	B	546	SER	2.7
1	A	143	ALA	2.7
1	B	140	ASN	2.6
1	A	4	SER	2.5
1	A	249	ILE	2.5
1	B	547	ALA	2.5
1	B	549	LYS	2.5
1	A	248	THR	2.4
1	A	394	LYS	2.3
1	B	323	TYR	2.2
1	A	267	LEU	2.0
1	A	550	LYS	2.0
1	A	274	LEU	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($\text{\AA}^2$)	Q<0.9
4	PEG	A	674	7/7	0.54	0.22	78,80,80,81	0
3	FMT	B	672	3/3	0.70	0.15	60,60,65,66	0
7	SO4	B	671	5/5	0.70	0.13	121,121,122,124	0
4	PEG	A	678	7/7	0.72	0.17	76,78,82,83	0
3	FMT	B	673	3/3	0.76	0.11	65,65,70,71	0
4	PEG	A	677	7/7	0.76	0.18	68,71,73,74	0
3	FMT	B	674	3/3	0.78	0.19	46,46,47,50	0
4	PEG	B	669	7/7	0.79	0.14	50,58,66,67	0
2	GOL	A	668	6/6	0.82	0.11	64,68,72,74	0
3	FMT	B	675	3/3	0.83	0.10	65,65,66,67	0
3	FMT	A	671	3/3	0.84	0.12	53,53,57,59	0
3	FMT	A	672	3/3	0.85	0.13	54,54,58,61	0
2	GOL	A	667	6/6	0.86	0.13	43,53,58,58	0
3	FMT	B	667	3/3	0.88	0.10	41,41,47,49	0
3	FMT	A	673	3/3	0.88	0.16	45,45,47,49	0
6	CL	A	676	1/1	0.89	0.11	63,63,63,63	0
3	FMT	A	669	3/3	0.90	0.17	48,48,51,53	0
3	FMT	B	668	3/3	0.92	0.08	43,43,45,47	0
3	FMT	A	670	3/3	0.94	0.09	44,44,45,47	0
5	MG	A	675	1/1	0.96	0.08	43,43,43,43	0
5	MG	B	670	1/1	0.97	0.05	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.