



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 AM GMT

PDB ID : 2WYS  
Title : HIGH RESOLUTION CRYSTALLOGRAPHIC STRUCTURE OF THE CLOSTRIDIUM THERMOCELLUM N-TERMINAL ENDO-1,4-BETA-D -XYLANASE 10B (XYN10B) CBM22-1-GH10 MODULES COMPLEXED WITH XYLOHEXAOSE  
Authors : Najmudin, S.; Pinheiro, B.A.; Romao, M.J.; Prates, J.A.M.; Fontes, C.M.G.A.  
Deposited on : 2009-11-20  
Resolution : 2.75 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

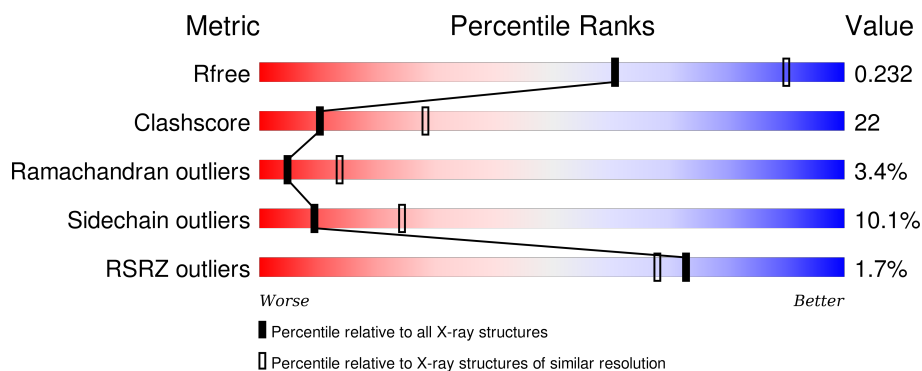
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	<div> <div> <div>2%</div> <div>57%</div> <div>31%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	540	<div> <div>2%</div> <div>58%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>

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	XYP	A	1001	-	-	X	-
3	XYP	A	1002	X	-	X	-
5	PO4	A	1555	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8545 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 ENDO-1,4-BETA-XYLANASE Y.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	Se	0	2	0
			4043	2538	688	799	8	10			
1	B	517	Total	C	N	O	S	Se	0	1	1
			4054	2543	692	802	8	9			

There are 44 discrepancies between the modelled and reference sequences:

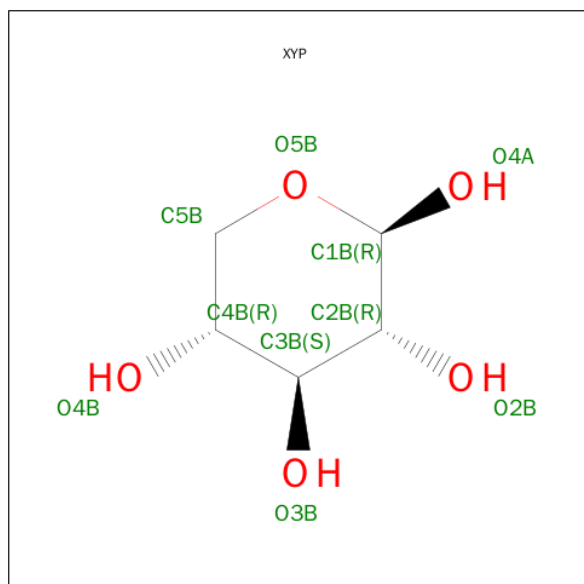
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	-	EXPRESSION TAG	UNP P51584
A	13	GLY	-	EXPRESSION TAG	UNP P51584
A	14	SER	-	EXPRESSION TAG	UNP P51584
A	15	SER	-	EXPRESSION TAG	UNP P51584
A	16	HIS	-	EXPRESSION TAG	UNP P51584
A	17	HIS	-	EXPRESSION TAG	UNP P51584
A	18	HIS	-	EXPRESSION TAG	UNP P51584
A	19	HIS	-	EXPRESSION TAG	UNP P51584
A	20	HIS	-	EXPRESSION TAG	UNP P51584
A	21	HIS	-	EXPRESSION TAG	UNP P51584
A	22	SER	-	EXPRESSION TAG	UNP P51584
A	23	SER	-	EXPRESSION TAG	UNP P51584
A	24	GLY	-	EXPRESSION TAG	UNP P51584
A	25	LEU	-	EXPRESSION TAG	UNP P51584
A	26	VAL	-	EXPRESSION TAG	UNP P51584
A	27	PRO	-	EXPRESSION TAG	UNP P51584
A	28	ARG	-	EXPRESSION TAG	UNP P51584
A	29	GLY	-	EXPRESSION TAG	UNP P51584
A	30	SER	-	EXPRESSION TAG	UNP P51584
A	31	HIS	-	EXPRESSION TAG	UNP P51584
A	32	MSE	-	EXPRESSION TAG	UNP P51584
A	337	ALA	GLU	ENGINEERED MUTATION	UNP P51584
B	12	MSE	-	EXPRESSION TAG	UNP P51584
B	13	GLY	-	EXPRESSION TAG	UNP P51584
B	14	SER	-	EXPRESSION TAG	UNP P51584

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	SER	-	EXPRESSION TAG	UNP P51584
B	16	HIS	-	EXPRESSION TAG	UNP P51584
B	17	HIS	-	EXPRESSION TAG	UNP P51584
B	18	HIS	-	EXPRESSION TAG	UNP P51584
B	19	HIS	-	EXPRESSION TAG	UNP P51584
B	20	HIS	-	EXPRESSION TAG	UNP P51584
B	21	HIS	-	EXPRESSION TAG	UNP P51584
B	22	SER	-	EXPRESSION TAG	UNP P51584
B	23	SER	-	EXPRESSION TAG	UNP P51584
B	24	GLY	-	EXPRESSION TAG	UNP P51584
B	25	LEU	-	EXPRESSION TAG	UNP P51584
B	26	VAL	-	EXPRESSION TAG	UNP P51584
B	27	PRO	-	EXPRESSION TAG	UNP P51584
B	28	ARG	-	EXPRESSION TAG	UNP P51584
B	29	GLY	-	EXPRESSION TAG	UNP P51584
B	30	SER	-	EXPRESSION TAG	UNP P51584
B	31	HIS	-	EXPRESSION TAG	UNP P51584
B	32	MSE	-	EXPRESSION TAG	UNP P51584
B	337	ALA	GLU	ENGINEERED MUTATION	UNP P51584

- Molecule 2 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			9	5	4		
2	B	1	Total	C	O	0	0
			9	5	4		

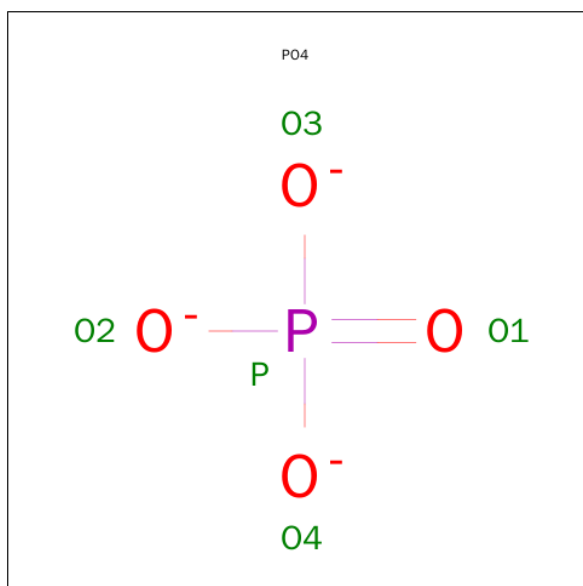
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			18	10	8		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Ca		0	0
			1	1			
4	A	3	Total	Ca		0	0
			3	3			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total	O	0	0
			151	151		
6	B	227	Total	O	0	0
			227	227		





S471	V335	K237
Q474	N336	T241
Y479	D341	Y243
K480	D342	Q244
	R345	S245
T492	T346	T248
S493	R347	N249
S494	Y348	T250
		N251
K497	G356	R252
A500	N359	Y254
	G360	Q268
P506	R361	
N507	S362	R274
	Q366	T277
T511		L278
W512	N371	V279
N523	I374	
N526	Y380	F289
Q527	A381	K290
A531	R382	D291
	K383	N292
I538	Y384	F293
W539		Q294
	N388	N295
W544	K390	T296
G545	C391	Q297
D546	I391	N298
G547	Y392	N299
	Y393	V300
P550	N394	S301
A551	D395	
	E398	V304
		N305
		D306
		Q307
	H402	R308
	K403	L309
	R404	E310
		S311
	D421	V312
	G422	T313
	Q426	K314
		N315
	D432	N316
		L320
	Q457	Q321
	E460	R322
	L461	P325
	D462	
	P466	A331
		V322

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.70Å 173.70Å 135.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.85 – 2.75 86.85 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.85-2.75) 98.9 (86.85-2.75)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.185 , 0.236 0.187 , 0.232	Depositor DCC
$R_{free}$ test set	3077 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60768 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, CA, PO4

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	0.99	2/4128 (0.0%)	0.94	5/5591 (0.1%)
1	B	1.06	5/4135 (0.1%)	0.98	5/5602 (0.1%)
All	All	1.03	7/8263 (0.1%)	0.96	10/11193 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
3	A	3	0
All	All	3	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	SER	C-N	-10.25	1.10	1.34
1	B	389	CYS	CB-SG	-7.09	1.70	1.82
1	B	86	GLU	CG-CD	6.00	1.60	1.51
1	B	348	TYR	CE2-CZ	5.56	1.45	1.38
1	B	86	GLU	CB-CG	5.51	1.62	1.52
1	B	42	GLU	CB-CG	5.31	1.62	1.52
1	A	473	GLN	CG-CD	5.13	1.62	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	SER	O-C-N	6.78	133.54	122.70
1	B	361	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	432	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	494	SER	CA-C-N	-5.89	104.23	117.20
1	A	258	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	274	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	462	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	404	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	308	ARG	NE-CZ-NH2	-5.10	117.75	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1002	XYP	C4B,C2B,C3B

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	SER	Peptide
1	B	494	SER	Peptide
1	B	80	SER	Peptide

## 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	4043	0	3849	173	0
1	B	4054	0	3848	160	0
2	A	10	0	10	6	0
2	B	28	0	25	6	0
3	A	18	0	15	6	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	151	0	0	26	0
6	B	227	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8545	0	7747	342	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 22.

All (342) 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:155:ALA:HA	6:A:2033:HOH:O	1.17	1.34
2:A:1001:XYP:O4B	3:A:1002:XYP:C5B	1.81	1.28
2:A:1001:XYP:C4B	3:A:1002:XYP:H5B2	1.68	1.24
1:B:492:THR:HG22	1:B:493:SER:H	1.05	1.19
1:B:157:ASN:HB3	6:B:2018:HOH:O	1.39	1.19
1:A:270:ASN:HB3	6:A:2068:HOH:O	1.44	1.18
1:B:241:THR:HB	1:B:316:MSE:HE1	1.16	1.15
1:A:119:TYR:HE1	1:A:128:ASN:HB3	1.10	1.12
1:B:241:THR:HB	1:B:316:MSE:CE	1.80	1.12
2:A:1001:XYP:O4B	3:A:1002:XYP:H5B2	0.96	1.10
1:A:85:SER:OG	1:A:87:LYS:HE2	1.51	1.10
1:B:493:SER:HA	1:B:494:SER:CB	1.80	1.10
1:B:49:CYS:HA	6:B:2005:HOH:O	1.49	1.09
1:A:119:TYR:CE1	1:A:128:ASN:HB3	1.88	1.08
1:A:158:ILE:CG2	1:A:159:THR:H	1.67	1.08
1:B:118:SER:HB3	1:B:129:LYS:HE2	1.34	1.05
1:B:85:SER:OG	1:B:87:LYS:HE2	1.58	1.02
1:A:289:PHE:HA	1:A:305:MSE:CE	1.89	1.02
1:A:119:TYR:HE2	1:A:152:PRO:HD2	1.25	1.00
1:A:121:ASP:HB3	1:A:124:THR:OG1	1.62	1.00
1:A:158:ILE:HG22	1:A:159:THR:N	1.78	0.96
1:A:434:ASN:HD22	1:A:435:GLY:H	1.04	0.95
1:A:288:PHE:O	1:A:305:MSE:HE1	1.66	0.95
1:B:361:ARG:HD3	6:B:2136:HOH:O	1.64	0.94
2:B:1002:XYP:HO4B	2:B:1003:XYP:C1B	1.72	0.94
1:A:312:TYR:CE1	1:A:316:MSE:HE3	2.04	0.93
1:B:492:THR:HG22	1:B:493:SER:N	1.82	0.93
1:B:493:SER:HA	1:B:494:SER:HB3	1.49	0.91
1:B:58:THR:HG22	6:B:2010:HOH:O	1.68	0.91
1:A:289:PHE:HA	1:A:305:MSE:HE1	1.53	0.91
1:A:158:ILE:CG2	1:A:159:THR:N	2.29	0.91
1:A:158:ILE:HG22	1:A:159:THR:H	1.30	0.90
1:B:120:LEU:HD12	1:B:121:ASP:N	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:XYP:O4B	2:B:1003:XYP:C2B	2.22	0.88
1:B:471:SER:H	1:B:474:GLN:HE21	1.21	0.88
1:A:492:THR:HG22	1:A:493:SER:H	1.36	0.88
1:A:141:GLU:HG2	6:A:2030:HOH:O	1.71	0.87
1:A:493:SER:HA	1:A:494:SER:CB	2.03	0.87
1:A:119:TYR:CE2	1:A:152:PRO:HD2	2.09	0.87
1:A:119:TYR:HE1	1:A:128:ASN:CB	1.88	0.86
1:A:270:ASN:HB2	6:A:2069:HOH:O	1.72	0.86
1:B:289:PHE:O	1:B:300:VAL:HG13	1.75	0.86
1:A:516:GLN:H	1:A:516:GLN:HE21	1.22	0.86
1:A:289:PHE:HA	1:A:305:MSE:HE3	1.58	0.83
1:A:44:ASN:OD1	1:A:325:PRO:HD2	1.79	0.83
2:B:1002:XYP:C4B	2:B:1003:XYP:C1B	2.58	0.82
1:A:129:LYS:HG2	1:A:130:GLU:H	1.44	0.81
2:A:1001:XYP:C4B	3:A:1002:XYP:C5B	2.53	0.81
1:A:89:PHE:CE2	1:A:214:VAL:HG22	2.17	0.80
1:B:119:TYR:HD1	1:B:120:LEU:N	1.80	0.80
1:B:128:ASN:O	1:B:129:LYS:HD2	1.82	0.79
1:B:122:SER:HA	6:B:2032:HOH:O	1.83	0.78
1:A:136:ASP:HB2	6:A:2029:HOH:O	1.83	0.78
1:A:158:ILE:HG23	1:A:159:THR:H	1.46	0.78
1:A:329:LEU:O	1:A:389:CYS:HB2	1.82	0.78
1:A:96:GLU:O	6:A:2021:HOH:O	2.02	0.78
1:B:241:THR:CB	1:B:316:MSE:CE	2.61	0.77
1:B:380:TYR:HE1	6:B:2146:HOH:O	1.66	0.77
1:A:193:ALA:HA	1:A:198:MSE:CE	2.16	0.76
1:A:347:ARG:HH11	1:A:348:TYR:HE1	1.34	0.76
1:A:155:ALA:C	1:A:156:VAL:HG22	2.05	0.76
1:A:434:ASN:ND2	1:A:435:GLY:H	1.83	0.75
1:B:241:THR:CB	1:B:316:MSE:HE1	2.08	0.75
1:A:434:ASN:HD22	1:A:435:GLY:N	1.82	0.75
1:B:41:PHE:O	1:B:69:ARG:HD3	1.85	0.75
1:B:251:ASN:HB3	6:B:2085:HOH:O	1.87	0.75
1:B:493:SER:HA	1:B:494:SER:OG	1.87	0.74
1:B:119:TYR:HD1	1:B:120:LEU:H	1.35	0.74
1:B:290:LYS:HA	1:B:298:ASN:O	1.88	0.74
1:A:478:LYS:O	1:A:482:VAL:HG23	1.88	0.73
1:B:492:THR:CG2	1:B:493:SER:H	1.88	0.73
1:B:254:VAL:HB	1:B:316:MSE:HE2	1.71	0.73
1:B:245:SER:HB3	6:B:2083:HOH:O	1.89	0.73
2:B:1002:XYP:O4B	2:B:1003:XYP:H2B	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:TYR:CD1	1:B:120:LEU:N	2.57	0.72
1:B:44:ASN:OD1	1:B:325:PRO:HD2	1.91	0.71
1:B:134:THR:O	6:B:2033:HOH:O	2.08	0.71
1:A:121:ASP:HA	6:A:2033:HOH:O	1.89	0.71
1:A:312:TYR:CZ	1:A:316:MSE:HE3	2.26	0.71
1:A:41:PHE:O	1:A:69:ARG:HD3	1.91	0.70
1:A:85:SER:OG	1:A:87:LYS:CE	2.35	0.70
1:A:234:ASN:HA	1:A:237:LYS:HD2	1.72	0.70
1:A:527[A]:GLN:OE1	6:A:2140:HOH:O	2.09	0.70
1:B:395:ASP:O	1:B:426:GLN:HG3	1.92	0.70
1:A:112:THR:HG23	1:A:136:ASP:OD1	1.92	0.70
1:B:278:LEU:HD13	1:B:313:ILE:HG12	1.72	0.70
1:B:347:ARG:HD3	6:B:2132:HOH:O	1.91	0.70
1:B:493:SER:CA	1:B:494:SER:CB	2.67	0.70
1:B:471:SER:H	1:B:474:GLN:NE2	1.89	0.70
1:A:137:VAL:HG22	1:A:143:THR:HG21	1.74	0.70
1:A:301:SER:HB3	1:A:304:VAL:HG23	1.74	0.69
1:B:108:THR:HA	6:B:2028:HOH:O	1.94	0.68
1:A:533:ASN:HA	1:A:536:ALA:HB3	1.76	0.68
1:A:144:GLU:HG3	1:A:145:ILE:N	2.09	0.68
1:A:312:TYR:CE1	1:A:316:MSE:CE	2.76	0.67
1:B:215:ASN:HB3	6:B:2066:HOH:O	1.94	0.67
1:B:493:SER:HB2	6:B:2208:HOH:O	1.94	0.66
1:A:493:SER:HA	1:A:494:SER:HB3	1.76	0.66
1:A:155:ALA:CA	6:A:2033:HOH:O	1.99	0.66
1:B:59:ALA:HB2	1:B:71:MSE:HE1	1.78	0.65
1:B:457:GLN:HG2	1:B:500:ALA:HB3	1.78	0.65
1:B:74:ILE:HG13	1:B:75:ASN:N	2.10	0.64
1:A:121:ASP:CB	1:A:124:THR:OG1	2.40	0.63
1:A:493:SER:HA	1:A:494:SER:OG	1.98	0.63
1:B:76:ARG:HH12	1:B:164:THR:HG23	1.64	0.63
1:A:155:ALA:O	1:A:156:VAL:HG22	1.98	0.63
1:A:89:PHE:CE2	1:A:214:VAL:CG2	2.82	0.62
1:B:241:THR:OG1	1:B:316:MSE:HE3	2.00	0.62
1:A:155:ALA:C	1:A:156:VAL:CG2	2.67	0.62
1:A:314:LYS:HG3	1:A:384:TYR:CE1	2.34	0.62
2:A:1001:XYP:O4B	3:A:1002:XYP:C4B	2.47	0.62
1:A:193:ALA:HA	1:A:198:MSE:HE3	1.80	0.61
1:B:224:LEU:HB2	6:B:2071:HOH:O	1.99	0.61
2:A:1001:XYP:C5B	3:A:1002:XYP:H5B2	2.30	0.61
1:A:433:MSE:CE	1:A:477:ASP:HB3	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HG3	1:B:347:ARG:HH11	1.66	0.60
1:A:55:THR:HG21	1:A:82:GLY:O	2.01	0.60
1:B:292:ASN:HB3	6:B:2103:HOH:O	1.99	0.60
1:B:221:ALA:O	6:B:2071:HOH:O	2.16	0.60
1:A:533:ASN:O	1:A:534:ALA:C	2.36	0.60
1:B:58:THR:HG23	1:B:322:ARG:NH1	2.17	0.60
1:A:127:GLU:HG3	1:B:126:GLU:OE1	2.02	0.60
1:A:516:GLN:HE21	1:A:516:GLN:N	1.97	0.59
1:A:49:CYS:HB3	1:A:257:ASN:OD1	2.03	0.59
1:B:347:ARG:HH11	1:B:347:ARG:CG	2.15	0.59
1:A:237:LYS:HE2	1:A:280:TRP:CZ3	2.37	0.59
1:B:234:ASN:HA	1:B:237:LYS:HD2	1.85	0.58
1:B:41:PHE:CD1	1:B:71:MSE:HE3	2.39	0.58
1:B:304:VAL:O	1:B:308:ARG:HG3	2.04	0.58
1:B:120:LEU:HD12	1:B:121:ASP:H	1.65	0.58
1:B:546:ASP:N	6:B:2226:HOH:O	2.22	0.58
1:A:359:ASN:HB2	1:A:361:ARG:HH21	1.69	0.58
1:A:162:ILE:HG22	1:A:170:PHE:CZ	2.39	0.58
1:A:44:ASN:OD1	1:A:325:PRO:CD	2.52	0.57
1:B:346:THR:CG2	6:B:2046:HOH:O	2.52	0.57
1:B:361:ARG:CD	6:B:2136:HOH:O	2.35	0.57
1:A:492:THR:HG22	1:A:493:SER:N	2.15	0.57
1:B:98:LYS:HB2	1:B:148:LYS:HE3	1.85	0.57
1:B:96:GLU:HA	1:B:149:TYR:O	2.06	0.56
1:B:480:LYS:HG2	1:B:538:ILE:HD11	1.88	0.56
1:A:129:LYS:HG2	1:A:130:GLU:N	2.19	0.56
1:B:249:ASN:O	1:B:307:GLN:HB3	2.06	0.56
1:B:314:LYS:HD2	1:B:384:TYR:CZ	2.40	0.56
1:B:241:THR:CB	1:B:316:MSE:HE3	2.33	0.55
1:A:442:TYR:CE2	1:A:482:VAL:HG13	2.41	0.55
1:A:76:ARG:HH22	1:A:164:THR:H	1.53	0.55
1:B:49:CYS:O	1:B:84:TYR:N	2.33	0.55
1:A:433:MSE:HE1	1:A:477:ASP:C	2.28	0.54
1:B:217:SER:HA	6:B:2020:HOH:O	2.06	0.54
1:B:84:TYR:HA	1:B:160:LEU:O	2.08	0.54
1:A:463:ILE:HG22	1:A:463:ILE:O	2.07	0.54
1:A:94:GLY:N	1:A:151:ALA:O	2.38	0.54
1:B:112:THR:O	1:B:164:THR:HA	2.07	0.54
1:B:233:GLU:O	1:B:237:LYS:HE3	2.08	0.53
1:A:63:GLU:O	1:A:142:TRP:HZ2	1.90	0.53
1:B:356:GLY:H	1:B:366:GLN:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:HA	6:B:2012:HOH:O	2.09	0.52
1:A:37:VAL:HB	1:A:177:ILE:HG13	1.91	0.52
1:B:388:ASN:HB3	6:B:2153:HOH:O	2.09	0.52
1:B:95:VAL:HB	1:B:97:TYR:CE2	2.44	0.52
1:A:300:VAL:CG2	1:A:305:MSE:HG2	2.40	0.52
1:B:336:ASN:OD1	1:B:394:ASN:HB3	2.09	0.52
1:B:56:TYR:O	1:B:57:LEU:HD12	2.10	0.52
1:A:76:ARG:NH2	1:A:164:THR:H	2.08	0.51
1:B:49:CYS:N	1:B:84:TYR:O	2.39	0.51
1:B:88:GLY:HA3	1:B:215:ASN:OD1	2.10	0.51
1:A:272:ALA:HB1	1:A:330:TYR:CD2	2.45	0.51
1:B:392:TYR:CE2	1:B:422:GLY:HA3	2.46	0.51
1:A:134:THR:HG22	6:A:2028:HOH:O	2.10	0.51
1:A:173:ASP:OD1	1:A:174:ASP:N	2.44	0.51
1:B:547:GLY:O	1:B:550:PRO:HD3	2.12	0.50
1:A:157:ASN:O	1:A:158:ILE:O	2.30	0.50
1:A:339:VAL:HG23	1:A:393:TYR:OH	2.11	0.50
1:B:493:SER:CA	1:B:494:SER:HB3	2.29	0.50
1:B:96:GLU:HG3	6:B:2022:HOH:O	2.10	0.50
1:B:471:SER:N	1:B:474:GLN:HE21	2.01	0.50
1:B:290:LYS:NZ	1:B:295:ASP:O	2.41	0.50
1:A:347:ARG:NH1	1:A:348:TYR:HE1	2.08	0.50
1:B:166:SER:OG	1:B:168:VAL:HG12	2.12	0.49
1:A:354:GLU:HB2	1:A:361:ARG:HG3	1.94	0.49
1:A:450:ILE:C	1:A:452:ILE:H	2.16	0.49
1:B:342:ASP:HA	6:B:2128:HOH:O	2.13	0.49
1:A:439:ILE:HD13	1:A:481:ALA:HB1	1.94	0.49
1:A:56:TYR:HE2	1:A:58:THR:HB	1.77	0.49
1:A:408:ALA:HB2	1:A:449:TYR:CE1	2.47	0.49
1:B:279:VAL:HB	1:B:335:VAL:HG22	1.93	0.49
1:B:195:LEU:HB3	1:B:205:VAL:HG11	1.94	0.49
1:B:206:GLY:HA3	1:B:229:SER:HB3	1.95	0.49
1:B:110:THR:CG2	1:B:138:VAL:HG12	2.43	0.49
1:B:207:SER:OG	1:B:208:VAL:N	2.46	0.49
1:A:112:THR:HG22	6:A:2028:HOH:O	2.12	0.48
1:B:187:THR:HA	6:B:2053:HOH:O	2.12	0.48
1:A:348:TYR:N	1:A:348:TYR:CD1	2.82	0.48
1:B:398:GLU:O	1:B:404:ARG:HB2	2.14	0.48
1:A:156:VAL:O	1:A:157:ASN:HB3	2.14	0.48
1:B:538:ILE:HG22	1:B:539:ILE:HD13	1.94	0.48
1:A:119:TYR:CD2	1:A:155:ALA:HB1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	1:B:322:ARG:HH12	1.77	0.48
1:B:119:TYR:O	1:B:127:GLU:OE1	2.31	0.48
1:B:181:GLY:HA3	6:B:2051:HOH:O	2.14	0.48
1:A:336:ASN:OD1	1:A:394:ASN:HB3	2.13	0.48
1:B:50:ASN:O	1:B:50:ASN:CG	2.52	0.47
1:B:305:MSE:O	1:B:306:ASP:C	2.50	0.47
1:B:460:GLU:OE1	2:B:1001:XYP:H1B	2.13	0.47
1:B:289:PHE:CE1	1:B:305:MSE:HE2	2.49	0.47
1:B:62:ASN:HA	1:B:67:GLY:O	2.14	0.47
1:A:157:ASN:N	6:A:2034:HOH:O	2.48	0.47
1:B:395:ASP:C	1:B:426:GLN:HG3	2.34	0.47
1:A:428:HIS:HD1	1:A:462:ASP:CG	2.16	0.47
1:B:342:ASP:O	1:B:345:ARG:HB2	2.15	0.47
1:A:456:VAL:O	1:A:498:VAL:HA	2.14	0.47
1:B:81:ASP:O	1:B:163:THR:HG22	2.15	0.47
1:B:162:ILE:HG22	1:B:170:PHE:CE1	2.49	0.47
1:A:480:LYS:HB2	1:A:534:ALA:HB1	1.96	0.47
1:B:292:ASN:ND2	1:B:294:GLN:HG3	2.30	0.47
1:B:92:ASP:HB2	1:B:95:VAL:CG2	2.45	0.47
1:A:238:PRO:HD3	1:A:277:THR:O	2.14	0.47
1:A:108:THR:HA	6:A:2026:HOH:O	2.15	0.47
1:B:300:VAL:HG23	1:B:301:SER:O	2.15	0.47
1:B:129:LYS:O	1:B:130:GLU:CG	2.63	0.46
1:A:152:PRO:O	1:A:154:THR:N	2.48	0.46
1:A:544:TRP:CD1	1:A:544:TRP:N	2.83	0.46
1:A:178:THR:HG23	6:A:2024:HOH:O	2.15	0.46
1:A:119:TYR:CE1	1:A:128:ASN:CB	2.74	0.46
1:A:410:ILE:HG22	1:A:411:CYS:N	2.31	0.46
1:A:202:TYR:HA	6:A:2043:HOH:O	2.16	0.46
1:A:528:PRO:HB3	1:A:532:TYR:CD2	2.51	0.46
1:A:279:VAL:HG13	1:A:364:TRP:CE2	2.51	0.46
1:B:219:ILE:O	1:B:223:ILE:HG12	2.16	0.46
1:A:158:ILE:O	1:A:159:THR:CB	2.64	0.45
1:A:348:TYR:N	1:A:348:TYR:HD1	2.14	0.45
1:A:162:ILE:CG2	1:A:170:PHE:CE1	2.98	0.45
1:A:473:GLN:HB3	6:A:2125:HOH:O	2.15	0.45
1:A:103:VAL:HB	1:A:113:PHE:CE2	2.52	0.45
1:B:222:LEU:HD13	1:B:526:ASN:HB3	1.98	0.45
1:A:433:MSE:HE1	1:A:477:ASP:HB3	1.99	0.45
1:A:203:PHE:HB2	1:A:500:ALA:HA	1.98	0.45
1:A:523:ASN:OD1	1:A:525:ASN:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:TRP:CE2	1:A:402:HIS:HE1	2.35	0.45
1:B:252:ILE:N	1:B:311:SER:OG	2.40	0.45
1:B:492:THR:CG2	1:B:493:SER:N	2.53	0.45
1:B:512:TRP:CZ3	2:B:1001:XYP:H5B1	2.51	0.45
1:A:160:LEU:HD12	1:A:161:SER:H	1.81	0.45
1:A:541:GLN:HA	1:A:544:TRP:CE2	2.52	0.45
1:A:392:TYR:CE2	1:A:422:GLY:HA3	2.51	0.45
1:B:76:ARG:HH22	1:B:164:THR:H	1.65	0.45
1:B:120:LEU:HD12	1:B:120:LEU:C	2.37	0.45
1:A:493:SER:HB2	6:A:2132:HOH:O	2.17	0.45
1:A:286:GLN:NE2	1:A:290:LYS:NZ	2.65	0.45
1:B:523:ASN:ND2	1:B:527[B]:GLN:HB2	2.32	0.45
1:A:119:TYR:OH	1:A:152:PRO:HG2	2.17	0.44
1:B:82:GLY:HA3	1:B:163:THR:HG22	1.99	0.44
1:B:316:MSE:O	1:B:320:ILE:HG13	2.16	0.44
1:A:179:ARG:HB2	6:A:2021:HOH:O	2.17	0.44
1:A:362:SER:HB3	1:A:365:VAL:HB	2.00	0.44
1:B:78:SER:C	1:B:80:SER:H	2.21	0.44
1:B:78:SER:O	1:B:80:SER:N	2.50	0.44
1:A:460:GLU:HG2	1:A:504:TRP:CZ3	2.52	0.44
1:A:335:VAL:HG21	1:A:374:ILE:HG23	1.99	0.44
1:A:156:VAL:N	6:A:2033:HOH:O	2.49	0.44
1:A:493:SER:CA	1:A:494:SER:CB	2.88	0.44
1:A:162:ILE:HG22	1:A:170:PHE:CE1	2.52	0.44
1:A:74:ILE:HG13	1:A:75:ASN:N	2.32	0.44
1:A:204:ARG:HG2	1:A:228:ASN:OD1	2.17	0.44
1:B:243:VAL:N	1:B:253:ARG:O	2.49	0.44
1:A:449:TYR:HA	1:A:452:ILE:HD12	2.00	0.44
1:A:471:SER:OG	1:A:474:GLN:HG3	2.18	0.44
1:A:493:SER:CB	6:A:2132:HOH:O	2.65	0.44
1:B:341:ASP:O	1:B:402:HIS:HE1	2.01	0.44
1:B:494:SER:HB2	1:B:497:LYS:HE2	2.00	0.43
1:B:162:ILE:HG22	1:B:170:PHE:CZ	2.53	0.43
1:A:98:LYS:O	1:A:177:ILE:HA	2.18	0.43
1:B:85:SER:OG	1:B:87:LYS:CE	2.49	0.43
1:B:382:ARG:NH2	1:B:421:ASP:OD1	2.45	0.43
1:A:159:THR:O	1:A:159:THR:HG22	2.14	0.43
1:A:193:ALA:CA	1:A:198:MSE:HE3	2.48	0.43
1:A:198:MSE:HE2	1:A:544:TRP:CH2	2.53	0.43
1:B:383:LYS:HD3	1:B:384:TYR:CZ	2.54	0.43
1:B:479:TYR:CD1	1:B:531:ALA:HB1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLY:O	1:B:85:SER:CB	2.66	0.43
1:B:41:PHE:HD1	1:B:71:MSE:HE3	1.83	0.43
1:B:507:ASN:HB2	1:B:523:ASN:O	2.18	0.43
1:A:395:ASP:O	1:A:426:GLN:HG3	2.18	0.43
1:A:347:ARG:HB3	1:A:348:TYR:CD1	2.54	0.43
1:A:463:ILE:HD12	1:A:479:TYR:CD2	2.54	0.43
1:A:489:ILE:O	6:A:2129:HOH:O	2.21	0.43
1:B:331:ALA:HA	1:B:390:LYS:O	2.19	0.43
1:A:56:TYR:O	1:A:57:LEU:HD12	2.18	0.43
1:A:216:ASN:N	6:A:2049:HOH:O	2.52	0.43
1:B:120:LEU:CD1	1:B:121:ASP:N	2.72	0.42
1:B:44:ASN:HA	6:B:2002:HOH:O	2.19	0.42
1:A:118:SER:HB3	1:A:129:LYS:HG3	2.00	0.42
1:A:152:PRO:C	1:A:154:THR:H	2.22	0.42
1:A:193:ALA:CA	1:A:198:MSE:CE	2.92	0.42
1:A:527[A]:GLN:NE2	6:A:2141:HOH:O	2.52	0.42
1:B:104:LYS:HD2	1:B:142:TRP:NE1	2.34	0.42
1:B:404:ARG:HD3	6:B:2160:HOH:O	2.20	0.42
1:A:464:SER:C	1:A:466:GLU:H	2.23	0.42
1:A:97:TYR:HB2	1:A:99:TYR:CE2	2.55	0.42
1:B:294:GLN:HE21	1:B:294:GLN:HA	1.85	0.42
1:B:341:ASP:O	1:B:402:HIS:CE1	2.72	0.42
1:B:119:TYR:O	1:B:127:GLU:CD	2.58	0.42
1:A:237:LYS:HE2	1:A:280:TRP:HZ3	1.80	0.41
1:B:110:THR:HG22	1:B:138:VAL:HG12	2.02	0.41
1:A:170:PHE:O	1:A:171:ILE:HG12	2.20	0.41
1:A:56:TYR:CE2	1:A:58:THR:HB	2.54	0.41
1:B:198:MSE:HG2	1:B:544:TRP:CE2	2.56	0.41
1:A:300:VAL:HG21	1:A:305:MSE:HE2	2.02	0.41
1:A:196:LYS:HB2	1:A:228:ASN:ND2	2.35	0.41
1:A:535:VAL:HA	1:A:538:ILE:HD12	2.02	0.41
1:B:50:ASN:N	6:B:2005:HOH:O	2.21	0.41
1:B:471:SER:OG	1:B:474:GLN:HG3	2.20	0.41
1:B:136:ASP:O	6:B:2035:HOH:O	2.22	0.41
1:A:541:GLN:C	1:A:543:GLU:H	2.23	0.41
1:A:223:ILE:H	1:A:223:ILE:HG12	1.70	0.41
1:A:245:SER:HB2	6:A:2057:HOH:O	2.20	0.41
1:A:540:PRO:O	1:A:543:GLU:HB2	2.20	0.41
1:B:292:ASN:OD1	1:B:297:GLY:HA3	2.21	0.41
1:B:113:PHE:HE2	1:B:170:PHE:CD1	2.39	0.41
1:A:275:GLY:HA3	1:A:332:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASN:HB3	6:A:2135:HOH:O	2.20	0.41
1:B:49:CYS:HB3	1:B:84:TYR:CE2	2.54	0.41
1:B:127:GLU:HB3	1:B:128:ASN:H	1.73	0.41
1:B:149:TYR:CG	1:B:150:LYS:N	2.88	0.41
1:B:104:LYS:HD2	1:B:142:TRP:CD1	2.55	0.41
1:B:76:ARG:HH12	1:B:164:THR:CG2	2.32	0.41
1:B:162:ILE:CG2	1:B:170:PHE:CE1	3.03	0.41
1:A:281:HIS:HB2	1:A:362:SER:HA	2.03	0.41
1:A:47:GLY:HA2	1:A:324:TYR:OH	2.21	0.41
1:B:115:LEU:O	1:B:132:ILE:HG13	2.21	0.41
1:B:53:VAL:HG22	1:B:53:VAL:O	2.21	0.41
1:A:112:THR:O	1:A:164:THR:HA	2.22	0.40
1:A:276:HIS:ND1	1:A:277:THR:HB	2.36	0.40
1:B:310:GLU:O	1:B:311:SER:C	2.59	0.40
1:A:286:GLN:HE21	1:A:290:LYS:NZ	2.19	0.40
1:A:75:ASN:ND2	1:A:75:ASN:O	2.54	0.40
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.87	0.40
1:B:371:ASN:HB3	1:B:374:ILE:HD12	2.03	0.40
1:A:537:SER:HB3	6:A:2143:HOH:O	2.21	0.40
1:B:173:ASP:OD1	1:B:174:ASP:N	2.55	0.40
1:A:331:ALA:HA	1:A:390:LYS:O	2.21	0.40
1:B:129:LYS:O	1:B:130:GLU:HG2	2.21	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	510/540 (94%)	427 (84%)	64 (12%)	19 (4%)	4	12
1	B	514/540 (95%)	451 (88%)	47 (9%)	16 (3%)	5	15
All	All	1024/1080 (95%)	878 (86%)	111 (11%)	35 (3%)	5	14

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	158	ILE
1	A	159	THR
1	A	494	SER
1	B	127	GLU
1	B	494	SER
1	A	153	LYS
1	A	542	SER
1	B	76	ARG
1	B	79	ALA
1	B	123	GLU
1	B	125	GLU
1	B	139	ALA
1	B	140	GLY
1	B	153	LYS
1	B	188	VAL
1	B	214	VAL
1	A	142	TRP
1	A	147	ALA
1	A	214	VAL
1	A	249	ASN
1	B	119	TYR
1	A	451	ASN
1	A	506	PRO
1	A	544	TRP
1	B	77	SER
1	B	506	PRO
1	A	104	LYS
1	A	77	SER
1	A	410	ILE
1	B	165	ASP
1	A	140	GLY
1	A	74	ILE
1	A	518	ALA
1	B	297	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/443 (98%)	387 (89%)	47 (11%)	8	21
1	B	433/443 (98%)	392 (90%)	41 (10%)	11	27
All	All	867/886 (98%)	779 (90%)	88 (10%)	9	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32[A]	MSE
1	A	32[B]	MSE
1	A	49	CYS
1	A	60	VAL
1	A	77	SER
1	A	86	GLU
1	A	95	VAL
1	A	104	LYS
1	A	106	ASN
1	A	108	THR
1	A	110	THR
1	A	112	THR
1	A	116	SER
1	A	119	TYR
1	A	122	SER
1	A	124	THR
1	A	128	ASN
1	A	130	GLU
1	A	143	THR
1	A	144	GLU
1	A	153	LYS
1	A	156	VAL
1	A	158	ILE
1	A	165	ASP
1	A	177	ILE
1	A	178	THR
1	A	203	PHE
1	A	214	VAL
1	A	261	SER
1	A	268	GLN
1	A	277	THR
1	A	303	SER
1	A	321	GLN

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Mol	Chain	Res	Type
1	A	332	TYR
1	A	340	SER
1	A	347	ARG
1	A	361	ARG
1	A	372	LYS
1	A	375	GLU
1	A	409	SER
1	A	434	ASN
1	A	480	LYS
1	A	494	SER
1	A	511	THR
1	A	516	GLN
1	A	533	ASN
1	A	535	VAL
1	B	33	ASP
1	B	51	LEU
1	B	58	THR
1	B	74	ILE
1	B	77	SER
1	B	78	SER
1	B	86	GLU
1	B	89	PHE
1	B	108	THR
1	B	115	LEU
1	B	119	TYR
1	B	120	LEU
1	B	124	THR
1	B	128	ASN
1	B	129	LYS
1	B	143	THR
1	B	150	LYS
1	B	157	ASN
1	B	178	THR
1	B	179	ARG
1	B	203	PHE
1	B	208	VAL
1	B	218	SER
1	B	245	SER
1	B	248	THR
1	B	268	GLN
1	B	277	THR
1	B	332	TYR

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Mol	Chain	Res	Type
1	B	346	THR
1	B	347	ARG
1	B	359	ASN
1	B	362	SER
1	B	382	ARG
1	B	388	ASN
1	B	421	ASP
1	B	462	ASP
1	B	466	GLU
1	B	480	LYS
1	B	494	SER
1	B	511	THR
1	B	512	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	294	GLN
1	A	388	ASN
1	A	402	HIS
1	A	416	ASN
1	A	434	ASN
1	A	447	GLN
1	A	516	GLN
1	A	541	GLN
1	B	128	ASN
1	B	294	GLN
1	B	298	ASN
1	B	474	GLN

### 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

2 carbohydrates 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$
3	XYP	A	1002	3	9,9,10	0.49	0	12,12,14	2.13	3 (25%)
3	XYP	A	1003	3	9,9,10	1.16	1 (11%)	12,12,14	1.62	2 (16%)

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	XYP	A	1002	3	3/3/3/4	0/0/14/17	0/1/1/1
3	XYP	A	1003	3	-	0/0/14/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	XYP	C4B-C3B	2.36	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	XYP	C4B-C3B-C2B	-5.50	105.80	111.24
3	A	1003	XYP	O3B-C3B-C2B	-2.08	106.24	110.00
3	A	1002	XYP	O2B-C2B-C1B	2.06	113.34	109.21
3	A	1002	XYP	C1B-C2B-C3B	2.95	113.03	109.54
3	A	1003	XYP	O4B-C4B-C3B	3.80	117.77	110.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1002	XYP	C4B

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Mol	Chain	Res	Type	Atom
3	A	1002	XYP	C2B
3	A	1002	XYP	C3B

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	XYP	6	0

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z  > 2$
2	XYP	A	1001	-	10,10,10	0.71	0	12,14,14	1.81	3 (25%)
5	PO4	A	1555	-	4,4,4	0.35	0	6,6,6	0.27	0
2	XYP	B	1001	2	10,10,10	0.97	0	12,14,14	0.90	1 (8%)
2	XYP	B	1002	2	9,9,10	1.17	1 (11%)	12,12,14	2.22	4 (33%)
2	XYP	B	1003	2	9,9,10	1.24	1 (11%)	12,12,14	2.45	7 (58%)
5	PO4	B	1553	-	4,4,4	0.40	0	6,6,6	0.30	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
2	XYP	A	1001	-	-	0/0/17/17	0/1/1/1
5	PO4	A	1555	-	-	0/0/0/0	0/0/0/0
2	XYP	B	1001	2	-	0/0/17/17	0/1/1/1
2	XYP	B	1002	2	-	0/0/14/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYP	B	1003	2	-	0/0/14/17	0/1/1/1
5	PO4	B	1553	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	XYP	C5B-C4B	2.02	1.57	1.52
2	B	1002	XYP	C2B-C3B	2.33	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	XYP	O3B-C3B-C4B	-3.58	103.54	110.00
2	B	1002	XYP	C1B-C2B-C3B	-3.08	105.90	109.54
2	A	1001	XYP	O5B-C5B-C4B	-2.54	106.73	110.86
2	B	1001	XYP	O3B-C3B-C4B	-2.38	105.70	110.00
2	A	1001	XYP	C4B-C3B-C2B	-2.16	107.37	111.04
2	B	1003	XYP	O3B-C3B-C2B	-2.02	106.35	110.00
2	B	1003	XYP	O5B-C1B-C2B	2.24	114.49	110.31
2	B	1002	XYP	O3B-C3B-C4B	2.56	114.63	110.00
2	B	1003	XYP	C5B-O5B-C1B	2.79	116.07	111.57
2	B	1003	XYP	C5B-C4B-C3B	3.10	113.21	109.54
2	B	1003	XYP	C4B-C3B-C2B	3.23	114.42	111.24
2	B	1003	XYP	C1B-C2B-C3B	3.28	113.42	109.54
2	B	1002	XYP	O3B-C3B-C2B	3.76	116.78	110.00
2	B	1003	XYP	O5B-C5B-C4B	3.83	117.46	110.31
2	B	1002	XYP	C5B-O5B-C1B	4.39	118.65	111.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	XYP	6	0
2	B	1001	XYP	2	0
2	B	1002	XYP	4	0
2	B	1003	XYP	4	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	504/540 (93%)	0.27	8 (1%) 74 70	42, 69, 106, 123	0
1	B	507/540 (93%)	0.15	9 (1%) 71 66	35, 55, 99, 122	0
All	All	1011/1080 (93%)	0.21	17 (1%) 73 68	35, 63, 103, 123	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	TYR	3.7
1	B	145	ILE	3.2
1	A	160	LEU	2.9
1	A	288	PHE	2.8
1	A	99	TYR	2.8
1	A	180	LYS	2.7
1	A	34	TYR	2.5
1	B	34	TYR	2.5
1	B	97	TYR	2.4
1	A	107	GLY	2.3
1	A	102	PHE	2.2
1	B	180	LYS	2.2
1	B	181	GLY	2.1
1	A	494	SER	2.1
1	B	60	VAL	2.1
1	B	147	ALA	2.0
1	B	170	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	XYP	A	1002	9/10	0.99	0.17	0.01	42,44,46,50	0
3	XYP	A	1003	9/10	0.96	0.12	-	55,70,73,73	0

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	A	1555	5/5	0.94	0.25	2.44	101,101,103,104	0
2	XYP	A	1001	10/10	0.97	0.19	0.55	49,53,55,60	0
2	XYP	B	1002	9/10	0.97	0.19	0.32	40,46,48,48	0
5	PO4	B	1553	5/5	0.93	0.17	-0.20	114,115,115,116	0
4	CA	B	1552	1/1	0.99	0.12	-0.83	58,58,58,58	0
2	XYP	B	1001	10/10	0.99	0.17	-0.84	40,42,44,44	0
4	CA	A	1552	1/1	0.91	0.13	-1.64	81,81,81,81	0
4	CA	A	1554	1/1	0.99	0.10	-2.30	62,62,62,62	0
4	CA	A	1553	1/1	0.88	0.14	-	95,95,95,95	0
2	XYP	B	1003	9/10	0.95	0.18	-	76,80,84,84	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.