



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:27 PM GMT

PDB ID : 1TPL  
Title : THE THREE-DIMENSIONAL STRUCTURE OF TYROSINE PHENOL-  
LYASE  
Authors : Antson, A.; Demidkina, T.; Dauter, Z.; Harutyunyan, E.; Wilson, K.  
Deposited on : 1992-11-25  
Resolution : 2.30 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

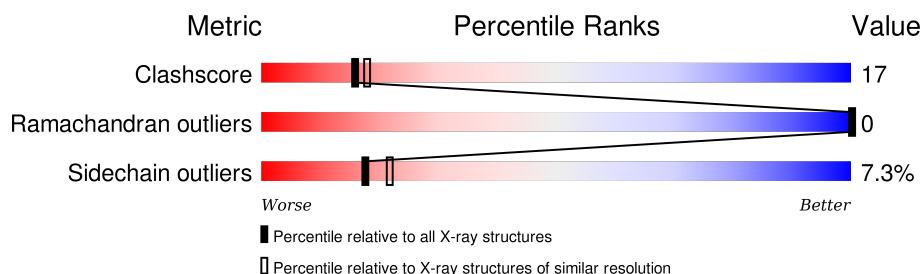
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	

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	SO4	A	458	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7194 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 TYROSINE PHENOL-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3361	2134	572	629	26			
1	B	426	Total	C	N	O	S	0	0	0
			3363	2136	573	628	26			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is water.

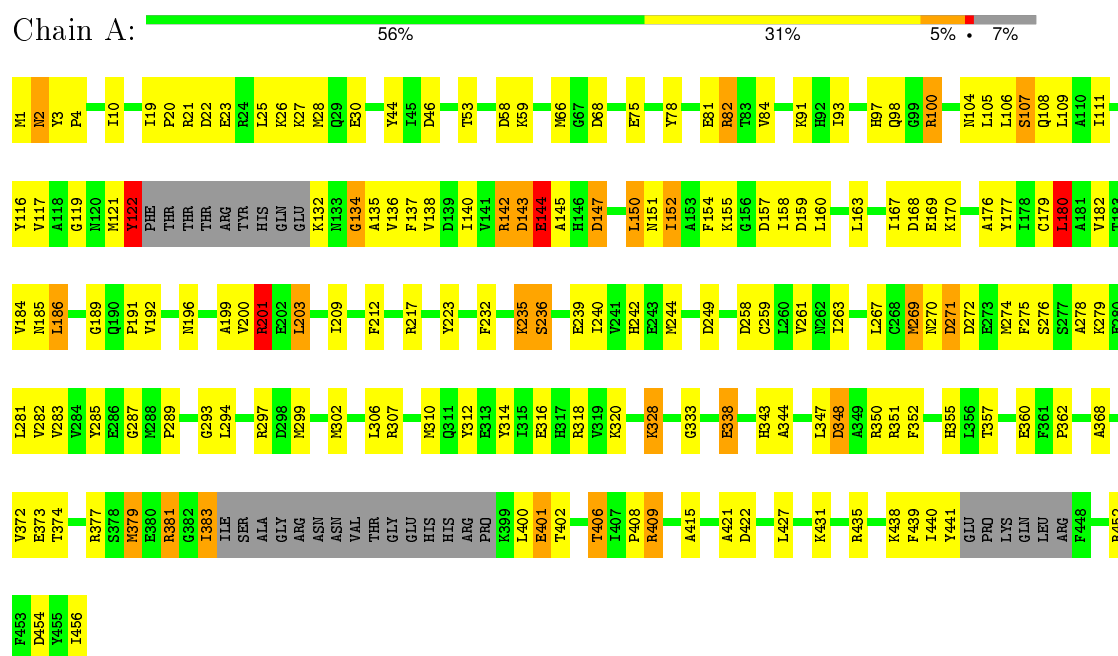
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	206	Total 206	O 206	0	0

### 3 Residue-property plots

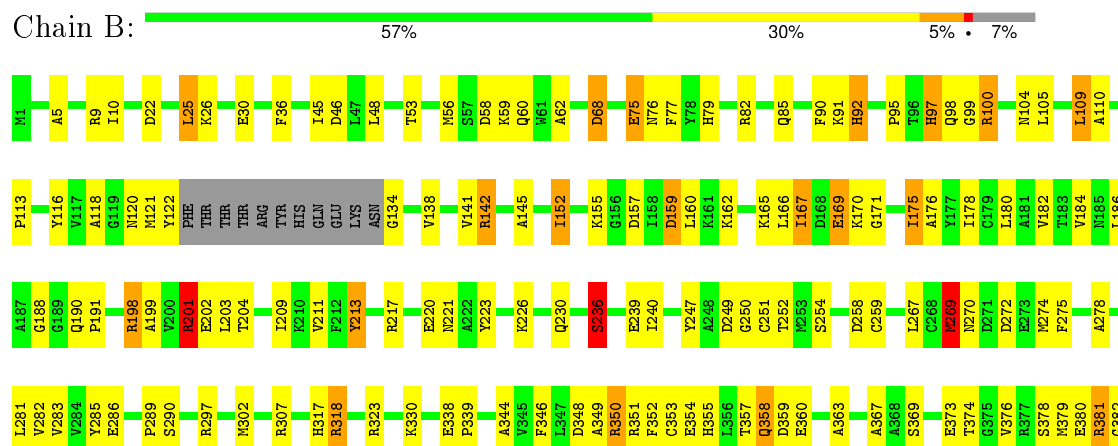
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: TYROSINE PHENOL-LYASE



#### • Molecule 1: TYROSINE PHENOL-LYASE



I383	I1E	SE	SE	ALA	GLY	ARG	ASN	ASN	VAL	TER	GLY	GLU	HIS	ARG	ARG	PRQ	K399	K400	R404	T405	T406	T407	P408	R409	R410	V420	A421	D422	I425	K426	Q429	H430	K431	E432	V440	V441	GLU	PRQ	LYS	GLN	R446	R447	F448	F449	T450	D454	Y455	T456
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.02Å 138.27Å 93.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.81	0/3423	1.69	56/4603 (1.2%)
1	B	0.81	0/3425	1.74	58/4606 (1.3%)
All	All	0.81	0/6848	1.71	114/9209 (1.2%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	NE-CZ-NH1	13.97	127.28	120.30
1	A	351	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	A	307	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	B	318	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	A	100	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	B	297	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	B	351	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	B	213	TYR	CB-CG-CD1	9.55	126.73	121.00
1	B	198	ARG	CD-NE-CZ	9.49	136.89	123.60
1	B	213	TYR	CB-CG-CD2	-9.42	115.35	121.00
1	B	350	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	297	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	B	198	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	58	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	58	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	A	377	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	201	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	B	58	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	B	440	ILE	C-N-CA	8.25	142.33	121.70
1	B	46	ASP	CB-CG-OD2	8.25	125.73	118.30
1	B	100	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	249	ASP	CB-CG-OD1	-8.12	110.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLU	CA-CB-CG	8.12	131.26	113.40
1	B	269	MET	N-CA-CB	7.93	124.87	110.60
1	B	455	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	A	258	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	159	ASP	CB-CG-OD1	7.45	125.01	118.30
1	B	307	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	351	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	46	ASP	CB-CG-OD2	7.38	124.94	118.30
1	B	409	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	B	62	ALA	CB-CA-C	7.17	120.86	110.10
1	B	82	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	169	GLU	CA-CB-CG	7.14	129.12	113.40
1	B	223	TYR	CB-CG-CD1	-7.02	116.79	121.00
1	A	271	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	100	ARG	CD-NE-CZ	6.90	133.26	123.60
1	B	258	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	223	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	A	379	MET	N-CA-CB	-6.69	98.57	110.60
1	A	122	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	44	TYR	CB-CG-CD1	6.58	124.95	121.00
1	A	186	LEU	CB-CA-C	6.51	122.57	110.20
1	B	186	LEU	CB-CA-C	6.43	122.42	110.20
1	A	338	GLU	OE1-CD-OE2	6.42	131.00	123.30
1	A	236	SER	CB-CA-C	-6.41	97.93	110.10
1	A	28	MET	CG-SD-CE	6.29	110.27	100.20
1	B	410	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	312	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	B	349	ALA	CB-CA-C	6.10	119.25	110.10
1	A	350	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	351	ARG	CD-NE-CZ	6.06	132.09	123.60
1	B	203	LEU	CB-CA-C	6.03	121.66	110.20
1	A	297	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	122	TYR	CA-CB-CG	6.00	124.79	113.40
1	B	269	MET	CA-CB-CG	5.99	123.49	113.30
1	A	409	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	B	455	TYR	CB-CG-CD2	5.97	124.58	121.00
1	A	297	ARG	CD-NE-CZ	-5.89	115.35	123.60
1	B	381	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	400	LEU	N-CA-CB	-5.84	98.72	110.40
1	A	66	MET	CA-CB-CG	-5.83	103.39	113.30
1	B	448	PHE	CA-C-N	-5.81	104.41	117.20
1	B	285	TYR	CB-CG-CD1	5.78	124.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ARG	CD-NE-CZ	5.76	131.67	123.60
1	B	449	PHE	CB-CA-C	5.69	121.79	110.40
1	B	201	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	236	SER	CB-CA-C	-5.66	99.36	110.10
1	A	348	ASP	CB-CA-C	5.65	121.69	110.40
1	A	217	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	92	HIS	CB-CA-C	-5.62	99.17	110.40
1	A	377	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	157	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	358	GLN	C-N-CA	5.58	135.66	121.70
1	A	168	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	143	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	220	GLU	CA-CB-CG	5.57	125.64	113.40
1	A	422	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	401	GLU	CG-CD-OE1	-5.51	107.28	118.30
1	A	310	MET	CG-SD-CE	5.51	109.01	100.20
1	A	374	THR	CA-CB-CG2	5.51	120.11	112.40
1	A	435	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	136	VAL	O-C-N	5.32	131.21	122.70
1	A	68	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	100	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	150	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	422	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	217	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	171	GLY	C-N-CA	5.25	134.82	121.70
1	A	81	GLU	CG-CD-OE2	-5.22	107.85	118.30
1	A	144	GLU	N-CA-CB	5.20	119.97	110.60
1	A	180	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	360	GLU	CG-CD-OE1	-5.18	107.94	118.30
1	A	360	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	B	323	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	B	350	ARG	CD-NE-CZ	5.17	130.84	123.60
1	B	318	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	A	81	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	203	LEU	CB-CA-C	5.16	120.00	110.20
1	A	82	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	367	ALA	CB-CA-C	5.14	117.81	110.10
1	A	22	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	432	GLU	CG-CD-OE1	5.13	128.55	118.30
1	B	97	HIS	CA-CB-CG	-5.12	104.89	113.60
1	A	152	ILE	N-CA-C	-5.08	97.28	111.00
1	A	409	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	68	ASP	CB-CA-C	5.06	120.52	110.40
1	A	134	GLY	C-N-CA	5.04	134.31	121.70
1	B	198	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	354	GLU	CB-CG-CD	5.02	127.74	114.20
1	A	144	GLU	OE1-CD-OE2	5.01	129.32	123.30
1	B	142	ARG	CG-CD-NE	5.01	122.33	111.80
1	B	157	ASP	CB-CG-OD1	5.01	122.81	118.30

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	3361	0	3319	113	0
1	B	3363	0	3323	117	0
2	A	10	0	0	2	0
2	B	10	0	0	0	0
3	A	244	0	0	13	0
3	B	206	0	0	25	2
All	All	7194	0	6642	228	2

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 (228) 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:441:TYR:CA	3:B:618:HOH:O	1.99	1.10
1:B:441:TYR:CB	3:B:618:HOH:O	1.97	1.09
1:B:441:TYR:HA	3:B:618:HOH:O	1.57	1.03
1:B:441:TYR:HB3	3:B:618:HOH:O	1.59	1.00
1:A:379:MET:HA	3:A:497:HOH:O	1.62	0.97
1:B:68:ASP:H	1:B:76:ASN:HD21	0.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASP:H	1:B:76:ASN:ND2	1.65	0.94
1:B:259:CYS:HB3	3:B:649:HOH:O	1.68	0.94
1:B:160:LEU:HD11	1:B:199:ALA:HB1	1.49	0.93
1:A:100:ARG:HH21	1:A:104:ASN:HB2	1.40	0.87
1:B:121:MET:HB2	1:B:184:VAL:HG23	1.57	0.85
1:B:68:ASP:N	1:B:76:ASN:HD21	1.76	0.84
1:A:134:GLY:HA3	3:A:668:HOH:O	1.77	0.83
1:A:150:LEU:HD22	1:A:151:ASN:H	1.47	0.78
1:A:2:ASN:HB2	3:A:678:HOH:O	1.84	0.77
1:A:145:ALA:HA	1:A:155:LYS:HG2	1.66	0.77
1:B:374:THR:O	3:B:552:HOH:O	2.02	0.77
1:B:75:GLU:HG3	3:B:522:HOH:O	1.86	0.75
1:A:271:ASP:HB3	1:A:274:MET:HB3	1.69	0.74
1:A:368:ALA:O	1:A:372:VAL:HG23	1.91	0.71
1:B:404:ARG:O	3:B:655:HOH:O	2.09	0.69
1:A:236:SER:HB2	1:A:239:GLU:HG3	1.73	0.69
1:B:178:ILE:HB	1:B:211:VAL:HG22	1.73	0.69
1:A:117:VAL:HG23	1:A:176:ALA:HB3	1.75	0.68
1:B:116:TYR:CZ	1:B:170:LYS:HG2	2.28	0.68
1:A:84:VAL:HG21	1:A:93:ILE:HD12	1.74	0.68
1:A:109:LEU:HD11	1:A:278:ALA:HB2	1.75	0.68
1:B:99:GLY:HA3	1:B:254:SER:HB2	1.75	0.68
1:B:357:THR:HB	1:B:360:GLU:HG3	1.75	0.68
1:B:338:GLU:HB3	1:B:339:PRO:HA	1.77	0.67
1:B:59:LYS:HD3	3:B:594:HOH:O	1.93	0.67
1:B:48:LEU:HD12	1:B:379:MET:HB2	1.75	0.67
1:B:204:THR:HB	1:B:209:ILE:HG22	1.77	0.66
1:A:151:ASN:HA	3:A:700:HOH:O	1.95	0.66
1:B:226:LYS:HB2	1:B:240:ILE:CD1	2.26	0.65
1:A:381:ARG:HG3	1:A:383:ILE:HD11	1.79	0.64
1:A:100:ARG:NH2	1:A:104:ASN:HB2	2.11	0.64
1:A:373:GLU:HB3	3:A:549:HOH:O	1.97	0.63
1:B:382:GLY:HA2	1:B:400:LEU:O	1.98	0.62
1:A:147:ASP:OD1	1:A:150:LEU:HB3	1.99	0.62
1:A:21:ARG:N	2:A:458:SO4:O3	2.31	0.62
1:B:122:TYR:N	3:B:635:HOH:O	2.32	0.62
1:B:97:HIS:H	1:B:97:HIS:HD1	1.48	0.62
1:A:106:LEU:HD23	1:A:107:SER:N	2.15	0.62
1:B:160:LEU:HD11	1:B:199:ALA:CB	2.27	0.62
1:B:383:ILE:HB	3:B:508:HOH:O	1.99	0.62
1:B:348:ASP:O	1:B:352:PHE:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:HG2	1:A:26:LYS:NZ	2.16	0.60
1:A:78:TYR:HB3	1:A:82:ARG:CZ	2.31	0.60
1:A:155:LYS:HD2	3:A:700:HOH:O	2.02	0.60
1:A:275:PHE:CZ	1:A:279:LYS:HD2	2.37	0.60
1:A:184:VAL:O	1:A:189:GLY:HA2	2.02	0.59
1:B:344:ALA:HB2	1:B:406:THR:HG23	1.83	0.59
1:A:383:ILE:HD12	3:A:664:HOH:O	2.02	0.59
1:A:294:LEU:HD23	1:A:299:MET:HG2	1.83	0.59
1:B:188:GLY:HA3	1:B:346:PHE:HE1	1.67	0.58
1:A:269:MET:HG3	1:A:274:MET:HG2	1.85	0.58
1:B:118:ALA:HB3	1:B:178:ILE:HD12	1.85	0.58
1:B:430:HIS:O	1:B:431:LYS:C	2.42	0.58
1:A:344:ALA:HB2	1:A:406:THR:HG23	1.86	0.58
1:A:242:HIS:HE1	3:A:610:HOH:O	1.85	0.57
1:B:100:ARG:HB2	3:B:533:HOH:O	2.04	0.57
1:A:116:TYR:O	1:A:176:ALA:N	2.33	0.57
1:A:232:PHE:HA	1:A:235:LYS:HG3	1.87	0.57
1:B:166:LEU:HG	1:B:175:ILE:HD11	1.86	0.57
1:A:105:LEU:O	1:A:109:LEU:HB2	2.04	0.56
1:B:431:LYS:HD2	3:B:646:HOH:O	2.04	0.56
1:B:353:CYS:HA	1:B:355:HIS:CE1	2.40	0.56
1:A:408:PRO:HB3	3:A:698:HOH:O	2.05	0.56
1:A:122:TYR:HD1	1:A:122:TYR:H	1.54	0.56
1:B:404:ARG:HB3	3:B:655:HOH:O	2.05	0.56
1:B:198:ARG:O	1:B:202:GLU:HG2	2.06	0.56
1:A:348:ASP:O	1:A:352:PHE:HB2	2.07	0.55
1:B:116:TYR:OH	1:B:170:LYS:HG2	2.06	0.55
1:A:373:GLU:HG3	1:A:427:LEU:HD21	1.87	0.55
1:A:272:ASP:O	1:A:275:PHE:HB3	2.06	0.55
1:B:121:MET:HB2	1:B:184:VAL:CG2	2.34	0.55
1:A:163:LEU:O	1:A:167:ILE:HG13	2.06	0.55
1:B:36:PHE:HB2	1:B:379:MET:HE3	1.89	0.55
1:B:376:VAL:HG21	1:B:420:VAL:HG22	1.89	0.54
1:B:155:LYS:NZ	1:B:338:GLU:O	2.40	0.54
1:A:106:LEU:HD21	1:A:177:TYR:OH	2.07	0.54
1:B:448:PHE:HB3	1:B:449:PHE:CD2	2.42	0.54
1:B:201:ARG:HA	1:B:201:ARG:HE	1.72	0.54
1:A:144:GLU:O	1:A:155:LYS:HE3	2.07	0.54
1:A:440:ILE:HG21	1:A:454:ASP:HB3	1.89	0.54
1:B:441:TYR:CD1	1:B:441:TYR:N	2.76	0.54
1:A:186:LEU:HD11	3:A:634:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:SER:HB2	1:A:239:GLU:CG	2.38	0.53
1:B:357:THR:HG22	1:B:359:ASP:H	1.73	0.53
1:A:150:LEU:HD22	1:A:151:ASN:N	2.20	0.53
1:B:45:ILE:HB	1:B:376:VAL:HG22	1.90	0.53
1:B:48:LEU:CD1	1:B:379:MET:HB2	2.37	0.53
1:A:53:THR:HG23	1:A:408:PRO:HB3	1.89	0.53
1:A:180:LEU:HD21	1:A:192:VAL:HG11	1.89	0.53
1:B:383:ILE:N	1:B:383:ILE:HD12	2.24	0.53
1:B:269:MET:HG2	1:B:274:MET:SD	2.49	0.52
1:A:23:GLU:O	1:A:27:LYS:HG2	2.10	0.52
1:A:362:PRO:HG2	1:A:401:GLU:OE1	2.10	0.52
1:A:381:ARG:HB3	1:A:383:ILE:HG12	1.91	0.52
1:A:142:ARG:HA	1:A:159:ASP:HB2	1.92	0.52
1:A:23:GLU:HG2	1:A:26:LYS:HZ1	1.75	0.51
1:A:201:ARG:HE	1:A:201:ARG:HA	1.74	0.51
1:A:106:LEU:HD21	1:A:177:TYR:CZ	2.45	0.51
1:A:167:ILE:HD13	1:A:209:ILE:HD12	1.93	0.51
1:B:105:LEU:O	1:B:109:LEU:HB2	2.11	0.51
1:A:373:GLU:CG	1:A:427:LEU:HD21	2.41	0.51
1:B:378:SER:HB3	1:B:405:LEU:HD23	1.93	0.51
1:B:77:PHE:HE1	1:B:95:PRO:HG3	1.76	0.51
1:A:121:MET:HG3	1:A:137:PHE:CZ	2.46	0.50
1:B:142:ARG:NH2	1:B:152:ILE:HD12	2.26	0.50
1:B:118:ALA:HB3	1:B:178:ILE:CD1	2.42	0.50
1:A:106:LEU:C	1:A:106:LEU:HD23	2.31	0.50
1:A:400:LEU:HD12	1:A:401:GLU:H	1.75	0.50
1:B:26:LYS:O	1:B:30:GLU:HG3	2.11	0.50
1:B:201:ARG:HE	1:B:201:ARG:CA	2.24	0.50
1:A:196:ASN:O	1:A:200:VAL:HG23	2.12	0.50
1:A:348:ASP:OD1	1:A:400:LEU:HD11	2.12	0.50
1:B:317:HIS:HD2	3:B:461:HOH:O	1.95	0.50
1:B:159:ASP:OD2	1:B:162:LYS:HG3	2.12	0.50
1:B:283:VAL:HG22	1:B:289:PRO:HD3	1.94	0.49
1:A:59:LYS:HD3	3:A:574:HOH:O	2.12	0.49
1:B:25:LEU:HD12	1:B:25:LEU:O	2.11	0.49
1:B:120:ASN:HA	1:B:141:VAL:HB	1.95	0.49
1:A:240:ILE:O	1:A:244:MET:HG3	2.12	0.49
1:B:155:LYS:HB2	3:B:525:HOH:O	2.12	0.49
1:B:440:ILE:HG12	1:B:454:ASP:HB2	1.93	0.49
1:A:121:MET:SD	1:A:179:CYS:SG	3.10	0.49
1:A:316:GLU:OE2	1:A:320:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD21	1:A:302:MET:HE1	1.95	0.48
1:B:302:MET:HG3	3:B:649:HOH:O	2.13	0.48
1:A:355:HIS:NE2	1:A:431:LYS:O	2.47	0.48
1:B:425:ILE:O	1:B:429:GLN:HG3	2.11	0.48
1:B:90:PHE:CE1	1:B:250:GLY:HA2	2.48	0.48
1:A:121:MET:H	1:A:121:MET:HG2	1.26	0.48
1:A:294:LEU:HD21	1:A:302:MET:CE	2.43	0.48
1:B:175:ILE:HD13	3:B:657:HOH:O	2.13	0.48
1:B:91:LYS:HG3	1:B:270:ASN:OD1	2.13	0.48
1:A:10:ILE:HG12	1:B:10:ILE:HG12	1.95	0.48
1:A:91:LYS:HD3	1:A:270:ASN:O	2.13	0.48
1:A:179:CYS:HA	1:A:212:PHE:O	2.14	0.48
1:B:190:GLN:OE1	1:B:190:GLN:HA	2.14	0.48
1:A:201:ARG:HA	1:A:201:ARG:NE	2.29	0.48
1:A:333:GLY:C	3:A:683:HOH:O	2.52	0.48
1:B:178:ILE:HB	1:B:211:VAL:CG2	2.43	0.47
1:A:283:VAL:HG22	1:A:289:PRO:HD3	1.96	0.47
1:B:145:ALA:HA	1:B:155:LYS:HG2	1.96	0.47
1:A:104:ASN:O	1:A:108:GLN:HG3	2.15	0.47
1:B:236:SER:HB3	1:B:239:GLU:H	1.80	0.47
1:A:109:LEU:HD11	1:A:278:ALA:CB	2.43	0.46
1:A:261:VAL:HG21	1:A:302:MET:HG3	1.97	0.46
1:B:109:LEU:HD21	1:B:278:ALA:HB2	1.97	0.46
1:A:169:GLU:HG3	1:A:170:LYS:HD2	1.97	0.46
1:B:213:TYR:O	1:B:251:CYS:HA	2.14	0.46
1:B:155:LYS:NZ	3:B:634:HOH:O	2.48	0.46
1:B:363:ALA:HB1	1:B:380:GLU:HB2	1.98	0.46
1:B:138:VAL:HG11	1:B:166:LEU:HD13	1.98	0.46
1:A:117:VAL:CG2	1:A:176:ALA:HB3	2.45	0.46
1:A:119:GLY:HA3	1:A:179:CYS:O	2.15	0.46
1:B:198:ARG:HG3	1:B:247:TYR:CE1	2.51	0.46
1:A:121:MET:SD	1:A:179:CYS:HB3	2.55	0.45
1:A:177:TYR:HE1	1:A:179:CYS:HB2	1.81	0.45
1:A:78:TYR:O	1:A:82:ARG:HD2	2.16	0.45
1:A:185:ASN:OD1	1:A:343:HIS:NE2	2.48	0.45
1:A:111:ILE:HG21	1:A:135:ALA:HB2	1.98	0.45
1:B:85:GLN:NE2	1:B:91:LYS:O	2.46	0.45
1:A:328:LYS:HD3	1:A:421:ALA:CB	2.47	0.45
1:B:259:CYS:CB	3:B:649:HOH:O	2.45	0.45
1:A:201:ARG:HE	1:A:201:ARG:CA	2.29	0.45
1:B:211:VAL:O	1:B:249:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:SER:O	1:B:373:GLU:HG2	2.17	0.45
1:A:98:GLN:HB2	3:A:673:HOH:O	2.17	0.45
1:A:20:PRO:HA	2:A:458:SO4:O3	2.17	0.44
1:A:415:ALA:HB1	1:B:5:ALA:HA	1.99	0.44
1:B:53:THR:HG23	1:B:408:PRO:HB3	1.99	0.44
1:A:281:LEU:O	1:A:285:TYR:HD1	2.00	0.44
1:B:352:PHE:O	1:B:431:LYS:HD2	2.17	0.44
1:B:79:HIS:HB3	3:B:516:HOH:O	2.18	0.44
1:A:381:ARG:HD2	1:A:381:ARG:HA	1.77	0.44
1:A:154:PHE:CD2	1:A:191:PRO:HB2	2.53	0.44
1:A:108:GLN:NE2	1:A:285:TYR:OH	2.51	0.44
1:B:116:TYR:CE1	1:B:170:LYS:HG2	2.51	0.44
1:B:97:HIS:NE2	1:B:98:GLN:NE2	2.57	0.43
1:A:160:LEU:HD21	1:A:199:ALA:HB1	1.99	0.43
1:B:379:MET:HB3	3:B:523:HOH:O	2.17	0.43
1:B:188:GLY:CA	1:B:346:PHE:HE1	2.30	0.43
1:A:26:LYS:O	1:A:30:GLU:HG3	2.18	0.43
1:B:252:THR:HG22	1:B:267:LEU:CD1	2.48	0.43
1:B:142:ARG:HA	1:B:159:ASP:HB2	1.99	0.43
1:B:191:PRO:HA	1:B:221:ASN:OD1	2.19	0.43
1:B:357:THR:O	1:B:358:GLN:C	2.57	0.43
1:B:407:ILE:HA	1:B:408:PRO:HD3	1.76	0.43
1:B:182:VAL:O	1:B:182:VAL:HG23	2.18	0.43
1:A:182:VAL:HG23	1:A:182:VAL:O	2.19	0.43
1:A:381:ARG:HB2	1:A:402:THR:OG1	2.19	0.43
1:A:440:ILE:O	1:A:440:ILE:HG13	2.18	0.43
1:B:167:ILE:HA	3:B:657:HOH:O	2.19	0.42
1:A:283:VAL:O	1:A:287:GLY:N	2.52	0.42
1:A:381:ARG:CG	1:A:383:ILE:HD11	2.46	0.42
1:A:314:TYR:OH	1:A:409:ARG:HD3	2.19	0.42
1:B:338:GLU:HB3	1:B:339:PRO:CA	2.48	0.42
1:A:438:LYS:HB3	1:A:456:ILE:HG22	2.01	0.42
1:B:56:MET:HA	1:B:60:GLN:OE1	2.20	0.42
1:A:347:LEU:O	1:A:402:THR:HA	2.20	0.42
1:B:353:CYS:HA	1:B:355:HIS:HE1	1.85	0.42
1:A:19:ILE:HA	1:A:20:PRO:HD3	1.80	0.42
1:A:97:HIS:HB3	1:A:293:GLY:O	2.20	0.42
1:A:236:SER:CB	1:A:239:GLU:H	2.32	0.41
1:A:3:TYR:HA	1:A:4:PRO:HD2	1.84	0.41
1:B:110:ALA:O	1:B:176:ALA:HB1	2.21	0.41
1:A:267:LEU:HD21	1:A:269:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:VAL:O	1:B:286:GLU:HB2	2.21	0.41
1:B:165:LYS:HG2	1:B:165:LYS:O	2.20	0.41
1:A:140:ILE:HG13	1:A:158:ILE:HG12	2.03	0.41
1:A:25:LEU:HD13	1:A:372:VAL:HG11	2.03	0.41
1:B:282:VAL:HG12	1:B:289:PRO:HA	2.02	0.41
1:A:282:VAL:HG12	1:A:289:PRO:HA	2.03	0.41
1:B:113:PRO:HB3	1:B:134:GLY:N	2.36	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.89	0.41
1:B:381:ARG:HA	1:B:381:ARG:HD2	1.88	0.41
1:B:166:LEU:CG	1:B:175:ILE:HD11	2.50	0.40
1:A:259:CYS:SG	1:A:306:LEU:HD13	2.62	0.40
1:B:77:PHE:CE1	1:B:95:PRO:HG3	2.56	0.40
1:B:9:ARG:HD2	3:B:652:HOH:O	2.22	0.40
1:B:92:HIS:HB3	1:B:275:PHE:CD1	2.56	0.40
1:B:422:ASP:O	1:B:426:LYS:HD2	2.20	0.40
1:B:440:ILE:HD12	1:B:440:ILE:O	2.21	0.40
1:B:350:ARG:NE	3:B:661:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:503:HOH:O	3:B:503:HOH:O[2_655]	0.62	1.58
3:B:471:HOH:O	3:B:471:HOH:O[2_655]	0.78	1.42

## 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	418/456 (92%)	396 (95%)	22 (5%)	0	100	100
1	B	418/456 (92%)	395 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	836/912 (92%)	791 (95%)	45 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	351/378 (93%)	322 (92%)	29 (8%)	14	17
1	B	351/378 (93%)	329 (94%)	22 (6%)	22	29
All	All	702/756 (93%)	651 (93%)	51 (7%)	17	22

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	75	GLU
1	A	107	SER
1	A	122	TYR
1	A	132	LYS
1	A	138	VAL
1	A	142	ARG
1	A	143	ASP
1	A	144	GLU
1	A	147	ASP
1	A	152	ILE
1	A	180	LEU
1	A	201	ARG
1	A	203	LEU
1	A	235	LYS
1	A	263	ILE
1	A	269	MET
1	A	276	SER
1	A	318	ARG

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Mol	Chain	Res	Type
1	A	328	LYS
1	A	338	GLU
1	A	357	THR
1	A	381	ARG
1	A	383	ILE
1	A	406	THR
1	A	439	PHE
1	A	441	TYR
1	A	452	ARG
1	B	22	ASP
1	B	25	LEU
1	B	104	ASN
1	B	109	LEU
1	B	152	ILE
1	B	167	ILE
1	B	169	GLU
1	B	175	ILE
1	B	201	ARG
1	B	230	GLN
1	B	236	SER
1	B	269	MET
1	B	272	ASP
1	B	281	LEU
1	B	290	SER
1	B	318	ARG
1	B	330	LYS
1	B	383	ILE
1	B	406	THR
1	B	441	TYR
1	B	448	PHE
1	B	450	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	190	GLN
1	A	311	GLN
1	B	39	ASN
1	B	76	ASN
1	B	98	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	317	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
2	SO4	A	457	-	4,4,4	0.97	0	6,6,6	0.46	0
2	SO4	A	458	-	4,4,4	1.26	0	6,6,6	0.65	0
2	SO4	B	457	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	B	458	-	4,4,4	1.28	0	6,6,6	0.33	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	SO4	A	457	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	458	-	-	0/0/0/0	0/0/0/0
2	SO4	B	457	-	-	0/0/0/0	0/0/0/0
2	SO4	B	458	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	458	SO4	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.