



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2024 – 01:36 pm BST

PDB ID : 5NHE  
Title : Crystal structure of xylose isomerase from *Piromyces* E2 in complex with two Cd<sup>2+</sup> ions and xylose  
Authors : Rozeboom, H.J.; Janssen, D.B.  
Deposited on : 2017-03-21  
Resolution : 1.86 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

<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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

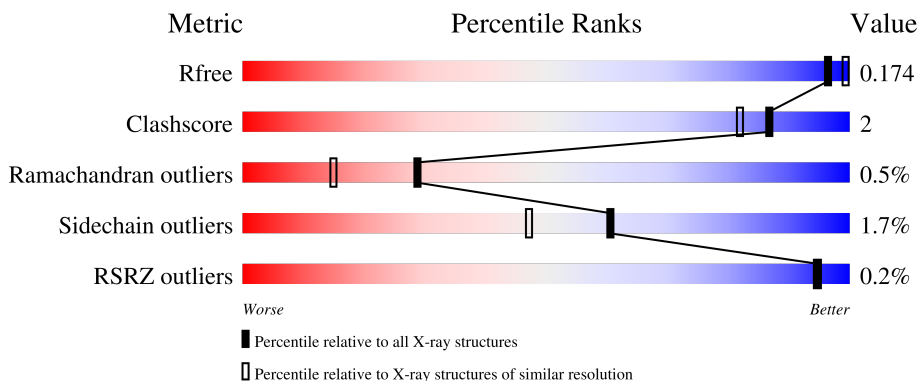
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	437	94% 5% .
1	B	437	95% 5%
1	C	437	95% . .
1	D	437	95% 5%

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
6	SO4	A	509	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15998 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.

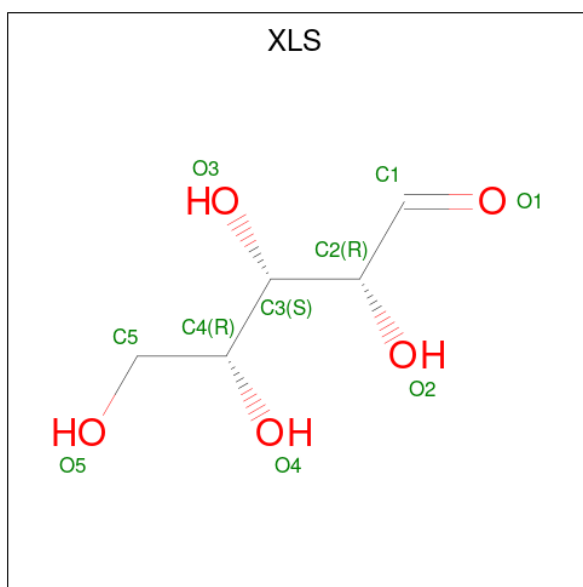
- Molecule 1 is a protein called Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3489	2215	584	669	21	0	3	0
1	B	436	3489	2214	584	670	21	0	3	0
1	C	436	3482	2210	583	668	21	0	2	0
1	D	436	3489	2214	584	670	21	0	3	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

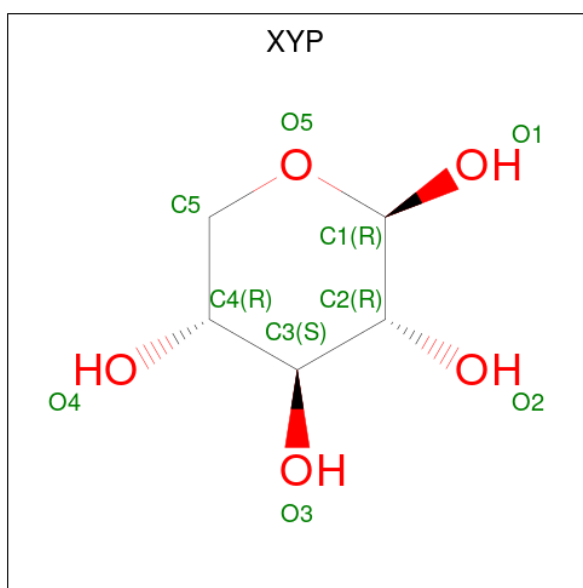
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 3	Cd 3	0	1
2	B	2	Total 3	Cd 3	0	1
2	C	2	Total 3	Cd 3	0	1
2	D	2	Total 3	Cd 3	0	1

- Molecule 3 is D-xylose (three-letter code: XLS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



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

- Molecule 4 is beta-D-xylopyranose (three-letter code: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



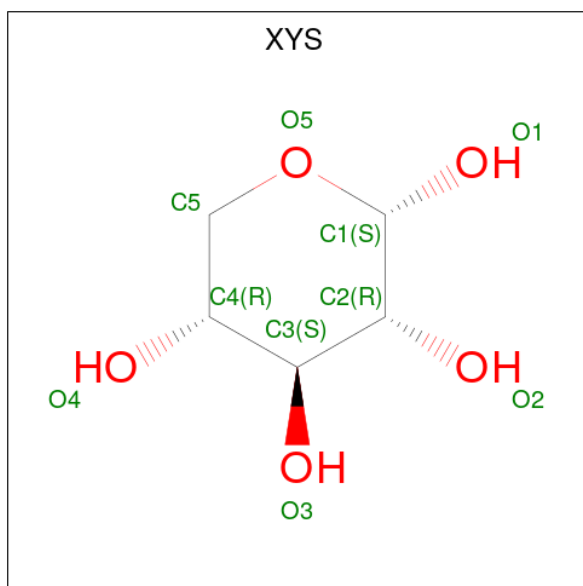
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	A	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	0
4	B	1	Total C O 10 5 5	0	0
4	B	1	Total C O 10 5 5	0	0
4	C	1	Total C O 10 5 5	0	0
4	C	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0

- Molecule 5 is alpha-D-xylopyranose (three-letter code: XYS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0
6	A	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	B	1	5	4	1	0	0
6	C	1	5	4	1	0	0
6	D	1	5	4	1	0	0
6	D	1	5	4	1	0	0
6	D	1	5	4	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	451	Total O 451 451	0	0
7	B	477	Total O 477 477	0	0
7	C	446	Total O 446 446	0	0
7	D	463	Total O 463 463	0	0



### 3 Residue-property plots [i](#)

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

- Molecule 1: Xylose isomerase

Chain A:  94% 5%



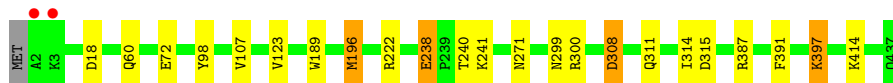
- Molecule 1: Xylose isomerase

Chain B:  95% 5%



- Molecule 1: Xylose isomerase

Chain C:  95% 5%



- Molecule 1: Xylose isomerase

Chain D:  95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.64Å 79.37Å 92.01Å 115.37° 89.97° 117.16°	Depositor
Resolution (Å)	45.10 – 1.86 45.16 – 1.86	Depositor EDS
% Data completeness (in resolution range)	88.2 (45.10-1.86) 88.3 (45.16-1.86)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.87Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.140 , 0.165 0.151 , 0.174	Depositor DCC
$R_{free}$ test set	6456 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for k,h,-h-k-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: XLS, XYS, CD, XYP, 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	0.58	1/3570 (0.0%)	0.73	5/4805 (0.1%)
1	B	0.59	1/3570 (0.0%)	0.73	2/4805 (0.0%)
1	C	0.58	0/3563	0.72	4/4795 (0.1%)
1	D	0.60	0/3570	0.72	3/4805 (0.1%)
All	All	0.59	2/14273 (0.0%)	0.73	14/19210 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	GLU	CD-OE1	-6.38	1.18	1.25
1	A	369	GLU	CD-OE1	-5.31	1.19	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	222	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	222	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	222	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	435	MET	CG-SD-CE	5.91	109.65	100.20
1	C	18	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	C	300	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	387	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	387	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	387	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	300	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	222	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	387	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	435	MET	CG-SD-CE	5.00	108.20	100.20

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	3489	0	3376	21	0
1	B	3489	0	3374	12	0
1	C	3482	0	3368	15	0
1	D	3489	0	3374	12	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	10	0	8	1	0
3	B	10	0	8	0	0
4	A	30	0	0	1	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	10	0	0	0	0
5	A	10	0	10	0	0
5	B	10	0	10	0	0
5	C	20	0	18	1	0
5	D	20	0	18	1	0
6	A	10	0	0	2	0
6	B	10	0	0	1	0
6	C	5	0	0	1	0
6	D	15	0	0	1	0
7	A	451	0	0	7	0
7	B	477	0	0	2	0
7	C	446	0	0	4	0
7	D	463	0	0	5	0
All	All	15998	0	13564	59	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 2.

All (59) 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:10:GLN:OE1	4:A:507:XYP:O3	1.99	0.79
1:A:60:GLN:HG2	1:C:60:GLN:HG2	1.68	0.76
1:B:196[B]:MET:CE	1:B:240:THR:HA	2.16	0.75
1:C:196[B]:MET:CE	1:C:240:THR:HA	2.17	0.74
1:A:196[B]:MET:CE	1:A:240:THR:HA	2.18	0.74
1:A:35:MET:HE2	1:A:376:GLN:HG2	1.68	0.73
1:B:196[B]:MET:HE1	1:B:240:THR:HA	1.69	0.73
1:C:196[A]:MET:SD	7:C:905:HOH:O	2.48	0.71
1:A:196[A]:MET:SD	7:A:888:HOH:O	2.48	0.71
1:B:196[B]:MET:HG2	7:D:684:HOH:O	1.91	0.70
6:B:507:SO4:O1	7:B:601:HOH:O	2.08	0.70
1:B:60:GLN:HG2	1:D:60:GLN:HG2	1.74	0.69
1:A:351:GLU:N	6:A:509:SO4:O1	2.24	0.69
6:A:509:SO4:O3	7:A:601:HOH:O	2.12	0.67
1:C:196[B]:MET:HE2	1:C:240:THR:HA	1.79	0.64
1:A:196[B]:MET:HE2	1:A:240:THR:HA	1.82	0.62
1:A:107:VAL:HB	1:A:123[A]:VAL:HG21	1.82	0.61
1:D:107:VAL:HB	1:D:123:VAL:HG21	1.82	0.60
3:A:503:XLS:C1	7:A:785:HOH:O	2.50	0.60
1:A:346:ASN:H	1:A:346:ASN:HD22	1.50	0.59
1:C:107:VAL:HB	1:C:123:VAL:HG21	1.84	0.59
7:A:675:HOH:O	1:C:196[B]:MET:HG2	2.01	0.59
1:B:107:VAL:HB	1:B:123:VAL:HG21	1.84	0.57
1:A:437:GLN:NE2	7:A:604:HOH:O	2.38	0.57
1:A:196[B]:MET:HG2	7:C:760:HOH:O	2.06	0.55
1:D:196[B]:MET:SD	1:D:240:THR:HA	2.48	0.54
1:A:196[B]:MET:HE1	1:A:240:THR:HA	1.91	0.52
1:D:2:ALA:HA	7:D:965:HOH:O	2.08	0.52
1:C:391:PHE:O	1:C:397:LYS:HE3	2.08	0.52
1:C:196[B]:MET:HE1	1:C:240:THR:HA	1.93	0.50
1:D:351:GLU:N	6:D:507:SO4:O4	2.39	0.50
1:B:238:GLU:OE1	1:B:308:ASP:HB2	2.12	0.50
1:D:196[A]:MET:HE3	7:D:828:HOH:O	2.12	0.49
1:D:238:GLU:OE1	1:D:308:ASP:HB2	2.11	0.49
1:A:238:GLU:OE1	1:A:308:ASP:HB2	2.13	0.49
1:C:238:GLU:OE1	1:C:308:ASP:HB2	2.12	0.49
1:C:196[A]:MET:HE3	7:C:852:HOH:O	2.12	0.49
1:B:299:ASN:HB2	1:B:311:GLN:O	2.15	0.47
1:C:196[B]:MET:HE3	1:C:196[B]:MET:HA	1.96	0.47
1:A:282:HIS:CD2	1:B:195:TYR:OH	2.69	0.46
7:B:729:HOH:O	1:D:196[A]:MET:HG2	2.15	0.46
1:C:299:ASN:HB2	1:C:311:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:HB2	1:A:311:GLN:O	2.15	0.46
1:D:299:ASN:HB2	1:D:311:GLN:O	2.16	0.46
1:A:437:GLN:CD	7:A:604:HOH:O	2.55	0.46
1:A:196[B]:MET:HE3	1:A:196[B]:MET:HA	2.00	0.44
1:D:343[A]:THR:HG22	1:D:347:SER:HB2	2.00	0.44
1:A:282:HIS:HD2	1:B:195:TYR:OH	2.01	0.44
1:B:343[A]:THR:HG22	1:B:347:SER:HB2	1.99	0.43
6:C:507:SO4:O3	7:C:601:HOH:O	2.21	0.43
1:B:196[A]:MET:HG2	7:D:684:HOH:O	2.19	0.42
1:D:210:MET:CE	7:D:860:HOH:O	2.68	0.42
1:C:98:TYR:OH	4:C:506:XYP:O1	2.18	0.42
1:A:140:TRP:HB3	1:A:185:ASN:HB2	2.02	0.42
1:D:258:HIS:HE1	5:D:504:XYS:O4	2.04	0.41
1:C:189:TRP:CD2	5:C:503:XYS:H2	2.56	0.41
1:A:196[B]:MET:SD	1:A:196[B]:MET:N	2.95	0.40
1:B:315:ASP:OD2	1:C:315:ASP:OD2	2.40	0.40
1:A:196[A]:MET:HE3	7:A:908:HOH:O	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	437/437 (100%)	428 (98%)	7 (2%)	2 (0%)	29	15
1	B	437/437 (100%)	427 (98%)	8 (2%)	2 (0%)	29	15
1	C	436/437 (100%)	428 (98%)	6 (1%)	2 (0%)	29	15
1	D	437/437 (100%)	428 (98%)	7 (2%)	2 (0%)	29	15
All	All	1747/1748 (100%)	1711 (98%)	28 (2%)	8 (0%)	29	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	GLU
1	B	238	GLU
1	C	238	GLU
1	D	238	GLU
1	A	314	ILE
1	B	314	ILE
1	C	314	ILE
1	D	314	ILE

### 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	360/358 (101%)	354 (98%)	6 (2%)	60	47
1	B	360/358 (101%)	352 (98%)	8 (2%)	52	36
1	C	359/358 (100%)	351 (98%)	8 (2%)	52	36
1	D	360/358 (101%)	354 (98%)	6 (2%)	60	47
All	All	1439/1432 (100%)	1411 (98%)	28 (2%)	60	43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196[A]	MET
1	A	196[B]	MET
1	A	241	LYS
1	A	271	ASN
1	A	346	ASN
1	A	414	LYS
1	B	72	GLU
1	B	121	LYS
1	B	196[A]	MET
1	B	196[B]	MET
1	B	241	LYS
1	B	271	ASN
1	B	397	LYS
1	B	414	LYS

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Mol	Chain	Res	Type
1	C	72	GLU
1	C	196[A]	MET
1	C	196[B]	MET
1	C	241	LYS
1	C	271	ASN
1	C	308	ASP
1	C	397	LYS
1	C	414	LYS
1	D	196[A]	MET
1	D	196[B]	MET
1	D	241	LYS
1	D	271	ASN
1	D	397	LYS
1	D	414	LYS

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

Mol	Chain	Res	Type
1	A	60	GLN
1	A	282	HIS
1	A	346	ASN
1	D	8	GLN
1	D	60	GLN
1	D	258	HIS
1	D	311	GLN
1	D	370	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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
5	XYS	D	504	-	10,10,10	0.95	0	14,14,14	1.08	1 (7%)
6	SO4	A	508	-	4,4,4	0.48	0	6,6,6	0.24	0
5	XYS	B	505	-	10,10,10	1.00	1 (10%)	14,14,14	1.45	3 (21%)
6	SO4	B	507	-	4,4,4	0.32	0	6,6,6	0.39	0
3	XLS	B	503	2	8,9,9	0.86	0	10,11,11	1.93	4 (40%)
5	XYS	C	505	-	10,10,10	0.96	0	14,14,14	1.25	0
5	XYS	D	503	2	10,10,10	1.37	2 (20%)	14,14,14	1.64	2 (14%)
4	XYP	B	506	-	10,10,10	0.50	0	14,14,14	1.20	2 (14%)
6	SO4	B	508	-	4,4,4	0.54	0	6,6,6	0.83	0
4	XYP	A	504	-	10,10,10	0.42	0	14,14,14	1.30	2 (14%)
6	SO4	D	508	-	4,4,4	0.47	0	6,6,6	0.50	0
4	XYP	C	506	-	10,10,10	1.18	2 (20%)	14,14,14	3.28	9 (64%)
3	XLS	A	503	2	8,9,9	0.46	0	10,11,11	0.92	0
4	XYP	A	507	-	10,10,10	0.60	0	14,14,14	1.19	2 (14%)
4	XYP	B	504	-	10,10,10	0.41	0	14,14,14	1.16	1 (7%)
6	SO4	D	507	-	4,4,4	0.53	0	6,6,6	0.40	0
4	XYP	A	506	-	10,10,10	0.50	0	14,14,14	0.91	0
4	XYP	D	505	-	10,10,10	0.87	0	14,14,14	2.43	4 (28%)
6	SO4	C	507	-	4,4,4	0.62	0	6,6,6	0.49	0
6	SO4	D	506	-	4,4,4	0.64	0	6,6,6	0.55	0
5	XYS	A	505	-	10,10,10	1.15	1 (10%)	14,14,14	1.79	3 (21%)
5	XYS	C	503	2	10,10,10	1.95	3 (30%)	14,14,14	2.35	5 (35%)
6	SO4	A	509	-	4,4,4	0.44	0	6,6,6	0.28	0
4	XYP	C	504	-	10,10,10	0.61	0	14,14,14	1.32	1 (7%)

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
5	XYS	D	503	2	-	-	0/1/1/1
4	XYP	D	505	-	-	-	0/1/1/1
5	XYS	D	504	-	-	-	0/1/1/1
4	XYP	B	506	-	-	-	0/1/1/1
5	XYS	B	505	-	-	-	0/1/1/1
4	XYP	C	506	-	-	-	0/1/1/1
5	XYS	A	505	-	-	-	0/1/1/1
3	XLS	A	503	2	-	6/10/12/12	-
5	XYS	C	503	2	-	-	0/1/1/1
4	XYP	A	507	-	-	-	0/1/1/1
4	XYP	B	504	-	-	-	0/1/1/1
4	XYP	A	504	-	-	-	0/1/1/1
3	XLS	B	503	2	-	5/10/12/12	-
5	XYS	C	505	-	-	-	0/1/1/1
4	XYP	C	504	-	-	-	0/1/1/1
4	XYP	A	506	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	XYS	O5-C1	4.46	1.49	1.43
5	D	503	XYS	O5-C1	2.91	1.47	1.43
4	C	506	XYP	C4-C3	2.73	1.56	1.52
5	C	503	XYS	C4-C3	2.68	1.56	1.52
5	A	505	XYS	C4-C3	2.35	1.56	1.52
5	B	505	XYS	C4-C3	2.19	1.55	1.52
5	D	503	XYS	O1-C1	2.18	1.46	1.39
4	C	506	XYP	O5-C1	2.07	1.46	1.43
5	C	503	XYS	O1-C1	2.03	1.46	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	XYP	C4-C3-C2	-5.69	101.05	110.89
4	D	505	XYP	C5-O5-C1	5.41	121.81	112.71
5	C	503	XYS	C5-C4-C3	4.91	115.70	109.67
4	D	505	XYP	O5-C5-C4	4.72	118.06	110.77
4	C	506	XYP	C5-C4-C3	-4.58	104.04	109.67
4	C	506	XYP	O2-C2-C3	4.38	120.47	110.35
4	C	504	XYP	C5-C4-C3	4.19	114.82	109.67
4	C	506	XYP	C5-O5-C1	4.16	119.70	112.71
5	A	505	XYS	O5-C5-C4	4.05	117.02	110.77
5	D	503	XYS	C5-C4-C3	4.01	114.60	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	506	XYP	O3-C3-C2	3.72	118.94	110.35
4	C	506	XYP	C1-C2-C3	-3.62	102.80	110.31
4	C	506	XYP	O5-C1-C2	3.55	114.71	109.43
5	A	505	XYS	C5-O5-C1	3.47	118.55	112.71
4	A	504	XYP	C5-C4-C3	3.40	113.84	109.67
4	C	506	XYP	O4-C4-C3	3.38	116.91	110.14
5	C	503	XYS	O5-C1-C2	3.31	114.35	109.43
3	B	503	XLS	O2-C2-C1	3.27	117.79	110.08
4	D	505	XYP	C4-C3-C2	-3.26	105.25	110.89
5	C	503	XYS	O3-C3-C4	3.24	116.21	109.99
5	B	505	XYS	O5-C5-C4	3.13	115.60	110.77
4	D	505	XYP	C1-C2-C3	-3.07	103.94	110.31
4	B	506	XYP	O5-C5-C4	-3.01	106.13	110.77
3	B	503	XLS	C5-C4-C3	-3.01	105.90	112.41
5	C	503	XYS	O1-C1-O5	2.98	117.49	109.72
5	D	503	XYS	O1-C1-O5	2.89	117.24	109.72
5	B	505	XYS	C5-O5-C1	2.83	117.46	112.71
5	C	503	XYS	O3-C3-C2	-2.82	103.83	110.35
5	A	505	XYS	O5-C1-C2	2.55	113.22	109.43
4	B	504	XYP	C4-C3-C2	-2.52	106.53	110.89
3	B	503	XLS	C3-C2-C1	-2.48	103.29	111.10
5	B	505	XYS	O5-C1-C2	2.46	113.08	109.43
4	A	507	XYP	C5-C4-C3	2.42	112.64	109.67
3	B	503	XLS	O4-C4-C5	2.39	114.74	109.14
4	A	507	XYP	O5-C1-C2	-2.18	106.19	109.43
4	C	506	XYP	O4-C4-C5	2.12	113.50	109.15
5	D	504	XYS	O2-C2-C1	-2.12	104.24	109.16
4	A	504	XYP	O4-C4-C3	-2.10	105.93	110.14
4	B	506	XYP	O4-C4-C3	-2.10	105.93	110.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	XLS	C2-C3-C4-C5
3	B	503	XLS	C2-C3-C4-O4
3	B	503	XLS	O3-C3-C4-C5
3	B	503	XLS	O3-C3-C4-O4
3	A	503	XLS	O3-C3-C4-C5
3	A	503	XLS	C2-C3-C4-C5
3	A	503	XLS	C3-C4-C5-O5
3	B	503	XLS	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
3	A	503	XLS	O3-C3-C4-O4
3	A	503	XLS	C2-C3-C4-O4
3	A	503	XLS	O4-C4-C5-O5

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	504	XYS	1	0
6	B	507	SO4	1	0
4	C	506	XYP	1	0
3	A	503	XLS	1	0
4	A	507	XYP	1	0
6	D	507	SO4	1	0
6	C	507	SO4	1	0
5	C	503	XYS	1	0
6	A	509	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 [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	436/437 (99%)	-0.36	1 (0%) 95   94	9, 15, 28, 47	0
1	B	436/437 (99%)	-0.38	0 100   100	9, 14, 28, 52	0
1	C	436/437 (99%)	-0.38	2 (0%) 91   91	9, 15, 28, 63	0
1	D	436/437 (99%)	-0.37	0 100   100	9, 14, 28, 37	0
All	All	1744/1748 (99%)	-0.37	3 (0%) 95   94	9, 15, 28, 63	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	4.6
1	A	2	ALA	3.1
1	C	3	LYS	3.0

### 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XYP	D	505	10/10	0.74	0.25	59,68,73,74	0
4	XYP	C	506	10/10	0.79	0.38	29,38,40,44	0
4	XYP	A	506	10/10	0.80	0.23	57,61,62,64	0
5	XYS	D	503	10/10	0.82	0.24	31,41,44,45	0
6	SO4	C	507	5/5	0.82	0.20	46,54,55,57	0
6	SO4	D	506	5/5	0.83	0.38	47,54,70,71	0
5	XYS	A	505	10/10	0.84	0.25	29,36,38,40	0
5	XYS	C	503	10/10	0.84	0.22	31,36,40,42	0
5	XYS	C	505	10/10	0.84	0.27	28,38,39,41	0
6	SO4	D	507	5/5	0.84	0.31	45,60,71,75	0
4	XYP	B	504	10/10	0.85	0.21	44,47,49,49	0
4	XYP	A	507	10/10	0.85	0.28	48,51,52,52	0
5	XYS	B	505	10/10	0.86	0.22	24,34,35,36	0
4	XYP	B	506	10/10	0.87	0.21	46,54,57,57	0
4	XYP	A	504	10/10	0.88	0.20	36,41,46,47	0
4	XYP	C	504	10/10	0.88	0.21	50,53,54,54	0
3	XLS	B	503	10/10	0.90	0.19	28,34,46,47	0
6	SO4	A	509	5/5	0.92	0.23	48,50,57,58	0
5	XYS	D	504	10/10	0.92	0.16	23,30,31,33	0
3	XLS	A	503	10/10	0.93	0.14	29,33,41,51	0
6	SO4	B	507	5/5	0.95	0.18	40,46,51,54	0
6	SO4	A	508	5/5	0.95	0.32	40,41,43,45	0
6	SO4	B	508	5/5	0.98	0.18	29,32,34,37	0
6	SO4	D	508	5/5	0.98	0.18	25,26,28,31	0
2	CD	A	501	1/1	1.00	0.03	16,16,16,16	1
2	CD	A	502[A]	1/1	1.00	0.05	15,15,15,15	1
2	CD	A	502[B]	1/1	1.00	0.05	30,30,30,30	1
2	CD	B	501	1/1	1.00	0.04	14,14,14,14	1
2	CD	B	502[A]	1/1	1.00	0.05	12,12,12,12	1
2	CD	B	502[B]	1/1	1.00	0.05	23,23,23,23	1
2	CD	C	501	1/1	1.00	0.03	14,14,14,14	1
2	CD	C	502[A]	1/1	1.00	0.04	14,14,14,14	1
2	CD	C	502[B]	1/1	1.00	0.04	24,24,24,24	1
2	CD	D	501	1/1	1.00	0.03	13,13,13,13	1
2	CD	D	502[A]	1/1	1.00	0.05	18,18,18,18	1
2	CD	D	502[B]	1/1	1.00	0.05	21,21,21,21	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.