



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:46 PM GMT

PDB ID : 4JFW  
Title : Crystal structure of a bacterial fucosidase with iminosugar inhibitor (2S,3S,4R,5S)-2-[N-(propylferrocene)]aminoethyl-5-methylpyrrolidine-3,4-diol  
Authors : Wright, D.W.; Davies, G.J.  
Deposited on : 2013-02-28  
Resolution : 2.10 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

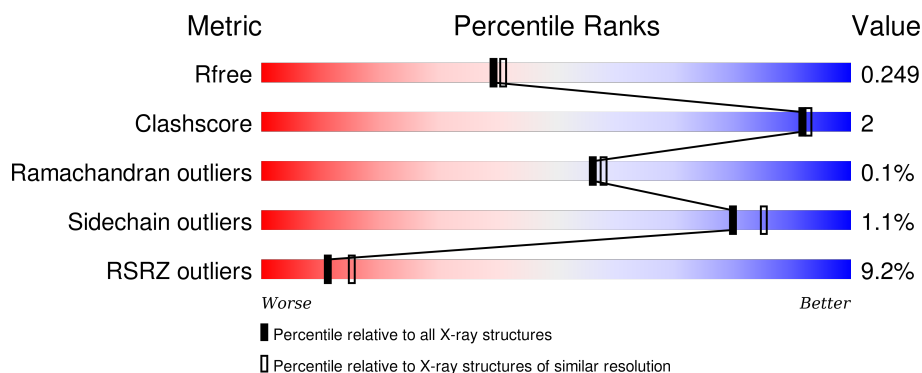
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	450	<div> <div>7%</div> <div>92%</div> <div>5%</div> </div>
1	B	450	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
1	C	450	<div> <div>10%</div> <div>92%</div> <div>6%</div> </div>
1	D	450	<div> <div>12%</div> <div>92%</div> <div>5%</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
3	SO4	B	503	-	-	X	-

## 2 Entry composition [i](#)

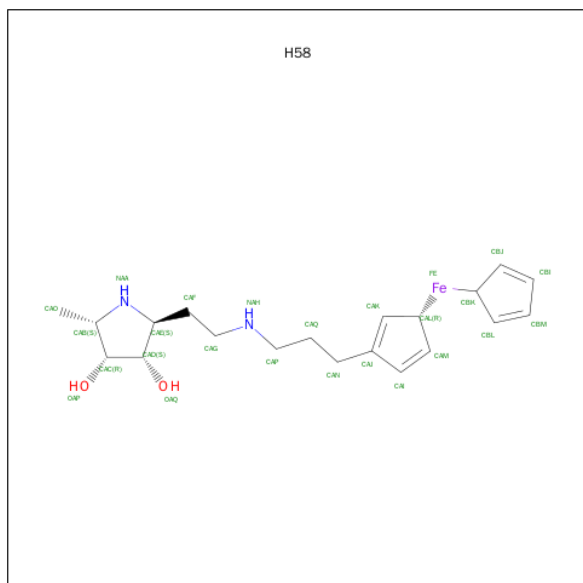
There are 5 unique types of molecules in this entry. The entry contains 14229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3491	2248	584	643	16			
1	B	439	Total	C	N	O	S	0	0	0
			3461	2227	578	640	16			
1	C	439	Total	C	N	O	S	0	0	0
			3460	2224	577	643	16			
1	D	438	Total	C	N	O	S	0	0	0
			3447	2215	576	640	16			

- Molecule 2 is (3ALPHA)-[3-({2-[(2S,3S,4R,5S)-3,4-DIHYDROXY-5-METHYLPYRROLIDIN-2-YL]ETHYL}AMINO)PROPYL]FERROCENE (three-letter code: H58) (formula: C<sub>20</sub>H<sub>30</sub>FeN<sub>2</sub>O<sub>2</sub>).



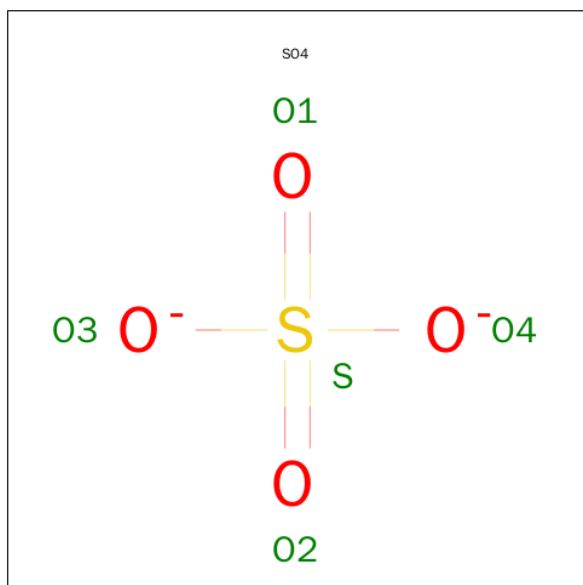
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			25	20	1	2	2		

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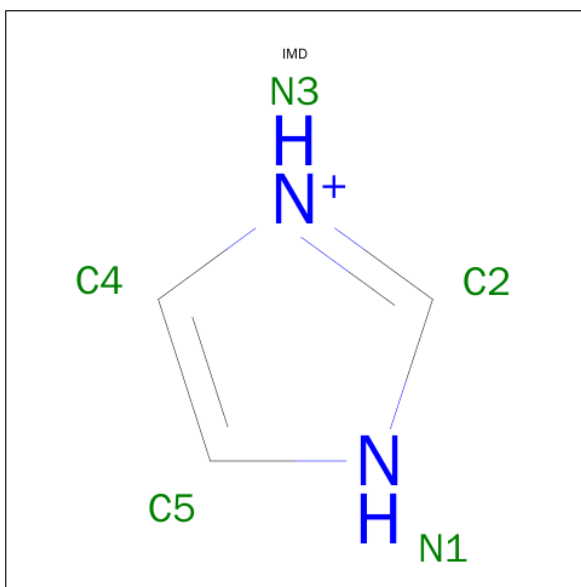
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			25	20	1	2	2	
2	C	1	Total	C	Fe	N	O	
			25	20	1	2	2	
2	D	1	Total	C	Fe	N	O	
			25	20	1	2	2	

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



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

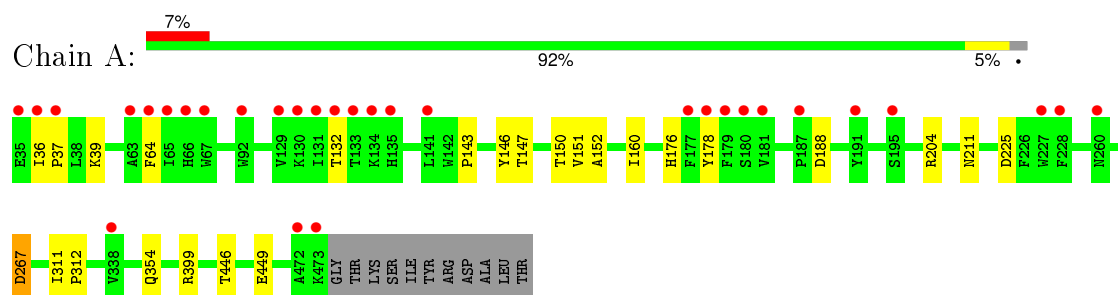
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	58	Total	O	0	0
			58	58		
5	C	38	Total	O	0	0
			38	38		
5	D	45	Total	O	0	0
			45	45		

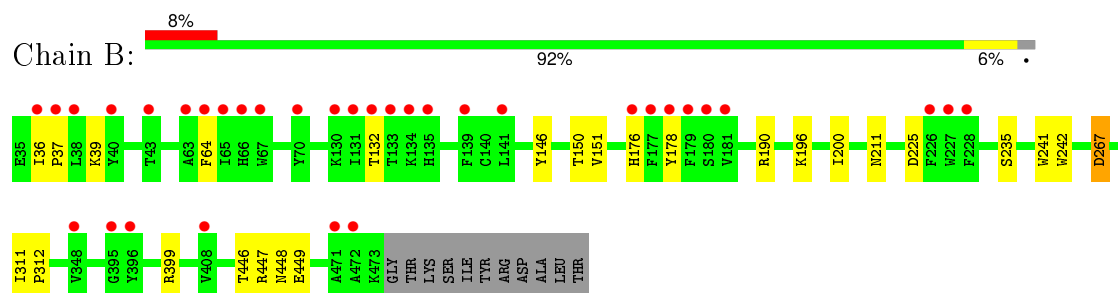
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

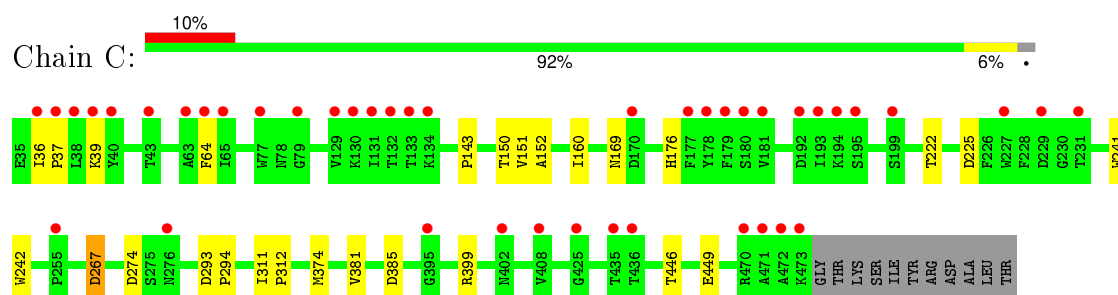
#### • Molecule 1: alpha-L-fucosidase



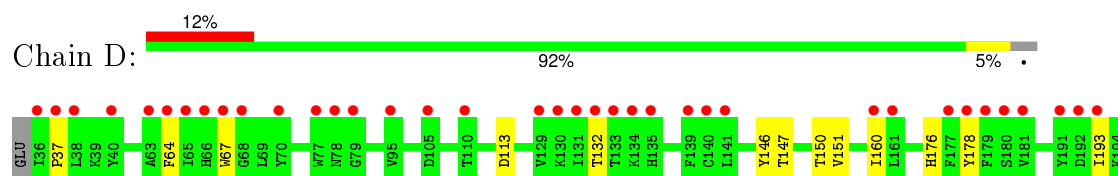
#### • Molecule 1: alpha-L-fucosidase

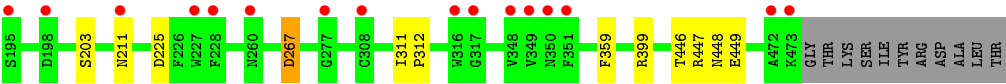


#### • Molecule 1: alpha-L-fucosidase



#### • Molecule 1: alpha-L-fucosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.51Å 189.98Å 97.54Å 90.00° 94.09° 90.00°	Depositor
Resolution (Å)	97.27 – 2.10 29.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (97.27-2.10) 99.9 (29.77-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0029	Depositor
R, $R_{free}$	0.207 , 0.244 0.213 , 0.249	Depositor DCC
$R_{free}$ test set	5986 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 118904 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: H58, IMD, 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	0.68	0/3598	0.73	1/4901 (0.0%)
1	B	0.66	0/3568	0.73	1/4869 (0.0%)
1	C	0.68	0/3567	0.73	2/4869 (0.0%)
1	D	0.67	0/3554	0.73	2/4850 (0.0%)
All	All	0.67	0/14287	0.73	6/19489 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	399	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	399	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	399	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	113	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	385	ASP	CB-CG-OD1	5.36	123.12	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3491	0	3257	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3461	0	3192	12	0
1	C	3460	0	3171	17	0
1	D	3447	0	3157	10	0
2	A	25	0	28	0	0
2	B	25	0	28	2	0
2	C	25	0	28	0	0
2	D	25	0	28	1	0
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	5	0	5	0	0
4	B	5	0	5	0	0
4	C	5	0	5	0	0
4	D	5	0	5	1	0
5	A	74	0	0	1	0
5	B	58	0	0	0	0
5	C	38	0	0	0	0
5	D	45	0	0	0	0
All	All	14229	0	12909	57	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 (57) 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:C:150:THR:HG22	1:C:152:ALA:H	1.34	0.89
1:A:150:THR:HG22	1:A:152:ALA:H	1.42	0.81
1:A:446:THR:HG22	1:A:449:GLU:HB3	1.76	0.67
1:B:446:THR:HG22	1:B:449:GLU:HB3	1.76	0.67
1:D:446:THR:HG22	1:D:449:GLU:HB3	1.77	0.66
1:C:446:THR:HG22	1:C:449:GLU:HB3	1.79	0.64
1:A:143:PRO:HA	1:A:150:THR:CG2	2.29	0.63
1:C:150:THR:HG22	1:C:152:ALA:N	2.13	0.60
1:C:143:PRO:HA	1:C:150:THR:CG2	2.33	0.59
1:C:176:HIS:CG	1:C:225:ASP:HB3	2.41	0.56
1:D:176:HIS:CG	1:D:225:ASP:HB3	2.42	0.55
2:D:501:H58:NAH	3:D:503:SO4:O2	2.40	0.54
1:A:176:HIS:CG	1:A:225:ASP:HB3	2.43	0.54
1:A:143:PRO:HA	1:A:150:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:HIS:CG	1:B:225:ASP:HB3	2.45	0.52
1:A:143:PRO:HA	1:A:150:THR:HG23	1.93	0.51
1:C:311:ILE:HB	1:C:312:PRO:HD3	1.93	0.50
1:D:193:ILE:O	1:D:193:ILE:HG23	2.11	0.50
1:C:143:PRO:HA	1:C:150:THR:HG23	1.95	0.49
1:A:188:ASP:OD2	1:A:204:ARG:NE	2.39	0.49
1:A:311:ILE:HB	1:A:312:PRO:HD3	1.96	0.48
1:C:143:PRO:HA	1:C:150:THR:HG21	1.96	0.47
1:A:267:ASP:N	1:A:267:ASP:OD1	2.47	0.47
1:D:267:ASP:OD1	1:D:267:ASP:N	2.46	0.47
1:B:36:ILE:HG23	1:B:37:PRO:HD2	1.96	0.46
1:B:267:ASP:OD1	1:B:267:ASP:N	2.48	0.46
1:C:36:ILE:HG23	1:C:37:PRO:HD2	1.97	0.46
1:D:311:ILE:HB	1:D:312:PRO:HD3	1.97	0.46
2:B:501:H58:H20	3:B:503:SO4:O4	2.17	0.45
1:B:311:ILE:HB	1:B:312:PRO:HD3	1.98	0.45
1:A:354:GLN:NE2	5:A:647:HOH:O	2.49	0.44
1:D:132:THR:HA	1:D:178:TYR:HB3	2.01	0.43
1:A:151:VAL:HG21	1:A:160:ILE:HG12	2.01	0.43
1:C:151:VAL:HG21	1:C:160:ILE:HG12	2.00	0.43
1:D:146:TYR:CZ	1:D:211:ASN:HB3	2.54	0.43
1:A:36:ILE:HG23	1:A:37:PRO:HD2	1.99	0.43
1:D:359:PHE:CZ	4:D:504:IMD:H4	2.54	0.43
1:A:39:LYS:N	1:A:267:ASP:OD2	2.44	0.42
1:D:151:VAL:HG21	1:D:160:ILE:HG12	2.00	0.42
1:B:196:LYS:O	1:B:200:ILE:HG12	2.19	0.42
1:D:447:ARG:O	1:D:448:ASN:HB2	2.20	0.42
1:B:241:TRP:CD2	1:B:242:TRP:N	2.88	0.42
1:B:447:ARG:O	1:B:448:ASN:HB2	2.21	0.41
1:B:132:THR:HA	1:B:178:TYR:HB3	2.02	0.41
1:C:241:TRP:CD2	1:C:242:TRP:N	2.88	0.41
1:C:39:LYS:N	1:C:267:ASP:OD2	2.49	0.41
1:C:293:ASP:HA	1:C:294:PRO:HD3	1.95	0.41
2:B:501:H58:NAH	3:B:503:SO4:O4	2.54	0.41
1:C:267:ASP:OD1	1:C:267:ASP:N	2.48	0.41
1:B:190:ARG:O	1:B:235:SER:CB	2.69	0.41
1:B:39:LYS:N	1:B:267:ASP:OD2	2.44	0.40
1:A:146:TYR:CZ	1:A:211:ASN:HB3	2.55	0.40
1:C:374:MET:HE1	1:C:381:VAL:HG11	2.03	0.40
1:C:169:ASN:ND2	1:C:222:THR:OG1	2.52	0.40
1:B:146:TYR:CZ	1:B:211:ASN:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:HA	1:A:178:TYR:HB3	2.04	0.40
1:C:274:ASP:C	1:C:274:ASP:OD1	2.60	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	437/450 (97%)	421 (96%)	16 (4%)	0	100	100
1	B	437/450 (97%)	422 (97%)	15 (3%)	0	100	100
1	C	437/450 (97%)	423 (97%)	14 (3%)	0	100	100
1	D	436/450 (97%)	419 (96%)	16 (4%)	1 (0%)	52	53
All	All	1747/1800 (97%)	1685 (96%)	61 (4%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	37	PRO

### 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	346/383 (90%)	343 (99%)	3 (1%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/383 (89%)	336 (99%)	4 (1%)	78	84
1	C	338/383 (88%)	336 (99%)	2 (1%)	90	94
1	D	337/383 (88%)	331 (98%)	6 (2%)	66	72
All	All	1361/1532 (89%)	1346 (99%)	15 (1%)	80	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	147	THR
1	A	267	ASP
1	B	64	PHE
1	B	150	THR
1	B	151	VAL
1	B	267	ASP
1	C	64	PHE
1	C	267	ASP
1	D	64	PHE
1	D	67	TRP
1	D	147	THR
1	D	150	THR
1	D	203	SER
1	D	267	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

15 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	H58	A	501	-	21,27,27	1.70	3 (14%)	17,36,36	1.61	4 (23%)
3	SO4	A	502	-	4,4,4	0.70	0	6,6,6	0.35	0
4	IMD	A	503	-	3,5,5	0.49	0	4,5,5	0.83	0
2	H58	B	501	-	21,27,27	1.72	3 (14%)	17,36,36	1.28	2 (11%)
3	SO4	B	502	-	4,4,4	0.48	0	6,6,6	0.18	0
3	SO4	B	503	-	4,4,4	0.71	0	6,6,6	0.59	0
4	IMD	B	504	-	3,5,5	0.62	0	4,5,5	0.33	0
2	H58	C	501	-	21,27,27	1.55	2 (9%)	17,36,36	1.19	2 (11%)
3	SO4	C	502	-	4,4,4	0.47	0	6,6,6	0.28	0
3	SO4	C	503	-	4,4,4	0.49	0	6,6,6	0.53	0
4	IMD	C	504	-	3,5,5	0.33	0	4,5,5	1.09	0
2	H58	D	501	-	21,27,27	1.63	3 (14%)	17,36,36	1.73	3 (17%)
3	SO4	D	502	-	4,4,4	0.53	0	6,6,6	0.39	0
3	SO4	D	503	-	4,4,4	0.40	0	6,6,6	0.21	0
4	IMD	D	504	-	3,5,5	0.53	0	4,5,5	0.79	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	H58	A	501	-	-	0/9/45/45	0/3/3/3
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
4	IMD	A	503	-	-	0/0/0/0	0/1/1/1
2	H58	B	501	-	-	0/9/45/45	0/3/3/3
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
3	SO4	B	503	-	-	0/0/0/0	0/0/0/0
4	IMD	B	504	-	-	0/0/0/0	0/1/1/1
2	H58	C	501	-	-	0/9/45/45	0/3/3/3
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	503	-	-	0/0/0/0	0/0/0/0
4	IMD	C	504	-	-	0/0/0/0	0/1/1/1
2	H58	D	501	-	-	0/9/45/45	0/3/3/3
3	SO4	D	502	-	-	0/0/0/0	0/0/0/0
3	SO4	D	503	-	-	0/0/0/0	0/0/0/0
4	IMD	D	504	-	-	0/0/0/0	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	H58	CAC-CAB	-3.43	1.48	1.53
2	D	501	H58	CAD-CAE	2.00	1.55	1.53
2	A	501	H58	CAD-CAE	2.20	1.55	1.53
2	C	501	H58	CAI-CAM	3.69	1.41	1.33
2	D	501	H58	CAI-CAM	3.84	1.41	1.33
2	B	501	H58	CAI-CAM	3.84	1.41	1.33
2	A	501	H58	CAI-CAM	3.94	1.41	1.33
2	C	501	H58	CAK-CAJ	5.46	1.42	1.33
2	B	501	H58	CAK-CAJ	5.59	1.42	1.33
2	D	501	H58	CAK-CAJ	5.60	1.42	1.33
2	A	501	H58	CAK-CAJ	5.94	1.43	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	H58	CAD-CAC-CAB	-3.36	97.25	103.15
2	C	501	H58	CAD-CAC-CAB	-3.29	97.35	103.15
2	D	501	H58	CAD-CAC-CAB	-2.95	97.96	103.15
2	B	501	H58	CAD-CAC-CAB	-2.73	98.35	103.15
2	A	501	H58	CAO-CAB-NAA	2.02	113.87	111.65
2	A	501	H58	CAC-CAD-CAE	2.18	106.81	103.17
2	C	501	H58	CAQ-CAN-CAJ	2.19	117.66	114.17
2	B	501	H58	CAO-CAB-NAA	2.78	114.70	111.65
2	D	501	H58	CAQ-CAN-CAJ	2.94	118.84	114.17
2	A	501	H58	CAQ-CAN-CAJ	4.16	120.78	114.17
2	D	501	H58	CAO-CAB-NAA	4.38	116.45	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	H58	2	0
3	B	503	SO4	2	0
2	D	501	H58	1	0
3	D	503	SO4	1	0
4	D	504	IMD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	439/450 (97%)	0.26	31 (7%)	19 26	30, 49, 68, 93	2 (0%)
1	B	439/450 (97%)	0.35	34 (7%)	16 22	33, 51, 75, 99	0
1	C	439/450 (97%)	0.48	43 (9%)	10 13	32, 53, 80, 100	1 (0%)
1	D	438/450 (97%)	0.65	53 (12%)	6 7	36, 56, 82, 107	1 (0%)
All	All	1755/1800 (97%)	0.43	161 (9%)	11 15	30, 52, 78, 107	4 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	TYR	7.7
1	C	472	ALA	7.0
1	B	178	TYR	6.9
1	D	132	THR	6.8
1	D	65	ILE	5.9
1	B	132	THR	5.8
1	A	178	TYR	5.6
1	A	36	ILE	5.5
1	D	133	THR	5.3
1	A	472	ALA	5.2
1	A	37	PRO	5.1
1	D	37	PRO	5.0
1	B	179	PHE	4.9
1	D	193	ILE	4.8
1	C	178	TYR	4.7
1	B	131	ILE	4.7
1	D	64	PHE	4.7
1	D	179	PHE	4.7
1	C	132	THR	4.6
1	B	65	ILE	4.5
1	D	131	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	132	THR	4.3
1	A	131	ILE	4.3
1	B	472	ALA	4.2
1	C	193	ILE	4.2
1	D	227	TRP	4.2
1	B	227	TRP	4.2
1	D	141	LEU	4.1
1	D	66	HIS	4.1
1	C	131	ILE	4.0
1	B	64	PHE	3.9
1	C	227	TRP	3.9
1	A	64	PHE	3.9
1	C	64	PHE	3.9
1	D	135	HIS	3.9
1	B	133	THR	3.8
1	D	134	LYS	3.8
1	B	471	ALA	3.8
1	A	65	ILE	3.7
1	D	79	GLY	3.7
1	B	36	ILE	3.7
1	C	37	PRO	3.7
1	D	177	PHE	3.6
1	B	134	LYS	3.6
1	D	130	LYS	3.6
1	D	228	PHE	3.6
1	D	195	SER	3.6
1	C	65	ILE	3.5
1	D	67	TRP	3.5
1	B	141	LEU	3.5
1	B	228	PHE	3.5
1	A	179	PHE	3.5
1	B	135	HIS	3.4
1	A	227	TRP	3.4
1	D	472	ALA	3.4
1	D	473	LYS	3.4
1	D	180	SER	3.4
1	B	130	LYS	3.3
1	B	180	SER	3.3
1	C	38	LEU	3.3
1	C	170	ASP	3.3
1	D	63	ALA	3.3
1	A	228	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	79	GLY	3.2
1	D	110	THR	3.2
1	D	40	TYR	3.2
1	D	348	VAL	3.1
1	C	36	ILE	3.1
1	C	40	TYR	3.1
1	B	66	HIS	3.0
1	C	402	ASN	3.0
1	B	40	TYR	3.0
1	C	473	LYS	3.0
1	C	133	THR	2.9
1	C	179	PHE	2.9
1	C	435	THR	2.9
1	C	276	ASN	2.9
1	D	36	ILE	2.9
1	D	129	VAL	2.9
1	A	133	THR	2.9
1	D	349	VAL	2.8
1	D	351	PHE	2.8
1	B	395	GLY	2.8
1	D	277	GLY	2.8
1	D	181	VAL	2.8
1	D	68	GLY	2.8
1	B	177	PHE	2.8
1	D	308	CYS	2.8
1	A	180	SER	2.8
1	B	181	VAL	2.8
1	C	255	PRO	2.7
1	D	95	VAL	2.7
1	D	317	GLY	2.7
1	D	78	ASN	2.7
1	C	39	LYS	2.7
1	D	70	TYR	2.6
1	C	408	VAL	2.6
1	B	67	TRP	2.6
1	D	191	TYR	2.6
1	C	129	VAL	2.6
1	C	425	GLY	2.6
1	A	130	LYS	2.6
1	B	396	TYR	2.6
1	B	176	HIS	2.6
1	B	43	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	470	ARG	2.5
1	D	192	ASP	2.5
1	D	316	TRP	2.5
1	B	408	VAL	2.5
1	A	66	HIS	2.5
1	C	43	THR	2.5
1	A	63	ALA	2.5
1	C	134	LYS	2.5
1	A	35	GLU	2.5
1	A	177	PHE	2.5
1	A	92	TRP	2.5
1	A	135	HIS	2.4
1	C	229	ASP	2.4
1	D	260	ASN	2.4
1	B	63	ALA	2.4
1	D	77	TRP	2.4
1	C	395	GLY	2.4
1	C	192	ASP	2.4
1	C	194	LYS	2.4
1	A	191	TYR	2.3
1	A	141	LEU	2.3
1	A	187	PRO	2.3
1	B	70	TYR	2.3
1	A	473	LYS	2.3
1	C	177	PHE	2.3
1	D	350	ASN	2.3
1	D	160	ILE	2.3
1	D	198	ASP	2.3
1	C	77	TRP	2.3
1	B	37	PRO	2.3
1	A	195	SER	2.2
1	D	38	LEU	2.2
1	C	436	THR	2.2
1	C	181	VAL	2.2
1	D	161	LEU	2.2
1	C	130	LYS	2.2
1	D	105	ASP	2.2
1	C	63	ALA	2.1
1	A	134	LYS	2.1
1	A	260	ASN	2.1
1	B	38	LEU	2.1
1	B	139	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	2.1
1	D	139	PHE	2.1
1	D	140	CYS	2.1
1	C	195	SER	2.1
1	B	348	VAL	2.1
1	D	211	ASN	2.1
1	A	67	TRP	2.0
1	C	471	ALA	2.0
1	B	226	PHE	2.0
1	A	129	VAL	2.0
1	C	231	THR	2.0
1	C	180	SER	2.0
1	A	181	VAL	2.0
1	C	199	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
4	IMD	C	504	5/5	0.92	0.26	1.52	62,66,70,73	5
4	IMD	A	503	5/5	0.93	0.24	1.19	71,75,77,81	0
2	H58	B	501	25/25	0.65	0.31	0.98	42,98,170,187	0
2	H58	A	501	25/25	0.69	0.26	0.78	37,91,157,172	0
2	H58	D	501	25/25	0.71	0.31	0.61	43,96,152,163	0
4	IMD	B	504	5/5	0.94	0.19	0.53	51,55,58,58	5
2	H58	C	501	25/25	0.86	0.21	0.44	35,85,116,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IMD	D	504	5/5	0.95	0.21	0.27	63,63,68,73	0
3	SO4	B	502	5/5	0.95	0.15	-	72,73,79,80	5
3	SO4	C	502	5/5	0.97	0.13	-	60,70,72,73	0
3	SO4	B	503	5/5	0.94	0.26	-	65,70,77,79	5
3	SO4	C	503	5/5	0.91	0.29	-	77,80,87,88	5
3	SO4	A	502	5/5	0.91	0.21	-	66,78,81,87	5
3	SO4	D	503	5/5	0.94	0.15	-	72,77,77,79	5
3	SO4	D	502	5/5	0.93	0.19	-	74,76,83,85	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.