



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:47 PM BST

PDB ID : 5YFC  
Title : Crystal structure of a new DPP III family member  
Authors : Xu, T.; Liu, J.  
Deposited on : 2017-09-20  
Resolution : 1.76 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

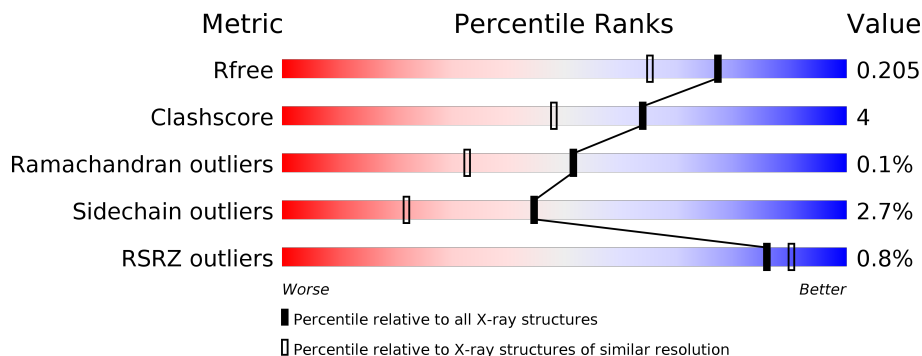
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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	703	
1	B	703	

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	804	-	-	X	-
2	SO4	B	803	-	-	X	-
5	TRS	A	811	-	X	X	-
5	TRS	B	810	-	X	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12724 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 Dipeptidyl peptidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	690	Total	C	N	O	S	0	36	0
			5581	3594	908	1071	8			
1	B	690	Total	C	N	O	S	0	35	0
			5580	3583	909	1080	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	696	LEU	-	expression tag	UNP B0S4Q0
A	697	GLU	-	expression tag	UNP B0S4Q0
A	698	HIS	-	expression tag	UNP B0S4Q0
A	699	HIS	-	expression tag	UNP B0S4Q0
A	700	HIS	-	expression tag	UNP B0S4Q0
A	701	HIS	-	expression tag	UNP B0S4Q0
A	702	HIS	-	expression tag	UNP B0S4Q0
A	703	HIS	-	expression tag	UNP B0S4Q0
B	696	LEU	-	expression tag	UNP B0S4Q0
B	697	GLU	-	expression tag	UNP B0S4Q0
B	698	HIS	-	expression tag	UNP B0S4Q0
B	699	HIS	-	expression tag	UNP B0S4Q0
B	700	HIS	-	expression tag	UNP B0S4Q0
B	701	HIS	-	expression tag	UNP B0S4Q0
B	702	HIS	-	expression tag	UNP B0S4Q0
B	703	HIS	-	expression tag	UNP B0S4Q0

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

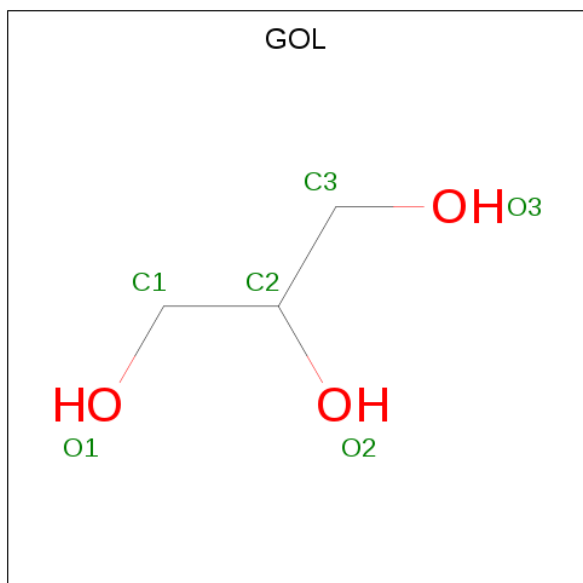


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

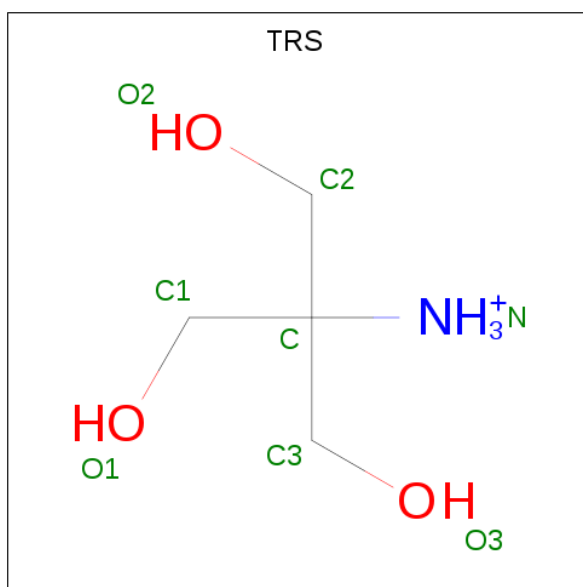
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	2	Total Cl 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0
5	B	1	8	4	1	3	0	0

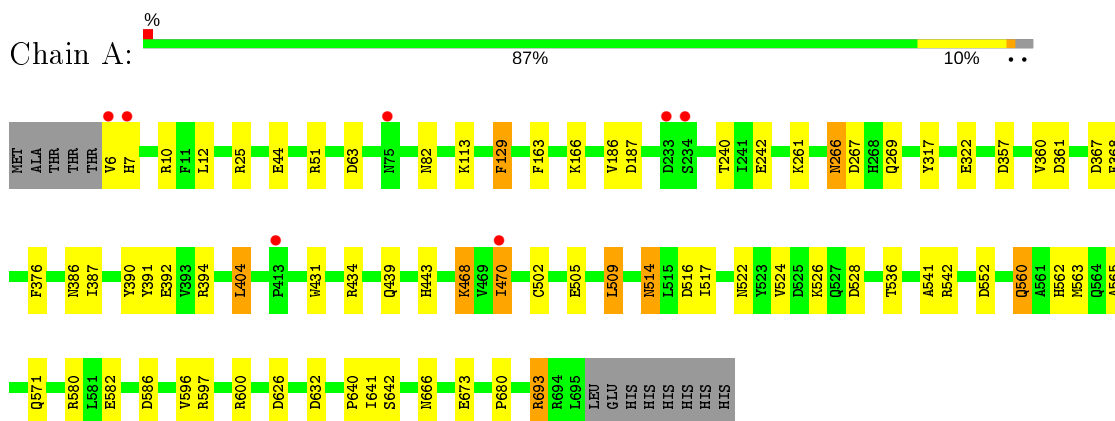
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	734	734	734	0	0
6	B	728	728	728	0	0

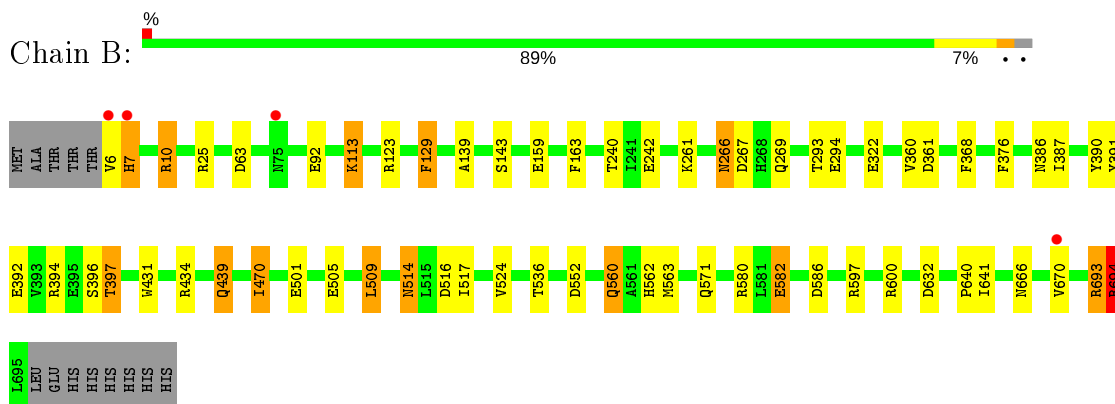
### 3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 3



- Molecule 1: Dipeptidyl peptidase 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.39Å 207.73Å 59.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.01 – 1.76 51.93 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.0 (59.01-1.76) 98.0 (51.93-1.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.67 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.152 , 0.198 0.165 , 0.205	Depositor DCC
$R_{free}$ test set	6535 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.1	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.479 for h,-k,-l 0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: GOL, TRS, SO4, CL

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	6/5804 (0.1%)	1.02	28/7874 (0.4%)
1	B	1.01	8/5803 (0.1%)	1.05	26/7874 (0.3%)
All	All	1.00	14/11607 (0.1%)	1.04	54/15748 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	GLU	CD-OE2	-6.30	1.18	1.25
1	A	582	GLU	CD-OE1	6.21	1.32	1.25
1	B	294	GLU	CD-OE2	-6.14	1.18	1.25
1	A	322	GLU	CD-OE2	-6.12	1.19	1.25
1	B	92[A]	GLU	CG-CD	6.07	1.61	1.51
1	B	92[B]	GLU	CG-CD	6.07	1.61	1.51
1	B	431	TRP	CB-CG	-5.84	1.39	1.50
1	B	582	GLU	CD-OE1	5.45	1.31	1.25
1	A	582	GLU	CD-OE2	-5.39	1.19	1.25
1	B	501	GLU	CD-OE1	5.11	1.31	1.25
1	A	431	TRP	CB-CG	-5.07	1.41	1.50
1	A	44	GLU	CD-OE1	-5.06	1.20	1.25
1	A	322	GLU	CD-OE1	5.04	1.31	1.25
1	B	322	GLU	CD-OE1	5.01	1.31	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25[A]	ARG	NE-CZ-NH1	-10.70	114.95	120.30
1	B	25[B]	ARG	NE-CZ-NH1	-10.70	114.95	120.30
1	A	693	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	B	693	ARG	NE-CZ-NH2	9.80	125.20	120.30
1	B	694	ARG	NE-CZ-NH1	8.56	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	580	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	B	10	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	394	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	597	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	580	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	B	394	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	A	509	LEU	CB-CG-CD2	7.89	124.41	111.00
1	B	600	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	10	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	267	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	B	10	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	25[A]	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	B	25[B]	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	B	267	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	B	600	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	693	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	10	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	404	LEU	CB-CG-CD1	6.70	122.39	111.00
1	B	361	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	B	586	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	63	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	361	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	509	LEU	CB-CG-CD2	6.41	121.89	111.00
1	B	693	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	63	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	129	PHE	CB-CG-CD1	6.05	125.04	120.80
1	B	694	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	187	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	528	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	92[A]	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	B	92[B]	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	A	600	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	600	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	586	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	367	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	129	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	B	123	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	187	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	129	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	B	434	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	626	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	361	ASP	CB-CG-OD1	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	25	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	361	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	582	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	A	542	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	434	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	113	LYS	CD-CE-NZ	5.01	123.22	111.70

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	5581	0	5669	49	0
1	B	5580	0	5636	48	0
2	A	35	0	0	3	0
2	B	35	0	0	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	8	0	11	6	0
5	B	8	0	11	7	0
6	A	734	0	0	10	0
6	B	728	0	0	9	0
All	All	12724	0	11343	95	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 4.

All (95) 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:439[B]:GLN:NE2	1:A:443[B]:HIS:ND1	1.90	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439[A]:GLN:OE1	1:B:505[A]:GLU:OE2	1.80	0.98
1:A:186[A]:VAL:HG11	1:A:317:TYR:CE1	2.05	0.92
1:A:541:ALA:HB1	1:A:596[A]:VAL:HG11	1.55	0.89
1:B:439[B]:GLN:NE2	6:B:901:HOH:O	1.99	0.86
1:B:396[A]:SER:OG	1:B:397[A]:THR:HG23	1.81	0.81
1:A:360[A]:VAL:HG11	6:A:941:HOH:O	1.81	0.80
1:A:439[B]:GLN:HE21	1:A:443[B]:HIS:CE1	1.99	0.79
1:B:360[A]:VAL:HG11	6:B:944:HOH:O	1.81	0.78
1:A:552[B]:ASP:OD1	6:A:901:HOH:O	2.06	0.74
1:A:468[A]:LYS:HD3	6:A:1559:HOH:O	1.88	0.73
1:A:571:GLN:HE22	1:A:640:PRO:HA	1.53	0.73
1:A:541:ALA:CB	1:A:596[A]:VAL:HG11	2.18	0.73
1:B:571:GLN:HE22	1:B:640:PRO:HA	1.54	0.72
1:A:470[B]:ILE:HA	6:A:945:HOH:O	1.89	0.71
1:A:439[A]:GLN:OE1	6:A:902:HOH:O	2.08	0.71
1:B:390:TYR:HA	5:B:810:TRS:H31	1.72	0.71
1:B:139:ALA:O	1:B:143[A]:SER:OG	2.09	0.70
1:B:6:VAL:HG13	1:B:159[A]:GLU:CD	2.12	0.70
1:B:391:TYR:H	5:B:810:TRS:C3	2.05	0.69
1:B:391:TYR:H	5:B:810:TRS:H32	1.58	0.69
1:A:642:SER:O	1:B:470[A]:ILE:HD11	1.95	0.67
1:A:390:TYR:HA	5:A:811:TRS:H32	1.76	0.67
1:B:470[B]:ILE:HA	6:B:941:HOH:O	1.94	0.66
1:B:396[A]:SER:OG	1:B:397[A]:THR:CG2	2.43	0.66
1:A:470[A]:ILE:HA	6:A:945:HOH:O	1.96	0.65
1:A:541:ALA:HB1	1:A:596[A]:VAL:CG1	2.28	0.63
1:A:391:TYR:N	5:A:811:TRS:H21	2.14	0.62
1:B:360[A]:VAL:CG1	6:B:944:HOH:O	2.42	0.60
1:B:7:HIS:CB	2:B:803:SO4:O4	2.50	0.59
1:B:694:ARG:HH11	1:B:694:ARG:HG2	1.66	0.59
1:A:186[A]:VAL:HG11	1:A:317:TYR:CZ	2.36	0.59
1:A:7:HIS:HB3	2:A:804:SO4:O2	2.01	0.59
1:B:6:VAL:HG12	1:B:10:ARG:NH2	2.18	0.57
1:B:470[A]:ILE:HA	6:B:941:HOH:O	2.05	0.56
1:B:560:GLN:NE2	1:B:563:MET:H	2.03	0.56
1:B:293:THR:HG23	1:B:397[A]:THR:HG21	1.88	0.56
1:A:360[A]:VAL:CG1	6:A:941:HOH:O	2.44	0.56
1:B:560:GLN:HE22	1:B:562:HIS:HB2	1.71	0.56
1:B:552[B]:ASP:OD1	6:B:902:HOH:O	2.17	0.56
1:A:166:LYS:NZ	2:A:807:SO4:O3	2.35	0.55
1:A:560:GLN:NE2	1:A:563:MET:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG12	1:B:10:ARG:HH22	1.70	0.55
1:A:571:GLN:NE2	1:A:641:ILE:H	2.05	0.55
1:B:571:GLN:NE2	1:B:641:ILE:H	2.05	0.55
1:B:560:GLN:HE21	1:B:563:MET:H	1.56	0.54
1:A:514:ASN:HD22	1:A:517:ILE:H	1.55	0.54
1:B:666:ASN:HD21	1:B:693:ARG:HE	1.55	0.54
1:A:560:GLN:HE22	1:A:562:HIS:HB2	1.74	0.53
1:B:514:ASN:HD22	1:B:517:ILE:H	1.56	0.52
1:B:509:LEU:HD22	1:B:536:THR:HG22	1.92	0.52
1:A:560:GLN:HE21	1:A:563:MET:H	1.58	0.51
1:B:266:ASN:ND2	1:B:269:GLN:H	2.08	0.51
1:A:163:PHE:CZ	1:A:552[B]:ASP:OD2	2.63	0.51
1:B:163:PHE:CZ	1:B:552[B]:ASP:OD2	2.63	0.51
1:B:240:THR:HG22	1:B:242[A]:GLU:HG3	1.92	0.51
1:B:391:TYR:H	5:B:810:TRS:H31	1.76	0.51
1:B:113:LYS:HE3	6:B:1354:HOH:O	2.12	0.50
1:B:632:ASP:OD1	6:B:903:HOH:O	2.18	0.50
1:A:666:ASN:HD21	1:A:693:ARG:HE	1.59	0.49
1:A:509:LEU:HD22	1:A:536:THR:HG22	1.93	0.49
1:B:7:HIS:HB2	2:B:803:SO4:O4	2.13	0.49
1:A:186[A]:VAL:HG11	1:A:317:TYR:CD1	2.48	0.48
1:B:582:GLU:OE2	1:B:597:ARG:NH2	2.40	0.48
1:A:266:ASN:ND2	1:A:269:GLN:H	2.11	0.48
1:A:632:ASP:OD1	6:A:904:HOH:O	2.19	0.48
1:A:7:HIS:CB	2:A:804:SO4:O2	2.61	0.48
1:B:7:HIS:HB3	2:B:803:SO4:O4	2.14	0.47
1:B:560:GLN:HE21	1:B:563:MET:HG2	1.79	0.47
1:A:113:LYS:HE3	6:A:1287:HOH:O	2.15	0.46
1:A:560:GLN:HE21	1:A:563:MET:HG2	1.81	0.46
1:B:391:TYR:N	5:B:810:TRS:H21	2.32	0.45
1:A:392[B]:GLU:H	5:A:811:TRS:H21	1.82	0.45
1:A:443[A]:HIS:ND1	1:A:505[A]:GLU:OE2	2.45	0.45
1:A:642:SER:O	1:B:470[A]:ILE:CD1	2.63	0.44
1:A:571:GLN:HE22	1:A:641:ILE:H	1.65	0.44
1:A:392[A]:GLU:H	5:A:811:TRS:H21	1.82	0.44
1:A:357:ASP:OD1	1:A:468[A]:LYS:HE3	2.17	0.44
1:B:571:GLN:HE22	1:B:641:ILE:H	1.66	0.43
1:B:396[A]:SER:HG	1:B:397[A]:THR:HG23	1.83	0.42
1:B:266:ASN:C	1:B:266:ASN:HD22	2.23	0.42
1:B:514:ASN:HD21	1:B:516:ASP:HB2	1.84	0.42
1:A:392[B]:GLU:H	5:A:811:TRS:C2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392[A]:GLU:H	5:A:811:TRS:C2	2.34	0.41
1:A:261:LYS:HD2	6:A:987:HOH:O	2.20	0.41
1:B:261:LYS:HD2	6:B:984:HOH:O	2.20	0.41
1:A:240:THR:HG22	1:A:242:GLU:HG3	2.03	0.41
1:A:514:ASN:HD21	1:A:516:ASP:HB2	1.85	0.41
1:B:392[A]:GLU:H	5:B:810:TRS:C2	2.34	0.41
1:B:392[B]:GLU:H	5:B:810:TRS:C2	2.34	0.41
1:A:502:CYS:HA	1:A:565:ALA:HB1	2.04	0.40
1:A:439[B]:GLN:HE22	1:A:505[B]:GLU:HG2	1.87	0.40
1:A:266:ASN:HD22	1:A:266:ASN:C	2.25	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	724/703 (103%)	708 (98%)	16 (2%)	0	100	100
1	B	724/703 (103%)	709 (98%)	14 (2%)	1 (0%)	51	33
All	All	1448/1406 (103%)	1417 (98%)	30 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	HIS

### 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	618/594 (104%)	597 (97%)	21 (3%)	37	14
1	B	618/594 (104%)	602 (97%)	16 (3%)	46	23
All	All	1236/1188 (104%)	1199 (97%)	37 (3%)	44	18

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	12[A]	LEU
1	A	12[B]	LEU
1	A	82	ASN
1	A	129	PHE
1	A	266	ASN
1	A	368	PHE
1	A	376	PHE
1	A	386	ASN
1	A	387	ILE
1	A	404	LEU
1	A	468[A]	LYS
1	A	468[B]	LYS
1	A	470[A]	ILE
1	A	470[B]	ILE
1	A	514	ASN
1	A	522	ASN
1	A	526	LYS
1	A	560	GLN
1	A	673	GLU
1	A	680	PRO
1	B	129	PHE
1	B	266	ASN
1	B	368	PHE
1	B	376	PHE
1	B	386	ASN
1	B	387	ILE
1	B	397[A]	THR
1	B	397[B]	THR
1	B	439[A]	GLN
1	B	439[B]	GLN
1	B	470[A]	ILE
1	B	470[B]	ILE

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Mol	Chain	Res	Type
1	B	514	ASN
1	B	560	GLN
1	B	670	VAL
1	B	694	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	151	GLN
1	A	266	ASN
1	A	386	ASN
1	A	401	ASN
1	A	514	ASN
1	A	560	GLN
1	A	571	GLN
1	A	666	ASN
1	A	675	GLN
1	B	100	GLN
1	B	266	ASN
1	B	386	ASN
1	B	401	ASN
1	B	514	ASN
1	B	560	GLN
1	B	571	GLN
1	B	666	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

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	804	-	4,4,4	0.41	0	6,6,6	0.52	0
2	SO4	A	804	-	4,4,4	0.56	0	6,6,6	0.59	0
2	SO4	B	805	-	4,4,4	0.75	0	6,6,6	0.61	0
2	SO4	A	803	-	4,4,4	0.64	0	6,6,6	0.26	0
5	TRS	B	810	-	7,7,7	1.86	2 (28%)	9,9,9	3.31	4 (44%)
4	GOL	B	809	-	5,5,5	0.78	0	5,5,5	0.65	0
2	SO4	A	807	-	4,4,4	0.53	0	6,6,6	0.40	0
2	SO4	B	802	-	4,4,4	0.33	0	6,6,6	0.89	0
2	SO4	A	806	-	4,4,4	0.54	0	6,6,6	0.83	0
5	TRS	A	811	-	7,7,7	2.16	2 (28%)	9,9,9	3.53	5 (55%)
2	SO4	B	806	-	4,4,4	0.50	0	6,6,6	0.61	0
2	SO4	B	801	-	4,4,4	0.69	0	6,6,6	0.77	0
2	SO4	A	801	-	4,4,4	0.84	0	6,6,6	0.71	0
2	SO4	B	803	-	4,4,4	0.53	0	6,6,6	0.82	0
2	SO4	A	805	-	4,4,4	0.43	0	6,6,6	0.71	0
2	SO4	A	802	-	4,4,4	0.60	0	6,6,6	0.63	0
4	GOL	A	810	-	5,5,5	0.65	0	5,5,5	0.70	0
2	SO4	B	807	-	4,4,4	0.23	0	6,6,6	0.24	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
5	TRS	A	811	-	-	8/9/9/9	-
5	TRS	B	810	-	-	6/9/9/9	-
4	GOL	A	810	-	-	1/4/4/4	-
4	GOL	B	809	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	811	TRS	O2-C2	-4.49	1.27	1.42
5	B	810	TRS	O2-C2	-3.51	1.30	1.42
5	B	810	TRS	O1-C1	2.23	1.49	1.42
5	A	811	TRS	O1-C1	2.01	1.48	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	810	TRS	O3-C3-C	6.04	130.12	111.00
5	A	811	TRS	C3-C-N	-5.75	90.81	107.98
5	B	810	TRS	O1-C1-C	5.71	129.08	111.00
5	A	811	TRS	O1-C1-C	5.60	128.73	111.00
5	A	811	TRS	O3-C3-C	4.52	125.31	111.00
5	A	811	TRS	C3-C-C1	3.88	122.85	110.81
5	B	810	TRS	C1-C-N	3.64	118.84	107.98
5	B	810	TRS	C3-C-N	-2.64	100.11	107.98
5	A	811	TRS	O2-C2-C	-2.08	104.39	111.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	810	TRS	N-C-C1-O1
5	B	810	TRS	C1-C-C2-O2
5	B	810	TRS	C3-C-C2-O2
5	B	810	TRS	N-C-C2-O2
5	A	811	TRS	C1-C-C2-O2
5	A	811	TRS	N-C-C2-O2
5	A	811	TRS	N-C-C3-O3
5	A	811	TRS	C2-C-C1-O1
5	A	811	TRS	C3-C-C1-O1
5	A	811	TRS	N-C-C1-O1
5	A	811	TRS	C1-C-C3-O3
5	A	811	TRS	C2-C-C3-O3
5	B	810	TRS	C2-C-C1-O1
5	B	810	TRS	C2-C-C3-O3
4	A	810	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	SO4	2	0
5	B	810	TRS	7	0
2	A	807	SO4	1	0
5	A	811	TRS	6	0
2	B	803	SO4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	690/703 (98%)	-0.39	7 (1%) 82 87	4, 9, 20, 55	0
1	B	690/703 (98%)	-0.41	4 (0%) 89 92	4, 9, 20, 52	0
All	All	1380/1406 (98%)	-0.40	11 (0%) 86 90	4, 9, 20, 55	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	HIS	2.8
1	B	7	HIS	2.8
1	A	6	VAL	2.6
1	A	413	PRO	2.6
1	B	6	VAL	2.6
1	A	75	ASN	2.3
1	B	75	ASN	2.2
1	A	470[A]	ILE	2.2
1	A	234	SER	2.1
1	B	670	VAL	2.1
1	A	233	ASP	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 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(Å <sup>2</sup> )	Q<0.9
2	SO4	B	805	5/5	0.81	0.15	38,41,47,48	0
2	SO4	B	806	5/5	0.84	0.19	46,49,53,58	0
2	SO4	A	805	5/5	0.84	0.18	50,50,54,55	0
5	TRS	B	810	8/8	0.85	0.18	17,19,25,31	0
3	CL	A	809	1/1	0.86	0.10	47,47,47,47	0
5	TRS	A	811	8/8	0.87	0.19	17,18,25,25	0
3	CL	B	808	1/1	0.91	0.08	44,44,44,44	0
4	GOL	B	809	6/6	0.92	0.21	16,20,20,21	0
2	SO4	A	806	5/5	0.92	0.12	33,45,48,49	0
2	SO4	A	803	5/5	0.92	0.16	32,43,44,48	0
2	SO4	B	802	5/5	0.94	0.14	28,34,42,44	0
2	SO4	A	802	5/5	0.94	0.13	29,36,40,51	0
4	GOL	A	810	6/6	0.94	0.19	15,19,20,21	0
2	SO4	B	801	5/5	0.95	0.13	18,19,26,28	0
2	SO4	B	804	5/5	0.95	0.18	35,43,48,51	0
2	SO4	B	803	5/5	0.96	0.13	34,35,39,39	0
2	SO4	A	804	5/5	0.96	0.14	32,33,39,40	0
2	SO4	A	807	5/5	0.96	0.13	39,42,45,47	0
2	SO4	A	801	5/5	0.96	0.10	16,19,25,26	0
2	SO4	B	807	5/5	0.96	0.14	39,43,46,48	0
3	CL	A	808	1/1	0.97	0.06	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.