



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2020 – 12:41 PM EDT

PDB ID : 6RS1  
Title : Dipeptide Gly-Pro binds to a glycolytic enzyme fructose biphosphate aldolase  
Authors : Shahar, A.; Zarivach, R.; Skirycz, A.; Wojciechowska, I.  
Deposited on : 2019-05-21  
Resolution : 1.90 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.8  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
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) : 2.8

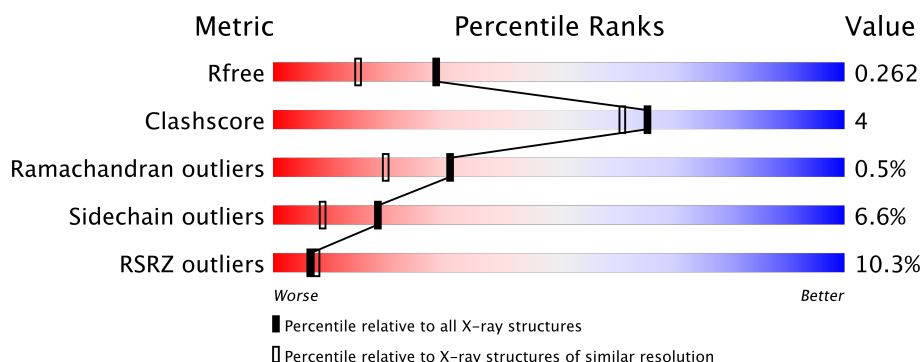
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	358	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	358	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	358	<div> <div>13%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	D	358	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10957 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 Fructose-bisphosphate aldolase 6, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	7	0
			2573	1628	443	493	9			
1	B	337	Total	C	N	O	S	0	6	0
			2575	1629	446	491	9			
1	C	337	Total	C	N	O	S	0	7	0
			2581	1631	447	494	9			
1	D	337	Total	C	N	O	S	0	5	0
			2569	1623	446	491	9			

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



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

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

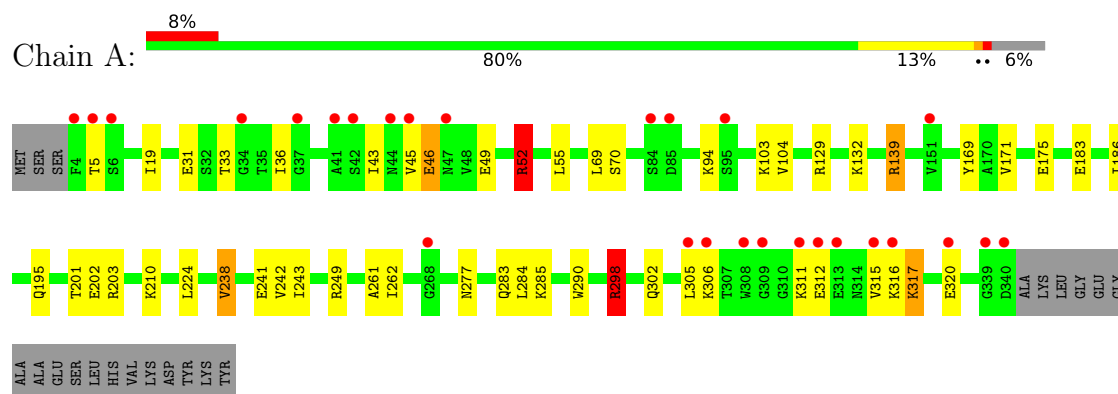
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	154	Total	O	0	0
			154	154		
3	C	135	Total	O	0	0
			135	135		
3	D	155	Total	O	0	0
			155	155		

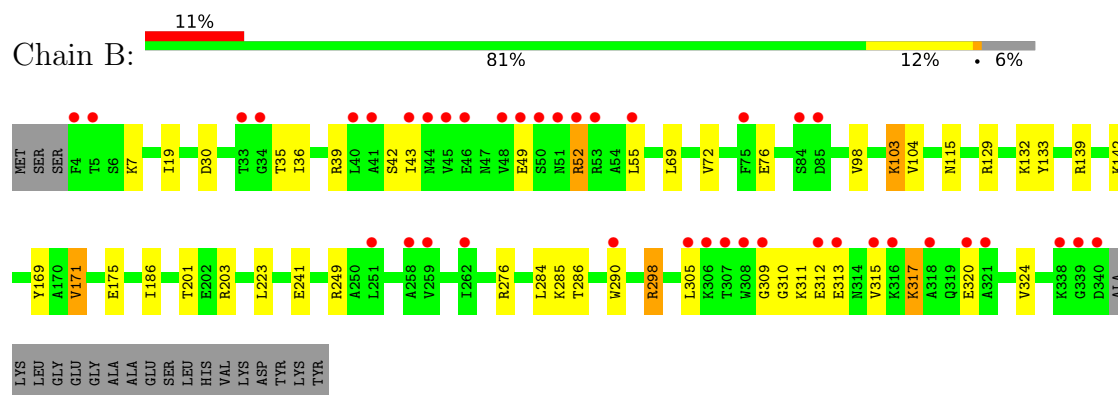
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

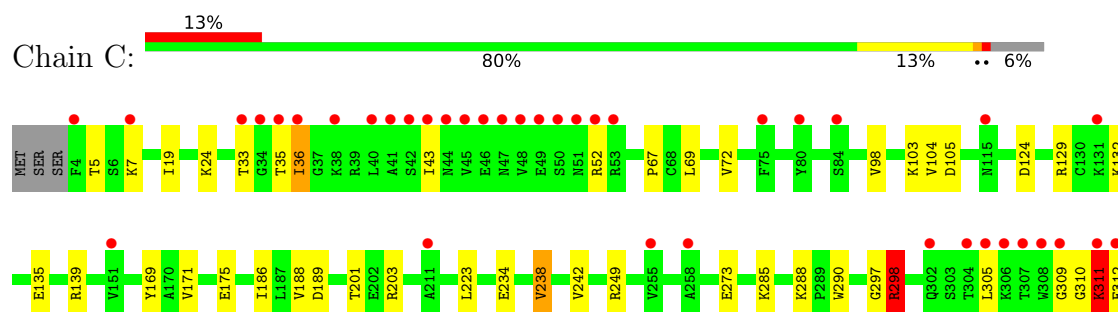
- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic

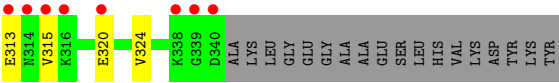


- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic

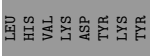
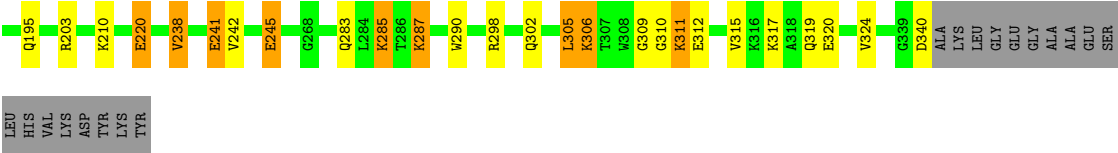
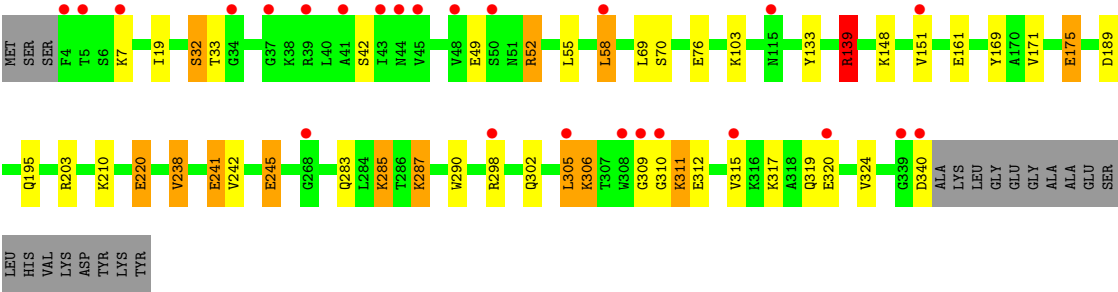
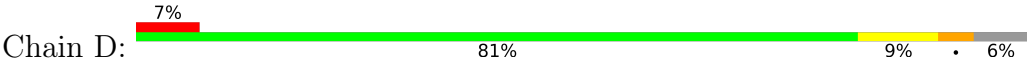


- Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic





● Molecule 1: Fructose-bisphosphate aldolase 6, cytosolic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.57Å 67.64Å 88.91Å 79.95° 73.13° 65.58°	Depositor
Resolution (Å)	48.37 – 1.90 48.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	71.1 (48.37-1.90) 95.4 (48.37-2.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.214 , 0.254 0.224 , 0.262	Depositor DCC
$R_{free}$ test set	4397 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.39% 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

### 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	0.82	6/2636 (0.2%)	0.82	5/3567 (0.1%)
1	B	0.70	0/2635	0.80	2/3565 (0.1%)
1	C	0.74	3/2644 (0.1%)	0.80	2/3577 (0.1%)
1	D	0.81	6/2626 (0.2%)	0.87	6/3553 (0.2%)
All	All	0.77	15/10541 (0.1%)	0.82	15/14262 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	15

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	GLU	CD-OE2	12.07	1.39	1.25
1	A	46[A]	GLU	CD-OE1	10.55	1.37	1.25
1	A	46[B]	GLU	CD-OE1	10.55	1.37	1.25
1	D	161	GLU	CD-OE1	7.43	1.33	1.25
1	D	161	GLU	CD-OE2	6.71	1.33	1.25
1	A	46[A]	GLU	CD-OE2	6.46	1.32	1.25
1	A	46[B]	GLU	CD-OE2	6.46	1.32	1.25
1	D	220	GLU	CD-OE1	-6.40	1.18	1.25
1	C	135	GLU	CD-OE1	6.14	1.32	1.25
1	A	183	GLU	CD-OE2	-5.75	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	GLU	CD-OE1	-5.75	1.19	1.25
1	A	202	GLU	CD-OE2	5.72	1.31	1.25
1	D	241	GLU	CD-OE1	5.71	1.31	1.25
1	C	234	GLU	CD-OE1	5.52	1.31	1.25
1	C	273	GLU	CD-OE2	5.51	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285[A]	LYS	CB-CA-C	8.57	127.54	110.40
1	D	285[C]	LYS	CB-CA-C	8.57	127.54	110.40
1	C	139	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	D	139	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	203	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	139	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	C	203	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	203	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	203	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	298	ARG	CB-CG-CD	5.76	126.57	111.60
1	A	139	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	139	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	298	ARG	CG-CD-NE	5.57	123.49	111.80
1	D	220	GLU	CA-CB-CG	5.34	125.16	113.40
1	A	139	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	52	ARG	Sidechain
1	B	249	ARG	Sidechain
1	B	39	ARG	Sidechain
1	B	52	ARG	Sidechain
1	C	249	ARG	Sidechain
1	C	298	ARG	Sidechain
1	C	311	LYS	Peptide
1	C	52	ARG	Sidechain
1	D	139	ARG	Sidechain
1	D	298	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	311	LYS	Peptide
1	D	52	ARG	Sidechain

## 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	2573	0	2638	26	0
1	B	2575	0	2641	26	0
1	C	2581	0	2642	20	0
1	D	2569	0	2628	25	0
2	A	10	0	0	0	0
2	B	15	0	0	1	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
3	A	170	0	0	2	0
3	B	154	0	0	3	0
3	C	135	0	0	2	0
3	D	155	0	0	6	0
All	All	10957	0	10549	92	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 (92) 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:284[B]:LEU:HD22	1:B:286:THR:CG2	2.03	0.89
1:A:243[B]:ILE:HD12	1:A:277:ASN:ND2	1.88	0.87
1:A:224:LEU:HB3	1:A:262[B]:ILE:HD12	1.55	0.86
1:B:19[B]:ILE:HD13	1:B:223:LEU:HD11	1.58	0.84
1:A:261:ALA:C	1:A:262[B]:ILE:HD13	2.01	0.81
1:C:297:GLY:HA3	1:C:298:ARG:HH11	1.45	0.80
1:B:284[B]:LEU:HD22	1:B:286:THR:HG22	1.73	0.68
1:A:261:ALA:O	1:A:262[B]:ILE:HD13	1.95	0.66
1:A:243[B]:ILE:HD12	1:A:277:ASN:CG	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLU:HA	1:D:52:ARG:NH1	2.12	0.64
1:A:49:GLU:HA	1:A:52:ARG:NH1	2.13	0.62
1:C:35:THR:OG1	2:C:401:SO4:O2	2.08	0.62
1:C:297:GLY:HA3	1:C:298:ARG:NH1	2.12	0.61
1:A:36:ILE:HG21	1:A:52:ARG:HD3	1.82	0.61
1:C:19[B]:ILE:HD13	1:C:223:LEU:HD11	1.83	0.61
1:D:302:GLN:HE21	1:D:306:LYS:CE	2.14	0.60
1:B:284[B]:LEU:HD22	1:B:286:THR:HG21	1.82	0.58
1:B:285:LYS:HB2	1:D:285[A]:LYS:HB2	1.85	0.58
1:A:283:GLN:OE1	3:A:501:HOH:O	2.18	0.57
1:A:317:LYS:O	1:A:320:GLU:HG2	2.04	0.57
1:D:238:VAL:HG13	1:D:242:VAL:HB	1.87	0.56
1:C:238:VAL:HG13	1:C:242:VAL:HB	1.87	0.56
1:D:189:ASP:OD2	3:D:501:HOH:O	2.18	0.55
1:D:148:LYS:HE2	3:D:532:HOH:O	2.05	0.55
1:B:317:LYS:O	1:B:320:GLU:HG2	2.06	0.55
1:A:238:VAL:HG13	1:A:242:VAL:HB	1.91	0.53
1:D:302:GLN:HE21	1:D:306:LYS:HE2	1.73	0.53
1:A:43:ILE:HD12	1:A:45:VAL:HG23	1.90	0.52
1:A:243[B]:ILE:HD12	1:A:277:ASN:HD21	1.73	0.51
1:A:302:GLN:HE22	1:A:306:LYS:HE3	1.76	0.51
1:B:285:LYS:CB	1:D:285[A]:LYS:HB2	2.40	0.51
1:D:245[A]:GLU:HG3	3:D:621:HOH:O	2.12	0.50
1:C:311:LYS:HG2	1:C:312:GLU:OE2	2.12	0.50
1:B:72:VAL:HG23	1:B:98:VAL:HG11	1.94	0.49
1:A:298:ARG:HD2	1:A:298:ARG:H	1.77	0.48
1:B:35:THR:OG1	2:B:403:SO4:O3	2.24	0.48
1:A:243[B]:ILE:HD11	3:A:508:HOH:O	2.14	0.47
1:B:285:LYS:HA	1:D:285[A]:LYS:HB2	1.96	0.47
1:B:142:LYS:HE3	3:B:553:HOH:O	2.13	0.47
1:B:76:GLU:OE2	1:B:133:TYR:OH	2.29	0.46
1:A:298:ARG:CD	1:A:298:ARG:H	2.29	0.46
1:A:210:LYS:HG2	1:D:210:LYS:HG2	1.98	0.46
1:D:32:SER:HB3	2:D:401:SO4:O1	2.17	0.45
1:A:31:GLU:CG	1:A:36:ILE:HD13	2.46	0.45
1:A:302:GLN:NE2	1:A:306:LYS:HE3	2.32	0.45
1:B:49:GLU:HA	1:B:52:ARG:NH1	2.30	0.45
1:D:283:GLN:OE1	3:D:502:HOH:O	2.21	0.45
1:B:312:GLU:HA	1:B:315:VAL:HG23	1.99	0.45
1:D:58:LEU:CD2	1:D:319:GLN:HG3	2.47	0.45
1:D:76:GLU:OE2	1:D:133:TYR:OH	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:CD1	1:C:201:THR:HA	2.47	0.44
1:B:285:LYS:CA	1:D:285[A]:LYS:HB2	2.47	0.44
1:B:186:ILE:CD1	1:B:201:THR:HA	2.48	0.44
1:B:36:ILE:HG21	1:B:52:ARG:HD2	1.99	0.44
1:C:72:VAL:HG23	1:C:98:VAL:HG11	2.00	0.43
1:A:186:ILE:CD1	1:A:201:THR:HA	2.48	0.43
1:C:320:GLU:O	1:C:324:VAL:HG23	2.18	0.43
1:D:139:ARG:HD3	3:D:544:HOH:O	2.18	0.43
1:C:285[B]:LYS:NZ	3:C:506:HOH:O	2.36	0.43
1:D:312:GLU:HA	1:D:315:VAL:HG23	2.01	0.43
1:C:124:ASP:OD1	3:C:501:HOH:O	2.22	0.43
1:A:171:VAL:O	1:A:175:GLU:HG3	2.19	0.43
1:C:171:VAL:O	1:C:175:GLU:HG3	2.19	0.42
1:C:132:LYS:HB3	1:C:132:LYS:HE3	1.93	0.42
1:B:104:VAL:O	1:B:129[A]:ARG:NH2	2.52	0.42
1:B:115:ASN:HB2	3:B:518:HOH:O	2.19	0.42
1:D:171:VAL:O	1:D:175:GLU:HG3	2.20	0.42
1:B:171:VAL:O	1:B:175:GLU:HG3	2.20	0.42
1:B:320:GLU:O	1:B:324:VAL:HG23	2.20	0.42
1:B:284[B]:LEU:CD2	1:B:286:THR:HB	2.50	0.41
1:D:58:LEU:CD2	1:D:319:GLN:CG	2.98	0.41
1:B:284[A]:LEU:HD23	1:B:284[A]:LEU:HA	1.94	0.41
1:C:36:ILE:O	1:C:36:ILE:HD13	2.20	0.41
1:C:43:ILE:HD12	1:C:43:ILE:HA	1.98	0.41
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.95	0.41
1:B:298:ARG:NH1	3:B:506:HOH:O	2.45	0.41
1:C:312:GLU:HA	1:C:315:VAL:HG23	2.01	0.41
1:B:43:ILE:HA	1:B:43:ILE:HD12	1.98	0.41
1:C:104:VAL:O	1:C:129[A]:ARG:NH2	2.52	0.41
1:C:24:LYS:HE3	1:C:67:PRO:O	2.21	0.41
1:C:288:LYS:HE2	1:C:288:LYS:HB2	1.93	0.41
1:D:55:LEU:HD11	1:D:305:LEU:CD2	2.51	0.41
1:A:19:ILE:HA	1:A:70:SER:HB2	2.03	0.40
1:A:312:GLU:HA	1:A:315:VAL:HG23	2.03	0.40
1:D:320:GLU:O	1:D:324:VAL:HG23	2.21	0.40
1:B:30:ASP:OD2	1:B:103:LYS:NZ	2.53	0.40
1:A:104:VAL:O	1:A:129:ARG:NH2	2.51	0.40
1:D:287:LYS:CG	3:D:557:HOH:O	2.70	0.40
1:D:19:ILE:HA	1:D:70:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	342/358 (96%)	330 (96%)	12 (4%)	0	100	100
1	B	341/358 (95%)	329 (96%)	10 (3%)	2 (1%)	27	15
1	C	342/358 (96%)	329 (96%)	11 (3%)	2 (1%)	27	15
1	D	340/358 (95%)	325 (96%)	12 (4%)	3 (1%)	19	8
All	All	1365/1432 (95%)	1313 (96%)	45 (3%)	7 (0%)	31	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	GLY
1	D	32	SER
1	B	309	GLY
1	C	309	GLY
1	C	310	GLY
1	D	310	GLY
1	D	309	GLY

### 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	275/284 (97%)	253 (92%)	22 (8%)	13	5
1	B	274/284 (96%)	258 (94%)	16 (6%)	22	12
1	C	275/284 (97%)	260 (94%)	15 (6%)	24	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	273/284 (96%)	252 (92%)	21 (8%)	14 6
All	All	1097/1136 (97%)	1023 (93%)	74 (7%)	18 8

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	33	THR
1	A	46[A]	GLU
1	A	46[B]	GLU
1	A	52	ARG
1	A	55	LEU
1	A	69	LEU
1	A	94	LYS
1	A	103	LYS
1	A	132	LYS
1	A	169	TYR
1	A	195	GLN
1	A	238	VAL
1	A	241	GLU
1	A	285[A]	LYS
1	A	285[B]	LYS
1	A	290	TRP
1	A	298	ARG
1	A	305	LEU
1	A	311	LYS
1	A	316	LYS
1	A	317	LYS
1	B	7	LYS
1	B	42	SER
1	B	55	LEU
1	B	69	LEU
1	B	103	LYS
1	B	132	LYS
1	B	169	TYR
1	B	171	VAL
1	B	241	GLU
1	B	276	ARG
1	B	290	TRP
1	B	298	ARG
1	B	305	LEU
1	B	311	LYS

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Mol	Chain	Res	Type
1	B	313	GLU
1	B	317	LYS
1	C	5	THR
1	C	7	LYS
1	C	33	THR
1	C	36	ILE
1	C	69	LEU
1	C	103	LYS
1	C	105	ASP
1	C	169	TYR
1	C	188	VAL
1	C	238	VAL
1	C	290	TRP
1	C	298	ARG
1	C	305	LEU
1	C	311	LYS
1	C	313	GLU
1	D	7	LYS
1	D	33	THR
1	D	42	SER
1	D	58	LEU
1	D	69	LEU
1	D	103	LYS
1	D	151	VAL
1	D	169	TYR
1	D	195	GLN
1	D	220	GLU
1	D	238	VAL
1	D	241	GLU
1	D	245[A]	GLU
1	D	245[B]	GLU
1	D	287	LYS
1	D	290	TRP
1	D	305	LEU
1	D	306	LYS
1	D	311	LYS
1	D	317	LYS
1	D	340	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	156	GLN
1	A	195	GLN
1	A	302	GLN
1	D	195	GLN
1	D	283	GLN
1	D	302	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 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	401	-	4,4,4	0.40	0	6,6,6	0.39	0
2	SO4	A	402	-	4,4,4	0.54	0	6,6,6	0.64	0
2	SO4	B	401	-	4,4,4	0.47	0	6,6,6	0.52	0
2	SO4	B	402	-	4,4,4	0.64	0	6,6,6	0.45	0
2	SO4	B	403	-	4,4,4	0.44	0	6,6,6	0.31	0
2	SO4	C	401	-	4,4,4	0.32	0	6,6,6	0.26	0
2	SO4	C	402	-	4,4,4	0.47	0	6,6,6	0.18	0
2	SO4	D	401	-	4,4,4	0.37	0	6,6,6	0.22	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	D	402	-	4,4,4	0.63	0	6,6,6	0.54	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.

No monomer is involved in short contacts.

## 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	337/358 (94%)	0.52	27 (8%) 12 14	5, 13, 55, 86	0
1	B	337/358 (94%)	0.79	40 (11%) 4 5	5, 15, 61, 80	0
1	C	337/358 (94%)	0.78	47 (13%) 2 2	5, 15, 64, 82	0
1	D	337/358 (94%)	0.58	25 (7%) 14 16	5, 14, 59, 73	0
All	All	1348/1432 (94%)	0.67	139 (10%) 6 7	5, 14, 60, 86	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	8.1
1	C	48	VAL	8.1
1	B	340	ASP	7.1
1	B	41	ALA	6.7
1	C	34	GLY	6.6
1	D	43	ILE	6.5
1	B	309	GLY	6.4
1	B	48	VAL	6.0
1	B	43	ILE	6.0
1	D	340	ASP	5.8
1	D	41	ALA	5.8
1	A	309	GLY	5.6
1	B	315	VAL	5.5
1	B	316	LYS	5.4
1	C	340	ASP	5.1
1	A	44	ASN	4.9
1	C	43	ILE	4.8
1	C	45	VAL	4.6
1	D	315	VAL	4.5
1	A	4	PHE	4.4
1	A	340	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	52	ARG	4.2
1	A	316	LYS	4.1
1	B	49	GLU	4.1
1	B	45	VAL	4.1
1	C	51	ASN	4.0
1	D	4	PHE	4.0
1	C	309	GLY	3.9
1	C	312	GLU	3.9
1	C	53	ARG	3.9
1	C	36	ILE	3.9
1	D	151	VAL	3.9
1	B	53	ARG	3.8
1	A	315	VAL	3.7
1	C	305	LEU	3.7
1	B	46	GLU	3.7
1	C	49	GLU	3.5
1	D	305	LEU	3.5
1	A	5	THR	3.5
1	C	46	GLU	3.5
1	B	51	ASN	3.4
1	A	313	GLU	3.4
1	C	44	ASN	3.3
1	D	308	TRP	3.3
1	D	44	ASN	3.3
1	C	320	GLU	3.3
1	C	42	SER	3.3
1	B	312	GLU	3.3
1	B	55	LEU	3.2
1	C	314	ASN	3.2
1	C	308	TRP	3.2
1	B	84	SER	3.2
1	B	313	GLU	3.1
1	B	34	GLY	3.1
1	D	50	SER	3.1
1	C	40	LEU	3.1
1	A	45	VAL	3.0
1	D	34	GLY	3.0
1	A	311	LYS	3.0
1	C	306	LYS	3.0
1	C	316	LYS	3.0
1	B	305	LEU	2.9
1	B	52	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	39	ARG	2.9
1	C	33	THR	2.9
1	A	151	VAL	2.9
1	D	309	GLY	2.9
1	D	115	ASN	2.9
1	D	48	VAL	2.8
1	B	318	ALA	2.8
1	B	321	ALA	2.8
1	B	320	GLU	2.8
1	C	313	GLU	2.8
1	A	42	SER	2.7
1	B	308	TRP	2.7
1	A	320	GLU	2.7
1	A	339	GLY	2.7
1	C	307	THR	2.7
1	A	95	SER	2.7
1	C	131	LYS	2.7
1	B	50	SER	2.7
1	A	268	GLY	2.6
1	D	5	THR	2.6
1	B	75	PHE	2.6
1	C	211	ALA	2.6
1	C	50	SER	2.6
1	B	85	ASP	2.6
1	C	84	SER	2.6
1	D	268	GLY	2.6
1	B	258	ALA	2.5
1	B	307	THR	2.5
1	D	37	GLY	2.5
1	C	7	LYS	2.5
1	C	4	PHE	2.5
1	A	305	LEU	2.5
1	D	310	GLY	2.5
1	B	40	LEU	2.5
1	C	115	ASN	2.5
1	A	6	SER	2.4
1	A	34	GLY	2.4
1	A	308	TRP	2.4
1	B	5	THR	2.4
1	C	35	THR	2.4
1	D	7	LYS	2.4
1	A	47	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	311	LYS	2.4
1	C	302	GLN	2.4
1	B	4	PHE	2.4
1	A	312	GLU	2.3
1	A	37	GLY	2.3
1	B	259	VAL	2.3
1	D	298	ARG	2.3
1	C	151	VAL	2.3
1	B	338	LYS	2.3
1	C	80	TYR	2.2
1	A	41	ALA	2.2
1	C	315	VAL	2.2
1	A	84	SER	2.2
1	D	320	GLU	2.2
1	B	306	LYS	2.2
1	B	339	GLY	2.2
1	C	258	ALA	2.2
1	C	75	PHE	2.1
1	B	251	LEU	2.1
1	B	290	TRP	2.1
1	B	44	ASN	2.1
1	D	45	VAL	2.1
1	C	304	THR	2.1
1	C	338	LYS	2.1
1	A	85	ASP	2.1
1	B	262	ILE	2.1
1	D	339	GLY	2.1
1	A	306	LYS	2.0
1	C	339	GLY	2.0
1	D	58	LEU	2.0
1	B	33	THR	2.0
1	C	47	ASN	2.0
1	C	38	LYS	2.0
1	C	255	VAL	2.0

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

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. 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
2	SO4	A	402	5/5	0.82	0.20	44,47,51,55	0
2	SO4	C	402	5/5	0.85	0.23	54,55,58,62	0
2	SO4	A	401	5/5	0.88	0.25	53,62,65,65	0
2	SO4	D	402	5/5	0.91	0.14	36,40,45,46	0
2	SO4	D	401	5/5	0.92	0.22	59,59,62,63	0
2	SO4	B	401	5/5	0.92	0.13	34,34,41,42	0
2	SO4	C	401	5/5	0.93	0.16	47,49,52,55	0
2	SO4	B	403	5/5	0.94	0.13	43,48,49,49	0
2	SO4	B	402	5/5	0.96	0.09	27,28,31,33	0

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

There are no such residues in this entry.