



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 07:59 AM EST

PDB ID : 1FBE  
Title : CRYSTALLOGRAPHIC STUDIES OF THE CATALYTIC MECHANISM OF  
THE NEUTRAL FORM OF FRUCTOSE-1,6-BISPHOSPHATASE  
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Deposited on : unknown  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

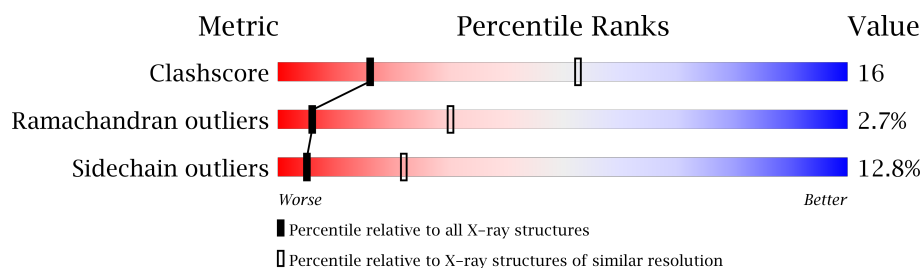
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5909 atoms, of which 1069 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 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	H	N	O	S	0	0	1
			2921	1520	530	403	453	15			
1	B	315	Total	C	H	N	O	S	0	0	1
			2938	1532	531	405	455	15			

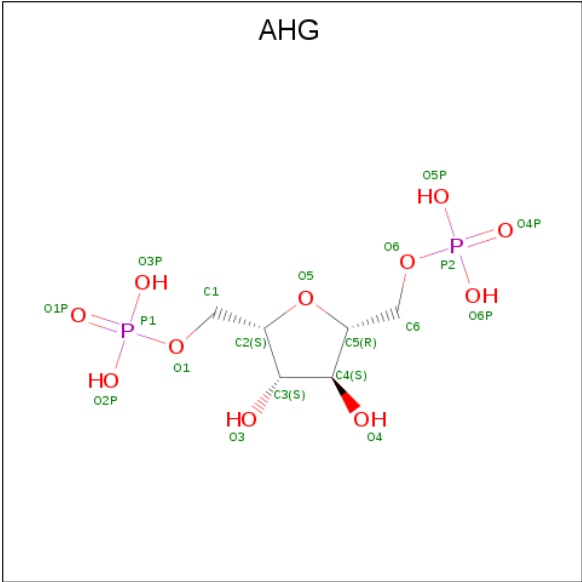
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	CONFLICT	UNP P00636
A	96	THR	SER	CONFLICT	UNP P00636
A	199	ASN	ASP	CONFLICT	UNP P00636
B	20	GLN	GLU	CONFLICT	UNP P00636
B	96	THR	SER	CONFLICT	UNP P00636
B	199	ASN	ASP	CONFLICT	UNP P00636

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2,5-ANHYDROGLUCITOL-1,6-BIPHOSPHATE (three-letter code: AHG) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>11</sub>P<sub>2</sub>).



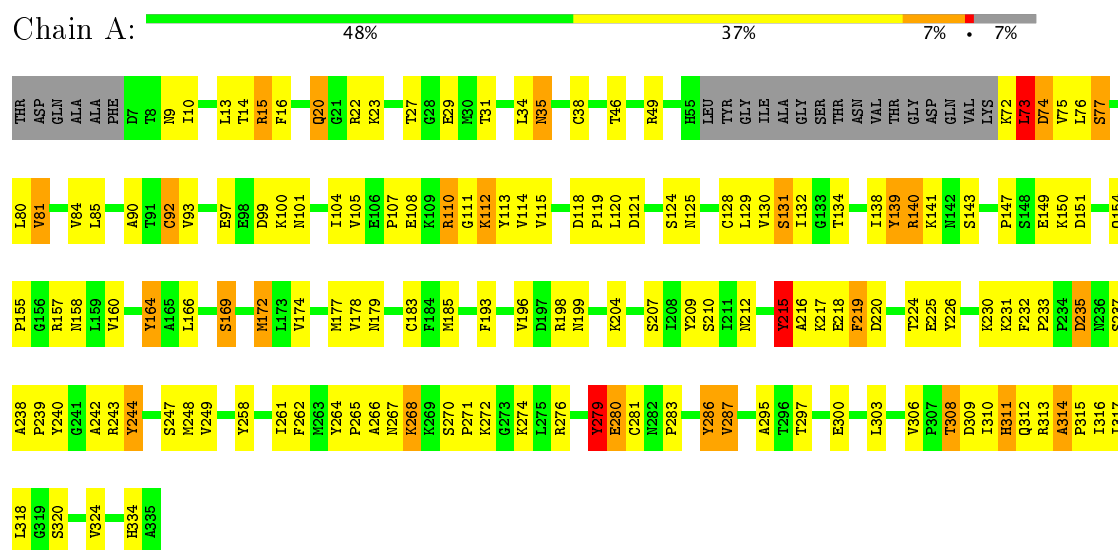
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	P	0	0
			23	6	4	11	2		
3	B	1	Total	C	H	O	P	0	0
			23	6	4	11	2		

### 3 Residue-property plots

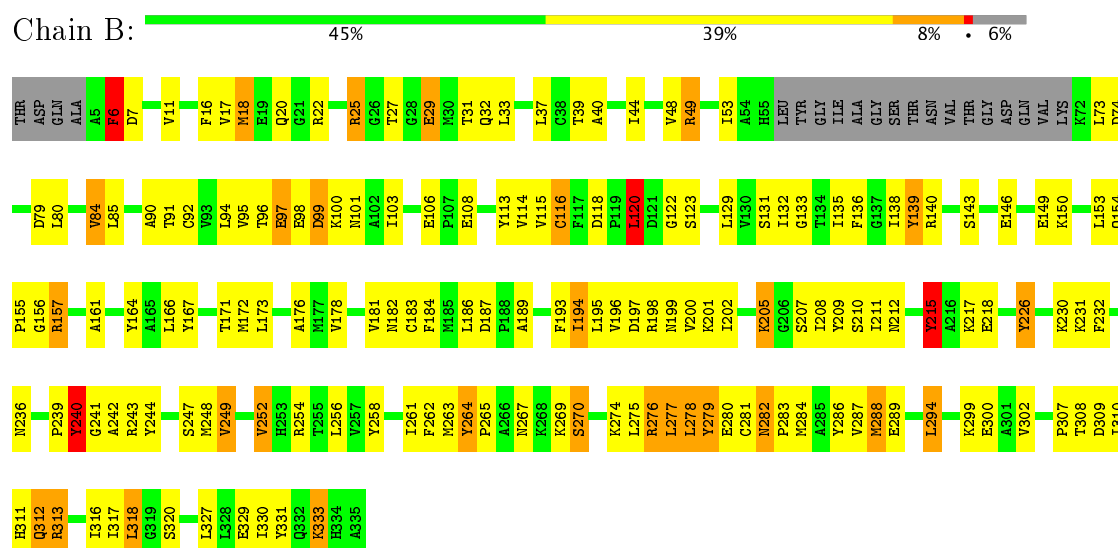
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



#### • Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.00 Å 132.00 Å 67.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.98	3/2430 (0.1%)	1.78	43/3286 (1.3%)
1	B	0.87	1/2447 (0.0%)	1.75	37/3309 (1.1%)
All	All	0.92	4/4877 (0.1%)	1.76	80/6595 (1.2%)

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	10
1	B	0	8
All	All	0	18

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	CD-OE1	-6.73	1.18	1.25
1	A	280	GLU	CD-OE2	-6.43	1.18	1.25
1	A	97	GLU	CD-OE2	5.62	1.31	1.25
1	B	97	GLU	CD-OE1	5.32	1.31	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	CB-CG-OD2	-20.98	99.41	118.30
1	B	313	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	B	97	GLU	OE1-CD-OE2	11.91	137.60	123.30
1	B	120	LEU	CA-C-N	-11.88	91.05	117.20
1	A	120	LEU	CA-C-N	-11.66	91.54	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	CA-CB-CG	10.98	137.56	113.40
1	B	120	LEU	O-C-N	9.84	138.45	122.70
1	A	15	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	B	49	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	243	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	B	167	TYR	CB-CG-CD1	-8.47	115.92	121.00
1	B	329	GLU	CA-CB-CG	8.04	131.10	113.40
1	B	18	MET	CA-CB-CG	-8.00	99.69	113.30
1	A	22	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	15	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	279	TYR	CB-CG-CD2	-7.81	116.32	121.00
1	B	195	LEU	CA-CB-CG	7.79	133.21	115.30
1	A	120	LEU	O-C-N	7.63	134.91	122.70
1	B	140	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	49	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	217	LYS	CA-CB-CG	7.38	129.63	113.40
1	B	25	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	139	TYR	CB-CG-CD1	-7.36	116.59	121.00
1	A	160	VAL	CG1-CB-CG2	-7.08	99.56	110.90
1	A	280	GLU	OE1-CD-OE2	-7.06	114.83	123.30
1	B	240	TYR	CB-CG-CD2	-6.92	116.84	121.00
1	A	49	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	118	ASP	OD1-CG-OD2	6.52	135.69	123.30
1	A	215	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	A	157	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	149	GLU	CA-CB-CG	6.41	127.50	113.40
1	A	164	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	B	167	TYR	CB-CG-CD2	6.29	124.77	121.00
1	B	97	GLU	CG-CD-OE2	-6.23	105.84	118.30
1	A	104	ILE	CA-C-N	-6.17	103.63	117.20
1	A	287	VAL	CA-CB-CG1	-6.14	101.69	110.90
1	A	196	VAL	CA-C-N	6.13	130.69	117.20
1	B	22	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	B	313	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	254	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	252	VAL	CA-CB-CG2	-5.94	101.99	110.90
1	B	157	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	173	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	112	LYS	CA-CB-CG	5.88	126.33	113.40
1	A	113	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	A	75	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	B	329	GLU	CB-CA-C	-5.71	98.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	SER	N-CA-C	-5.65	95.75	111.00
1	A	20	GLN	CB-CG-CD	5.56	126.05	111.60
1	A	308	THR	CA-CB-CG2	-5.51	104.68	112.40
1	A	198	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	314	ALA	CB-CA-C	-5.47	101.89	110.10
1	B	92	CYS	CA-CB-SG	-5.47	104.15	114.00
1	A	311	HIS	CA-CB-CG	5.46	122.88	113.60
1	A	121	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	177	MET	CG-SD-CE	-5.36	91.62	100.20
1	B	232	PHE	N-CA-C	-5.33	96.60	111.00
1	A	35	ASN	CA-CB-CG	-5.32	101.70	113.40
1	A	226	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	B	39	THR	CA-CB-CG2	5.29	119.81	112.40
1	A	219	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	B	215	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	286	TYR	CB-CG-CD2	5.28	124.17	121.00
1	B	318	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	333	LYS	CA-CB-CG	5.22	124.88	113.40
1	A	81	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	B	193	PHE	N-CA-C	-5.20	96.95	111.00
1	A	118	ASP	N-CA-CB	5.16	119.89	110.60
1	A	14	THR	CA-CB-CG2	-5.16	105.17	112.40
1	B	118	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	140	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	154	GLN	CA-CB-CG	5.12	124.67	113.40
1	B	288	MET	CA-CB-CG	-5.11	104.62	113.30
1	B	25	ARG	CA-CB-CG	5.10	124.61	113.40
1	A	287	VAL	CA-CB-CG2	5.08	118.52	110.90
1	A	247	SER	N-CA-C	-5.07	97.30	111.00
1	A	132	ILE	CB-CA-C	-5.04	101.51	111.60
1	A	110	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	B	287	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	B	264	TYR	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	16	PHE	Sidechain
1	A	164	TYR	Sidechain
1	A	193	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	215	TYR	Sidechain
1	A	220	ASP	Peptide
1	A	240	TYR	Sidechain
1	A	244	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	279	TYR	Sidechain
1	B	106	GLU	Peptide
1	B	120	LEU	Mainchain
1	B	164	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain
1	B	258	TYR	Sidechain
1	B	279	TYR	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	2391	530	2448	67	0
1	B	2407	531	2462	93	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	19	4	10	1	0
3	B	19	4	10	5	0
All	All	4840	1069	4930	157	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 16.

All (157) 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:252:VAL:HG11	1:B:284:MET:SD	2.21	0.80
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.66	0.78
1:B:327:LEU:HD12	1:B:330:ILE:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:CYS:HB3	1:B:316:ILE:HD12	1.68	0.75
1:B:226:TYR:HE2	1:B:261:ILE:HG21	1.51	0.75
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.71	0.73
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.71	0.71
1:A:185:MET:SD	1:B:53:ILE:HG13	2.32	0.69
1:B:209:TYR:HA	1:B:261:ILE:HG22	1.73	0.69
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.07	0.69
1:B:96:THR:HB	1:B:99:ASP:HB2	1.75	0.67
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.35	0.67
1:A:155:PRO:HD2	1:A:158:ASN:HD22	1.59	0.66
1:A:107:PRO:HA	1:A:110:ARG:HG3	1.79	0.64
1:B:29:GLU:HA	1:B:32:GLN:OE1	1.99	0.62
1:B:44:ILE:O	1:B:48:VAL:HG23	2.01	0.60
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.83	0.60
3:A:336:AHG:H2	3:A:336:AHG:O3P	1.99	0.60
1:B:96:THR:HG22	1:B:97:GLU:N	2.18	0.59
1:B:226:TYR:CE2	1:B:261:ILE:HG21	2.36	0.59
1:B:150:LYS:HA	1:B:153:LEU:HD12	1.83	0.59
1:B:95:VAL:HB	1:B:116:CYS:HB2	1.84	0.58
1:A:112:LYS:HD2	1:A:140:ARG:NH2	2.19	0.58
1:B:288:MET:HG3	1:B:318:LEU:HD22	1.86	0.57
1:A:90:ALA:HA	1:A:111:GLY:HA3	1.86	0.57
1:B:187:ASP:HB2	1:B:194:ILE:HD11	1.86	0.57
1:A:172:MET:SD	1:A:183:CYS:HB3	2.46	0.56
1:B:274:LYS:NZ	3:B:336:AHG:H61	2.21	0.56
1:A:209:TYR:CZ	1:A:242:ALA:HB2	2.40	0.56
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.41	0.56
1:A:281:CYS:SG	1:A:314:ALA:HB3	2.46	0.55
1:B:96:THR:HG22	1:B:98:GLU:H	1.70	0.55
1:A:15:ARG:HH11	1:A:15:ARG:HG2	1.71	0.55
1:B:182:ASN:ND2	1:B:198:ARG:HA	2.21	0.55
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.89	0.55
1:A:9:ASN:HD21	1:A:15:ARG:HH21	1.54	0.54
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.88	0.54
1:B:176:ALA:HB2	1:B:181:VAL:HG13	1.89	0.54
1:B:252:VAL:HG21	1:B:284:MET:CG	2.38	0.54
1:A:114:VAL:O	1:A:138:ILE:HA	2.07	0.54
1:A:92:CYS:HA	1:A:105:VAL:HB	1.89	0.54
1:B:330:ILE:HG23	1:B:333:LYS:NZ	2.22	0.54
1:B:11:VAL:HG12	1:B:16:PHE:HB2	1.90	0.54
1:A:283:PRO:O	1:A:287:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:SER:HB3	1:B:262:PHE:HA	1.90	0.53
1:A:81:VAL:HA	1:A:84:VAL:HG22	1.91	0.53
1:A:81:VAL:O	1:A:85:LEU:HG	2.08	0.53
1:B:136:PHE:O	1:B:283:PRO:HB3	2.09	0.53
1:B:120:LEU:HG	1:B:132:ILE:HD12	1.90	0.53
1:A:248:MET:CE	1:A:280:GLU:HB3	2.39	0.52
1:A:31:THR:O	1:A:35:ASN:HB2	2.10	0.52
1:B:277:LEU:HB3	1:B:312:GLN:O	2.11	0.51
1:A:209:TYR:CE1	1:A:242:ALA:HB2	2.45	0.51
1:A:212:ASN:HB2	1:A:244:TYR:CE2	2.45	0.51
1:B:263:MET:HG2	1:B:317:ILE:HG23	1.93	0.51
1:B:166:LEU:O	1:B:171:THR:HA	2.11	0.51
1:B:94:LEU:HB2	1:B:103:ILE:HD13	1.92	0.51
1:B:171:THR:HB	1:B:186:LEU:HD23	1.93	0.50
1:B:248:MET:N	3:B:336:AHG:O3	2.44	0.50
1:B:205:LYS:HB2	1:B:205:LYS:NZ	2.27	0.50
1:B:289:GLU:HG2	1:B:294:LEU:HA	1.94	0.50
1:A:235:ASP:HB2	1:A:237:SER:OG	2.12	0.49
1:B:330:ILE:HA	1:B:333:LYS:HG2	1.93	0.49
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.94	0.49
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.47	0.49
1:B:103:ILE:HD12	1:B:103:ILE:H	1.77	0.49
1:B:116:CYS:SG	1:B:278:LEU:HD13	2.52	0.49
1:B:288:MET:HG3	1:B:318:LEU:HD13	1.94	0.49
1:B:280:GLU:O	1:B:283:PRO:HD2	2.13	0.49
1:A:179:ASN:H	1:A:179:ASN:ND2	2.11	0.48
1:B:154:GLN:O	1:B:307:PRO:HG3	2.14	0.48
1:B:210:SER:N	1:B:261:ILE:O	2.47	0.48
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.96	0.48
1:B:276:ARG:NH1	1:B:313:ARG:HD3	2.29	0.48
1:B:252:VAL:HG21	1:B:284:MET:HG2	1.95	0.48
1:A:74:ASP:HA	1:A:77:SER:OG	2.13	0.48
1:A:128:CYS:O	1:A:129:LEU:HB2	2.14	0.47
1:A:141:LYS:HG3	1:A:151:ASP:OD1	2.14	0.47
1:A:20:GLN:O	1:A:23:LYS:HB2	2.14	0.47
1:A:248:MET:HE1	1:A:280:GLU:HB3	1.96	0.47
1:A:286:TYR:HA	1:A:303:LEU:HD11	1.95	0.47
1:A:297:THR:HG22	1:A:315:PRO:O	2.14	0.47
1:B:122:GLY:H	3:B:336:AHG:P1	2.37	0.47
1:A:215:TYR:HB2	1:A:219:PHE:CE1	2.50	0.47
1:A:210:SER:HB3	1:A:262:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASP:HB3	1:A:312:GLN:HB3	1.96	0.47
1:B:202:ILE:HG12	1:B:320:SER:OG	2.14	0.47
1:B:252:VAL:HG21	1:B:284:MET:SD	2.55	0.47
1:B:242:ALA:O	1:B:243:ARG:HG2	2.15	0.47
1:A:232:PHE:CD2	1:B:217:LYS:HG2	2.50	0.46
1:A:274:LYS:O	1:A:313:ARG:HD3	2.14	0.46
1:A:317:ILE:HG22	1:A:324:VAL:HG13	1.98	0.46
1:B:181:VAL:O	1:B:200:VAL:HG23	2.16	0.46
1:B:95:VAL:HG11	1:B:278:LEU:HD12	1.97	0.46
1:B:155:PRO:HB3	1:B:307:PRO:HD3	1.97	0.46
1:B:299:LYS:HG3	1:B:300:GLU:H	1.80	0.45
1:B:183:CYS:HB2	1:B:197:ASP:HB2	1.98	0.45
1:B:274:LYS:HZ3	3:B:336:AHG:H61	1.81	0.45
1:A:204:LYS:O	1:A:320:SER:HB3	2.16	0.45
1:A:231:LYS:O	1:A:239:PRO:HB3	2.16	0.45
1:B:275:LEU:O	1:B:281:CYS:SG	2.75	0.45
1:B:80:LEU:O	1:B:84:VAL:HG22	2.16	0.45
1:A:115:VAL:HG22	1:A:138:ILE:HG12	1.99	0.45
1:B:29:GLU:HB3	1:B:113:TYR:HE2	1.82	0.45
1:A:13:LEU:HD13	1:A:38:CYS:SG	2.56	0.44
1:A:72:LYS:HG2	1:A:73:LEU:H	1.81	0.44
1:B:90:ALA:O	1:B:113:TYR:HB2	2.16	0.44
1:B:269:LYS:O	1:B:270:SER:HB2	2.17	0.44
1:A:80:LEU:O	1:A:84:VAL:HG13	2.17	0.44
1:B:37:LEU:HD21	1:B:136:PHE:CE2	2.53	0.44
1:B:161:ALA:HA	1:B:286:TYR:HE2	1.83	0.44
1:B:187:ASP:CB	1:B:194:ILE:HD11	2.48	0.44
1:B:226:TYR:HB2	1:B:327:LEU:HD13	1.99	0.44
1:B:231:LYS:O	1:B:239:PRO:HB3	2.18	0.44
1:B:282:ASN:HD22	1:B:302:VAL:HG12	1.82	0.44
1:A:267:ASN:O	1:A:271:PRO:HA	2.18	0.43
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.52	0.43
1:A:218:GLU:HB3	1:A:268:LYS:HD2	1.99	0.43
1:B:197:ASP:HB3	1:B:200:VAL:HG22	2.00	0.43
1:B:330:ILE:HG23	1:B:333:LYS:HZ3	1.83	0.43
1:A:119:PRO:HA	1:A:134:THR:HG23	2.00	0.43
1:B:230:LYS:HB3	1:B:240:TYR:HB2	2.01	0.43
1:B:308:THR:HB	1:B:312:GLN:HG3	2.00	0.43
1:A:100:LYS:HG3	1:A:101:ASN:H	1.84	0.43
1:A:232:PHE:CZ	1:B:217:LYS:HA	2.54	0.43
1:B:282:ASN:HA	1:B:282:ASN:HD22	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:O	1:B:20:GLN:HB2	2.19	0.43
1:B:288:MET:SD	1:B:318:LEU:HD13	2.59	0.42
1:B:122:GLY:N	3:B:336:AHG:O2P	2.51	0.42
1:A:295:ALA:CB	1:A:318:LEU:HB3	2.49	0.42
1:B:208:ILE:HA	1:B:241:GLY:O	2.19	0.42
1:A:169:SER:O	1:B:49:ARG:HA	2.20	0.42
1:A:310:ILE:HG13	1:A:311:HIS:N	2.34	0.42
1:B:115:VAL:HG13	1:B:138:ILE:HG12	2.01	0.42
1:B:226:TYR:HB2	1:B:327:LEU:CD1	2.50	0.42
1:A:233:PRO:HD3	1:A:239:PRO:HG3	2.01	0.42
1:B:244:TYR:HE1	1:B:262:PHE:HE1	1.68	0.42
1:A:29:GLU:HB3	1:A:90:ALA:HB1	2.02	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.81	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.70	0.42
1:A:212:ASN:O	1:A:219:PHE:HZ	2.02	0.42
1:A:281:CYS:SG	1:A:316:ILE:HD12	2.59	0.42
1:B:243:ARG:NH1	1:B:243:ARG:HG2	2.35	0.41
1:B:261:ILE:HA	1:B:261:ILE:HD12	1.93	0.41
1:A:266:ALA:HB1	1:A:271:PRO:O	2.20	0.41
1:A:166:LEU:HD13	1:A:249:VAL:HG12	2.02	0.41
1:A:238:ALA:HA	1:A:239:PRO:HD3	1.93	0.41
1:B:187:ASP:OD1	1:B:189:ALA:HB3	2.20	0.41
1:B:172:MET:HA	1:B:184:PHE:O	2.21	0.41
1:A:141:LYS:HE3	1:A:143:SER:O	2.20	0.41
1:A:266:ALA:H	1:A:315:PRO:HB3	1.86	0.41
1:B:309:ASP:O	1:B:312:GLN:HB2	2.21	0.41
1:A:209:TYR:HA	1:A:261:ILE:HG23	2.03	0.40
1:B:215:TYR:HE2	1:B:264:TYR:HH	1.65	0.40
1:A:130:VAL:HG12	1:A:131:SER:O	2.21	0.40
1:A:112:LYS:HD2	1:A:140:ARG:HH21	1.87	0.40
1:B:6:PHE:HA	1:B:6:PHE:HD1	1.66	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	309/335 (92%)	276 (89%)	31 (10%)	2 (1%)	28	70
1	B	311/335 (93%)	257 (83%)	39 (12%)	15 (5%)	2	16
All	All	620/670 (92%)	533 (86%)	70 (11%)	17 (3%)	6	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	B	27	THR
1	B	73	LEU
1	B	100	LYS
1	B	276	ARG
1	A	92	CYS
1	B	156	GLY
1	B	157	ARG
1	B	199	ASN
1	B	270	SER
1	B	277	LEU
1	B	178	VAL
1	B	236	ASN
1	B	6	PHE
1	B	74	ASP
1	B	256	LEU
1	B	31	THR

### 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	261/278 (94%)	227 (87%)	34 (13%)	5	21
1	B	262/278 (94%)	229 (87%)	33 (13%)	5	23
All	All	523/556 (94%)	456 (87%)	67 (13%)	5	22

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	27	THR
1	A	46	THR
1	A	73	LEU
1	A	74	ASP
1	A	76	LEU
1	A	77	SER
1	A	99	ASP
1	A	108	GLU
1	A	124	SER
1	A	131	SER
1	A	140	ARG
1	A	147	PRO
1	A	150	LYS
1	A	169	SER
1	A	172	MET
1	A	178	VAL
1	A	199	ASN
1	A	207	SER
1	A	224	THR
1	A	225	GLU
1	A	230	LYS
1	A	235	ASP
1	A	264	TYR
1	A	265	PRO
1	A	268	LYS
1	A	270	SER
1	A	272	LYS
1	A	276	ARG
1	A	279	TYR
1	A	300	GLU
1	A	306	VAL
1	A	308	THR
1	A	334	HIS
1	B	6	PHE
1	B	7	ASP
1	B	18	MET
1	B	25	ARG
1	B	29	GLU
1	B	33	LEU
1	B	79	ASP
1	B	84	VAL

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Mol	Chain	Res	Type
1	B	91	THR
1	B	99	ASP
1	B	101	ASN
1	B	108	GLU
1	B	116	CYS
1	B	123	SER
1	B	129	LEU
1	B	131	SER
1	B	135	ILE
1	B	143	SER
1	B	146	GLU
1	B	149	GLU
1	B	194	ILE
1	B	196	VAL
1	B	201	LYS
1	B	205	LYS
1	B	207	SER
1	B	249	VAL
1	B	265	PRO
1	B	278	LEU
1	B	279	TYR
1	B	282	ASN
1	B	294	LEU
1	B	312	GLN
1	B	331	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	158	ASN
1	A	179	ASN
1	A	199	ASN
1	B	182	ASN
1	B	282	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
3	AHG	A	336	2	19,19,19	0.65	0	29,29,29	0.86	1 (3%)
3	AHG	B	336	2	19,19,19	0.63	0	29,29,29	0.89	1 (3%)

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
3	AHG	A	336	2	-	0/12/28/28	0/1/1/1
3	AHG	B	336	2	-	0/12/28/28	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	336	AHG	O2P-P1-O1P	2.18	119.01	110.50
3	B	336	AHG	O2P-P1-O1P	2.28	119.43	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	336	AHG	1	0
3	B	336	AHG	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.