



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:54 AM UTC

PDB ID : 3ENV / pdb\_00003env  
Title : Substrate and inhibitor complexes of ribose 5-phosphate isomerase from *Vibrio vulnificus* YJ016  
Authors : Min, K.; Kwon, T.H.; Kim, T.G.  
Deposited on : 2008-09-26  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

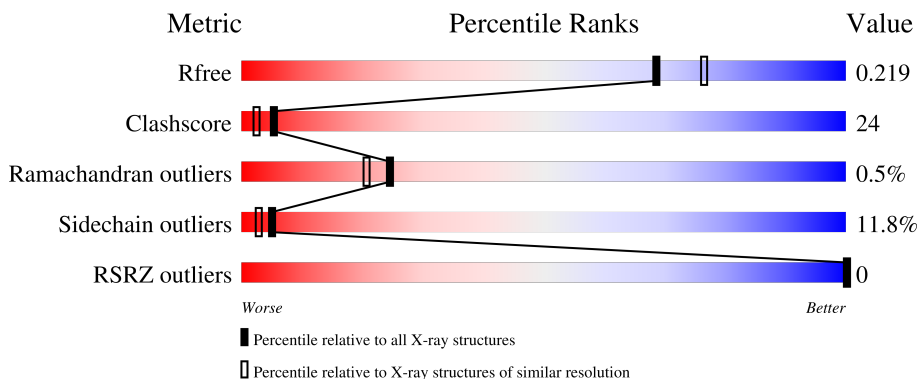
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	235	
1	B	235	

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	ABF	A	1269	X	X	-	-
2	ABF	B	1269	X	X	-	-

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3360 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 Ribose-5-phosphate isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1602	1010	266	318	8	0	0	0
1	B	217	1602	1010	266	318	8	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

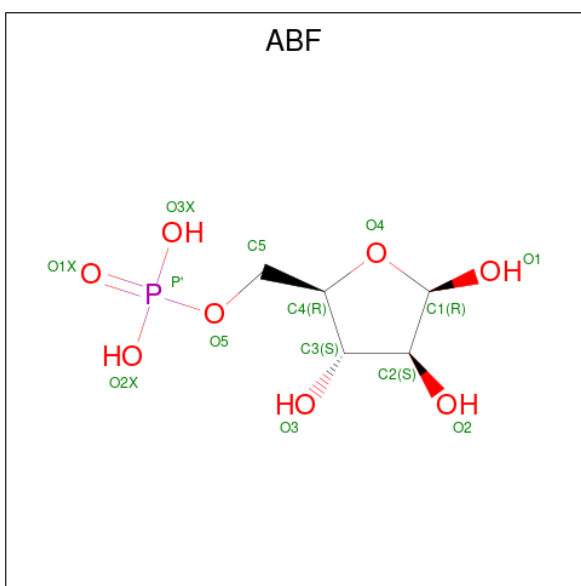
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	expression tag	UNP Q7MHL9
A	-15	SER	-	expression tag	UNP Q7MHL9
A	-14	HIS	-	expression tag	UNP Q7MHL9
A	-13	MET	-	expression tag	UNP Q7MHL9
A	-12	ALA	-	expression tag	UNP Q7MHL9
A	-11	SER	-	expression tag	UNP Q7MHL9
A	-10	MET	-	expression tag	UNP Q7MHL9
A	-9	THR	-	expression tag	UNP Q7MHL9
A	-8	GLY	-	expression tag	UNP Q7MHL9
A	-7	GLY	-	expression tag	UNP Q7MHL9
A	-6	GLN	-	expression tag	UNP Q7MHL9
A	-5	GLN	-	expression tag	UNP Q7MHL9
A	-4	MET	-	expression tag	UNP Q7MHL9
A	-3	GLY	-	expression tag	UNP Q7MHL9
A	-2	ARG	-	expression tag	UNP Q7MHL9
A	-1	GLY	-	expression tag	UNP Q7MHL9
A	0	SER	-	expression tag	UNP Q7MHL9
B	-16	GLY	-	expression tag	UNP Q7MHL9
B	-15	SER	-	expression tag	UNP Q7MHL9
B	-14	HIS	-	expression tag	UNP Q7MHL9
B	-13	MET	-	expression tag	UNP Q7MHL9
B	-12	ALA	-	expression tag	UNP Q7MHL9
B	-11	SER	-	expression tag	UNP Q7MHL9
B	-10	MET	-	expression tag	UNP Q7MHL9
B	-9	THR	-	expression tag	UNP Q7MHL9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q7MHL9
B	-7	GLY	-	expression tag	UNP Q7MHL9
B	-6	GLN	-	expression tag	UNP Q7MHL9
B	-5	GLN	-	expression tag	UNP Q7MHL9
B	-4	MET	-	expression tag	UNP Q7MHL9
B	-3	GLY	-	expression tag	UNP Q7MHL9
B	-2	ARG	-	expression tag	UNP Q7MHL9
B	-1	GLY	-	expression tag	UNP Q7MHL9
B	0	SER	-	expression tag	UNP Q7MHL9

- Molecule 2 is 5-O-phosphono-beta-D-arabinofuranose (CCD ID: ABF) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		

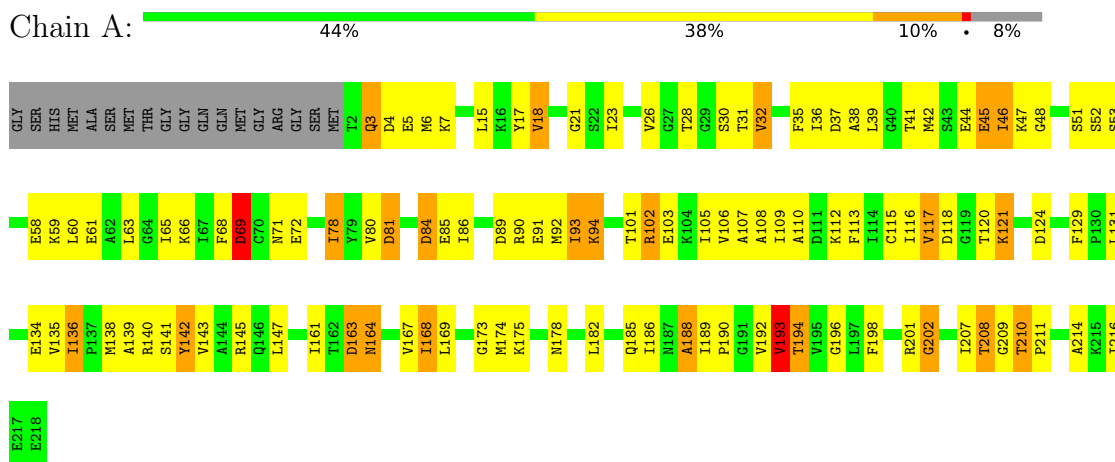
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	71	Total	O	0	0
			71	71		

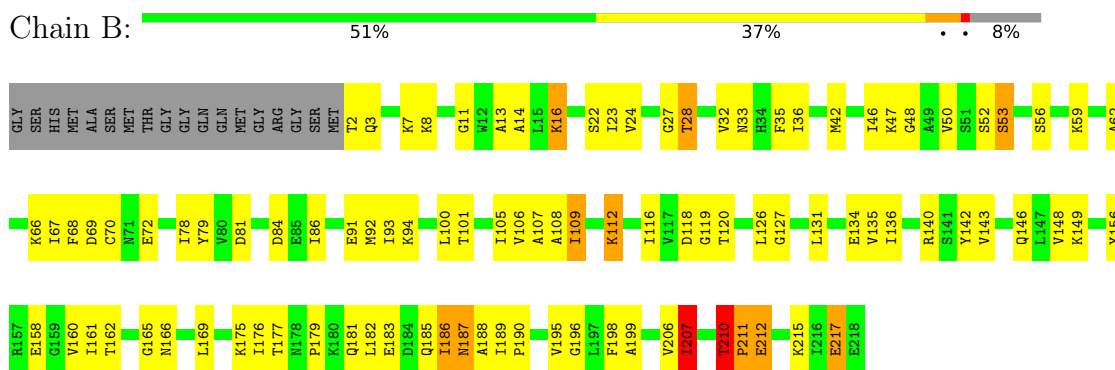
### 3 Residue-property plots [i](#)

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: Ribose-5-phosphate isomerase A



- Molecule 1: Ribose-5-phosphate isomerase A



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.02Å 77.02Å 190.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.00-2.00) 99.9 (25.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.67 (at 1.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.238 , 0.314 0.213 , 0.219	Depositor DCC
$R_{free}$ test set	2710 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtrriage
Anisotropy	0.810	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.080 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.097 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.079 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$ 0.079 for $-h,2/3^*h+1/3^*k+1/3^*l,4/3^*h+8/3^*k-1/3^*l$ 0.085 for $1/3^*h+2/3^*k-1/3^*l,-k,-8/3^*h-4/3^*k-1/3^*l$ 0.097 for $-1/3^*h-2/3^*k+1/3^*l,-2/3^*h-1/3^*k-1/3^*l,4/3^*h-4/3^*k-1/3^*l$ 0.367 for $-h-k,k,-l$	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: ABF

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	1.33	4/1622 (0.2%)	1.50	26/2195 (1.2%)
1	B	1.39	5/1622 (0.3%)	1.43	9/2195 (0.4%)
All	All	1.36	9/3244 (0.3%)	1.47	35/4390 (0.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	VAL	CA-CB	8.59	1.62	1.55
1	A	188	ALA	CA-CB	-7.39	1.43	1.54
1	B	8	LYS	CA-C	-6.37	1.45	1.52
1	B	162	THR	CA-CB	6.18	1.62	1.53
1	B	210	THR	CA-CB	5.67	1.61	1.53
1	B	24	VAL	CA-CB	5.47	1.60	1.54
1	A	110	ALA	CA-CB	5.40	1.61	1.53
1	A	202	GLY	N-CA	5.36	1.48	1.44
1	B	84	ASP	N-CA	-5.14	1.39	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	VAL	N-CA-C	-8.06	102.58	110.72
1	A	121	LYS	N-CA-C	7.83	122.94	113.23
1	A	210	THR	CA-C-N	7.71	127.76	119.28
1	A	210	THR	C-N-CA	7.71	127.76	119.28
1	B	127	GLY	N-CA-C	7.39	123.28	114.48
1	B	53	SER	N-CA-C	7.29	121.28	109.40
1	A	124	ASP	N-CA-C	-6.77	103.92	112.93
1	A	168	ILE	N-CA-C	6.35	117.06	108.17
1	A	143	VAL	N-CA-C	-6.23	104.27	110.62
1	A	78	ILE	N-CA-C	6.22	118.89	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	TYR	N-CA-C	-6.17	104.24	110.97
1	B	131	LEU	N-CA-C	-6.06	102.15	109.72
1	A	193	VAL	N-CA-C	-6.00	105.84	111.48
1	B	107	ALA	N-CA-C	5.99	117.48	111.07
1	B	52	SER	N-CA-C	-5.91	105.66	112.92
1	A	193	VAL	N-CA-CB	5.85	117.36	111.57
1	A	173	GLY	N-CA-C	5.82	123.68	115.30
1	A	32	VAL	CB-CA-C	-5.80	102.86	112.26
1	A	129	PHE	CA-C-N	5.80	125.81	119.89
1	A	129	PHE	C-N-CA	5.80	125.81	119.89
1	A	94	LYS	N-CA-C	5.69	118.49	109.50
1	A	147	LEU	N-CA-C	5.64	117.43	111.28
1	B	207	ILE	CB-CA-C	-5.61	105.50	112.45
1	A	53	SER	CA-C-N	5.53	127.73	120.60
1	A	53	SER	C-N-CA	5.53	127.73	120.60
1	A	84	ASP	N-CA-C	-5.51	106.23	113.12
1	A	81	ASP	N-CA-C	-5.44	100.66	108.60
1	A	136	ILE	N-CA-C	-5.42	103.64	108.95
1	A	69	ASP	CA-C-N	5.35	127.70	120.38
1	A	69	ASP	C-N-CA	5.35	127.70	120.38
1	B	207	ILE	N-CA-C	5.28	114.82	106.32
1	A	182	LEU	N-CA-C	-5.23	105.64	112.23
1	A	35	PHE	N-CA-C	-5.21	105.67	112.23
1	B	93	ILE	N-CA-CB	5.15	117.94	111.46
1	A	107	ALA	N-CA-C	5.10	118.28	111.75

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	1602	0	1627	95	0
1	B	1602	0	1627	70	1
2	A	14	0	0	0	0
2	B	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	57	0	0	8	1
3	B	71	0	0	8	0
All	All	3360	0	3254	156	1

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 24.

All (156) 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:2:THR:HG23	1:B:120:THR:HG23	1.46	0.96
1:A:21:GLY:N	1:A:45:GLU:O	2.11	0.84
1:A:134:GLU:HB3	1:A:193:VAL:HG22	1.60	0.83
1:A:164:ASN:H	1:A:164:ASN:HD22	1.26	0.83
1:B:2:THR:CG2	1:B:120:THR:HG23	2.07	0.83
1:B:161:ILE:HD12	1:B:165:GLY:HA2	1.60	0.82
1:B:2:THR:HG21	1:B:119:GLY:H	1.43	0.82
1:A:164:ASN:H	1:A:164:ASN:ND2	1.78	0.81
1:B:28:THR:OG1	1:B:53:SER:HB2	1.82	0.80
1:A:15:LEU:HD22	1:A:38:ALA:HB1	1.60	0.80
1:A:139:ALA:HB2	1:B:105:ILE:HD13	1.64	0.80
1:B:35:PHE:HB2	3:B:1333:HOH:O	1.81	0.80
1:A:94:LYS:HZ2	1:A:113:PHE:HZ	1.31	0.78
1:A:210:THR:HB	1:A:211:PRO:HD2	1.67	0.77
1:B:183:GLU:O	1:B:187:ASN:HB2	1.85	0.77
1:A:44:GLU:H	1:A:44:GLU:CD	1.94	0.75
1:A:105:ILE:HB	3:A:1320:HOH:O	1.87	0.72
1:A:3:GLN:HG3	1:A:6:MET:H	1.53	0.72
1:B:53:SER:HB3	1:B:56:SER:HB2	1.71	0.71
1:A:142:TYR:HB2	1:B:109:ILE:HD11	1.73	0.70
1:B:91:GLU:OE1	1:B:179:PRO:HG2	1.93	0.69
1:A:32:VAL:O	1:A:36:ILE:HG13	1.93	0.69
1:B:78:ILE:HG22	1:B:112:LYS:HB3	1.75	0.68
1:B:50:VAL:HG22	1:B:68:PHE:O	1.94	0.68
1:A:69:ASP:OD2	1:A:71:ASN:N	2.28	0.67
1:B:94:LYS:HD3	1:B:198:PHE:CD2	2.30	0.66
1:B:112:LYS:HB2	1:B:112:LYS:HZ3	1.60	0.66
1:A:134:GLU:HB3	1:A:193:VAL:CG2	2.25	0.66
1:A:208:THR:O	1:A:214:ALA:HB1	1.96	0.65
1:A:210:THR:HB	1:A:211:PRO:CD	2.26	0.65
1:B:2:THR:HG21	1:B:119:GLY:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:C	1:A:188:ALA:H	2.05	0.64
1:A:116:ILE:HG22	1:A:207:ILE:HB	1.79	0.64
1:A:207:ILE:HG12	1:A:216:ILE:HG23	1.81	0.63
1:B:116:ILE:HD13	3:B:1333:HOH:O	1.98	0.63
1:A:164:ASN:ND2	1:A:164:ASN:N	2.45	0.63
1:B:23:ILE:HG13	1:B:47:LYS:HB3	1.80	0.62
1:B:146:GLN:NE2	3:B:1279:HOH:O	2.28	0.62
1:A:135:VAL:HG21	1:A:169:LEU:HD12	1.81	0.61
1:A:84:ASP:O	1:A:121:LYS:HD2	1.99	0.61
1:B:2:THR:OG1	1:B:3:GLN:N	2.30	0.61
1:B:210:THR:O	1:B:212:GLU:N	2.34	0.61
1:A:23:ILE:HG13	1:A:47:LYS:HB3	1.82	0.61
1:A:89:ASP:O	1:A:90:ARG:HB2	2.01	0.61
1:B:13:ALA:O	1:B:16:LYS:HG3	2.00	0.60
1:A:208:THR:HG22	1:A:209:GLY:H	1.67	0.58
1:A:17:TYR:HE2	1:A:207:ILE:HD11	1.68	0.58
1:B:100:LEU:HD11	1:B:196:GLY:HA2	1.85	0.58
1:A:18:VAL:CG2	1:A:46:ILE:HD11	2.33	0.58
1:A:108:ALA:HB2	1:B:190:PRO:HG2	1.87	0.57
1:A:134:GLU:CB	1:A:193:VAL:HG22	2.34	0.56
1:B:176:ILE:O	1:B:176:ILE:HG22	2.06	0.56
1:A:117:VAL:O	1:A:208:THR:HA	2.06	0.56
1:A:66:LYS:NZ	1:A:68:PHE:CZ	2.73	0.55
1:A:103:GLU:HG2	3:A:1325:HOH:O	2.06	0.55
1:A:7:LYS:HD3	1:A:30:SER:HB2	1.89	0.54
1:A:117:VAL:HG12	1:A:208:THR:HG23	1.89	0.54
1:A:23:ILE:CG1	1:A:47:LYS:HB3	2.38	0.54
1:A:163:ASP:N	1:A:163:ASP:OD1	2.39	0.54
1:B:143:VAL:HG22	1:B:189:ILE:HG22	1.89	0.54
1:B:185:GLN:O	1:B:188:ALA:HB3	2.08	0.54
1:B:126:LEU:HB2	1:B:176:ILE:HB	1.90	0.53
1:A:78:ILE:HG22	1:A:112:LYS:HB2	1.90	0.53
1:B:33:ASN:HA	1:B:36:ILE:HD12	1.90	0.53
1:A:136:ILE:HD13	1:A:193:VAL:HG12	1.89	0.53
1:B:211:PRO:HB2	1:B:212:GLU:OE1	2.09	0.53
1:A:120:THR:HG22	1:A:120:THR:O	2.08	0.52
1:A:163:ASP:OD1	1:A:164:ASN:ND2	2.43	0.52
1:B:11:GLY:HA2	3:B:1333:HOH:O	2.10	0.52
1:B:79:TYR:CD1	1:B:106:VAL:HG12	2.45	0.52
1:A:4:ASP:HA	1:A:7:LYS:HD2	1.91	0.52
1:A:39:LEU:HD23	1:A:60:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HG2	1:B:108:ALA:HB2	1.92	0.51
1:B:14:ALA:HB3	3:B:1333:HOH:O	2.11	0.51
1:B:182:LEU:O	1:B:186:ILE:HG13	2.10	0.51
1:A:134:GLU:CD	1:A:193:VAL:HG21	2.36	0.50
1:A:167:VAL:O	1:A:168:ILE:HD13	2.11	0.50
1:A:3:GLN:NE2	3:A:1307:HOH:O	2.38	0.50
1:A:42:MET:O	1:A:46:ILE:HD13	2.12	0.50
1:A:178:ASN:OD1	3:A:1275:HOH:O	2.20	0.50
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.27	0.50
1:A:189:ILE:HB	1:A:192:VAL:HG23	1.94	0.49
1:B:91:GLU:HB3	1:B:199:ALA:HA	1.95	0.49
1:B:146:GLN:O	3:B:1335:HOH:O	2.20	0.49
1:B:210:THR:O	1:B:211:PRO:C	2.56	0.49
1:A:26:VAL:HB	1:A:51:SER:HB2	1.95	0.49
1:B:156:TYR:CD2	1:B:158:GLU:HG2	2.48	0.49
1:A:118:ASP:OD1	1:A:118:ASP:C	2.56	0.49
1:A:193:VAL:CG2	1:A:194:THR:N	2.76	0.49
1:B:146:GLN:NE2	1:B:149:LYS:HE2	2.28	0.48
1:B:11:GLY:HA2	1:B:116:ILE:HD12	1.94	0.48
1:B:101:THR:OG1	1:B:134:GLU:OE1	2.26	0.47
1:A:23:ILE:HA	1:A:48:GLY:O	2.14	0.47
1:B:78:ILE:HA	1:B:112:LYS:O	2.14	0.47
1:B:94:LYS:HD3	1:B:198:PHE:CG	2.49	0.47
1:A:60:LEU:O	1:A:63:LEU:HB2	2.15	0.47
1:A:108:ALA:CB	1:B:190:PRO:HG2	2.45	0.47
1:B:48:GLY:HA3	1:B:68:PHE:HE2	1.80	0.47
1:A:18:VAL:HG22	1:A:42:MET:HE2	1.96	0.47
1:A:131:LEU:HD23	1:A:174:MET:CE	2.45	0.47
1:B:206:VAL:HB	1:B:217:GLU:HG2	1.96	0.47
1:A:86:ILE:HA	1:A:91:GLU:O	2.15	0.46
1:A:136:ILE:CD1	1:A:193:VAL:HG12	2.45	0.46
1:A:102:ARG:O	1:A:106:VAL:HG23	2.15	0.46
1:B:66:LYS:HD3	1:B:68:PHE:CZ	2.50	0.45
1:A:58:GLU:HA	1:A:61:GLU:OE2	2.16	0.45
1:A:186:ILE:C	1:A:188:ALA:N	2.70	0.45
1:A:201:ARG:NH1	1:A:202:GLY:O	2.51	0.44
1:A:42:MET:O	1:A:42:MET:HG3	2.18	0.44
1:B:187:ASN:HD22	1:B:187:ASN:HA	1.60	0.44
1:B:207:ILE:O	1:B:207:ILE:HG22	2.17	0.44
1:A:103:GLU:CG	3:A:1325:HOH:O	2.64	0.44
1:B:182:LEU:HA	1:B:185:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASP:HB2	1:A:93:ILE:HG22	1.99	0.43
1:A:117:VAL:N	1:A:207:ILE:O	2.42	0.43
1:A:138:MET:O	1:B:70:CYS:HB2	2.18	0.43
1:A:198:PHE:CD1	1:A:198:PHE:N	2.86	0.43
1:B:53:SER:HB3	1:B:56:SER:CB	2.46	0.43
1:A:109:ILE:HD11	1:B:142:TYR:HB2	2.00	0.43
1:A:193:VAL:HG23	1:A:194:THR:N	2.33	0.43
1:B:22:SER:O	1:B:46:ILE:HB	2.19	0.43
1:A:85:GLU:O	1:A:92:MET:HA	2.18	0.42
1:A:142:TYR:CE1	1:A:189:ILE:CG2	3.03	0.42
1:A:7:LYS:HA	1:A:31:THR:HG23	2.01	0.42
1:B:140:ARG:HD2	1:B:156:TYR:CG	2.54	0.42
1:B:135:VAL:O	1:B:166:ASN:HB3	2.19	0.42
1:B:183:GLU:OE2	3:B:1274:HOH:O	2.21	0.42
1:A:18:VAL:HG21	1:A:46:ILE:HD11	2.02	0.42
1:B:27:GLY:HA3	1:B:81:ASP:CG	2.45	0.42
1:A:81:ASP:O	1:A:115:CYS:HA	2.20	0.42
1:B:7:LYS:HE2	3:B:1300:HOH:O	2.19	0.42
1:A:52:SER:CB	3:A:1325:HOH:O	2.68	0.41
1:A:37:ASP:OD1	1:A:59:LYS:NZ	2.43	0.41
1:A:142:TYR:CD2	1:B:109:ILE:HG13	2.54	0.41
1:A:185:GLN:O	1:A:188:ALA:HB3	2.20	0.41
1:B:94:LYS:HD3	1:B:198:PHE:CE2	2.55	0.41
1:B:210:THR:C	1:B:212:GLU:N	2.78	0.41
1:A:84:ASP:O	1:A:121:LYS:CD	2.66	0.41
1:A:120:THR:O	1:A:120:THR:CG2	2.68	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.21	0.41
1:A:189:ILE:HA	1:A:190:PRO:HD3	1.94	0.41
1:B:140:ARG:HD2	1:B:156:TYR:CD1	2.55	0.41
1:A:65:ILE:O	1:A:65:ILE:HG22	2.19	0.41
1:A:32:VAL:O	1:A:32:VAL:HG12	2.20	0.41
1:B:2:THR:OG1	1:B:118:ASP:HB2	2.21	0.41
1:B:59:LYS:O	1:B:62:ALA:HB3	2.20	0.41
1:B:92:MET:HB2	1:B:198:PHE:HB2	2.03	0.41
1:B:156:TYR:HA	1:B:169:LEU:HD23	2.02	0.41
1:A:94:LYS:HB2	1:A:198:PHE:CE1	2.56	0.40
1:B:69:ASP:O	1:B:72:GLU:HB2	2.21	0.40
1:A:51:SER:OG	1:A:52:SER:N	2.54	0.40
1:A:52:SER:HB2	3:A:1325:HOH:O	2.20	0.40
1:A:113:PHE:HB2	1:A:201:ARG:NH2	2.35	0.40
1:A:101:THR:HG21	1:B:136:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HA	3:A:1320:HOH:O	2.21	0.40
1:A:131:LEU:HD23	1:A:174:MET:HE1	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ARG:NH2	3:A:1276:HOH:O[2_455]	2.17	0.03

## 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	215/235 (92%)	201 (94%)	13 (6%)	1 (0%)	24	21
1	B	215/235 (92%)	206 (96%)	8 (4%)	1 (0%)	24	21
All	All	430/470 (92%)	407 (95%)	21 (5%)	2 (0%)	24	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLY
1	B	211	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	170/182 (93%)	150 (88%)	20 (12%)	5	3
1	B	170/182 (93%)	150 (88%)	20 (12%)	5	3
All	All	340/364 (93%)	300 (88%)	40 (12%)	5	3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	GLU
1	A	18	VAL
1	A	28	THR
1	A	41	THR
1	A	45	GLU
1	A	46	ILE
1	A	69	ASP
1	A	72	GLU
1	A	80	VAL
1	A	93	ILE
1	A	102	ARG
1	A	117	VAL
1	A	161	ILE
1	A	163	ASP
1	A	164	ASN
1	A	175	LYS
1	A	193	VAL
1	A	194	THR
1	A	208	THR
1	B	16	LYS
1	B	28	THR
1	B	32	VAL
1	B	42	MET
1	B	67	ILE
1	B	86	ILE
1	B	109	ILE
1	B	112	LYS
1	B	160	VAL
1	B	175	LYS
1	B	177	THR
1	B	181	GLN
1	B	186	ILE
1	B	187	ASN
1	B	195	VAL

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Mol	Chain	Res	Type
1	B	207	ILE
1	B	210	THR
1	B	212	GLU
1	B	215	LYS
1	B	217	GLU

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

Mol	Chain	Res	Type
1	A	71	ASN
1	A	164	ASN
1	A	178	ASN
1	A	187	ASN
1	A	200	HIS
1	B	166	ASN
1	B	187	ASN
1	B	200	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	ABF	A	1269	-	14,14,14	4.24	9 (64%)	19,21,21	3.96	12 (63%)
2	ABF	B	1269	-	14,14,14	4.06	8 (57%)	19,21,21	3.92	12 (63%)

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	ABF	A	1269	-	4/4/5/5	6/6/22/22	0/1/1/1
2	ABF	B	1269	-	4/4/5/5	6/6/22/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1269	ABF	C1-C2	-11.42	1.39	1.52
2	B	1269	ABF	C1-C2	-11.21	1.39	1.52
2	B	1269	ABF	C3-C4	-5.65	1.38	1.53
2	A	1269	ABF	O4-C1	-5.54	1.36	1.43
2	B	1269	ABF	C3-C2	-5.28	1.39	1.53
2	A	1269	ABF	C3-C2	-4.96	1.39	1.53
2	A	1269	ABF	C3-C4	-4.88	1.40	1.53
2	B	1269	ABF	O4-C1	-3.75	1.38	1.43
2	A	1269	ABF	O4-C4	-3.42	1.37	1.45
2	A	1269	ABF	P'-O3X	3.09	1.66	1.54
2	B	1269	ABF	O4-C4	-3.07	1.38	1.45
2	B	1269	ABF	O3-C3	-2.75	1.36	1.43
2	B	1269	ABF	O2-C2	-2.52	1.36	1.43
2	A	1269	ABF	P'-O2X	2.43	1.63	1.54
2	A	1269	ABF	O2-C2	-2.30	1.37	1.43
2	B	1269	ABF	P'-O2X	2.19	1.62	1.54
2	A	1269	ABF	P'-O5	2.10	1.66	1.60

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1269	ABF	O1-C1-O4	10.41	124.38	111.12
2	B	1269	ABF	O1-C1-O4	10.00	123.86	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1269	ABF	O2-C2-C1	5.71	127.73	111.85
2	A	1269	ABF	O3-C3-C4	5.55	127.02	111.08
2	B	1269	ABF	O3-C3-C4	5.04	125.57	111.08
2	A	1269	ABF	O2-C2-C3	4.98	127.78	111.82
2	A	1269	ABF	O2-C2-C1	4.95	125.62	111.85
2	B	1269	ABF	O3-C3-C2	4.49	126.22	111.82
2	A	1269	ABF	C5-C4-C3	4.47	131.29	115.21
2	A	1269	ABF	O3-C3-C2	4.38	125.85	111.82
2	B	1269	ABF	C5-C4-C3	4.18	130.26	115.21
2	B	1269	ABF	C1-C2-C3	4.14	107.38	102.29
2	B	1269	ABF	O2-C2-C3	4.07	124.88	111.82
2	B	1269	ABF	O1-C1-C2	3.89	128.13	110.25
2	B	1269	ABF	O4-C4-C5	3.82	121.56	109.33
2	A	1269	ABF	O4-C1-C2	3.69	109.79	104.67
2	B	1269	ABF	O5-P'-O1X	3.56	116.07	106.44
2	A	1269	ABF	C1-C2-C3	3.51	106.61	102.29
2	A	1269	ABF	O1-C1-C2	3.39	125.83	110.25
2	A	1269	ABF	O4-C4-C5	3.36	120.09	109.33
2	A	1269	ABF	O5-P'-O1X	3.25	115.22	106.44
2	B	1269	ABF	C2-C3-C4	2.90	108.20	102.61
2	B	1269	ABF	O4-C1-C2	2.41	108.01	104.67
2	A	1269	ABF	C2-C3-C4	2.34	107.13	102.61

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1269	ABF	C3
2	A	1269	ABF	C1
2	A	1269	ABF	C4
2	A	1269	ABF	C2
2	B	1269	ABF	C3
2	B	1269	ABF	C1
2	B	1269	ABF	C4
2	B	1269	ABF	C2

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1269	ABF	C5-O5-P'-O1X
2	A	1269	ABF	C5-O5-P'-O3X
2	B	1269	ABF	C5-O5-P'-O1X
2	B	1269	ABF	C5-O5-P'-O2X

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Mol	Chain	Res	Type	Atoms
2	B	1269	ABF	C5-O5-P'-O3X
2	A	1269	ABF	O4-C4-C5-O5
2	B	1269	ABF	C3-C4-C5-O5
2	A	1269	ABF	C3-C4-C5-O5
2	A	1269	ABF	C4-C5-O5-P'
2	B	1269	ABF	C4-C5-O5-P'
2	A	1269	ABF	C5-O5-P'-O2X
2	B	1269	ABF	O4-C4-C5-O5

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 [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	217/235 (92%)	-1.38	0 <a href="#">100</a> <a href="#">100</a>	2, 6, 21, 31	0
1	B	217/235 (92%)	-1.44	0 <a href="#">100</a> <a href="#">100</a>	2, 4, 14, 25	0
All	All	434/470 (92%)	-1.41	0 <a href="#">100</a> <a href="#">100</a>	2, 4, 19, 31	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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	ABF	A	1269	14/14	0.97	0.11	31,36,37,38	0
2	ABF	B	1269	14/14	0.98	0.08	25,30,31,33	0

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

There are no such residues in this entry.