



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:30 AM UTC

PDB ID : 1FPK / pdb_00001fpk
Title : FRUCTOSE-1,6-BISPHOSPHATASE (D-FRUCTOSE-1,6-BISPHOSPHAT
E 1-PHOSPHOHYDROLASE) COMPLEXED WITH THALLIUM IONS (10
MM)
Authors : Villeret, V.; Lipscomb, W.N.
Deposited on : 1995-06-02
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

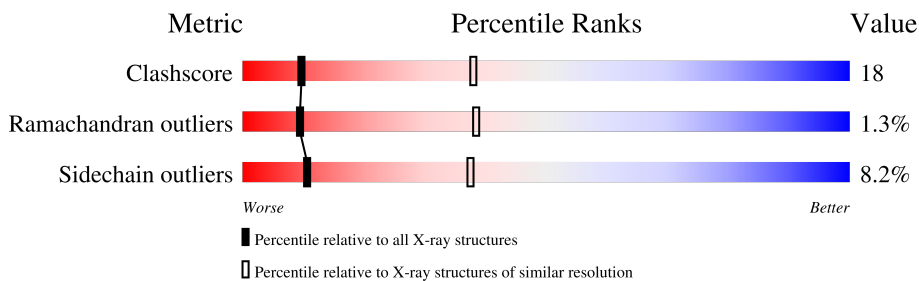
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Note EDS was not executed.

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4786 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-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2390	1520	402	453	15			
1	B	312	Total	C	N	O	S	0	0	0
			2390	1520	402	453	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 THALLIUM (I) ION (CCD ID: TL) (formula: Tl).

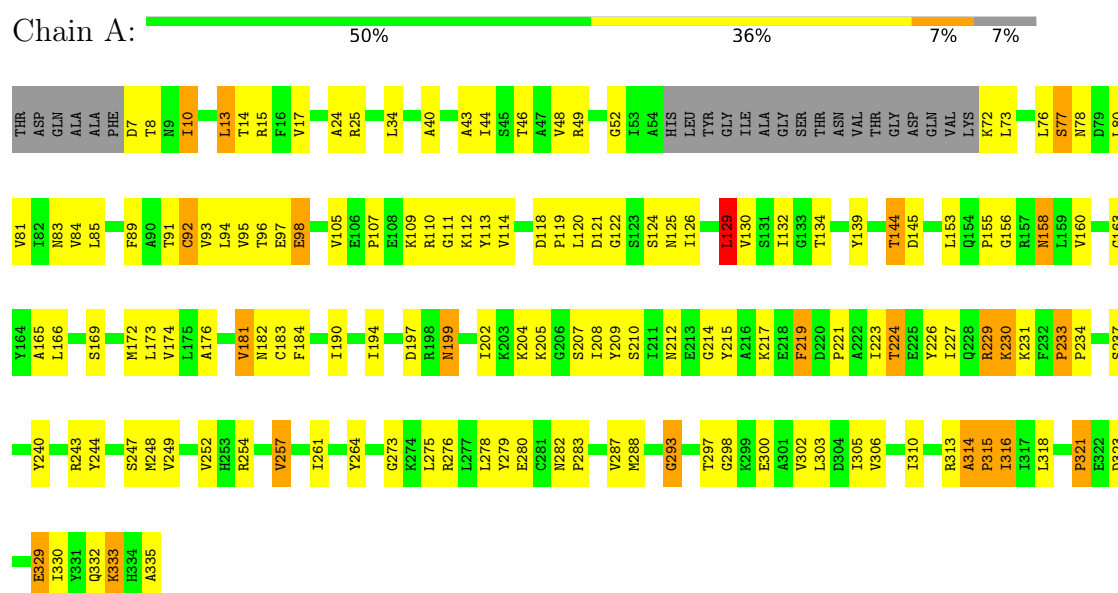
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Tl	0	0
			3	3		
2	B	3	Total	Tl	0	0
			3	3		

3 Residue-property plots

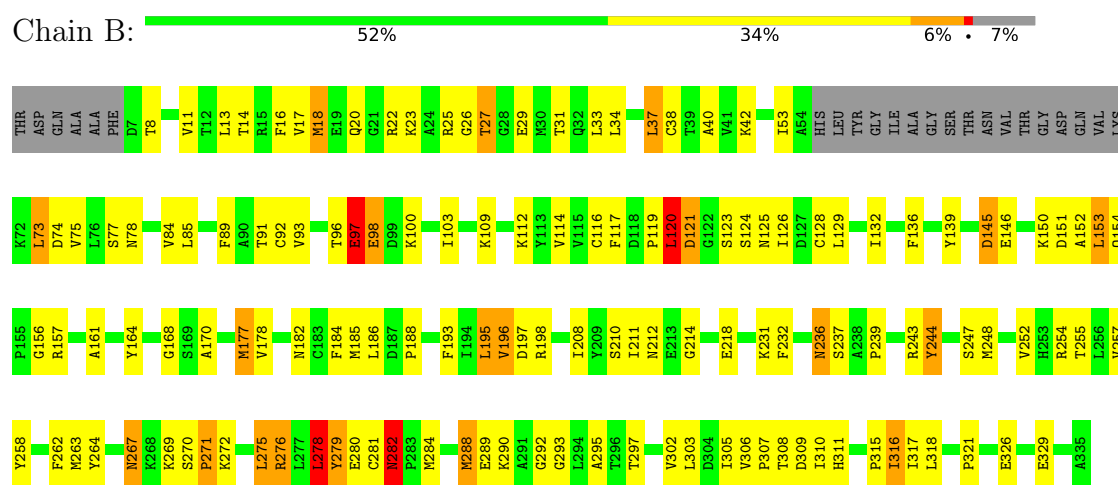
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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, α , β , γ	132.60 Å 132.60 Å 67.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	73.0 (8.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.226 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: TL

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	0.89	1/2429 (0.0%)	1.33	28/3284 (0.9%)
1	B	0.90	3/2429 (0.1%)	1.34	32/3284 (1.0%)
All	All	0.89	4/4858 (0.1%)	1.33	60/6568 (0.9%)

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	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	LEU	CA-C	-9.48	1.43	1.53
1	A	233	PRO	CA-C	6.55	1.58	1.52
1	B	282	ASN	CA-C	6.13	1.59	1.52
1	B	121	ASP	N-CA	-5.47	1.39	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	LYS	N-CA-C	-13.86	96.45	113.50
1	B	112	LYS	N-CA-C	9.93	125.22	113.20
1	A	118	ASP	N-CA-C	-9.25	93.70	109.15
1	A	207	SER	N-CA-C	9.25	123.29	112.93
1	B	117	PHE	N-CA-C	8.89	122.95	108.99
1	B	29	GLU	N-CA-C	-8.29	102.19	111.14
1	B	97	GLU	N-CA-C	-8.05	102.59	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	PRO	N-CA-C	-7.95	98.40	111.68
1	A	112	LYS	N-CA-C	7.75	122.58	113.20
1	B	20	GLN	N-CA-C	-7.73	101.76	112.12
1	A	144	THR	N-CA-C	7.71	122.45	112.89
1	A	76	LEU	N-CA-C	-7.62	102.92	111.07
1	A	25	ARG	N-CA-C	-7.30	101.89	111.02
1	A	98	GLU	N-CA-C	7.04	121.12	112.54
1	B	214	GLY	N-CA-C	-6.97	104.04	113.37
1	A	257	VAL	N-CA-C	6.73	118.34	111.00
1	B	33	LEU	N-CA-C	-6.73	103.56	111.03
1	A	293	GLY	N-CA-C	-6.59	103.53	112.57
1	A	219	PHE	N-CA-C	6.55	118.75	110.24
1	A	273	GLY	N-CA-C	-6.47	103.23	112.81
1	B	270	SER	N-CA-C	-6.41	94.92	108.39
1	B	125	ASN	N-CA-C	6.31	120.44	112.87
1	B	75	VAL	N-CA-C	-6.30	104.61	110.53
1	B	236	ASN	N-CA-C	6.30	124.21	110.80
1	B	23	LYS	N-CA-C	-6.24	104.93	112.54
1	A	121	ASP	N-CA-C	6.12	119.22	109.24
1	A	158	ASN	N-CA-C	6.04	120.49	113.18
1	B	193	PHE	N-CA-C	-6.04	100.01	109.25
1	B	247	SER	N-CA-C	-6.00	98.08	108.69
1	A	247	SER	N-CA-C	-5.97	97.22	107.61
1	B	14	THR	N-CA-C	-5.91	104.75	111.07
1	A	15	ARG	N-CA-C	-5.73	105.04	111.28
1	B	272	LYS	N-CA-C	-5.72	104.71	112.26
1	B	329	GLU	CB-CA-C	-5.70	101.85	110.92
1	B	315	PRO	N-CA-C	-5.58	103.08	111.57
1	B	26	GLY	N-CA-C	-5.54	100.05	113.18
1	A	113	TYR	N-CA-C	5.54	118.75	109.95
1	A	181	VAL	N-CA-C	-5.52	100.38	108.11
1	A	278	LEU	N-CA-C	5.52	118.01	111.33
1	B	271	PRO	N-CA-C	5.48	121.76	113.81
1	B	16	PHE	N-CA-C	5.45	116.90	111.07
1	A	329	GLU	N-CA-C	-5.43	105.28	111.14
1	B	309	ASP	N-CA-C	-5.42	99.61	108.76
1	A	297	THR	N-CA-C	-5.38	106.49	113.16
1	B	150	LYS	N-CA-C	-5.36	105.09	111.69
1	B	237	SER	N-CA-C	-5.36	101.74	109.29
1	A	24	ALA	N-CA-C	-5.31	106.57	113.16
1	B	8	THR	N-CA-C	5.30	119.36	113.01
1	A	208	ILE	N-CA-C	5.20	115.76	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	THR	N-CA-C	5.19	121.85	110.80
1	B	308	THR	N-CA-C	5.17	120.24	113.88
1	B	278	LEU	N-CA-C	5.13	121.74	110.80
1	A	83	ASN	N-CA-C	5.13	116.56	111.07
1	B	177	MET	N-CA-C	-5.10	102.60	109.95
1	B	267	ASN	N-CA-C	-5.09	99.22	108.65
1	A	129	LEU	N-CA-C	5.06	118.76	112.58
1	B	119	PRO	N-CA-C	5.03	120.44	113.65
1	B	145	ASP	N-CA-C	5.03	121.51	110.80
1	A	314	ALA	N-CA-C	5.01	114.58	108.11
1	A	298	GLY	N-CA-C	-5.01	107.74	114.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	LEU	Mainchain
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	2390	0	2448	89	0
1	B	2390	0	2448	86	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	4786	0	4896	170	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 18.

All (170) 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:248:MET:HE3	1:A:275:LEU:HD22	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:HB3	1:B:267:ASN:HB2	1.59	0.85
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.60	0.81
1:B:182:ASN:ND2	1:B:198:ARG:HA	1.97	0.79
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.67	0.77
1:A:275:LEU:HD12	1:A:275:LEU:H	1.52	0.75
1:B:248:MET:HE3	1:B:275:LEU:HD22	1.71	0.73
1:B:276:ARG:HG2	1:B:280:GLU:OE2	1.90	0.72
1:A:92:CYS:HA	1:A:105:VAL:HB	1.71	0.71
1:B:288:MET:HG3	1:B:318:LEU:HB2	1.75	0.69
1:B:121:ASP:O	1:B:132:ILE:HB	1.94	0.67
1:B:154:GLN:O	1:B:307:PRO:HG2	1.94	0.65
1:A:264:TYR:CG	1:A:275:LEU:HD11	2.33	0.64
1:B:211:ILE:HD12	1:B:263:MET:HB2	1.79	0.64
1:A:264:TYR:CB	1:A:275:LEU:HD11	2.29	0.63
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.33	0.63
1:B:275:LEU:HB2	1:B:281:CYS:SG	2.40	0.62
1:B:74:ASP:HB3	1:B:120:LEU:HB3	1.81	0.61
1:B:96:THR:HG22	1:B:98:GLU:H	1.66	0.60
1:B:243:ARG:O	1:B:244:TYR:HB2	2.01	0.60
1:A:7:ASP:HB3	1:A:10:ILE:HG23	1.83	0.60
1:B:93:VAL:HB	1:B:114:VAL:HG13	1.82	0.60
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.84	0.60
1:A:96:THR:HG22	1:A:98:GLU:H	1.67	0.59
1:B:267:ASN:O	1:B:271:PRO:HA	2.03	0.59
1:B:18:MET:O	1:B:22:ARG:HB3	2.02	0.59
1:A:155:PRO:HD2	1:A:158:ASN:HD22	1.68	0.58
1:A:248:MET:HE3	1:A:275:LEU:CD2	2.29	0.58
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.86	0.58
1:A:264:TYR:HB3	1:A:275:LEU:HD11	1.85	0.57
1:A:226:TYR:HD1	1:A:330:ILE:HD12	1.69	0.57
1:A:125:ASN:HB3	1:A:130:VAL:HB	1.86	0.57
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.03	0.57
1:A:17:VAL:HG11	1:A:34:LEU:HD12	1.87	0.57
1:A:210:SER:HB2	1:A:254:ARG:HH22	1.70	0.57
1:A:48:VAL:HG11	1:A:132:ILE:HD11	1.86	0.56
1:B:276:ARG:O	1:B:280:GLU:HB2	2.05	0.56
1:B:252:VAL:HG11	1:B:284:MET:SD	2.45	0.56
1:A:125:ASN:OD1	1:A:130:VAL:HG21	2.06	0.56
1:A:276:ARG:HD3	1:A:280:GLU:OE2	2.06	0.55
1:B:275:LEU:HD12	1:B:275:LEU:H	1.71	0.55
1:B:264:TYR:HB3	1:B:275:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB3	1:A:80:LEU:HD21	1.87	0.55
1:A:275:LEU:HD13	1:A:316:ILE:CG2	2.36	0.55
1:B:231:LYS:O	1:B:239:PRO:HB3	2.06	0.55
1:B:11:VAL:HG11	1:B:195:LEU:HD23	1.89	0.55
1:B:282:ASN:ND2	1:B:302:VAL:HG12	2.22	0.54
1:B:116:CYS:SG	1:B:278:LEU:HD13	2.47	0.54
1:A:91:THR:HB	1:A:94:LEU:HD21	1.89	0.54
1:B:212:ASN:HB2	1:B:244:TYR:CE2	2.43	0.54
1:A:264:TYR:HB3	1:A:275:LEU:CD1	2.38	0.54
1:B:116:CYS:SG	1:B:278:LEU:CD1	2.96	0.54
1:A:172:MET:HE2	1:B:129:LEU:HD11	1.90	0.53
1:A:283:PRO:O	1:A:287:VAL:HG23	2.09	0.53
1:A:215:TYR:HB2	1:A:219:PHE:CE1	2.44	0.53
1:B:170:ALA:HB1	1:B:185:MET:HE2	1.91	0.53
1:A:231:LYS:O	1:A:233:PRO:HD3	2.10	0.52
1:A:229:ARG:HG3	1:A:230:LYS:HD2	1.90	0.52
1:A:202:ILE:HD12	1:A:288:MET:HE1	1.91	0.52
1:A:210:SER:HB2	1:A:254:ARG:NH2	2.25	0.52
1:A:126:ILE:HG12	1:A:132:ILE:HD13	1.92	0.52
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.92	0.51
1:B:89:PHE:HA	1:B:109:LYS:O	2.10	0.51
1:B:275:LEU:HD13	1:B:316:ILE:HG22	1.91	0.51
1:A:212:ASN:HB2	1:A:244:TYR:CE2	2.46	0.51
1:A:129:LEU:HD21	1:B:170:ALA:HB3	1.93	0.51
1:A:77:SER:O	1:A:81:VAL:HG23	2.11	0.51
1:B:100:LYS:O	1:B:310:ILE:HD11	2.10	0.51
1:B:96:THR:HG22	1:B:97:GLU:N	2.27	0.50
1:B:161:ALA:HB2	1:B:177:MET:HG2	1.92	0.50
1:A:89:PHE:CE1	1:A:109:LYS:HG2	2.46	0.50
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.94	0.50
1:B:74:ASP:HA	1:B:77:SER:OG	2.11	0.50
1:A:156:GLY:C	1:A:303:LEU:HD22	2.36	0.50
1:B:114:VAL:HG11	1:B:152:ALA:HA	1.93	0.50
1:A:119:PRO:HA	1:A:134:THR:HG23	1.93	0.50
1:B:170:ALA:CB	1:B:185:MET:HE2	2.42	0.50
1:A:13:LEU:HA	1:A:184:PHE:CE2	2.46	0.50
1:A:85:LEU:HB3	1:A:91:THR:HG21	1.94	0.49
1:B:17:VAL:HG21	1:B:34:LEU:HD12	1.93	0.49
1:B:289:GLU:HA	1:B:293:GLY:O	2.13	0.49
1:B:168:GLY:C	1:B:170:ALA:H	2.19	0.49
1:A:282:ASN:HD22	1:A:302:VAL:HG12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:CB	1:B:267:ASN:HB2	2.36	0.49
1:B:302:VAL:HG21	1:B:316:ILE:HD12	1.94	0.48
1:B:126:ILE:O	1:B:129:LEU:HD23	2.14	0.48
1:B:252:VAL:O	1:B:255:THR:HB	2.13	0.48
1:A:13:LEU:HD12	1:A:184:PHE:CE1	2.49	0.47
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.97	0.47
1:A:209:TYR:HA	1:A:261:ILE:CG2	2.45	0.47
1:A:210:SER:CB	1:A:254:ARG:HH22	2.27	0.47
1:B:248:MET:HE3	1:B:275:LEU:CD2	2.41	0.47
1:A:165:ALA:HA	1:A:172:MET:O	2.15	0.47
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.81	0.46
1:A:95:VAL:HG13	1:A:310:ILE:HD13	1.97	0.46
1:A:288:MET:CG	1:A:318:LEU:HD13	2.44	0.46
1:A:288:MET:HG3	1:A:318:LEU:HD13	1.96	0.46
1:A:282:ASN:ND2	1:A:302:VAL:HG12	2.31	0.46
1:B:212:ASN:HB2	1:B:244:TYR:CZ	2.50	0.46
1:B:156:GLY:HA3	1:B:303:LEU:HD22	1.98	0.46
1:B:164:TYR:CD2	1:B:284:MET:HE1	2.51	0.45
1:A:7:ASP:O	1:A:10:ILE:HG12	2.16	0.45
1:A:107:PRO:HA	1:A:110:ARG:HG3	1.97	0.45
1:A:293:GLY:HA2	1:A:321:PRO:HD3	1.98	0.45
1:B:37:LEU:HD21	1:B:136:PHE:CG	2.51	0.45
1:A:209:TYR:HA	1:A:261:ILE:HG23	1.96	0.45
1:B:211:ILE:HG13	1:B:263:MET:O	2.16	0.45
1:B:269:LYS:HD3	1:B:269:LYS:HA	1.66	0.45
1:B:297:THR:CG2	1:B:305:ILE:HD11	2.47	0.45
1:A:13:LEU:HD12	1:A:184:PHE:CD1	2.51	0.45
1:A:190:ILE:HD11	1:A:194:ILE:HD11	1.98	0.45
1:A:223:ILE:O	1:A:227:ILE:HG13	2.17	0.45
1:B:168:GLY:C	1:B:170:ALA:N	2.73	0.44
1:A:276:ARG:HA	1:A:313:ARG:HA	1.99	0.44
1:A:44:ILE:HG21	1:A:120:LEU:HD13	1.99	0.44
1:A:97:GLU:HG3	1:A:279:TYR:CE2	2.53	0.44
1:B:186:LEU:O	1:B:188:PRO:HD3	2.18	0.44
1:B:257:VAL:HG23	1:B:258:TYR:N	2.33	0.44
1:A:212:ASN:HB2	1:A:244:TYR:CZ	2.53	0.44
1:B:13:LEU:HD12	1:B:184:PHE:CG	2.52	0.44
1:B:37:LEU:HD21	1:B:136:PHE:CD2	2.52	0.44
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.18	0.44
1:B:145:ASP:HB2	1:B:146:GLU:H	1.53	0.44
1:B:17:VAL:HG21	1:B:34:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:HD12	1:B:196:VAL:N	2.32	0.44
1:B:74:ASP:CB	1:B:120:LEU:HB3	2.47	0.43
1:A:122:GLY:O	1:A:125:ASN:HB2	2.17	0.43
1:A:332:GLN:HA	1:A:335:ALA:HB3	1.99	0.43
1:B:178:VAL:HA	1:B:290:LYS:HE3	2.00	0.43
1:B:103:ILE:H	1:B:103:ILE:HD12	1.83	0.43
1:A:329:GLU:O	1:A:333:LYS:N	2.51	0.43
1:A:257:VAL:HG21	1:B:128:CYS:HA	2.00	0.43
1:A:316:ILE:HD11	1:A:318:LEU:HD23	1.99	0.43
1:B:243:ARG:HB3	1:B:254:ARG:NH1	2.33	0.43
1:B:254:ARG:O	1:B:254:ARG:HG2	2.18	0.43
1:A:40:ALA:HB2	1:A:84:VAL:HG21	2.00	0.43
1:A:182:ASN:ND2	1:A:199:ASN:H	2.16	0.43
1:A:230:LYS:HG3	1:A:240:TYR:CG	2.54	0.43
1:B:297:THR:HG21	1:B:305:ILE:HD11	2.01	0.43
1:A:221:PRO:HA	1:A:224:THR:HG22	2.01	0.42
1:A:288:MET:HG3	1:A:318:LEU:HB2	2.00	0.42
1:A:72:LYS:O	1:A:73:LEU:C	2.62	0.42
1:A:233:PRO:HA	1:A:234:PRO:HD2	1.88	0.42
1:B:292:GLY:O	1:B:321:PRO:HD3	2.19	0.42
1:A:275:LEU:HD13	1:A:316:ILE:HG21	2.00	0.42
1:B:289:GLU:HG2	1:B:293:GLY:O	2.18	0.42
1:A:217:LYS:HB3	1:B:232:PHE:CD2	2.54	0.42
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.55	0.42
1:A:163:GLY:HA3	1:A:174:VAL:O	2.20	0.42
1:B:38:CYS:O	1:B:42:LYS:HG3	2.18	0.42
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.80	0.42
1:A:155:PRO:HG3	1:A:306:VAL:HG22	2.02	0.42
1:B:153:LEU:HB3	1:B:307:PRO:O	2.20	0.41
1:A:302:VAL:O	1:A:305:ILE:HD12	2.19	0.41
1:A:91:THR:O	1:A:111:GLY:N	2.48	0.41
1:B:96:THR:O	1:B:311:HIS:HE1	2.04	0.41
1:B:161:ALA:CB	1:B:177:MET:HG2	2.50	0.41
1:B:295:ALA:HA	1:B:317:ILE:O	2.21	0.41
1:A:13:LEU:HD13	1:A:173:LEU:HD13	2.02	0.41
1:A:176:ALA:HA	1:A:181:VAL:HA	2.02	0.41
1:A:210:SER:HA	1:A:243:ARG:O	2.21	0.41
1:B:53:ILE:O	1:B:53:ILE:HG22	2.21	0.41
1:B:97:GLU:HA	1:B:279:TYR:CZ	2.55	0.41
1:B:210:SER:HB3	1:B:262:PHE:HD1	1.86	0.41
1:A:248:MET:O	1:A:252:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:HA	1:B:307:PRO:HD3	1.76	0.40
1:A:205:LYS:HA	1:A:323:ASP:OD1	2.22	0.40
1:A:214:GLY:O	1:B:239:PRO:HB2	2.21	0.40
1:B:93:VAL:HG21	1:B:151:ASP:HB2	2.02	0.40
1:A:184:PHE:HA	1:A:194:ILE:O	2.21	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	308/335 (92%)	284 (92%)	21 (7%)	3 (1%)	12	45
1	B	308/335 (92%)	265 (86%)	38 (12%)	5 (2%)	7	34
All	All	616/670 (92%)	549 (89%)	59 (10%)	8 (1%)	9	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	27	THR
1	B	244	TYR
1	A	92	CYS
1	B	236	ASN
1	B	153	LEU
1	A	52	GLY
1	A	321	PRO
1	B	25	ARG

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%)	240 (92%)	21 (8%)	11	38
1	B	261/278 (94%)	239 (92%)	22 (8%)	10	37
All	All	522/556 (94%)	479 (92%)	43 (8%)	10	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	10	ILE
1	A	13	LEU
1	A	14	THR
1	A	46	THR
1	A	49	ARG
1	A	77	SER
1	A	124	SER
1	A	129	LEU
1	A	144	THR
1	A	145	ASP
1	A	160	VAL
1	A	169	SER
1	A	199	ASN
1	A	204	LYS
1	A	224	THR
1	A	229	ARG
1	A	230	LYS
1	A	237	SER
1	A	300	GLU
1	A	316	ILE
1	B	18	MET
1	B	31	THR
1	B	37	LEU
1	B	73	LEU
1	B	91	THR
1	B	92	CYS

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	98	GLU
1	B	123	SER
1	B	124	SER
1	B	157	ARG
1	B	195	LEU
1	B	196	VAL
1	B	197	ASP
1	B	208	ILE
1	B	275	LEU
1	B	276	ARG
1	B	278	LEU
1	B	282	ASN
1	B	288	MET
1	B	316	ILE
1	B	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	158	ASN
1	A	182	ASN
1	A	199	ASN
1	A	282	ASN
1	B	154	GLN
1	B	182	ASN
1	B	282	ASN
1	B	334	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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

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.