



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:48 PM UTC

PDB ID : 1B57 / pdb_00001b57
Title : CLASS II FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE IN COMPLEX
WITH PHOSPHOGLYCOLOHYDROXAMATE
Authors : Hall, D.R.; Hunter, W.N.
Deposited on : 1999-01-12
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

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
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

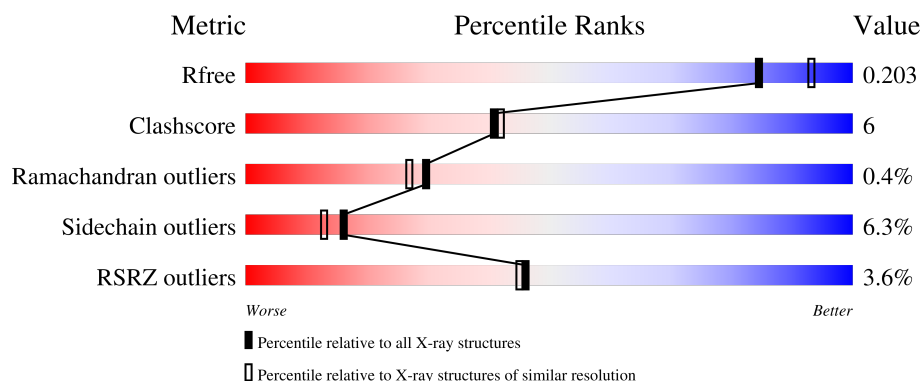
1 Overall quality at a glance

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 ≥ 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	3% 70% 21% ...
1	B	358	4% 73% 19% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5503 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 PROTEIN (FRUCTOSE-BISPHOSPHATE ALDOLASE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2624	1665	440	509	10			
1	B	346	Total	C	N	O	S	0	0	0
			2624	1665	440	509	10			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	3	Total	Zn	0	0
			3	3		

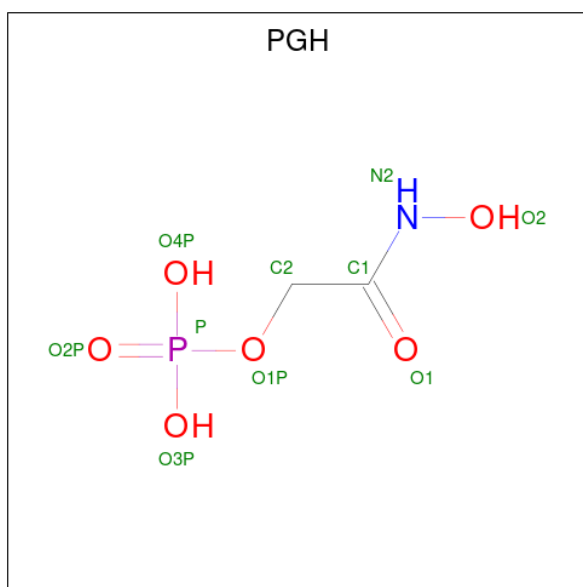
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: C₂H₆NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
5	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

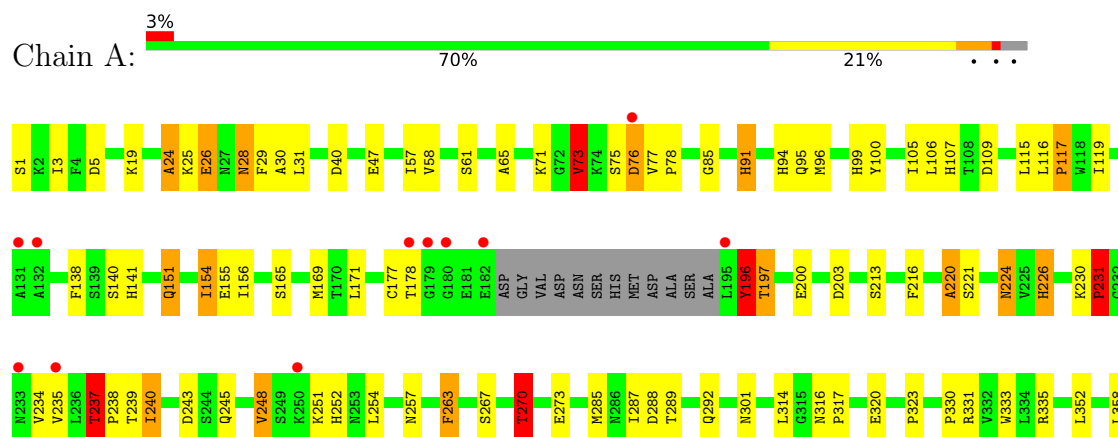
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	113	Total	O	0	0
			113	113		
6	B	112	Total	O	0	0
			112	112		

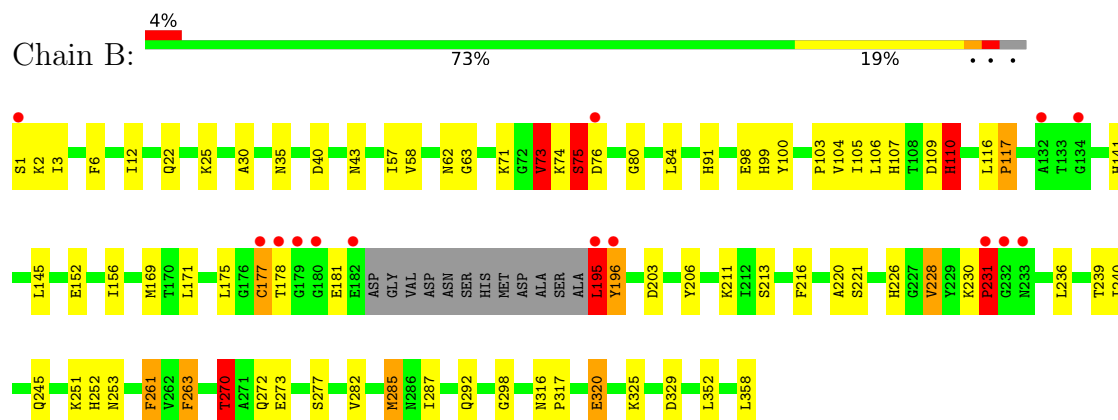
3 Residue-property plots [i](#)

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: PROTEIN (FRUCTOSE-BISPHOSPHATE ALDOLASE II)



• Molecule 1: PROTEIN (FRUCTOSE-BISPHOSPHATE ALDOLASE II)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.24Å 78.24Å 289.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.5 (30.00-2.00) 76.1 (30.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.230 (Not available) , 0.203	Depositor DCC
R_{free} test set	2691 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5503	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ZN, NA, PGH

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	0.86	0/2683	1.67	45/3648 (1.2%)
1	B	0.88	0/2683	1.73	39/3648 (1.1%)
All	All	0.87	0/5366	1.70	84/7296 (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	18
1	B	0	13
All	All	0	31

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	THR	N-CA-CB	-10.29	98.33	111.09
1	B	263	PHE	CA-CB-CG	10.12	123.92	113.80
1	A	73	VAL	CB-CA-C	-9.56	98.99	111.13
1	B	104	VAL	CA-C-N	-8.57	112.56	123.19
1	B	104	VAL	C-N-CA	-8.57	112.56	123.19
1	A	99	HIS	CA-CB-CG	-8.08	105.72	113.80
1	B	213	SER	N-CA-CB	-8.04	103.72	111.27
1	B	73	VAL	CB-CA-C	-8.03	102.46	111.45
1	A	40	ASP	CA-CB-CG	-7.77	104.83	112.60
1	A	91	HIS	CA-CB-CG	-7.44	106.36	113.80
1	B	75	SER	N-CA-CB	7.34	122.38	110.42
1	A	231	PRO	N-CA-C	7.23	127.37	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ASN	CA-C-N	7.04	127.79	119.98
1	B	62	ASN	C-N-CA	7.04	127.79	119.98
1	B	107	HIS	N-CA-CB	-6.92	100.10	111.66
1	B	320	GLU	CB-CA-C	-6.87	99.00	110.68
1	A	26	GLU	CB-CA-C	6.73	124.52	110.32
1	A	230	LYS	CA-C-N	6.65	128.15	119.84
1	A	230	LYS	C-N-CA	6.65	128.15	119.84
1	B	40	ASP	CA-CB-CG	-6.58	106.02	112.60
1	B	195	LEU	CA-C-N	6.58	132.86	122.21
1	B	195	LEU	C-N-CA	6.58	132.86	122.21
1	B	75	SER	CA-C-O	6.53	127.35	120.36
1	B	58	VAL	CA-C-N	-6.32	112.21	122.82
1	B	58	VAL	C-N-CA	-6.32	112.21	122.82
1	A	252	HIS	CA-CB-CG	-6.27	107.53	113.80
1	A	234	VAL	N-CA-CB	6.23	118.50	111.21
1	B	99	HIS	CA-CB-CG	-6.21	107.59	113.80
1	B	110	HIS	CA-CB-CG	-6.09	107.70	113.80
1	B	292	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	A	73	VAL	N-CA-CB	6.02	125.27	111.30
1	A	154	ILE	CB-CG1-CD1	6.00	126.41	113.80
1	A	237	THR	CA-CB-CG2	6.00	120.70	110.50
1	A	76	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	213	SER	N-CA-CB	-5.99	105.64	111.27
1	A	5	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	19	LYS	N-CA-CB	5.94	118.62	110.01
1	A	237	THR	CA-C-N	5.93	125.61	119.56
1	A	237	THR	C-N-CA	5.93	125.61	119.56
1	A	107	HIS	N-CA-CB	-5.87	101.85	111.66
1	A	238	PRO	CA-C-N	5.86	128.93	120.38
1	A	238	PRO	C-N-CA	5.86	128.93	120.38
1	B	270	THR	OG1-CB-CG2	5.84	120.97	109.30
1	A	58	VAL	CA-C-N	-5.83	113.02	122.82
1	A	58	VAL	C-N-CA	-5.83	113.02	122.82
1	A	26	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	238	PRO	CA-C-O	5.70	127.33	119.18
1	B	73	VAL	N-CA-CB	5.68	122.07	111.15
1	A	138	PHE	CA-C-O	-5.68	114.58	121.28
1	B	35	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	270	THR	N-CA-CB	-5.64	102.30	110.36
1	A	220	ALA	O-C-N	-5.63	116.64	123.29
1	A	28	ASN	CA-C-N	-5.58	113.44	122.36
1	A	28	ASN	C-N-CA	-5.58	113.44	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	331	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	B	74	LYS	CA-C-N	-5.46	115.51	122.77
1	B	74	LYS	C-N-CA	-5.46	115.51	122.77
1	B	228	VAL	N-CA-CB	-5.44	103.57	111.52
1	A	335	ARG	CD-NE-CZ	5.44	132.02	124.40
1	B	181	GLU	CA-CB-CG	5.42	124.95	114.10
1	B	100	TYR	N-CA-C	-5.38	106.72	113.28
1	A	237	THR	CB-CA-C	5.37	120.01	111.15
1	A	263	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	243	ASP	CA-C-N	-5.29	111.53	120.58
1	A	243	ASP	C-N-CA	-5.29	111.53	120.58
1	A	196	TYR	CA-C-O	-5.29	115.48	121.72
1	B	253	ASN	CA-CB-CG	-5.29	107.31	112.60
1	B	298	GLY	O-C-N	-5.29	117.11	122.19
1	B	63	GLY	CA-C-N	5.26	125.78	120.00
1	B	63	GLY	C-N-CA	5.26	125.78	120.00
1	B	231	PRO	N-CA-C	5.25	123.28	112.47
1	A	226	HIS	CA-CB-CG	-5.23	108.57	113.80
1	B	329	ASP	CA-C-N	5.23	125.53	119.47
1	B	329	ASP	C-N-CA	5.23	125.53	119.47
1	A	140	SER	N-CA-CB	-5.17	103.02	111.66
1	B	43	ASN	CA-C-O	-5.17	115.07	120.55
1	A	95	GLN	CA-CB-CG	5.13	124.36	114.10
1	B	22	GLN	CB-CG-CD	-5.09	103.94	112.60
1	B	84	LEU	CA-C-O	-5.09	115.03	120.42
1	A	240	ILE	CB-CA-C	-5.06	105.40	111.88
1	A	270	THR	N-CA-CB	-5.04	102.20	110.41
1	A	224	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	94	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	PRO	Mainchain
1	A	151	GLN	Mainchain
1	A	156	ILE	Mainchain
1	A	165	SER	Mainchain
1	A	177	CYS	Mainchain
1	A	197	THR	Mainchain
1	A	220	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	24	ALA	Mainchain
1	A	248	VAL	Mainchain
1	A	25	LYS	Mainchain
1	A	267	SER	Mainchain
1	A	301	ASN	Mainchain
1	A	320	GLU	Mainchain
1	A	333	TRP	Mainchain
1	A	47	GLU	Mainchain
1	A	61	SER	Mainchain
1	A	73	VAL	Mainchain
1	A	96	MET	Mainchain
1	B	1	SER	Mainchain
1	B	117	PRO	Mainchain
1	B	175	LEU	Mainchain
1	B	195	LEU	Mainchain
1	B	196	TYR	Mainchain
1	B	220	ALA	Mainchain
1	B	231	PRO	Mainchain
1	B	25	LYS	Mainchain
1	B	261	PHE	Mainchain
1	B	285	MET	Mainchain
1	B	320	GLU	Mainchain
1	B	6	PHE	Mainchain
1	B	98	GLU	Mainchain

5.2 Too-close contacts [i](#)

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	2624	0	2520	33	0
1	B	2624	0	2520	36	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	1	0
5	A	10	0	3	1	0
5	B	10	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	113	0	0	1	0
6	B	112	0	0	2	0
All	All	5503	0	5046	67	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 6.

All (67) 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:270:THR:HG22	1:A:273:GLU:H	1.28	0.98
1:B:270:THR:HG22	1:B:273:GLU:H	1.26	0.97
1:B:12:ILE:HD11	1:B:103:PRO:HB2	1.59	0.84
1:A:77:VAL:HB	1:A:78:PRO:HD2	1.62	0.80
1:B:203:ASP:OD2	1:B:251:LYS:NZ	2.18	0.73
1:B:203:ASP:CG	1:B:251:LYS:HZ2	1.97	0.73
1:B:251:LYS:NZ	1:B:252:HIS:NE2	2.37	0.70
1:A:316:ASN:HB2	1:A:317:PRO:CD	2.21	0.70
1:B:270:THR:HG23	1:B:272:GLN:H	1.58	0.68
1:A:285:MET:HE3	1:A:287:ILE:HD11	1.78	0.65
1:A:316:ASN:HB2	1:A:317:PRO:HD2	1.81	0.62
1:B:203:ASP:OD1	1:B:251:LYS:NZ	2.32	0.61
1:B:141:HIS:CD2	1:B:169:MET:HE1	2.36	0.59
1:A:100:TYR:CE1	1:B:73:VAL:HG13	2.40	0.56
1:B:270:THR:HB	1:B:273:GLU:OE1	2.05	0.56
1:A:178:THR:HG21	1:A:226:HIS:CE1	2.41	0.56
1:B:203:ASP:CG	1:B:251:LYS:NZ	2.62	0.55
1:B:30:ALA:HB3	1:B:352:LEU:HD22	1.90	0.53
1:A:65:ALA:O	1:A:85:GLY:HA3	2.09	0.53
1:A:285:MET:CE	1:A:287:ILE:HD11	2.39	0.52
1:A:24:ALA:HB1	1:A:29:PHE:O	2.11	0.51
1:B:270:THR:CG2	1:B:272:GLN:H	2.23	0.51
1:B:116:LEU:N	1:B:117:PRO:CD	2.74	0.50
1:B:178:THR:HG21	1:B:226:HIS:CE1	2.47	0.49
1:B:277:SER:HB3	1:B:282:VAL:HG21	1.93	0.49
1:B:195:LEU:O	1:B:196:TYR:HD1	1.96	0.48
1:B:285:MET:HE3	1:B:287:ILE:HD11	1.96	0.48
1:B:251:LYS:HG2	1:B:252:HIS:CD2	2.48	0.48
1:A:196:TYR:N	1:A:196:TYR:CD1	2.82	0.48
1:A:245:GLN:CD	1:A:257:ASN:HA	2.37	0.48
1:B:230:LYS:HA	1:B:231:PRO:HD3	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:HB2	1:B:317:PRO:CD	2.44	0.47
1:A:91:HIS:CE1	6:A:437:HOH:O	2.67	0.47
1:A:203:ASP:OD1	1:A:251:LYS:NZ	2.47	0.47
1:B:177:CYS:HB3	6:B:393:HOH:O	2.13	0.47
1:A:316:ASN:CB	1:A:317:PRO:CD	2.89	0.46
1:A:200:GLU:H	1:A:200:GLU:CD	2.24	0.46
1:A:237:THR:HG22	1:A:240:ILE:HG12	1.97	0.46
1:A:30:ALA:HB3	1:A:352:LEU:HD22	1.97	0.45
1:B:75:SER:OG	1:B:80:GLY:HA3	2.16	0.45
1:A:203:ASP:CG	1:A:251:LYS:HZ2	2.23	0.45
1:A:116:LEU:N	1:A:117:PRO:CD	2.79	0.45
1:A:196:TYR:N	1:A:196:TYR:HD1	2.14	0.45
1:A:1:SER:HB3	4:A:365:CL:CL	2.54	0.45
1:A:314:LEU:HD23	1:A:323:PRO:HA	1.99	0.45
1:A:109:ASP:OD2	5:A:359:PGH:O2	2.34	0.44
1:A:248:VAL:HG12	1:A:254:LEU:HD12	1.98	0.44
1:A:171:LEU:O	1:A:216:PHE:HA	2.18	0.44
1:B:245:GLN:HG2	1:B:261:PHE:HE2	1.83	0.44
1:B:57:ILE:HG12	1:B:105:ILE:HB	2.00	0.43
1:A:57:ILE:HG12	1:A:105:ILE:HB	2.00	0.43
1:B:3:ILE:HB	1:B:358:LEU:HA	2.01	0.42
1:A:141:HIS:CD2	1:A:169:MET:HE1	2.55	0.42
1:A:151:GLN:O	1:A:155:GLU:HG3	2.20	0.42
1:B:171:LEU:O	1:B:216:PHE:HA	2.18	0.42
1:B:251:LYS:HG2	1:B:252:HIS:NE2	2.34	0.42
1:B:240:ILE:HG23	6:B:407:HOH:O	2.19	0.42
1:B:236:LEU:HD12	1:B:273:GLU:HB3	2.02	0.41
1:A:289:THR:OG1	1:B:325:LYS:NZ	2.52	0.41
1:A:3:ILE:HB	1:A:358:LEU:HA	2.02	0.41
1:A:288:ASP:O	1:A:292:GLN:HG3	2.21	0.41
1:B:109:ASP:OD2	5:B:359:PGH:O2	2.38	0.41
1:B:109:ASP:O	1:B:110:HIS:C	2.64	0.41
1:B:145:LEU:CD1	1:B:156:ILE:HB	2.51	0.41
1:B:206:TYR:CD2	1:B:206:TYR:C	2.99	0.40
1:A:115:LEU:C	1:A:117:PRO:HD2	2.46	0.40
1:B:178:THR:HG21	1:B:226:HIS:ND1	2.35	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%)	328 (96%)	13 (4%)	1 (0%)	36	35
1	B	342/358 (96%)	332 (97%)	8 (2%)	2 (1%)	21	17
All	All	684/716 (96%)	660 (96%)	21 (3%)	3 (0%)	30	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	PRO
1	B	231	PRO
1	B	110	HIS

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	276/296 (93%)	255 (92%)	21 (8%)	12	9
1	B	276/296 (93%)	262 (95%)	14 (5%)	21	19
All	All	552/592 (93%)	517 (94%)	35 (6%)	16	13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	28	ASN
1	A	31	LEU

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Mol	Chain	Res	Type
1	A	71	LYS
1	A	73	VAL
1	A	75	SER
1	A	76	ASP
1	A	106	LEU
1	A	119	ILE
1	A	154	ILE
1	A	196	TYR
1	A	197	THR
1	A	221	SER
1	A	224	ASN
1	A	231	PRO
1	A	235	VAL
1	A	237	THR
1	A	239	THR
1	A	263	PHE
1	A	270	THR
1	A	330	PRO
1	B	2	LYS
1	B	71	LYS
1	B	73	VAL
1	B	75	SER
1	B	76	ASP
1	B	106	LEU
1	B	152	GLU
1	B	177	CYS
1	B	211	LYS
1	B	221	SER
1	B	228	VAL
1	B	239	THR
1	B	263	PHE
1	B	270	THR

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

Mol	Chain	Res	Type
1	A	62	ASN
1	A	79	GLN
1	A	95	GLN
1	B	62	ASN
1	B	79	GLN
1	B	99	HIS

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Mol	Chain	Res	Type
1	B	272	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 10 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
5	PGH	A	359	2,3	9,9,9	1.55	2 (22%)	10,12,12	2.09	2 (20%)
5	PGH	B	359	2,3	9,9,9	2.23	1 (11%)	10,12,12	3.55	4 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGH	A	359	2,3	-	4/8/8/8	-
5	PGH	B	359	2,3	-	4/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	359	PGH	C1-N2	5.91	1.38	1.32
5	A	359	PGH	C1-N2	3.22	1.35	1.32
5	A	359	PGH	P-O1P	-2.18	1.53	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	359	PGH	O2-N2-C1	-9.63	105.56	119.79
5	A	359	PGH	O2-N2-C1	-4.53	113.10	119.79
5	A	359	PGH	O1-C1-N2	-3.75	118.67	123.27
5	B	359	PGH	O1-C1-N2	-3.09	119.47	123.27
5	B	359	PGH	C2-C1-N2	-2.78	111.62	116.41
5	B	359	PGH	O1-C1-C2	2.03	125.24	119.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	359	PGH	N2-C1-C2-O1P
5	A	359	PGH	O1-C1-N2-O2
5	A	359	PGH	C2-O1P-P-O2P
5	B	359	PGH	N2-C1-C2-O1P
5	B	359	PGH	O1-C1-N2-O2
5	B	359	PGH	C2-O1P-P-O2P
5	A	359	PGH	O1-C1-C2-O1P
5	B	359	PGH	O1-C1-C2-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	359	PGH	1	0
5	B	359	PGH	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	346/358 (96%)	-0.20	11 (3%) 50 49	12, 24, 48, 68	0
1	B	346/358 (96%)	-0.15	14 (4%) 42 41	11, 23, 48, 68	0
All	All	692/716 (96%)	-0.17	25 (3%) 46 45	11, 24, 48, 68	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	LEU	6.0
1	B	195	LEU	5.1
1	A	178	THR	4.5
1	A	179	GLY	3.8
1	B	232	GLY	3.8
1	A	132	ALA	3.7
1	B	180	GLY	3.5
1	B	182	GLU	3.4
1	B	76	ASP	3.4
1	A	233	ASN	3.3
1	B	1	SER	3.2
1	B	233	ASN	3.1
1	A	180	GLY	3.1
1	A	235	VAL	2.8
1	B	178	THR	2.8
1	B	177	CYS	2.7
1	B	231	PRO	2.7
1	A	131	ALA	2.6
1	B	179	GLY	2.5
1	B	134	GLY	2.5
1	B	196	TYR	2.3
1	A	250	LYS	2.2
1	A	76	ASP	2.2
1	B	132	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	GLU	2.1

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, 95th 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 ²)	Q<0.9
2	ZN	B	362	1/1	0.95	0.05	47,47,47,47	0
2	ZN	A	362	1/1	0.96	0.05	49,49,49,49	0
4	CL	A	365	1/1	0.96	0.07	22,22,22,22	0
3	NA	A	364	1/1	0.98	0.04	22,22,22,22	0
3	NA	B	364	1/1	0.98	0.04	21,21,21,21	0
2	ZN	A	363	1/1	0.98	0.06	28,28,28,28	0
2	ZN	A	361	1/1	0.99	0.04	30,30,30,30	0
2	ZN	B	361	1/1	0.99	0.03	28,28,28,28	0
5	PGH	A	359	10/10	0.99	0.04	18,20,21,22	0
5	PGH	B	359	10/10	0.99	0.05	14,16,17,20	0
2	ZN	B	360	1/1	1.00	0.01	17,17,17,17	0
2	ZN	A	360	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.