



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 PM UTC

PDB ID : 5LDZ / pdb_00005ldz
Title : Quadruple space group ambiguity due to rotational and translational non-crystallographic symmetry in human liver fructose-1,6-bisphosphatase
Authors : Ruf, A.; Tetaz, T.; Schott, B.; Joseph, C.; Rudolph, M.G.
Deposited on : 2016-06-29
Resolution : 2.20 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

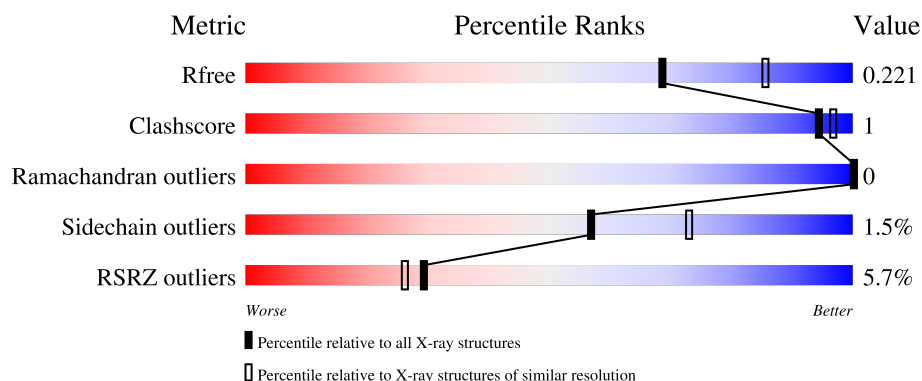
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	338	5% 87% 5% 8%
1	B	338	5% 87% 5% 8%
1	C	338	5% 85% 7% 8%
1	D	338	6% 87% 6% 7%
1	E	338	5% 86% 6% 8%

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Mol	Chain	Length	Quality of chain
1	F	338	6% 88% •7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15173 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.

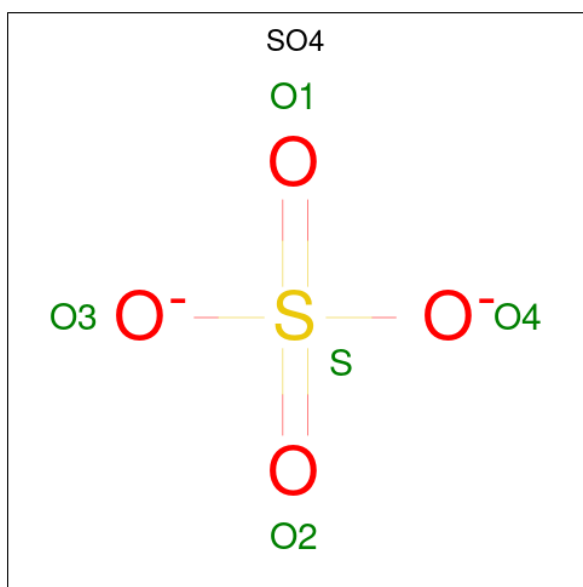
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2388	1522	396	453	17			
1	B	312	Total	C	N	O	S	0	7	0
			2446	1555	407	467	17			
1	C	311	Total	C	N	O	S	0	0	0
			2383	1519	394	453	17			
1	D	313	Total	C	N	O	S	0	7	0
			2459	1564	410	468	17			
1	E	311	Total	C	N	O	S	0	0	0
			2388	1522	396	453	17			
1	F	314	Total	C	N	O	S	0	7	0
			2464	1567	411	469	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	1
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

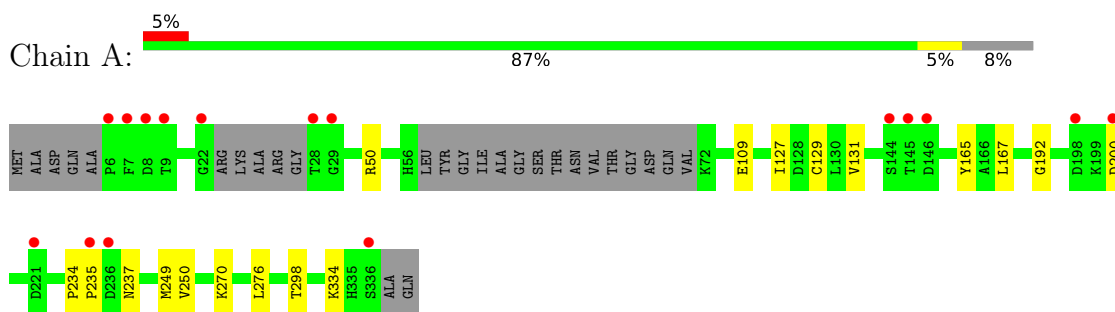
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	86	Total 86	O 86	0	0
5	C	73	Total 73	O 73	0	0
5	D	83	Total 83	O 83	0	0
5	E	85	Total 85	O 85	0	0
5	F	80	Total 80	O 80	0	0

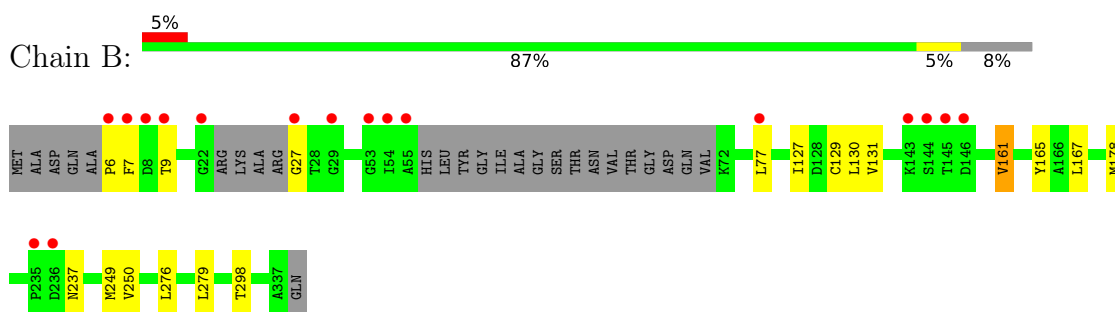
3 Residue-property plots [i](#)

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.

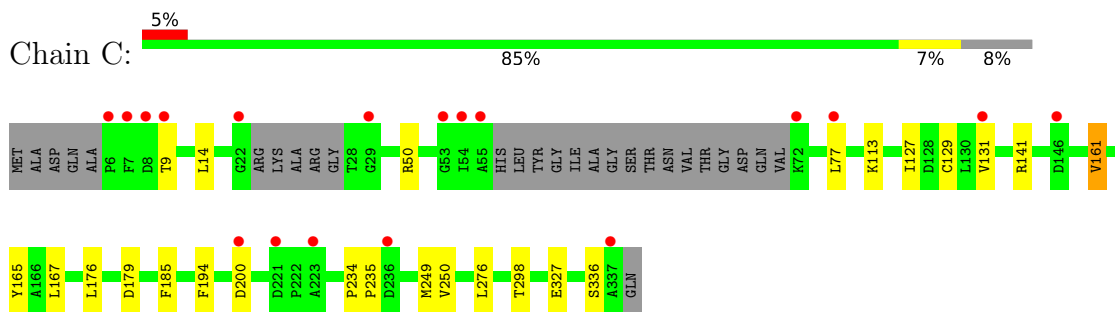
- Molecule 1: Fructose-1,6-bisphosphatase 1



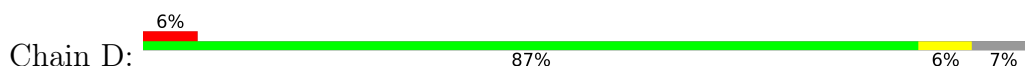
- Molecule 1: Fructose-1,6-bisphosphatase 1

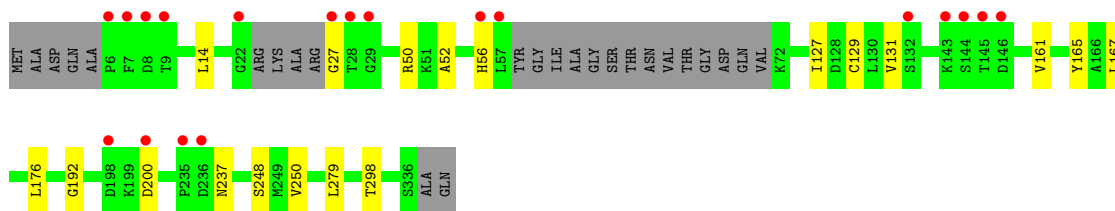


- Molecule 1: Fructose-1,6-bisphosphatase 1

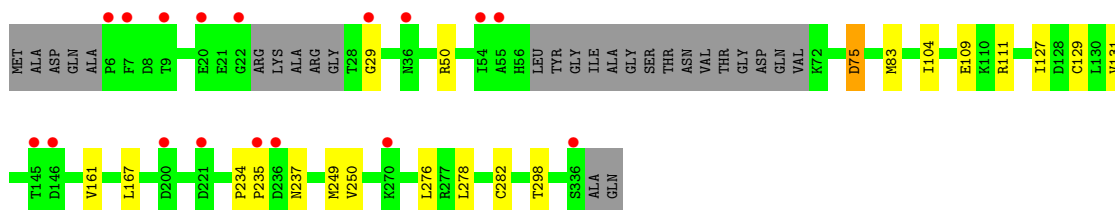
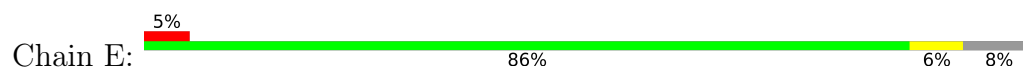


- Molecule 1: Fructose-1,6-bisphosphatase 1

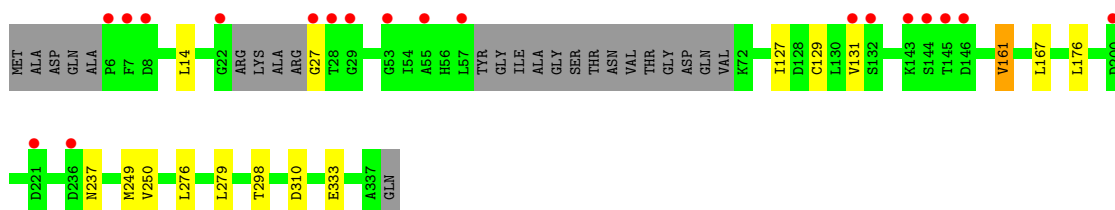
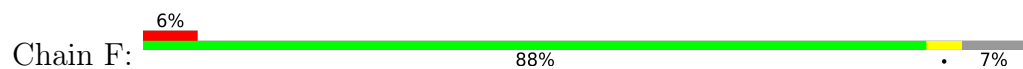




● Molecule 1: Fructose-1,6-bisphosphatase 1



● Molecule 1: Fructose-1,6-bisphosphatase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.52Å 121.52Å 316.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 2.20 39.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.80-2.20) 99.9 (39.80-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.20Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.206 , 0.239 (Not available) , 0.221	Depositor DCC
R_{free} test set	6091 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtrriage
Anisotropy	0.597	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15173	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0632e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, CL, ZN

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	0.83	0/2431	1.18	4/3284 (0.1%)
1	B	0.83	1/2488 (0.0%)	1.19	6/3359 (0.2%)
1	C	0.83	0/2425	1.22	7/3276 (0.2%)
1	D	0.83	0/2502	1.19	8/3378 (0.2%)
1	E	0.84	0/2431	1.19	3/3284 (0.1%)
1	F	0.83	0/2507	1.20	8/3385 (0.2%)
All	All	0.83	1/14784 (0.0%)	1.19	36/19966 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	MET	SD-CE	5.01	1.92	1.79

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	VAL	N-CA-C	-7.23	105.59	111.81
1	F	161	VAL	N-CA-C	-6.92	105.86	111.81
1	C	161	VAL	N-CA-C	-6.90	105.88	111.81
1	D	161	VAL	N-CA-C	-6.54	106.18	111.81
1	B	27	GLY	CA-C-N	6.54	129.04	120.28
1	B	27	GLY	C-N-CA	6.54	129.04	120.28
1	A	200	ASP	CA-C-N	5.80	128.34	120.63
1	A	200	ASP	C-N-CA	5.80	128.34	120.63
1	A	298	THR	N-CA-C	-5.77	106.24	113.28
1	C	336	SER	CA-C-N	5.65	131.87	121.70
1	C	336	SER	C-N-CA	5.65	131.87	121.70
1	C	179	ASP	CA-CB-CG	5.59	118.19	112.60
1	E	237	ASN	CA-CB-CG	5.55	118.15	112.60
1	B	298	THR	N-CA-C	-5.50	106.57	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	THR	N-CA-C	-5.49	106.59	113.28
1	B	237	ASN	CA-CB-CG	5.46	118.06	112.60
1	D	237	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	237	ASN	CA-CB-CG	5.42	118.02	112.60
1	E	298	THR	N-CA-C	-5.40	106.69	113.28
1	F	27	GLY	CA-C-N	5.34	127.44	120.28
1	F	27	GLY	C-N-CA	5.34	127.44	120.28
1	F	333	GLU	CA-C-N	5.32	127.41	120.28
1	F	333	GLU	C-N-CA	5.32	127.41	120.28
1	C	298	THR	N-CA-C	-5.31	106.80	113.28
1	B	279	LEU	N-CA-C	5.31	117.06	111.28
1	D	27	GLY	CA-C-N	5.25	127.31	120.28
1	D	27	GLY	C-N-CA	5.25	127.31	120.28
1	F	237	ASN	CA-CB-CG	5.24	117.84	112.60
1	F	279	LEU	N-CA-C	5.22	116.65	111.07
1	D	279	LEU	N-CA-C	5.13	116.95	111.36
1	C	200	ASP	CA-C-N	5.09	127.41	120.63
1	C	200	ASP	C-N-CA	5.09	127.41	120.63
1	D	200	ASP	CA-C-N	5.07	127.37	120.63
1	D	200	ASP	C-N-CA	5.07	127.37	120.63
1	E	75	ASP	CA-CB-CG	5.07	117.67	112.60
1	F	298	THR	N-CA-C	-5.06	106.95	113.23

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	2388	0	2420	7	0
1	B	2446	0	2482	8	0
1	C	2383	0	2418	10	0
1	D	2459	0	2495	6	0
1	E	2388	0	2420	7	0
1	F	2464	0	2500	4	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	20	0	0	0	0
3	B	35	0	0	0	0
3	C	25	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	0	0
3	F	25	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	81	0	0	0	0
5	B	86	0	0	0	0
5	C	73	0	0	0	0
5	D	83	0	0	0	0
5	E	85	0	0	1	0
5	F	80	0	0	0	0
All	All	15173	0	14735	38	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 1.

All (38) 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:167:LEU:HD13	1:A:250:VAL:HG12	1.92	0.51
1:F:14:LEU:HD21	1:F:176:LEU:HD22	1.94	0.49
1:B:167:LEU:HD13	1:B:250:VAL:HG12	1.94	0.49
1:E:129:CYS:SG	1:E:131:VAL:HB	2.53	0.48
1:F:167:LEU:HD13	1:F:250:VAL:HG12	1.95	0.48
1:C:167:LEU:HD13	1:C:250:VAL:HG12	1.95	0.48
1:D:167:LEU:HD13	1:D:250:VAL:HG12	1.96	0.47
1:A:129:CYS:SG	1:A:131:VAL:HB	2.55	0.46
1:D:129:CYS:SG	1:D:131:VAL:HB	2.56	0.45
1:E:167:LEU:HD13	1:E:250:VAL:HG12	1.98	0.45
1:B:9:THR:HG22	1:C:77:LEU:HD12	1.97	0.44
1:B:129:CYS:SG	1:B:131:VAL:HB	2.58	0.44
1:C:129:CYS:SG	1:C:131:VAL:HB	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HD11	1:D:176:LEU:HD22	2.01	0.43
1:D:52:ALA:O	1:D:56:HIS:HB3	2.18	0.43
1:C:249:MET:HE3	1:C:276:LEU:HD13	1.99	0.43
1:E:83:MET:HE1	1:E:104:ILE:HD13	2.00	0.43
1:A:249:MET:HE3	1:A:276:LEU:HD13	2.00	0.42
1:F:129:CYS:SG	1:F:131:VAL:HB	2.58	0.42
1:B:6:PRO:HB2	1:B:7:PHE:H	1.71	0.42
1:A:234:PRO:HA	1:A:235:PRO:HD3	1.96	0.42
1:A:192:GLY:HA3	1:D:192:GLY:HA3	2.02	0.42
1:C:14:LEU:HD11	1:C:176:LEU:HD22	2.00	0.42
1:A:167:LEU:HD23	1:B:130:LEU:HD12	2.01	0.42
1:C:185:PHE:HB3	1:C:194:PHE:HB3	2.01	0.42
1:E:278:LEU:HA	1:E:282:CYS:HB2	2.02	0.42
1:A:165:TYR:CD1	1:A:250:VAL:HG13	2.55	0.41
1:D:165:TYR:CD1	1:D:250:VAL:HG13	2.55	0.41
1:C:234:PRO:HA	1:C:235:PRO:HD3	1.99	0.41
1:E:234:PRO:HA	1:E:235:PRO:HD3	1.97	0.41
1:E:249:MET:HE3	1:E:276:LEU:HD13	2.01	0.41
1:E:29:GLY:HA2	5:E:568:HOH:O	2.21	0.41
1:F:249:MET:HE3	1:F:276:LEU:HD13	2.02	0.41
1:B:77:LEU:HD12	1:C:9:THR:HG22	2.03	0.40
1:B:165:TYR:CD1	1:B:250:VAL:HG13	2.56	0.40
1:C:165:TYR:CD1	1:C:250:VAL:HG13	2.56	0.40
1:B:249:MET:HE3	1:B:276:LEU:HD13	2.03	0.40
1:C:113:LYS:HD3	1:C:141:ARG:HE	1.85	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	305/338 (90%)	297 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	313/338 (93%)	307 (98%)	6 (2%)	0	100	100
1	C	305/338 (90%)	298 (98%)	7 (2%)	0	100	100
1	D	314/338 (93%)	305 (97%)	9 (3%)	0	100	100
1	E	305/338 (90%)	297 (97%)	8 (3%)	0	100	100
1	F	315/338 (93%)	308 (98%)	7 (2%)	0	100	100
All	All	1857/2028 (92%)	1812 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	263/281 (94%)	258 (98%)	5 (2%)	50	66
1	B	269/281 (96%)	267 (99%)	2 (1%)	76	87
1	C	262/281 (93%)	258 (98%)	4 (2%)	57	73
1	D	271/281 (96%)	268 (99%)	3 (1%)	65	79
1	E	263/281 (94%)	257 (98%)	6 (2%)	44	59
1	F	271/281 (96%)	268 (99%)	3 (1%)	65	79
All	All	1599/1686 (95%)	1576 (99%)	23 (1%)	57	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	109	GLU
1	A	127	ILE
1	A	270	LYS
1	A	334	LYS
1	B	127	ILE
1	B	161	VAL
1	C	50	ARG

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Mol	Chain	Res	Type
1	C	127	ILE
1	C	161	VAL
1	C	327	GLU
1	D	50	ARG
1	D	127	ILE
1	D	248	SER
1	E	50	ARG
1	E	75	ASP
1	E	109	GLU
1	E	111	ARG
1	E	127	ILE
1	E	161	VAL
1	F	127	ILE
1	F	161	VAL
1	F	310	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	B	36	ASN
1	B	102	HIS
1	C	33	GLN
1	C	36	ASN
1	C	102	HIS
1	D	33	GLN
1	D	102	HIS
1	D	155	GLN
1	D	159	ASN
1	E	33	GLN
1	E	102	HIS
1	F	33	GLN
1	F	102	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 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	SO4	E	404	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	F	403	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	C	406	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	A	406	-	4,4,4	0.16	0	6,6,6	0.26	0
3	SO4	A	404	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	E	405	-	4,4,4	0.38	0	6,6,6	0.14	0
3	SO4	A	403	-	4,4,4	0.37	0	6,6,6	0.27	0
3	SO4	C	404	-	4,4,4	0.33	0	6,6,6	0.26	0
3	SO4	F	404	-	4,4,4	0.29	0	6,6,6	0.33	0
3	SO4	B	404	-	4,4,4	0.36	0	6,6,6	0.25	0
3	SO4	B	407[B]	-	4,4,4	0.32	0	6,6,6	0.11	0
3	SO4	D	404	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	D	403	-	4,4,4	0.27	0	6,6,6	0.42	0
3	SO4	D	405	-	4,4,4	0.27	0	6,6,6	0.38	0
3	SO4	F	402	-	4,4,4	0.29	0	6,6,6	0.40	0
3	SO4	B	405	-	4,4,4	0.16	0	6,6,6	0.45	0
3	SO4	F	405	-	4,4,4	0.27	0	6,6,6	0.43	0
3	SO4	B	402	-	4,4,4	0.36	0	6,6,6	0.37	0
3	SO4	B	406	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	B	403	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	F	406	-	4,4,4	0.25	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	405	-	4,4,4	0.40	0	6,6,6	0.19	0
3	SO4	B	408	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	C	405	-	4,4,4	0.37	0	6,6,6	0.25	0
3	SO4	C	402	-	4,4,4	0.27	0	6,6,6	0.35	0
3	SO4	E	406	-	4,4,4	0.27	0	6,6,6	0.30	0
3	SO4	E	403	-	4,4,4	0.22	0	6,6,6	0.37	0
3	SO4	D	406	-	4,4,4	0.29	0	6,6,6	0.31	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	311/338 (92%)	0.20	16 (5%)	33	30	27, 40, 78, 127	0
1	B	312/338 (92%)	0.19	17 (5%)	31	28	22, 38, 73, 122	7 (2%)
1	C	311/338 (92%)	0.21	18 (5%)	29	25	25, 40, 76, 116	0
1	D	313/338 (92%)	0.25	19 (6%)	27	24	23, 39, 78, 123	7 (2%)
1	E	311/338 (92%)	0.27	17 (5%)	30	27	27, 41, 81, 149	0
1	F	314/338 (92%)	0.27	19 (6%)	27	24	23, 40, 79, 115	7 (2%)
All	All	1872/2028 (92%)	0.23	106 (5%)	29	26	22, 40, 78, 149	21 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	144[A]	SER	8.4
1	D	144[A]	SER	8.0
1	B	22	GLY	7.9
1	D	143[A]	LYS	7.8
1	F	143[A]	LYS	7.3
1	C	22	GLY	6.9
1	F	22	GLY	6.9
1	E	22	GLY	6.4
1	D	22	GLY	6.3
1	A	146	ASP	5.7
1	A	22	GLY	5.7
1	F	57	LEU	5.5
1	D	27	GLY	5.5
1	B	143[A]	LYS	5.4
1	C	146	ASP	5.1
1	A	145	THR	5.0
1	F	27	GLY	4.9
1	D	146[A]	ASP	4.9
1	F	55	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	145[A]	THR	4.6
1	B	7	PHE	4.4
1	C	55	ALA	4.4
1	B	27	GLY	4.4
1	C	337	ALA	4.4
1	D	236	ASP	4.4
1	A	236	ASP	4.4
1	E	236	ASP	4.4
1	F	6	PRO	4.1
1	C	6	PRO	4.0
1	F	146[A]	ASP	3.9
1	A	200	ASP	3.9
1	B	146[A]	ASP	3.9
1	E	146	ASP	3.8
1	F	7	PHE	3.8
1	D	57	LEU	3.8
1	B	145[A]	THR	3.7
1	C	236	ASP	3.6
1	E	6	PRO	3.6
1	A	29	GLY	3.6
1	E	7	PHE	3.6
1	E	200	ASP	3.6
1	B	53	GLY	3.5
1	E	55	ALA	3.5
1	C	29	GLY	3.5
1	C	7	PHE	3.5
1	B	236	ASP	3.5
1	B	29	GLY	3.4
1	D	28	THR	3.4
1	B	6	PRO	3.3
1	F	132	SER	3.2
1	C	54	ILE	3.2
1	A	7	PHE	3.1
1	D	29	GLY	3.1
1	F	29	GLY	3.1
1	A	144	SER	3.1
1	D	145[A]	THR	3.0
1	B	55	ALA	3.0
1	C	8	ASP	2.9
1	E	336	SER	2.9
1	B	54	ILE	2.9
1	C	200	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	235	PRO	2.8
1	E	54	ILE	2.8
1	B	8	ASP	2.8
1	F	236	ASP	2.8
1	E	145	THR	2.7
1	D	132	SER	2.7
1	E	29	GLY	2.7
1	A	235	PRO	2.7
1	D	235	PRO	2.7
1	D	8	ASP	2.6
1	A	336	SER	2.6
1	C	221	ASP	2.6
1	D	200	ASP	2.6
1	A	6	PRO	2.6
1	E	270	LYS	2.6
1	D	9	THR	2.6
1	D	7	PHE	2.5
1	D	56	HIS	2.5
1	C	53	GLY	2.5
1	B	9	THR	2.4
1	E	221	ASP	2.4
1	C	9	THR	2.4
1	F	200	ASP	2.3
1	A	9	THR	2.3
1	D	6	PRO	2.3
1	E	235	PRO	2.3
1	A	8	ASP	2.3
1	A	198	ASP	2.3
1	F	28	THR	2.3
1	B	144[A]	SER	2.3
1	E	36	ASN	2.2
1	C	72	LYS	2.2
1	D	198	ASP	2.2
1	F	221	ASP	2.2
1	C	131	VAL	2.1
1	F	53	GLY	2.1
1	E	9	THR	2.1
1	A	221	ASP	2.1
1	F	8	ASP	2.1
1	A	28	THR	2.1
1	B	77	LEU	2.1
1	F	131	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	20	GLU	2.0
1	C	223	ALA	2.0
1	C	77	LEU	2.0

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
3	SO4	C	405	5/5	0.60	0.18	101,102,102,106	0
3	SO4	F	405	5/5	0.60	0.20	103,103,105,106	0
3	SO4	D	406	5/5	0.62	0.17	110,111,112,113	0
3	SO4	F	406	5/5	0.69	0.11	128,129,130,131	0
3	SO4	E	405	5/5	0.72	0.14	113,114,114,114	0
3	SO4	E	406	5/5	0.73	0.14	97,98,98,98	0
3	SO4	E	404	5/5	0.73	0.10	103,103,104,104	0
3	SO4	C	406	5/5	0.73	0.10	132,132,133,133	0
3	SO4	A	406	5/5	0.76	0.15	108,110,111,111	0
3	SO4	B	406	5/5	0.78	0.09	124,125,125,125	0
3	SO4	B	405	5/5	0.79	0.14	84,85,86,87	0
3	SO4	F	404	5/5	0.79	0.12	93,93,94,94	0
3	SO4	B	404	5/5	0.79	0.12	92,92,95,96	0
3	SO4	D	405	5/5	0.79	0.12	88,89,91,92	0
3	SO4	B	408	5/5	0.80	0.15	116,118,119,119	0
3	SO4	A	405	5/5	0.81	0.12	90,91,91,94	0
3	SO4	B	403	5/5	0.83	0.09	98,99,100,101	0
3	SO4	F	403	5/5	0.84	0.07	105,106,106,106	0
3	SO4	D	404	5/5	0.85	0.09	100,101,102,102	0
3	SO4	C	404	5/5	0.85	0.12	103,103,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	403	5/5	0.87	0.07	101,102,102,103	0
3	SO4	B	407[B]	5/5	0.88	0.11	87,87,88,89	5
3	SO4	A	404	5/5	0.88	0.07	103,103,103,104	0
3	SO4	E	403	5/5	0.91	0.12	57,58,60,65	0
4	CL	B	409	1/1	0.91	0.16	78,78,78,78	0
4	CL	D	407	1/1	0.91	0.12	78,78,78,78	0
3	SO4	F	402	5/5	0.92	0.11	55,55,55,59	0
3	SO4	D	403	5/5	0.93	0.12	49,50,52,57	0
3	SO4	A	403	5/5	0.94	0.10	54,54,59,60	0
4	CL	F	407	1/1	0.94	0.09	73,73,73,73	0
3	SO4	C	402	5/5	0.95	0.10	49,50,55,55	0
3	SO4	B	402	5/5	0.96	0.08	52,54,56,59	0
2	ZN	D	402	1/1	0.99	0.02	41,41,41,41	0
2	ZN	E	401	1/1	0.99	0.03	50,50,50,50	0
2	ZN	E	402	1/1	0.99	0.03	38,38,38,38	0
2	ZN	A	401	1/1	0.99	0.03	49,49,49,49	0
2	ZN	A	402	1/1	0.99	0.04	38,38,38,38	0
2	ZN	B	401	1/1	0.99	0.05	48,48,48,48	0
2	ZN	C	401	1/1	0.99	0.05	50,50,50,50	0
2	ZN	D	401	1/1	1.00	0.04	47,47,47,47	0
2	ZN	F	401	1/1	1.00	0.05	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.