



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:33 AM BST

PDB ID : 6IO4
Title : Silver-bound Glyceraldehyde-3-phosphate dehydrogenase A
Authors : Wang, H.; Sun, H.; Wang, M.
Deposited on : 2018-10-29
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

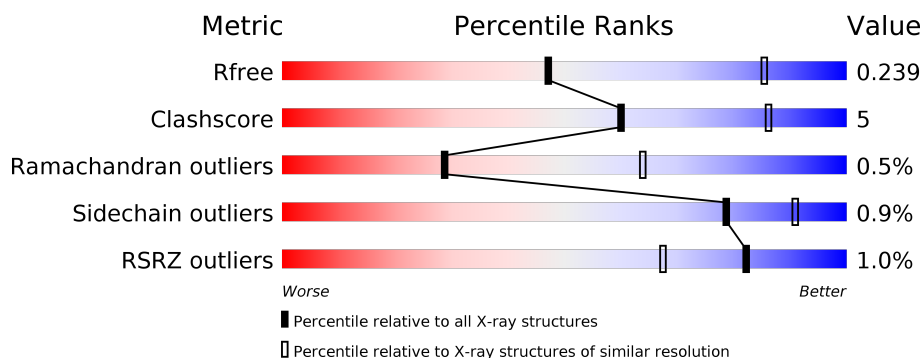
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.






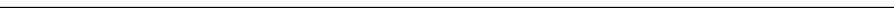
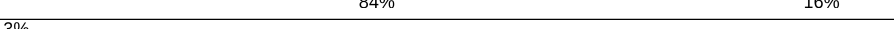




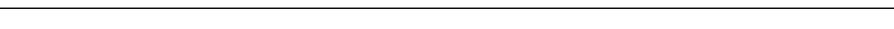
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	329	<div> <div>88%</div> <div>12%</div> </div>
1	B	329	<div> <div>87%</div> <div>13%</div> </div>
1	C	329	<div> <div>89%</div> <div>10%</div> </div>
1	D	329	<div> <div>90%</div> <div>10%</div> </div>
1	E	329	<div> <div>88%</div> <div>12%</div> </div>
1	F	329	<div> <div>86%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	329	 90% 10%
1	H	329	 % 87% 13%
1	I	329	 3% 88% 12%
1	J	329	 84% 16%
1	K	329	 3% 91% 9%
1	L	329	 87% 12%
1	M	329	 2% 88% 12%
1	N	329	 5% 88% 12%
1	O	329	 89% 11%
1	P	329	 86% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38671 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 Glyceraldehyde-3-phosphate dehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2405	1519	412	464	10			
1	B	329	Total	C	N	O	S	0	0	0
			2428	1532	414	472	10			
1	C	329	Total	C	N	O	S	0	0	0
			2405	1519	412	464	10			
1	D	329	Total	C	N	O	S	0	0	0
			2428	1532	414	472	10			
1	E	329	Total	C	N	O	S	0	1	0
			2411	1522	415	464	10			
1	F	329	Total	C	N	O	S	0	0	0
			2428	1532	414	472	10			
1	G	329	Total	C	N	O	S	0	1	0
			2410	1522	415	463	10			
1	H	329	Total	C	N	O	S	0	0	0
			2421	1528	413	470	10			
1	I	329	Total	C	N	O	S	0	1	0
			2405	1519	414	462	10			
1	J	329	Total	C	N	O	S	0	0	0
			2425	1530	413	472	10			
1	K	329	Total	C	N	O	S	0	0	0
			2393	1510	411	462	10			
1	L	329	Total	C	N	O	S	0	0	0
			2428	1532	414	472	10			
1	M	329	Total	C	N	O	S	0	1	0
			2408	1520	414	464	10			
1	N	329	Total	C	N	O	S	0	0	0
			2424	1529	414	471	10			
1	O	329	Total	C	N	O	S	0	1	0
			2411	1522	415	464	10			
1	P	329	Total	C	N	O	S	0	0	0
			2425	1530	413	472	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	ASP	engineered mutation	UNP P0A9B2
B	78	GLY	ASP	engineered mutation	UNP P0A9B2
C	78	GLY	ASP	engineered mutation	UNP P0A9B2
D	78	GLY	ASP	engineered mutation	UNP P0A9B2
E	78	GLY	ASP	engineered mutation	UNP P0A9B2
F	78	GLY	ASP	engineered mutation	UNP P0A9B2
G	78	GLY	ASP	engineered mutation	UNP P0A9B2
H	78	GLY	ASP	engineered mutation	UNP P0A9B2
I	78	GLY	ASP	engineered mutation	UNP P0A9B2
J	78	GLY	ASP	engineered mutation	UNP P0A9B2
K	78	GLY	ASP	engineered mutation	UNP P0A9B2
L	78	GLY	ASP	engineered mutation	UNP P0A9B2
M	78	GLY	ASP	engineered mutation	UNP P0A9B2
N	78	GLY	ASP	engineered mutation	UNP P0A9B2
O	78	GLY	ASP	engineered mutation	UNP P0A9B2
P	78	GLY	ASP	engineered mutation	UNP P0A9B2

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Ag 1 1	0	0
2	G	1	Total Ag 1 1	0	0
2	J	1	Total Ag 1 1	0	0
2	D	1	Total Ag 1 1	0	0
2	K	1	Total Ag 1 1	0	0
2	E	1	Total Ag 1 1	0	0
2	H	1	Total Ag 1 1	0	0
2	B	1	Total Ag 1 1	0	0
2	I	1	Total Ag 1 1	0	0
2	C	1	Total Ag 1 1	0	0
2	A	1	Total Ag 1 1	0	0

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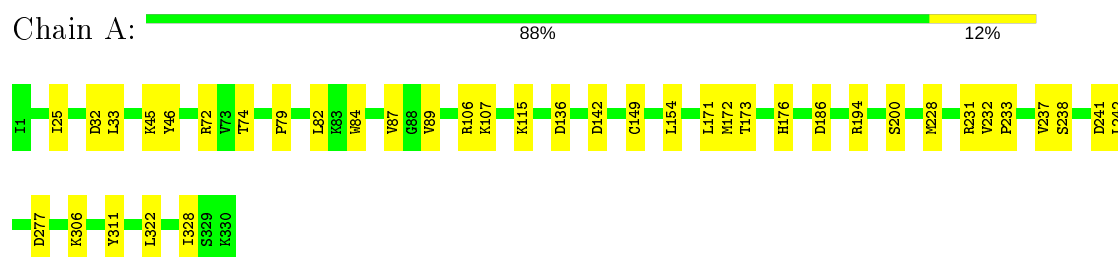
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	1	Total 1	Ag 1	0	0
2	O	1	Total 1	Ag 1	0	0
2	L	1	Total 1	Ag 1	0	0
2	F	1	Total 1	Ag 1	0	0
2	M	1	Total 1	Ag 1	0	0

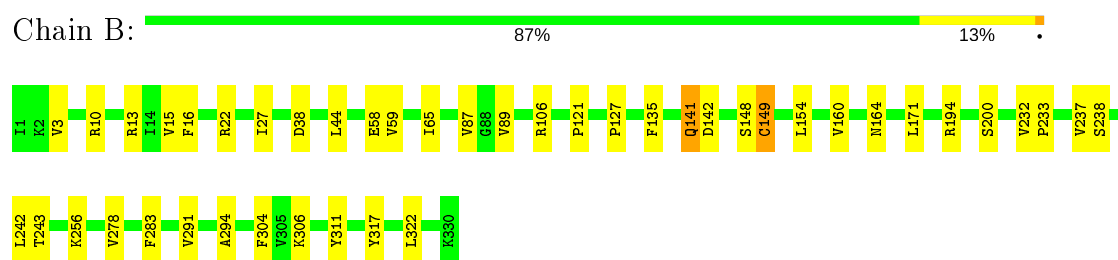
3 Residue-property plots

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 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.

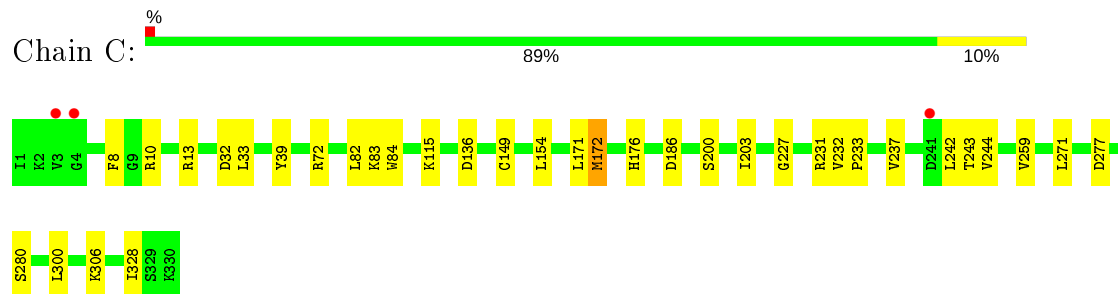
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



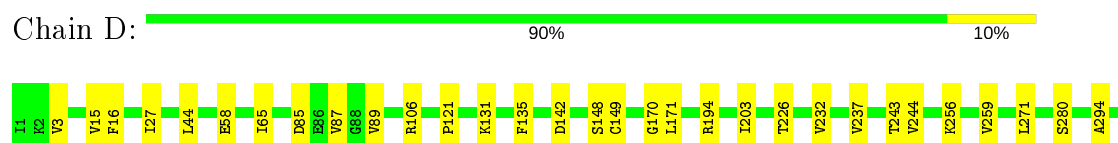
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



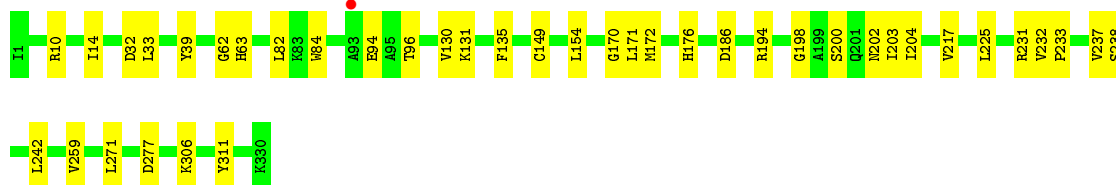
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A





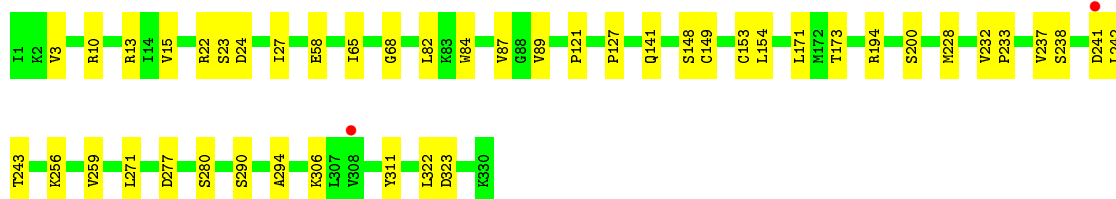
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain E: 88% 12%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain F: 86% 14%



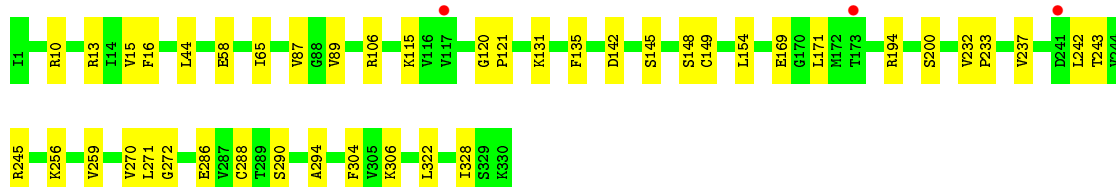
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain G: 90% 10%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

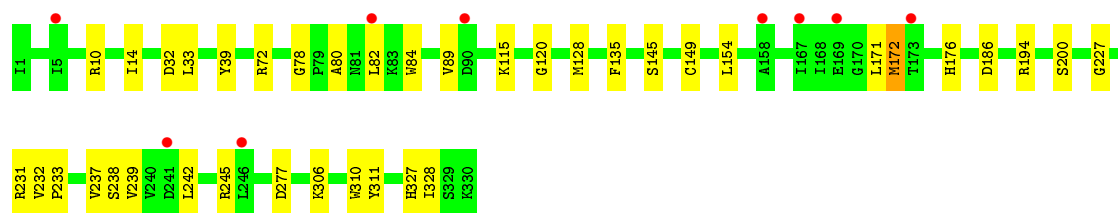
Chain H: 87% 13%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

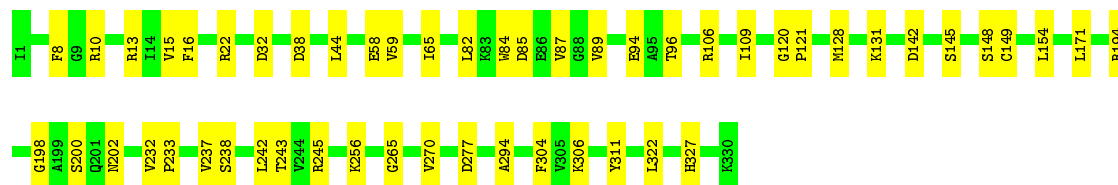
Chain I: 3% 88% 12%





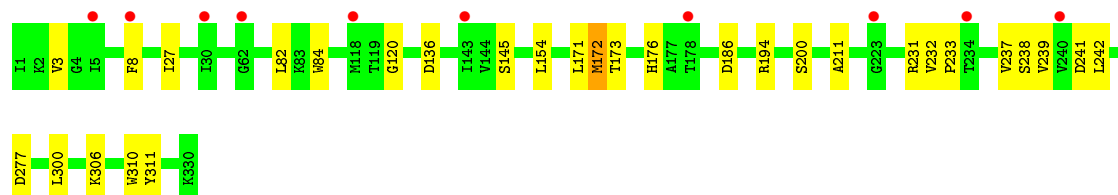
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain J: 84% 16%



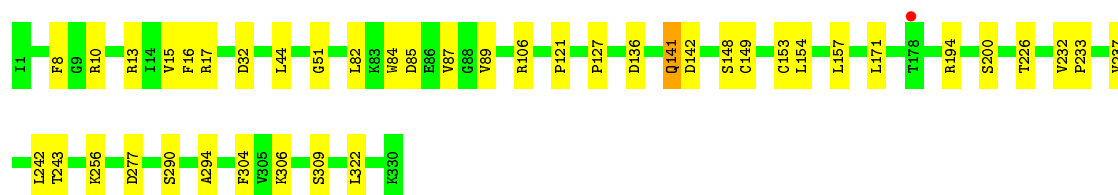
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain K: 3% 91% 9%



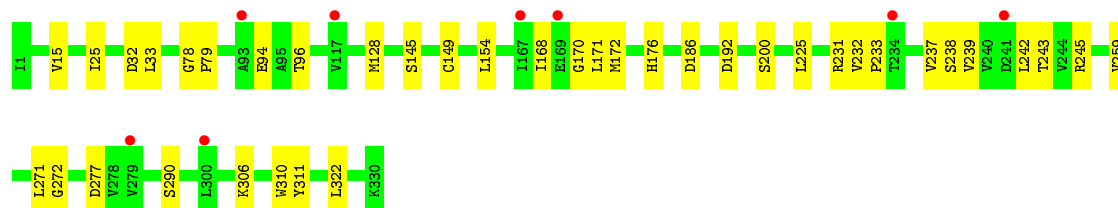
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain L: 87% 12%

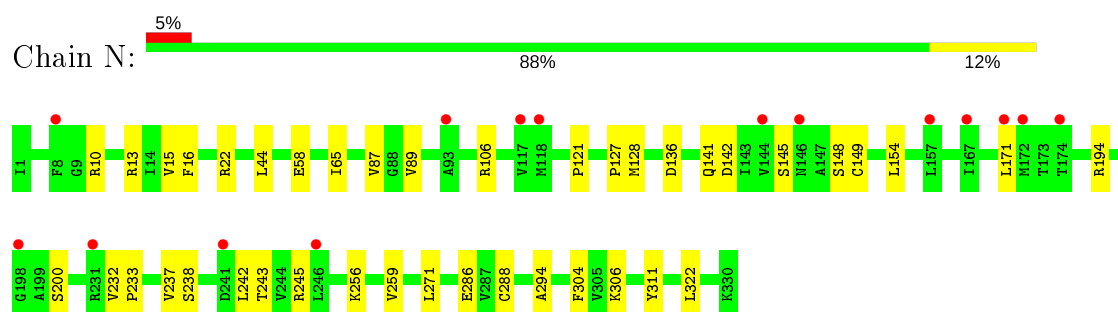


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

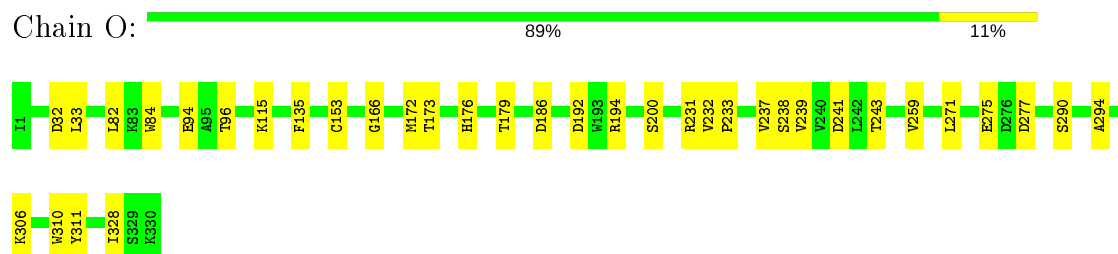
Chain M: 2% 88% 12%



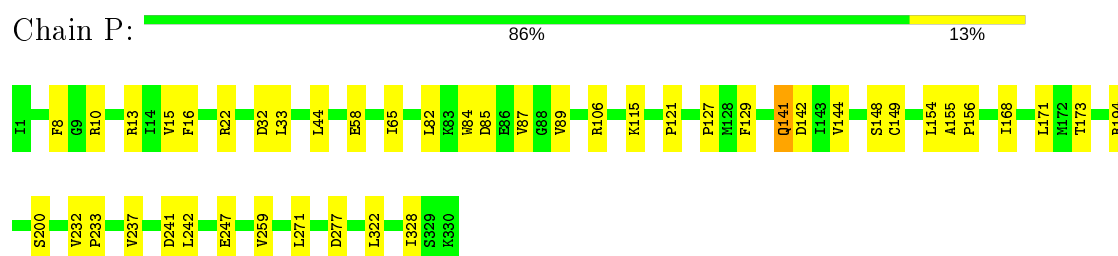
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.99Å 110.02Å 139.71Å 87.66° 86.94° 87.26°	Depositor
Resolution (Å)	87.77 – 3.10 139.41 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.2 (87.77-3.10) 90.3 (139.41-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.14_3260:001)	Depositor
R, R_{free}	0.175 , 0.240 0.174 , 0.239	Depositor DCC
R_{free} test set	4138 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38671	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: AG

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	0.24	0/2443	0.43	0/3321
1	B	0.24	0/2466	0.43	0/3348
1	C	0.24	0/2443	0.43	0/3321
1	D	0.24	0/2466	0.42	0/3348
1	E	0.24	0/2454	0.43	0/3335
1	F	0.24	0/2466	0.43	0/3348
1	G	0.24	0/2453	0.42	0/3335
1	H	0.24	0/2459	0.42	0/3340
1	I	0.24	0/2448	0.42	0/3329
1	J	0.24	0/2463	0.42	0/3345
1	K	0.24	0/2431	0.42	0/3307
1	L	0.24	0/2466	0.43	0/3348
1	M	0.24	0/2451	0.42	0/3332
1	N	0.24	0/2462	0.42	0/3345
1	O	0.24	0/2454	0.42	0/3335
1	P	0.24	0/2463	0.43	0/3345
All	All	0.24	0/39288	0.42	0/53382

There are no bond length outliers.

There are no bond angle outliers.

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	2405	0	2350	24	0
1	B	2428	0	2382	26	0
1	C	2405	0	2350	22	0
1	D	2428	0	2382	25	0
1	E	2411	0	2359	24	0
1	F	2428	0	2382	31	0
1	G	2410	0	2359	21	0
1	H	2421	0	2372	25	0
1	I	2405	0	2351	24	0
1	J	2425	0	2376	34	0
1	K	2393	0	2324	19	0
1	L	2428	0	2382	26	0
1	M	2408	0	2353	26	0
1	N	2424	0	2376	27	0
1	O	2411	0	2359	19	0
1	P	2425	0	2376	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	1	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
All	All	38671	0	37833	335	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 5.

All (335) 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:E:171:LEU:HG	1:F:306:LYS:HE2	1.75	0.69
1:G:176:HIS:HB3	1:G:231[B]:ARG:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:HIS:HB3	1:M:231[B]:ARG:HD3	1.77	0.67
1:A:154:LEU:HD11	1:A:242:LEU:HD13	1.77	0.66
1:P:15:VAL:HG13	1:P:322:LEU:HD11	1.78	0.66
1:F:127:PRO:HG3	1:F:141:GLN:HE21	1.60	0.65
1:M:171:LEU:HG	1:N:306:LYS:HE2	1.78	0.65
1:I:176:HIS:HB3	1:I:231[B]:ARG:HD3	1.80	0.64
1:A:277:ASP:HB3	1:B:194:ARG:HG2	1.78	0.64
1:L:127:PRO:HG3	1:L:141:GLN:HE21	1.64	0.63
1:P:58:GLU:HG2	1:P:65:ILE:HB	1.81	0.63
1:L:200:SER:HA	1:L:233:PRO:HB3	1.82	0.62
1:J:15:VAL:HG13	1:J:322:LEU:HD11	1.82	0.61
1:H:154:LEU:HD11	1:H:242:LEU:HD13	1.83	0.60
1:M:171:LEU:HD23	1:N:243:THR:HG23	1.83	0.60
1:E:306:LYS:HB2	1:F:171:LEU:HD13	1.83	0.60
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.82	0.60
1:I:277:ASP:HB3	1:J:194:ARG:HG2	1.83	0.60
1:L:10:ARG:HH11	1:L:13:ARG:HH21	1.48	0.60
1:M:277:ASP:HB3	1:N:194:ARG:HG2	1.83	0.59
1:E:171:LEU:HD23	1:F:243:THR:HG23	1.84	0.58
1:C:306:LYS:HB2	1:D:171:LEU:HD13	1.85	0.58
1:D:131:LYS:N	1:D:135:PHE:CE1	2.72	0.58
1:F:121:PRO:HG3	1:F:148:SER:HB3	1.86	0.58
1:D:256:LYS:HD2	1:D:294:ALA:HB1	1.84	0.58
1:K:194:ARG:HG2	1:L:277:ASP:HB3	1.85	0.58
1:J:87:VAL:HG23	1:J:89:VAL:HG23	1.85	0.58
1:K:200:SER:HA	1:K:233:PRO:HB3	1.86	0.58
1:N:106:ARG:NH1	1:N:142:ASP:OD2	2.37	0.58
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.84	0.57
1:L:87:VAL:HG23	1:L:89:VAL:HG23	1.86	0.57
1:O:277:ASP:HB3	1:P:194:ARG:HG2	1.86	0.57
1:E:306:LYS:HE2	1:F:171:LEU:HB3	1.86	0.57
1:M:200:SER:HA	1:M:233:PRO:HB3	1.87	0.57
1:E:277:ASP:HB3	1:F:194:ARG:HG2	1.87	0.56
1:H:10:ARG:HH11	1:H:13:ARG:HH21	1.53	0.56
1:N:121:PRO:HG3	1:N:148:SER:HB3	1.87	0.56
1:E:154:LEU:HD11	1:E:242:LEU:HD13	1.86	0.56
1:L:15:VAL:HG13	1:L:322:LEU:HD11	1.86	0.56
1:J:106:ARG:NH1	1:J:142:ASP:OD2	2.38	0.56
1:I:120:GLY:O	1:I:145:SER:OG	2.24	0.56
1:I:171:LEU:HD23	1:J:243:THR:HG23	1.86	0.56
1:G:171:LEU:HD23	1:H:243:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PRO:HG3	1:D:148:SER:HB3	1.88	0.55
1:H:121:PRO:HG3	1:H:148:SER:HB3	1.88	0.55
1:P:22:ARG:HD3	1:P:322:LEU:HD23	1.88	0.55
1:D:131:LYS:HA	1:D:135:PHE:CD1	2.40	0.55
1:C:200:SER:HA	1:C:233:PRO:HB3	1.88	0.55
1:F:15:VAL:HG13	1:F:322:LEU:HD11	1.88	0.55
1:M:306:LYS:HB2	1:N:171:LEU:HD13	1.88	0.55
1:A:306:LYS:HB2	1:B:171:LEU:HD13	1.89	0.55
1:C:277:ASP:HB3	1:D:194:ARG:HG2	1.88	0.55
1:F:87:VAL:HG23	1:F:89:VAL:HG23	1.88	0.54
1:K:232:VAL:HG11	1:L:232:VAL:HG11	1.89	0.54
1:O:176:HIS:HB3	1:O:231[B]:ARG:HD3	1.88	0.54
1:I:306:LYS:HE2	1:J:171:LEU:HB3	1.89	0.54
1:M:306:LYS:HE2	1:N:171:LEU:HB3	1.89	0.54
1:P:10:ARG:HH11	1:P:13:ARG:HH21	1.56	0.54
1:D:106:ARG:NH1	1:D:142:ASP:OD2	2.40	0.54
1:I:128:MET:HG2	1:I:145:SER:HB3	1.89	0.54
1:C:280:SER:HB3	1:D:203:ILE:H	1.73	0.54
1:C:72:ARG:NH2	1:C:83:LYS:O	2.42	0.54
1:I:32:ASP:OD1	1:I:33:LEU:N	2.40	0.54
1:K:176:HIS:HB3	1:K:231:ARG:HD3	1.90	0.54
1:I:200:SER:HA	1:I:233:PRO:HB3	1.90	0.53
1:N:87:VAL:HG23	1:N:89:VAL:HG23	1.91	0.53
1:L:121:PRO:HG3	1:L:148:SER:HB3	1.90	0.53
1:E:200:SER:HA	1:E:233:PRO:HB3	1.91	0.53
1:M:192:ASP:OD2	1:M:231[A]:ARG:NH2	2.33	0.53
1:B:127:PRO:HG3	1:B:141:GLN:HE21	1.74	0.53
1:B:200:SER:HA	1:B:233:PRO:HB3	1.90	0.53
1:N:128:MET:HG2	1:N:145:SER:HB3	1.91	0.53
1:G:171:LEU:HG	1:H:306:LYS:HE2	1.91	0.52
1:F:154:LEU:HD11	1:F:242:LEU:HD13	1.91	0.52
1:H:87:VAL:HG23	1:H:89:VAL:HG23	1.92	0.52
1:P:8:PHE:N	1:P:32:ASP:OD2	2.43	0.52
1:H:259:VAL:HG13	1:H:271:LEU:HD21	1.90	0.52
1:B:87:VAL:HG23	1:B:89:VAL:HG23	1.92	0.52
1:F:259:VAL:HG13	1:F:271:LEU:HD21	1.90	0.52
1:B:121:PRO:HG3	1:B:148:SER:HB3	1.91	0.52
1:H:120:GLY:O	1:H:145:SER:OG	2.27	0.52
1:D:87:VAL:HG23	1:D:89:VAL:HG23	1.92	0.52
1:J:22:ARG:HD3	1:J:322:LEU:HD23	1.92	0.51
1:A:232:VAL:HG11	1:B:232:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:HG13	1:B:322:LEU:HD11	1.92	0.51
1:G:179:THR:OG1	1:G:231[B]:ARG:NH1	2.41	0.51
1:M:168:ILE:HD12	1:M:245:ARG:HG2	1.91	0.51
1:H:200:SER:HA	1:H:233:PRO:HB3	1.91	0.51
1:P:32:ASP:OD1	1:P:33:LEU:N	2.43	0.51
1:B:10:ARG:HH11	1:B:13:ARG:HH21	1.59	0.51
1:N:22:ARG:HD3	1:N:322:LEU:HD23	1.93	0.51
1:M:272:GLY:N	1:M:290:SER:O	2.36	0.51
1:L:154:LEU:HD11	1:L:242:LEU:HD13	1.93	0.51
1:A:171:LEU:HG	1:B:306:LYS:HE2	1.91	0.50
1:O:32:ASP:OD1	1:O:33:LEU:N	2.44	0.50
1:A:306:LYS:HE2	1:B:171:LEU:HB3	1.93	0.50
1:M:32:ASP:OD1	1:M:33:LEU:N	2.45	0.50
1:K:171:LEU:HD23	1:L:243:THR:HG23	1.94	0.50
1:N:10:ARG:HH11	1:N:13:ARG:HH21	1.59	0.50
1:A:106:ARG:NH1	1:A:142:ASP:OD2	2.42	0.49
1:N:149:CYS:HG	2:N:401:AG:AG	1.80	0.49
1:K:173:THR:O	1:K:241:ASP:N	2.44	0.49
1:K:277:ASP:HB3	1:L:194:ARG:HG3	1.95	0.49
1:N:154:LEU:HD11	1:N:242:LEU:HD13	1.95	0.49
1:F:173:THR:HB	1:F:241:ASP:HB3	1.94	0.49
1:H:106:ARG:NH1	1:H:142:ASP:OD2	2.45	0.49
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.48	0.49
1:B:106:ARG:NH1	1:B:142:ASP:OD2	2.45	0.49
1:C:115:LYS:HD3	1:C:328:ILE:HD12	1.95	0.49
1:I:245:ARG:HD2	1:J:245:ARG:HD2	1.95	0.49
1:N:259:VAL:HG13	1:N:271:LEU:HD21	1.94	0.49
1:F:10:ARG:HH11	1:F:13:ARG:HH21	1.59	0.49
1:I:171:LEU:HG	1:J:306:LYS:HE2	1.95	0.49
1:G:32:ASP:OD1	1:G:33:LEU:N	2.44	0.49
1:A:171:LEU:HD23	1:B:243:THR:HG23	1.95	0.49
1:O:306:LYS:HB2	1:P:171:LEU:HD13	1.94	0.49
1:P:87:VAL:HG23	1:P:89:VAL:HG23	1.94	0.49
1:M:245:ARG:HD2	1:N:245:ARG:HD2	1.94	0.49
1:H:272:GLY:N	1:H:290:SER:O	2.41	0.48
1:N:256:LYS:HD2	1:N:294:ALA:HB1	1.94	0.48
1:B:22:ARG:HD3	1:B:322:LEU:HD23	1.93	0.48
1:H:115:LYS:NZ	1:H:328:ILE:O	2.45	0.48
1:I:115:LYS:HD3	1:I:328:ILE:HD12	1.96	0.48
1:K:306:LYS:HB2	1:L:171:LEU:HD13	1.96	0.48
1:I:306:LYS:HB2	1:J:171:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:LEU:HD11	1:J:242:LEU:HD13	1.95	0.48
1:J:256:LYS:HD2	1:J:294:ALA:HB1	1.94	0.48
1:C:171:LEU:HD23	1:D:243:THR:HG23	1.95	0.48
1:E:176:HIS:HB3	1:E:231[B]:ARG:HD3	1.96	0.48
1:N:15:VAL:HG13	1:N:322:LEU:HD11	1.96	0.48
1:E:232:VAL:HG11	1:F:232:VAL:HG11	1.94	0.48
1:J:106:ARG:HD3	1:J:109:ILE:HD12	1.96	0.48
1:P:259:VAL:HG13	1:P:271:LEU:HD21	1.95	0.48
1:F:58:GLU:HG2	1:F:65:ILE:HB	1.95	0.47
1:J:82:LEU:HD13	1:J:84:TRP:CZ2	2.48	0.47
1:N:127:PRO:HG3	1:N:141:GLN:HE21	1.78	0.47
1:L:106:ARG:NH1	1:L:142:ASP:OD2	2.47	0.47
1:L:256:LYS:HD2	1:L:294:ALA:HB1	1.95	0.47
1:N:200:SER:HA	1:N:233:PRO:HB3	1.95	0.47
1:C:232:VAL:HG11	1:D:232:VAL:HG11	1.96	0.47
1:G:259:VAL:HG13	1:G:271:LEU:HD21	1.96	0.47
1:G:232:VAL:HG11	1:H:232:VAL:HG11	1.96	0.47
1:G:200:SER:HA	1:G:233:PRO:HB3	1.95	0.47
1:B:58:GLU:HG2	1:B:65:ILE:HB	1.95	0.47
1:F:22:ARG:HD3	1:F:322:LEU:HD23	1.96	0.47
1:E:94:GLU:OE2	1:E:96:THR:OG1	2.23	0.47
1:J:94:GLU:OE2	1:J:96:THR:OG1	2.27	0.47
1:P:173:THR:HB	1:P:241:ASP:HB3	1.96	0.47
1:P:84:TRP:HB3	1:P:89:VAL:HB	1.97	0.47
1:B:256:LYS:HD2	1:B:294:ALA:HB1	1.96	0.47
1:D:131:LYS:CA	1:D:135:PHE:CE1	2.98	0.47
1:O:179:THR:OG1	1:O:231[B]:ARG:NH1	2.48	0.47
1:J:121:PRO:HG3	1:J:148:SER:HB3	1.96	0.47
1:P:200:SER:HA	1:P:233:PRO:HB3	1.96	0.47
1:P:115:LYS:NZ	1:P:328:ILE:O	2.39	0.47
1:I:171:LEU:HB2	1:J:304:PHE:CE2	2.50	0.46
1:G:154:LEU:HD11	1:G:242:LEU:HD13	1.98	0.46
1:G:72:ARG:NH2	1:G:83:LYS:O	2.49	0.46
1:M:128:MET:HG2	1:M:145:SER:HB3	1.98	0.46
1:M:170:GLY:HA3	1:M:225:LEU:HD23	1.96	0.46
1:N:58:GLU:HG2	1:N:65:ILE:HB	1.97	0.46
1:G:245:ARG:HD2	1:H:245:ARG:HD2	1.97	0.46
1:I:78:GLY:O	1:I:80:ALA:N	2.43	0.46
1:G:306:LYS:HB2	1:H:171:LEU:HD13	1.98	0.46
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.51	0.46
1:K:120:GLY:O	1:K:145:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:GLU:HG2	1:H:65:ILE:HB	1.98	0.46
1:I:135:PHE:O	1:I:327:HIS:NE2	2.48	0.46
1:O:200:SER:HA	1:O:233:PRO:HB3	1.97	0.46
1:P:84:TRP:CE3	1:P:89:VAL:HG21	2.51	0.46
1:J:131:LYS:HG2	1:J:270:VAL:HG21	1.98	0.46
1:A:200:SER:HA	1:A:233:PRO:HB3	1.98	0.46
1:E:198:GLY:O	1:E:202:ASN:ND2	2.41	0.46
1:I:72:ARG:NH1	1:I:82:LEU:O	2.49	0.46
1:M:171:LEU:HB2	1:N:304:PHE:CE2	2.51	0.46
1:D:131:LYS:HB2	1:D:135:PHE:CZ	2.51	0.45
1:M:171:LEU:HA	1:M:171:LEU:HD12	1.82	0.45
1:P:168:ILE:HD11	1:P:247:GLU:HA	1.99	0.45
1:C:10:ARG:HH11	1:C:13:ARG:NH2	2.15	0.45
1:F:153:CYS:HA	1:F:290:SER:HB2	1.99	0.45
1:I:232:VAL:HG11	1:J:232:VAL:HG11	1.98	0.45
1:A:32:ASP:OD1	1:A:33:LEU:N	2.48	0.45
1:D:58:GLU:HG2	1:D:65:ILE:HB	1.98	0.45
1:C:203:ILE:H	1:D:280:SER:HB3	1.82	0.45
1:I:154:LEU:HD11	1:I:242:LEU:HD13	1.97	0.45
1:A:79:PRO:HB2	1:A:107:LYS:HB2	1.98	0.45
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.52	0.45
1:G:243:THR:HG23	1:H:171:LEU:HD12	1.99	0.45
1:J:85:ASP:OD1	1:J:85:ASP:N	2.50	0.45
1:O:243:THR:HG23	1:P:171:LEU:HD12	1.99	0.45
1:D:15:VAL:HG13	1:D:322:LEU:HD11	1.99	0.44
1:E:203:ILE:H	1:F:280:SER:HB3	1.82	0.44
1:K:136:ASP:OD1	1:K:136:ASP:N	2.50	0.44
1:K:239:VAL:HB	1:K:310:TRP:CE3	2.52	0.44
1:B:154:LEU:HD11	1:B:242:LEU:HD13	1.99	0.44
1:E:238:SER:HB2	1:E:311:TYR:CZ	2.52	0.44
1:F:3:VAL:HB	1:F:27:ILE:HD13	1.99	0.44
1:H:15:VAL:HG13	1:H:322:LEU:HD11	1.98	0.44
1:J:58:GLU:HG2	1:J:65:ILE:HB	1.99	0.44
1:K:171:LEU:HB2	1:L:304:PHE:CE2	2.52	0.44
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.53	0.44
1:P:121:PRO:HG3	1:P:148:SER:HB3	1.98	0.44
1:B:38:ASP:HA	1:B:59:VAL:HG21	1.99	0.44
1:P:85:ASP:N	1:P:85:ASP:OD1	2.51	0.44
1:F:24:ASP:OD1	1:F:24:ASP:N	2.49	0.44
1:G:171:LEU:HB2	1:H:304:PHE:CE2	2.53	0.44
1:J:10:ARG:HH11	1:J:13:ARG:HH21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PHE:CE2	1:B:44:LEU:HD11	2.52	0.44
1:J:120:GLY:O	1:J:145:SER:OG	2.32	0.44
1:O:259:VAL:HG13	1:O:271:LEU:HD21	2.00	0.44
1:E:259:VAL:HG13	1:E:271:LEU:HD21	2.00	0.44
1:F:238:SER:HB2	1:F:311:TYR:CZ	2.52	0.44
1:J:238:SER:HB2	1:J:311:TYR:CZ	2.53	0.44
1:L:8:PHE:N	1:L:32:ASP:OD2	2.48	0.44
1:O:194:ARG:HG2	1:P:277:ASP:HB3	1.99	0.44
1:C:306:LYS:HE2	1:D:171:LEU:HB3	1.99	0.43
1:O:153:CYS:HA	1:O:290:SER:HB2	2.00	0.43
1:L:17:ARG:NH2	1:L:51:GLY:O	2.49	0.43
1:O:173:THR:O	1:O:241:ASP:N	2.51	0.43
1:F:22:ARG:NH1	1:F:323:ASP:OD1	2.50	0.43
1:A:194:ARG:NH1	1:B:278:VAL:O	2.50	0.43
1:F:84:TRP:HB3	1:F:89:VAL:HB	2.01	0.43
1:F:68:GLY:HA3	1:J:265:GLY:HA2	1.99	0.43
1:G:120:GLY:O	1:G:145:SER:OG	2.32	0.43
1:H:256:LYS:HD2	1:H:294:ALA:HB1	2.00	0.43
1:K:300:LEU:HD23	1:L:226:THR:HG22	2.01	0.43
1:M:259:VAL:HG13	1:M:271:LEU:HD21	1.99	0.43
1:M:25:ILE:HG21	1:M:322:LEU:HD12	2.00	0.43
1:M:15:VAL:HG13	1:M:322:LEU:HD21	2.01	0.43
1:E:130:VAL:HG23	1:E:217:VAL:HG11	2.00	0.43
1:F:23:SER:HB2	1:J:327:HIS:ND1	2.34	0.43
1:E:204:ILE:HB	1:E:231[B]:ARG:HB2	2.01	0.43
1:J:38:ASP:HA	1:J:59:VAL:HG21	2.00	0.43
1:C:242:LEU:HG	1:C:244:VAL:HG13	2.01	0.43
1:D:3:VAL:HB	1:D:27:ILE:HD13	2.01	0.43
1:I:239:VAL:HB	1:I:310:TRP:CE3	2.54	0.43
1:A:228:MET:HE3	1:A:228:MET:HB2	1.97	0.43
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.54	0.43
1:C:243:THR:HG23	1:D:171:LEU:HD12	2.00	0.43
1:J:198:GLY:O	1:J:202:ASN:ND2	2.44	0.43
1:K:171:LEU:HG	1:L:306:LYS:HE2	2.00	0.43
1:O:232:VAL:HG11	1:P:232:VAL:HG11	2.01	0.43
1:G:238:SER:HB2	1:G:311:TYR:CZ	2.54	0.43
1:K:238:SER:HB2	1:K:311:TYR:CZ	2.54	0.43
1:O:115:LYS:HD3	1:O:328:ILE:HD12	1.99	0.43
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.54	0.42
1:G:277:ASP:HB3	1:H:194:ARG:HG2	2.00	0.42
1:J:128:MET:HG2	1:J:145:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:129:PHE:HD2	1:P:144:VAL:HG13	1.84	0.42
1:C:259:VAL:HG13	1:C:271:LEU:HD21	2.01	0.42
1:C:32:ASP:OD1	1:C:33:LEU:N	2.47	0.42
1:D:85:ASP:N	1:D:85:ASP:OD1	2.51	0.42
1:E:194:ARG:HG3	1:F:277:ASP:HB3	2.00	0.42
1:N:286:GLU:HG3	1:N:288:CYS:H	1.84	0.42
1:E:170:GLY:HA3	1:E:225:LEU:HD23	2.01	0.42
1:H:16:PHE:CE2	1:H:44:LEU:HD11	2.54	0.42
1:L:153:CYS:HA	1:L:290:SER:HB2	2.01	0.42
1:C:171:LEU:HA	1:C:171:LEU:HD12	1.82	0.42
1:L:85:ASP:OD1	1:L:85:ASP:N	2.51	0.42
1:N:16:PHE:CE2	1:N:44:LEU:HD11	2.54	0.42
1:P:84:TRP:HE3	1:P:89:VAL:HG21	1.84	0.42
1:D:170:GLY:HA3	1:D:244:VAL:HG12	2.00	0.42
1:P:154:LEU:HD11	1:P:242:LEU:HD13	2.01	0.42
1:D:259:VAL:HG13	1:D:271:LEU:HD21	2.01	0.42
1:F:84:TRP:CE3	1:F:89:VAL:HG21	2.54	0.42
1:I:238:SER:HB2	1:I:311:TYR:CZ	2.55	0.42
1:L:157:LEU:HD22	1:L:309:SER:HB2	2.02	0.42
1:M:238:SER:HB2	1:M:311:TYR:CZ	2.55	0.42
1:O:238:SER:HB2	1:O:311:TYR:CZ	2.55	0.42
1:A:45:LYS:HD2	1:A:46:TYR:CE2	2.55	0.42
1:D:16:PHE:CE2	1:D:44:LEU:HD11	2.55	0.42
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.54	0.42
1:C:172:MET:HG3	1:C:227:GLY:HA3	2.01	0.42
1:K:154:LEU:HD11	1:K:242:LEU:HD13	2.01	0.42
1:F:256:LYS:HD2	1:F:294:ALA:HB1	2.02	0.42
1:M:232:VAL:HG11	1:N:232:VAL:HG11	2.01	0.42
1:A:136:ASP:OD1	1:A:136:ASP:N	2.53	0.41
1:A:87:VAL:HG13	1:A:89:VAL:HG23	2.02	0.41
1:B:3:VAL:HB	1:B:27:ILE:HD13	2.02	0.41
1:E:62:GLY:O	1:E:63:HIS:ND1	2.53	0.41
1:P:106:ARG:NH1	1:P:142:ASP:OD2	2.53	0.41
1:C:154:LEU:HD11	1:C:242:LEU:HD13	2.01	0.41
1:E:171:LEU:HA	1:E:171:LEU:HD12	1.82	0.41
1:P:127:PRO:HG3	1:P:141:GLN:HE21	1.85	0.41
1:B:160:VAL:O	1:B:164:ASN:ND2	2.38	0.41
1:C:300:LEU:HD23	1:D:226:THR:HG22	2.02	0.41
1:E:10:ARG:O	1:E:14:ILE:HG12	2.20	0.41
1:O:239:VAL:HB	1:O:310:TRP:CE3	2.56	0.41
1:A:72:ARG:HD3	1:A:74:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HB2	1:B:304:PHE:CE2	2.55	0.41
1:F:84:TRP:HE3	1:F:89:VAL:HG21	1.85	0.41
1:G:172:MET:HG3	1:G:227:GLY:HA3	2.02	0.41
1:H:286:GLU:HG3	1:H:288:CYS:H	1.86	0.41
1:I:10:ARG:O	1:I:14:ILE:HG12	2.20	0.41
1:I:194:ARG:HG3	1:J:277:ASP:HB3	2.03	0.41
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.55	0.41
1:E:32:ASP:OD1	1:E:33:LEU:N	2.47	0.41
1:J:200:SER:HA	1:J:233:PRO:HB3	2.02	0.41
1:K:82:LEU:HD13	1:K:84:TRP:CZ2	2.56	0.41
1:A:115:LYS:HD3	1:A:328:ILE:HD12	2.03	0.41
1:D:131:LYS:HA	1:D:135:PHE:CE1	2.56	0.41
1:J:10:ARG:HA	1:J:10:ARG:HD2	1.88	0.41
1:M:239:VAL:HB	1:M:310:TRP:CE3	2.56	0.41
1:M:78:GLY:HA2	1:M:79:PRO:HD3	1.95	0.41
1:A:25:ILE:HD12	1:A:322:LEU:HB3	2.02	0.41
1:L:136:ASP:OD1	1:L:136:ASP:N	2.53	0.41
1:N:238:SER:HB2	1:N:311:TYR:CZ	2.56	0.41
1:G:300:LEU:HD13	1:H:169:GLU:HB2	2.02	0.41
1:M:243:THR:HG23	1:N:171:LEU:HD12	2.02	0.41
1:B:149:CYS:HB3	1:B:317:TYR:HB2	2.03	0.41
1:K:3:VAL:HB	1:K:27:ILE:HD13	2.03	0.41
1:B:238:SER:HB2	1:B:311:TYR:CZ	2.56	0.41
1:L:82:LEU:HD13	1:L:84:TRP:CZ2	2.56	0.41
1:O:192:ASP:OD2	1:O:231[A]:ARG:NH2	2.50	0.41
1:E:131:LYS:HD2	1:E:135:PHE:CE2	2.55	0.40
1:F:200:SER:HA	1:F:233:PRO:HB3	2.01	0.40
1:H:131:LYS:HG2	1:H:270:VAL:HG21	2.03	0.40
1:I:172:MET:HG3	1:I:227:GLY:HA3	2.03	0.40
1:A:173:THR:O	1:A:241:ASP:N	2.54	0.40
1:J:8:PHE:N	1:J:32:ASP:OD2	2.49	0.40
1:K:172:MET:HG2	1:K:211:ALA:HB2	2.02	0.40
1:L:16:PHE:CE2	1:L:44:LEU:HD11	2.56	0.40
1:M:154:LEU:HD11	1:M:242:LEU:HD13	2.02	0.40
1:O:275:GLU:HG2	1:O:294:ALA:HB3	2.03	0.40
1:G:87:VAL:HG13	1:G:89:VAL:HG23	2.03	0.40
1:C:136:ASP:OD1	1:C:136:ASP:N	2.54	0.40
1:I:84:TRP:HB3	1:I:89:VAL:HB	2.04	0.40
1:J:16:PHE:CE2	1:J:44:LEU:HD11	2.57	0.40
1:L:10:ARG:HA	1:L:10:ARG:HD2	1.86	0.40
1:O:94:GLU:OE2	1:O:96:THR:OG1	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:155:ALA:HB3	1:P:156:PRO:HD3	2.02	0.40
1:P:16:PHE:CE2	1:P:44:LEU:HD11	2.57	0.40
1:B:283:PHE:CE1	1:B:291:VAL:HG11	2.57	0.40
1:M:94:GLU:OE2	1:M:96:THR:OG1	2.27	0.40
1:N:136:ASP:N	1:N:136:ASP:OD1	2.55	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	327/329 (99%)	305 (93%)	20 (6%)	2 (1%)	25	59
1	B	327/329 (99%)	304 (93%)	22 (7%)	1 (0%)	41	73
1	C	327/329 (99%)	307 (94%)	18 (6%)	2 (1%)	25	59
1	D	327/329 (99%)	305 (93%)	21 (6%)	1 (0%)	41	73
1	E	328/329 (100%)	309 (94%)	17 (5%)	2 (1%)	25	59
1	F	327/329 (99%)	303 (93%)	23 (7%)	1 (0%)	41	73
1	G	328/329 (100%)	310 (94%)	16 (5%)	2 (1%)	25	59
1	H	327/329 (99%)	309 (94%)	17 (5%)	1 (0%)	41	73
1	I	328/329 (100%)	304 (93%)	22 (7%)	2 (1%)	25	59
1	J	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	K	327/329 (99%)	308 (94%)	17 (5%)	2 (1%)	25	59
1	L	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	M	328/329 (100%)	308 (94%)	18 (6%)	2 (1%)	25	59
1	N	327/329 (99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	O	328/329 (100%)	311 (95%)	14 (4%)	3 (1%)	17	52
1	P	327/329 (99%)	308 (94%)	18 (6%)	1 (0%)	41	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5237/5264 (100%)	4909 (94%)	303 (6%)	25 (0%)	29	64

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	ASP
1	G	186	ASP
1	M	186	ASP
1	A	186	ASP
1	E	186	ASP
1	F	237	VAL
1	H	237	VAL
1	I	186	ASP
1	I	237	VAL
1	K	186	ASP
1	B	237	VAL
1	C	237	VAL
1	E	237	VAL
1	G	237	VAL
1	K	237	VAL
1	L	237	VAL
1	N	237	VAL
1	O	237	VAL
1	P	237	VAL
1	A	237	VAL
1	D	237	VAL
1	J	237	VAL
1	M	237	VAL
1	O	186	ASP
1	O	166	GLY

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	239/263 (91%)	237 (99%)	2 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	246/263 (94%)	243 (99%)	3 (1%)	71	88
1	C	239/263 (91%)	235 (98%)	4 (2%)	60	83
1	D	246/263 (94%)	245 (100%)	1 (0%)	91	96
1	E	240/263 (91%)	237 (99%)	3 (1%)	69	87
1	F	246/263 (94%)	244 (99%)	2 (1%)	81	92
1	G	240/263 (91%)	238 (99%)	2 (1%)	81	92
1	H	245/263 (93%)	243 (99%)	2 (1%)	81	92
1	I	239/263 (91%)	236 (99%)	3 (1%)	69	87
1	J	246/263 (94%)	245 (100%)	1 (0%)	91	96
1	K	236/263 (90%)	234 (99%)	2 (1%)	81	92
1	L	246/263 (94%)	244 (99%)	2 (1%)	81	92
1	M	240/263 (91%)	238 (99%)	2 (1%)	81	92
1	N	246/263 (94%)	246 (100%)	0	100	100
1	O	240/263 (91%)	238 (99%)	2 (1%)	81	92
1	P	246/263 (94%)	244 (99%)	2 (1%)	81	92
All	All	3880/4208 (92%)	3847 (99%)	33 (1%)	78	91

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	CYS
1	A	172	MET
1	B	135	PHE
1	B	141	GLN
1	B	149	CYS
1	C	8	PHE
1	C	39	TYR
1	C	149	CYS
1	C	172	MET
1	D	149	CYS
1	E	39	TYR
1	E	149	CYS
1	E	172	MET
1	F	149	CYS
1	F	228	MET
1	G	149	CYS
1	G	172	MET

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Mol	Chain	Res	Type
1	H	135	PHE
1	H	149	CYS
1	I	39	TYR
1	I	149	CYS
1	I	172	MET
1	J	149	CYS
1	K	8	PHE
1	K	172	MET
1	L	141	GLN
1	L	149	CYS
1	M	149	CYS
1	M	172	MET
1	O	135	PHE
1	O	172	MET
1	P	141	GLN
1	P	149	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 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

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	329/329 (100%)	-0.08	0 100 100	51, 85, 115, 149	0
1	B	329/329 (100%)	-0.19	0 100 100	49, 73, 106, 133	0
1	C	329/329 (100%)	-0.08	3 (0%) 84 69	51, 85, 123, 140	0
1	D	329/329 (100%)	-0.10	0 100 100	46, 75, 111, 150	0
1	E	329/329 (100%)	-0.01	1 (0%) 94 88	65, 90, 127, 165	0
1	F	329/329 (100%)	-0.01	2 (0%) 89 78	57, 87, 118, 141	0
1	G	329/329 (100%)	-0.05	0 100 100	52, 89, 125, 157	0
1	H	329/329 (100%)	0.03	3 (0%) 84 69	53, 103, 135, 167	0
1	I	329/329 (100%)	0.17	9 (2%) 54 31	60, 120, 155, 187	0
1	J	329/329 (100%)	0.02	0 100 100	56, 89, 129, 153	0
1	K	329/329 (100%)	0.28	10 (3%) 50 27	71, 120, 158, 174	0
1	L	329/329 (100%)	-0.03	1 (0%) 94 88	57, 84, 120, 167	0
1	M	329/329 (100%)	0.21	8 (2%) 59 37	66, 121, 155, 198	0
1	N	329/329 (100%)	0.29	15 (4%) 32 16	69, 123, 162, 197	0
1	O	329/329 (100%)	-0.11	0 100 100	56, 81, 120, 161	0
1	P	329/329 (100%)	-0.12	0 100 100	53, 71, 95, 146	0
All	All	5264/5264 (100%)	0.01	52 (0%) 82 67	46, 90, 143, 198	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	241	ASP	5.8
1	N	93	ALA	3.9
1	N	144	VAL	3.8
1	N	241	ASP	3.6
1	K	62	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	118	MET	3.4
1	K	8	PHE	3.2
1	K	5	ILE	3.2
1	N	167	ILE	3.1
1	I	173	THR	2.9
1	M	241	ASP	2.9
1	I	167	ILE	2.9
1	I	246	LEU	2.9
1	I	82	LEU	2.8
1	M	169	GLU	2.8
1	K	223	GLY	2.7
1	N	171	LEU	2.7
1	N	198	GLY	2.7
1	N	172	MET	2.6
1	I	158	ALA	2.5
1	M	300	LEU	2.5
1	K	143	ILE	2.5
1	K	178	THR	2.5
1	L	178	THR	2.5
1	N	174	THR	2.5
1	N	118	MET	2.4
1	M	279	VAL	2.4
1	H	241	ASP	2.4
1	K	30	ILE	2.4
1	H	117	VAL	2.3
1	N	231	ARG	2.3
1	E	93	ALA	2.3
1	K	234	THR	2.3
1	I	169	GLU	2.3
1	H	173	THR	2.3
1	K	240	VAL	2.2
1	N	246	LEU	2.2
1	M	234	THR	2.2
1	I	90	ASP	2.2
1	M	117	VAL	2.2
1	M	93	ALA	2.2
1	C	241	ASP	2.2
1	F	241	ASP	2.2
1	I	5	ILE	2.1
1	M	167	ILE	2.1
1	C	3	VAL	2.1
1	N	8	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	146	ASN	2.1
1	N	117	VAL	2.0
1	N	157	LEU	2.0
1	F	308	VAL	2.0
1	C	4	GLY	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 monosaccharides 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	AG	P	401	1/1	0.84	0.43	175,175,175,175	1
2	AG	N	401	1/1	0.90	0.19	98,98,98,98	1
2	AG	K	401	1/1	0.93	0.20	101,101,101,101	1
2	AG	I	401	1/1	0.95	0.14	92,92,92,92	1
2	AG	L	401	1/1	0.96	0.32	144,144,144,144	0
2	AG	M	401	1/1	0.96	0.15	82,82,82,82	1
2	AG	A	401	1/1	0.96	0.27	112,112,112,112	1
2	AG	G	401	1/1	0.96	0.28	129,129,129,129	1
2	AG	B	401	1/1	0.96	0.36	154,154,154,154	1
2	AG	F	401	1/1	0.96	0.23	112,112,112,112	1
2	AG	E	401	1/1	0.97	0.19	96,96,96,96	1
2	AG	D	401	1/1	0.97	0.27	112,112,112,112	1
2	AG	J	401	1/1	0.97	0.28	113,113,113,113	1
2	AG	O	401	1/1	0.98	0.15	76,76,76,76	1
2	AG	H	401	1/1	0.98	0.11	82,82,82,82	1
2	AG	C	401	1/1	0.99	0.18	79,79,79,79	1

6.5 Other polymers [i](#)

There are no such residues in this entry.