wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 08:46 AM EDT

PDB ID	:	8EU4
Title	:	Escherichia coli pyruvate kinase A301S
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Deposited on	:	2022-10-18
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

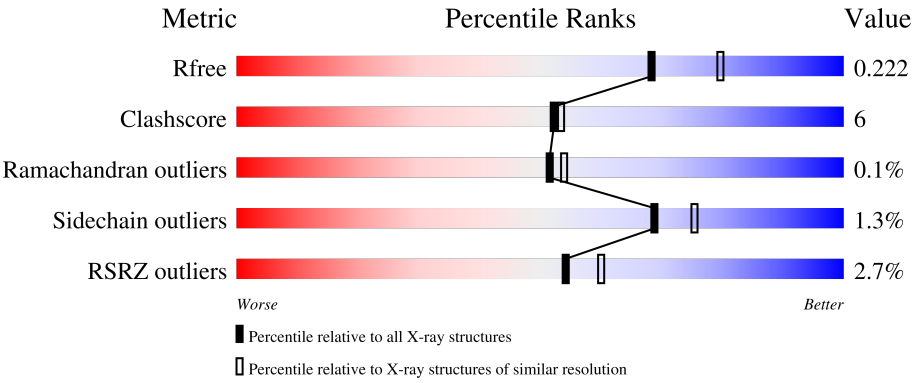
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 <=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	470	6% 88% 10%
1	B	470	88% 11%
1	C	470	3% 87% 10%
1	D	470	% 87% 10%
1	E	470	% 86% 12%

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Mol	Chain	Length	Quality of chain
1	F	470	8% 82% 15%
1	G	470	% 86% 12%
1	H	470	2% 86% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 57299 atoms, of which 28463 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.

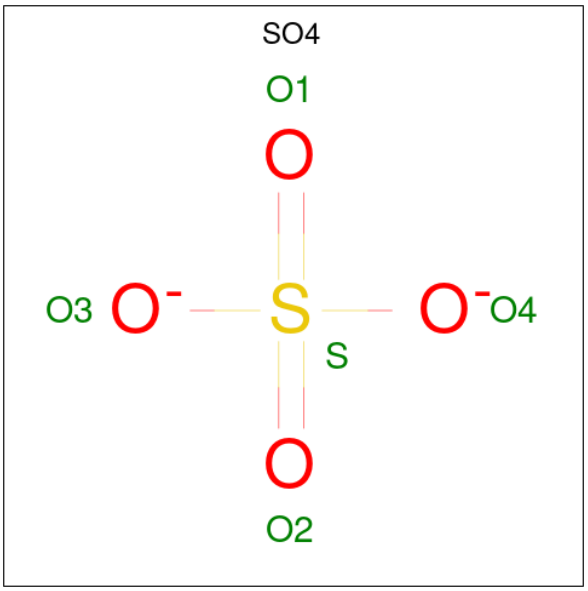
- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	462	Total	C	H	N	O	S	0	0	0
			7003	2155	3542	600	682	24			
1	E	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	D	462	Total	C	H	N	O	S	0	0	0
			7030	2161	3562	601	682	24			
1	G	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	B	462	Total	C	H	N	O	S	0	0	0
			7047	2164	3573	604	682	24			
1	F	461	Total	C	H	N	O	S	0	0	0
			6991	2152	3538	596	681	24			
1	H	462	Total	C	H	N	O	S	0	0	0
			7030	2161	3562	601	682	24			
1	C	462	Total	C	H	N	O	S	0	0	0
			6998	2155	3540	597	682	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	SER	ALA	engineered mutation	UNP A0A0A0G552
E	301	SER	ALA	engineered mutation	UNP A0A0A0G552
D	301	SER	ALA	engineered mutation	UNP A0A0A0G552
G	301	SER	ALA	engineered mutation	UNP A0A0A0G552
B	301	SER	ALA	engineered mutation	UNP A0A0A0G552
F	301	SER	ALA	engineered mutation	UNP A0A0A0G552
H	301	SER	ALA	engineered mutation	UNP A0A0A0G552
C	301	SER	ALA	engineered mutation	UNP A0A0A0G552

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0
3	E	153	Total O 153 153	0	0
3	D	146	Total O 146 146	0	0
3	G	157	Total O 157 157	0	0

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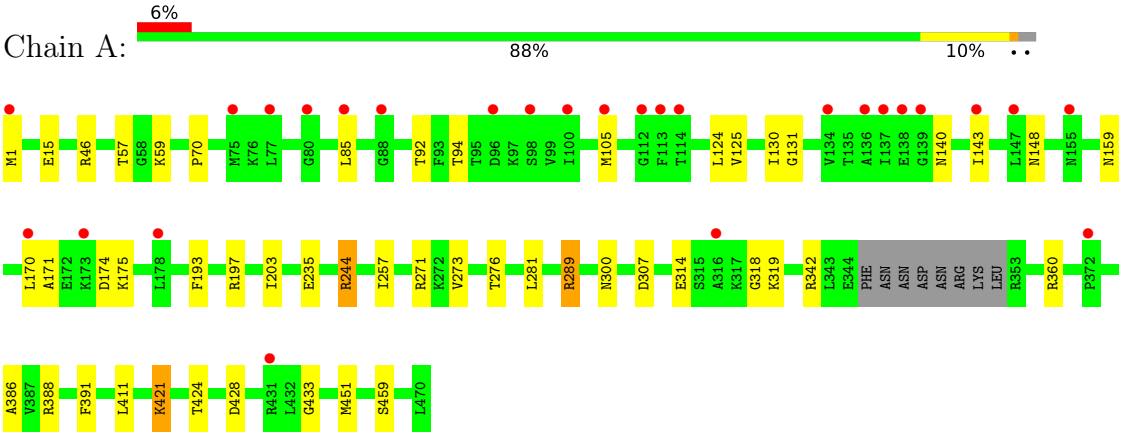
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	169	Total O 169 169	0	0
3	F	103	Total O 103 103	0	0
3	H	114	Total O 114 114	0	0
3	C	120	Total O 120 120	0	0

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.

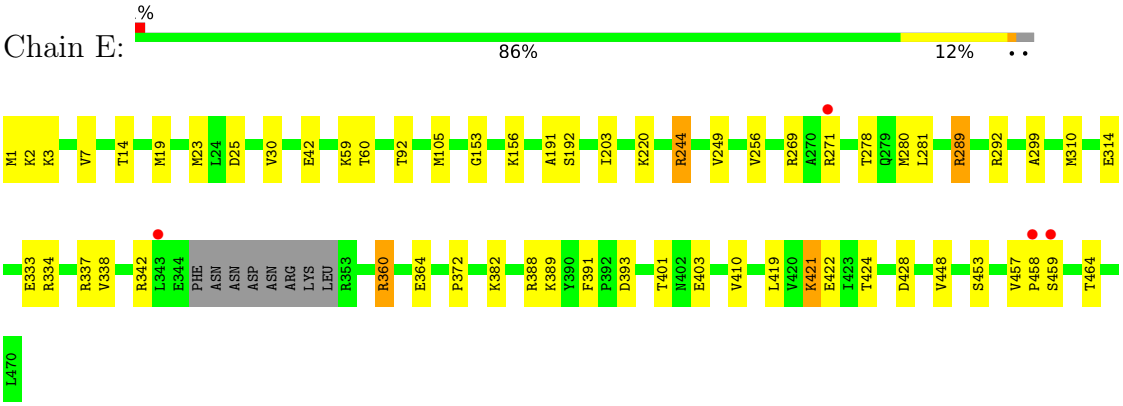
• Molecule 1: Pyruvate kinase

Chain A:



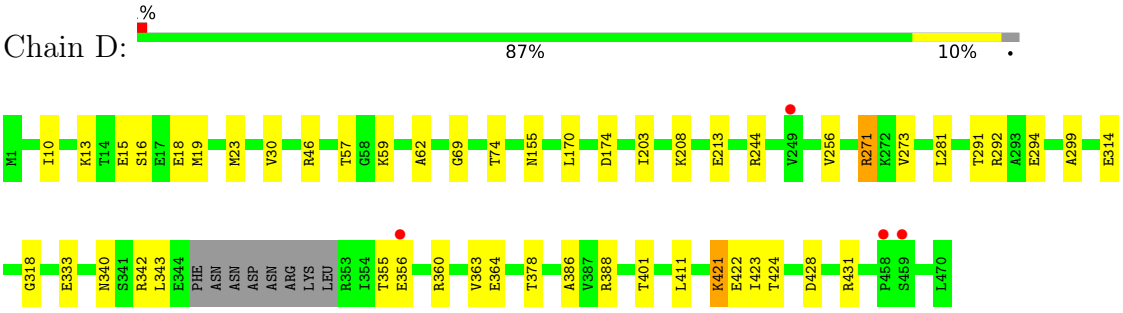
• Molecule 1: Pyruvate kinase

Chain E:



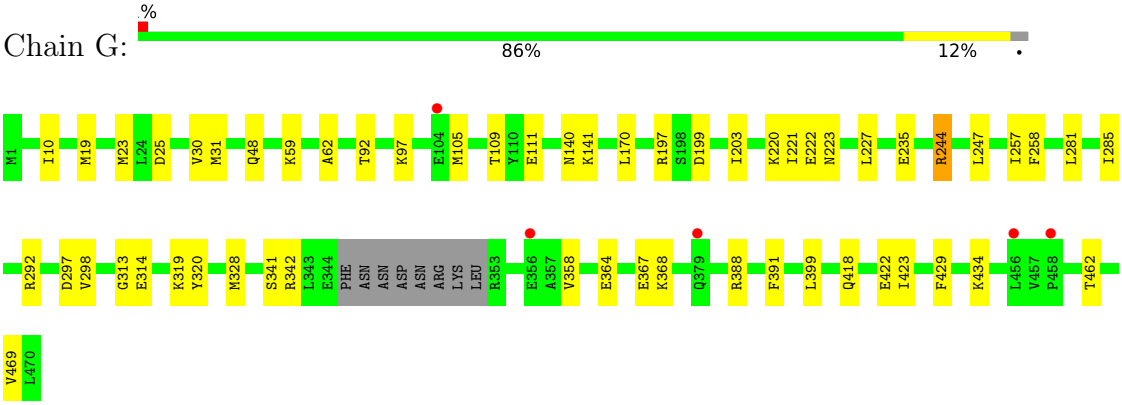
• Molecule 1: Pyruvate kinase

Chain D:



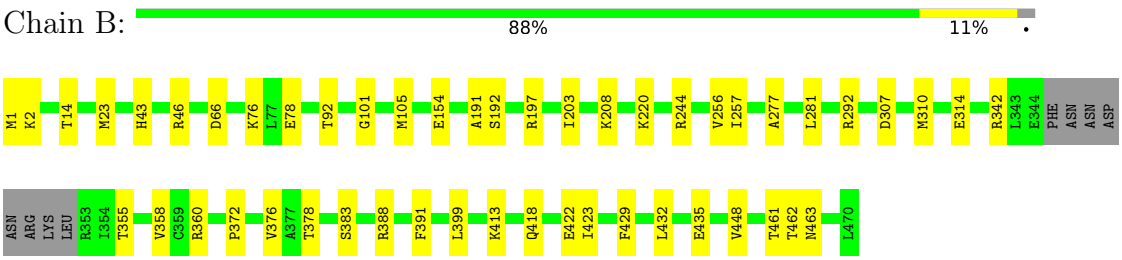
• Molecule 1: Pyruvate kinase

Chain G:



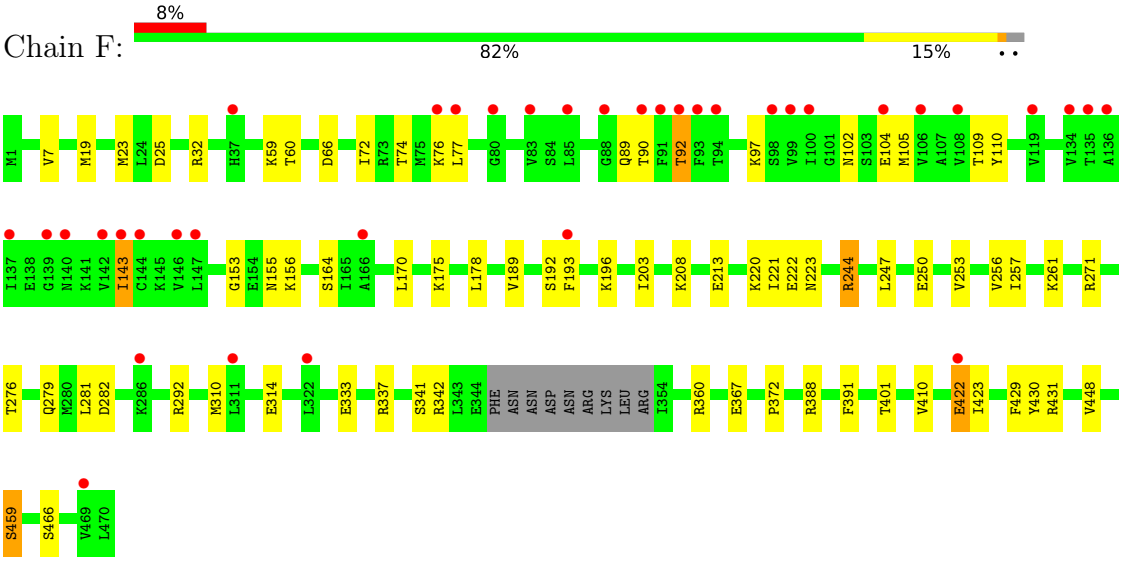
• Molecule 1: Pyruvate kinase

Chain B:



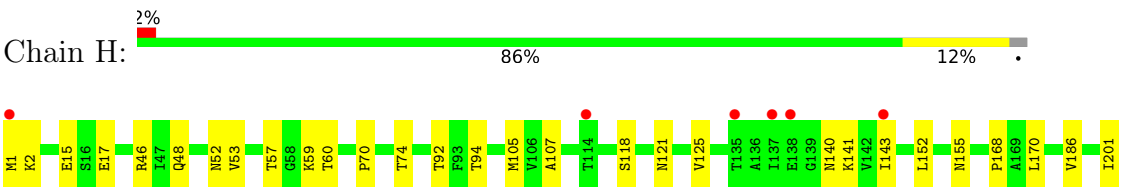
• Molecule 1: Pyruvate kinase

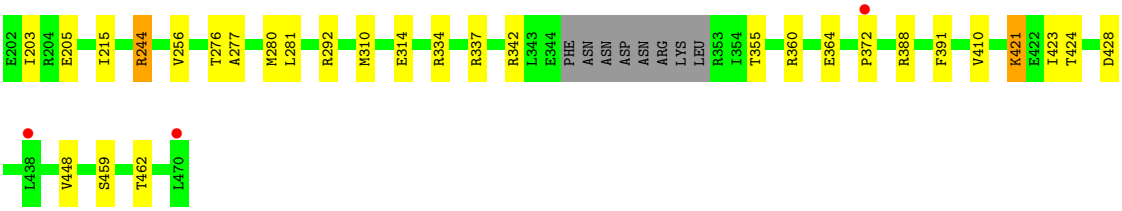
Chain F:



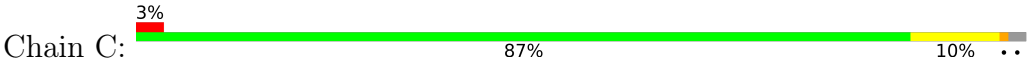
• Molecule 1: Pyruvate kinase

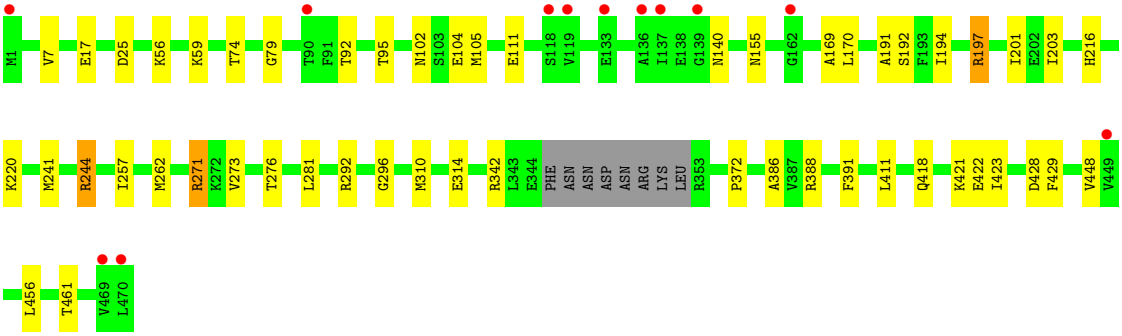
Chain H:





• Molecule 1: Pyruvate kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	129.33Å 74.47Å 240.83Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	48.17 – 2.10 48.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.17-2.10) 99.8 (48.17-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.224 0.199 , 0.222	Depositor DCC
R_{free} test set	13639 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.080 for h,-k,-l	Depositor
Outliers	9 of 267878 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	57299	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.99 % 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 2.1787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.31	0/3495	0.58	1/4713 (0.0%)
1	B	0.33	0/3508	0.58	0/4728
1	C	0.30	0/3492	0.55	0/4710
1	D	0.34	0/3502	0.60	0/4721
1	E	0.35	0/3508	0.59	0/4728
1	F	0.37	1/3487 (0.0%)	0.61	1/4703 (0.0%)
1	G	0.33	0/3508	0.58	0/4728
1	H	0.31	0/3502	0.59	0/4721
All	All	0.33	1/28002 (0.0%)	0.59	2/37752 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	ILE	CG1-CD1	-5.79	1.10	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	92	THR	OG1-CB-CG2	6.54	125.05	110.00
1	A	307	ASP	CB-CG-OD1	-6.24	112.69	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	271	ARG	Sidechain

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	3461	3542	3542	38	0
1	B	3474	3573	3573	34	0
1	C	3458	3540	3540	34	1
1	D	3468	3562	3562	41	0
1	E	3474	3573	3573	47	1
1	F	3453	3538	3538	55	0
1	G	3474	3573	3573	42	0
1	H	3468	3562	3562	41	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	104	0	0	1	0
3	B	169	0	0	2	0
3	C	120	0	0	0	0
3	D	146	0	0	1	0
3	E	153	0	0	1	0
3	F	103	0	0	3	0
3	G	157	0	0	3	0
3	H	114	0	0	1	0
All	All	28836	28463	28463	311	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 311 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:F:175:LYS:NZ	3:F:601:HOH:O	2.03	0.83
1:D:15:GLU:OE1	1:D:46:ARG:NH1	2.12	0.82
1:D:57:THR:HG21	1:D:59:LYS:HE3	1.65	0.78
1:F:72:ILE:HD12	1:F:110:TYR:HB2	1.64	0.77
1:E:14:THR:HA	1:E:19:MET:HG2	1.66	0.77

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:GLU:OE2	1:C:79:GLY:H[2_554]	1.56	0.04

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	458/470 (97%)	449 (98%)	9 (2%)	0	100	100
1	B	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	C	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	D	458/470 (97%)	449 (98%)	9 (2%)	0	100	100
1	E	458/470 (97%)	451 (98%)	7 (2%)	0	100	100
1	F	457/470 (97%)	444 (97%)	11 (2%)	2 (0%)	34	32
1	G	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
1	H	458/470 (97%)	450 (98%)	8 (2%)	0	100	100
All	All	3663/3760 (97%)	3593 (98%)	68 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	459	SER

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Mol	Chain	Res	Type
1	F	422	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	379/390 (97%)	373 (98%)	6 (2%)	62	69
1	B	382/390 (98%)	378 (99%)	4 (1%)	76	82
1	C	379/390 (97%)	370 (98%)	9 (2%)	49	53
1	D	381/390 (98%)	377 (99%)	4 (1%)	76	82
1	E	382/390 (98%)	377 (99%)	5 (1%)	69	75
1	F	379/390 (97%)	374 (99%)	5 (1%)	69	75
1	G	382/390 (98%)	380 (100%)	2 (0%)	88	92
1	H	381/390 (98%)	377 (99%)	4 (1%)	76	82
All	All	3045/3120 (98%)	3006 (99%)	39 (1%)	69	75

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	421	LYS
1	C	388	ARG
1	H	459	SER
1	C	244	ARG
1	C	421	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	F	501	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	E	501	-	4,4,4	0.17	0	6,6,6	0.26	0
2	SO4	C	501	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	G	501	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	H	501	-	4,4,4	0.12	0	6,6,6	0.12	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	SO4	1	0
2	A	501	SO4	1	0
2	D	501	SO4	1	0

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, 95^{th} 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	462/470 (98%)	0.36	27 (5%) 23 28	14, 28, 56, 70	0
1	B	462/470 (98%)	0.00	0 100 100	13, 23, 36, 50	0
1	C	462/470 (98%)	0.24	12 (2%) 56 61	14, 29, 43, 55	0
1	D	462/470 (98%)	0.05	4 (0%) 84 86	13, 25, 39, 55	0
1	E	462/470 (98%)	0.06	4 (0%) 84 86	12, 23, 36, 53	0
1	F	461/470 (98%)	0.44	37 (8%) 12 16	14, 28, 62, 72	0
1	G	462/470 (98%)	0.06	5 (1%) 80 84	13, 24, 39, 50	0
1	H	462/470 (98%)	0.25	9 (1%) 66 71	12, 28, 42, 65	0
All	All	3695/3760 (98%)	0.18	98 (2%) 54 60	12, 26, 46, 72	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	134	VAL	8.6
1	A	136	ALA	6.4
1	A	112	GLY	5.5
1	F	139	GLY	5.2
1	F	77	LEU	5.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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, 95^{th} 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	SO4	D	501	5/5	0.97	0.13	27,29,30,31	0
2	SO4	F	501	5/5	0.97	0.11	20,22,24,25	0
2	SO4	A	501	5/5	0.98	0.08	23,24,31,31	0
2	SO4	E	501	5/5	0.98	0.08	21,23,26,27	0
2	SO4	H	501	5/5	0.98	0.08	24,27,33,33	0
2	SO4	G	501	5/5	0.99	0.07	22,23,24,28	0
2	SO4	B	501	5/5	0.99	0.09	24,26,27,30	0
2	SO4	C	501	5/5	0.99	0.08	22,25,27,31	0

6.5 Other polymers (i)

There are no such residues in this entry.