wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:19 PM GMT

PDB ID	:	1JR3
Title	:	Crystal Structure of the Processivity Clamp Loader Gamma Complex of E. coli DNA Polymerase III
Authors	:	Jeruzalmi, D.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2001-08-10
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

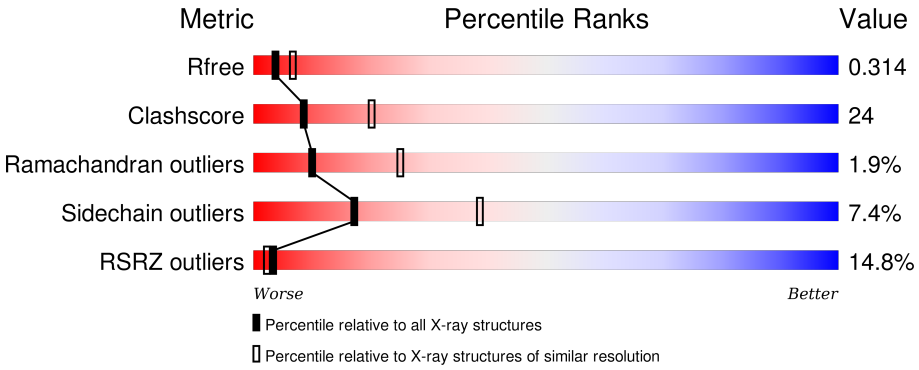
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	373	18% 58% 38%
1	B	373	18% 59% 35%
1	C	373	11% 61% 31% 5%
2	D	343	9% 56% 36% 5%
3	E	334	16% 62% 34%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1500	-	-	X	-
5	SO4	B	2500	-	-	X	-
5	SO4	C	5500	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13845 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 DNA polymerase III subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			
1	B	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
1	C	366	Total	C	N	O	S	0	0	0
			2850	1793	514	527	16			

- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	338	Total	C	N	O	S	0	0	0
			2687	1702	488	487	10			

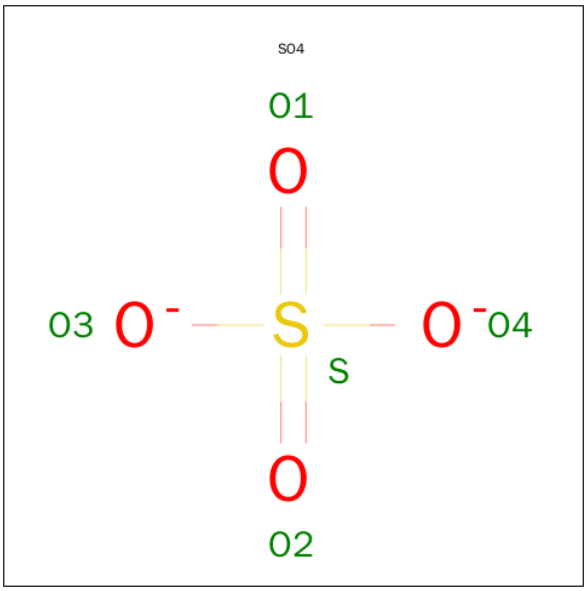
- Molecule 3 is a protein called DNA polymerase III, delta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



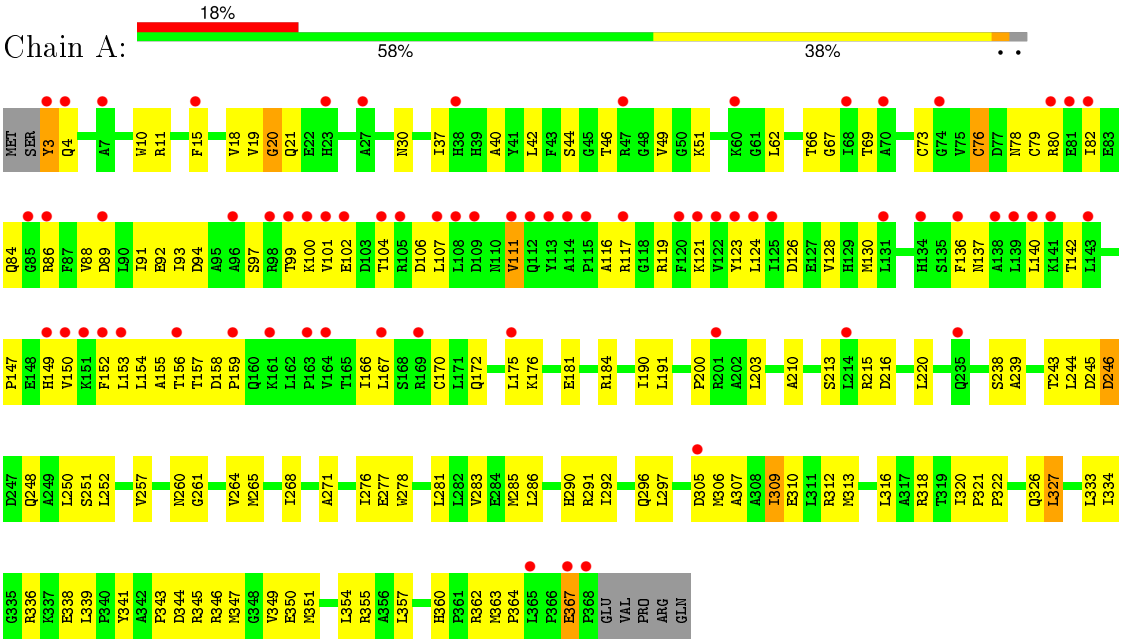
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

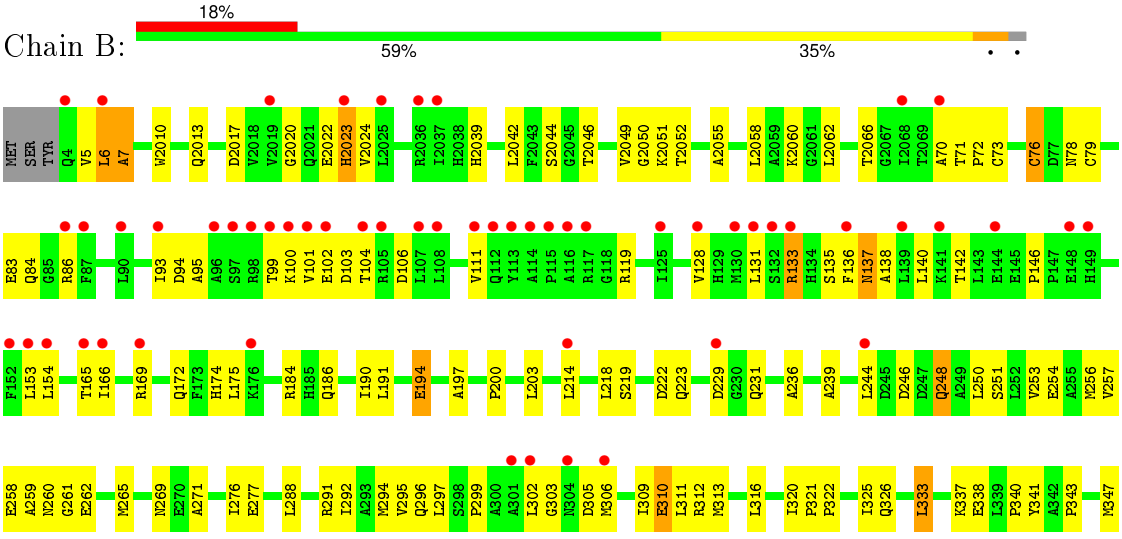
- Molecule 1: DNA polymerase III subunit gamma

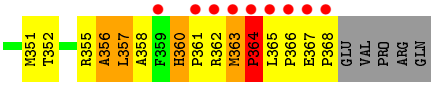
Chain A:



- Molecule 1: DNA polymerase III subunit gamma

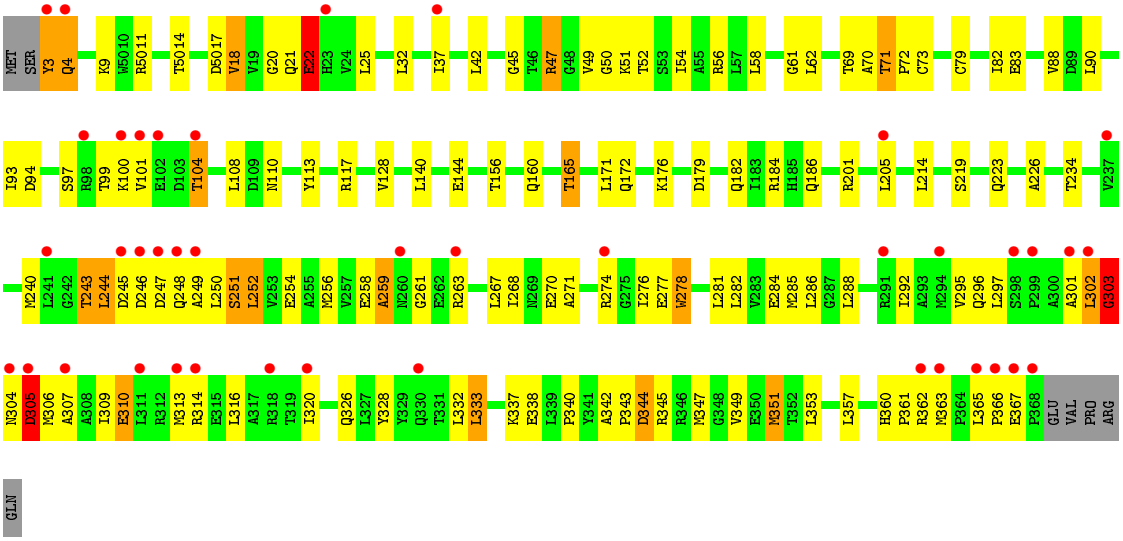
Chain B:





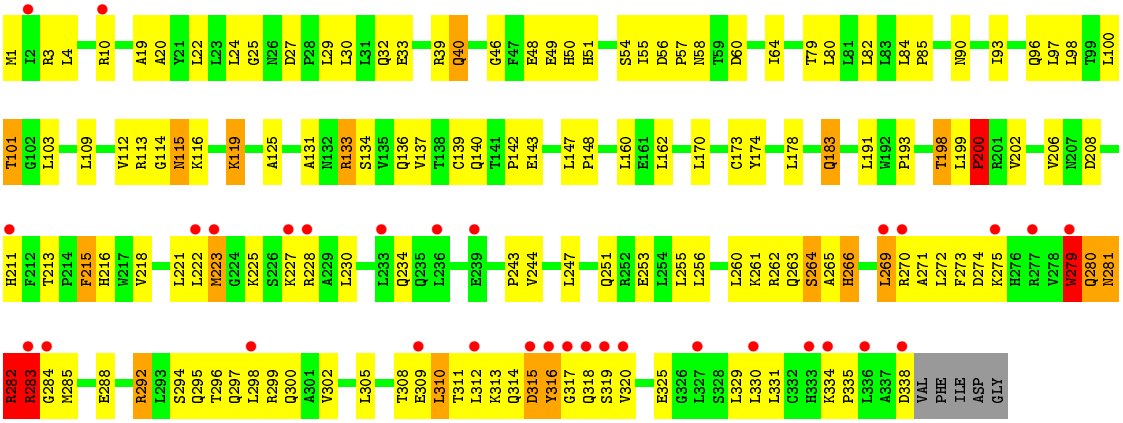
• Molecule 1: DNA polymerase III subunit gamma

Chain C:



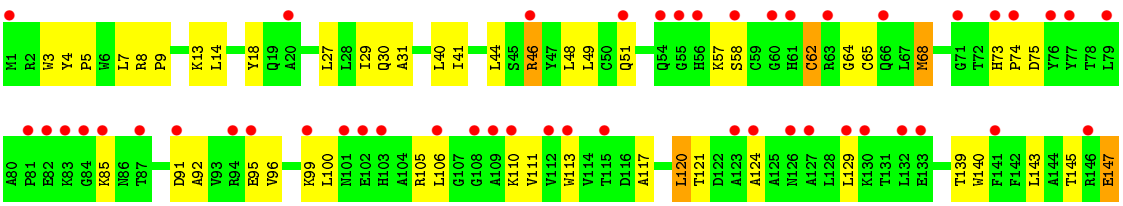
• Molecule 2: DNA polymerase III, delta subunit

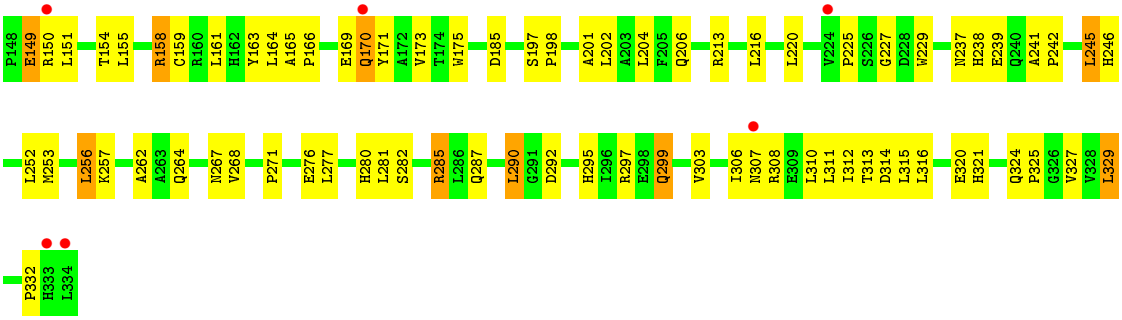
Chain D:



• Molecule 3: DNA polymerase III, delta' subunit

Chain E:




P148 E149 R150 L151 T154 L155 R158 C159 R160 L161 H162 Y163 L164 A165 P166 E169 Q170 Y171 A172 V173 T174 W175 D185 S197 P198 A201 L202 A203 L204 F205 Q206 R213 L216 L220 W224 P225 S226 G227 D228 W229 N237 H238 E239 Q240 A241 P242 L245 H246
L252 M253 L256 K257 A262 A263 Q264 N267 V268 P271 E276 L277 H280 L281 S282 R285 L286 Q287 L290 G291 D292 H295 I296 R297 E298 Q299 V303 I306 N307 R308 E309 L310 L311 I312 T313 D314 L315 L316 E320 H321 Q324 P325 G326 V327 V328 L329
P332 H333 L334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.70Å 95.86Å 285.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.70 90.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.70) 76.9 (90.87-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	13.60	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.304 0.286 , 0.314	Depositor DCC
R_{free} test set	2839 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 71.5	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 60122 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13845	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.48	0/2898	0.74	2/3930 (0.1%)
1	B	0.66	7/2885 (0.2%)	0.95	14/3912 (0.4%)
1	C	0.57	0/2898	0.88	10/3930 (0.3%)
2	D	0.85	8/2735 (0.3%)	0.93	10/3716 (0.3%)
3	E	0.49	0/2666	0.70	0/3639
All	All	0.62	15/14082 (0.1%)	0.85	36/19127 (0.2%)

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	B	0	1
2	D	0	4
All	All	0	5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	315	ASP	CB-CG	29.10	2.12	1.51
1	B	133	ARG	CZ-NH2	-10.95	1.18	1.33
2	D	310	LEU	CG-CD2	-9.05	1.18	1.51
1	B	363	MET	CG-SD	8.99	2.04	1.81
1	B	363	MET	SD-CE	8.90	2.27	1.77

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	MET	CG-SD-CE	17.06	127.49	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	283	ARG	C-N-CA	12.38	148.31	122.30
1	C	244	LEU	CB-CG-CD2	-11.83	90.88	111.00
2	D	280	GLN	C-N-CA	11.46	150.36	121.70
1	B	133	ARG	NE-CZ-NH1	10.92	125.76	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2023	HIS	Sidechain
2	D	280	GLN	Peptide
2	D	281	ASN	Mainchain
2	D	282	ARG	Mainchain
2	D	319	SER	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	2850	0	2896	158	0
1	B	2838	0	2887	195	0
1	C	2850	0	2895	133	1
2	D	2687	0	2741	146	1
3	E	2601	0	2603	100	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	5	0	0	7	0
5	B	5	0	0	2	0
5	C	5	0	0	3	0
All	All	13845	0	14022	664	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 24.

The worst 5 of 664 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:B:363:MET:SD	1:B:363:MET:CG	2.04	1.45
1:C:304:ASN:ND2	2:D:234:GLN:OE1	1.61	1.30
1:B:363:MET:SD	1:B:363:MET:CE	2.27	1.21
1:C:94:ASP:H	1:C:100:LYS:NZ	1.40	1.17
2:D:315:ASP:CB	2:D:315:ASP:CG	2.12	1.16

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:C:117:ARG:NH2	2:D:281:ASN:ND2[4_486]	1.70	0.50

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	364/373 (98%)	335 (92%)	23 (6%)	6 (2%)	12 30
1	B	363/373 (97%)	325 (90%)	28 (8%)	10 (3%)	6 15
1	C	364/373 (98%)	334 (92%)	22 (6%)	8 (2%)	8 22
2	D	336/343 (98%)	307 (91%)	22 (6%)	7 (2%)	9 23
3	E	332/334 (99%)	301 (91%)	29 (9%)	2 (1%)	30 59
All	All	1759/1796 (98%)	1602 (91%)	124 (7%)	33 (2%)	10 25

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	GLY
1	A	104	THR
1	A	111	VAL
1	A	364	PRO
1	B	2022	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	303/310 (98%)	288 (95%)	15 (5%)	30 60
1	B	302/310 (97%)	289 (96%)	13 (4%)	35 66
1	C	303/310 (98%)	280 (92%)	23 (8%)	16 37
2	D	287/291 (99%)	261 (91%)	26 (9%)	12 26
3	E	270/270 (100%)	239 (88%)	31 (12%)	7 16
All	All	1465/1491 (98%)	1357 (93%)	108 (7%)	17 39

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	344	ASP
2	D	143	GLU
3	E	256	LEU
1	C	357	LEU
2	D	101	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	105	HIS
2	D	204	GLN
3	E	280	HIS
2	D	136	GLN
2	D	211	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	SO4	A	1500	-	4,4,4	3.35	2 (50%)	6,6,6	0.97	1 (16%)
5	SO4	B	2500	-	4,4,4	3.29	2 (50%)	6,6,6	0.98	0
5	SO4	C	5500	-	4,4,4	3.32	2 (50%)	6,6,6	0.96	0

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	SO4	A	1500	-	-	0/0/0/0	0/0/0/0
5	SO4	B	2500	-	-	0/0/0/0	0/0/0/0
5	SO4	C	5500	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1500	SO4	O3-S	-5.14	1.28	1.47
5	C	5500	SO4	O3-S	-4.99	1.29	1.47
5	B	2500	SO4	O3-S	-4.73	1.30	1.47
5	A	1500	SO4	O1-S	4.11	1.61	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5500	SO4	O1-S	4.31	1.61	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1500	SO4	O4-S-O3	2.05	117.32	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	SO4	7	0
5	B	2500	SO4	2	0
5	C	5500	SO4	3	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	366/373 (98%)	1.10	69 (18%) 2 1	32, 76, 152, 173	0
1	B	365/373 (97%)	1.31	66 (18%) 2 1	27, 75, 159, 190	0
1	C	366/373 (98%)	0.89	41 (11%) 7 5	27, 62, 129, 156	0
2	D	338/343 (98%)	0.82	32 (9%) 10 8	38, 69, 121, 142	0
3	E	334/334 (100%)	1.14	54 (16%) 3 2	30, 67, 156, 161	0
All	All	1769/1796 (98%)	1.05	262 (14%) 3 2	27, 69, 151, 190	0

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	PRO	18.8
1	B	365	LEU	15.7
1	B	368	PRO	15.4
1	B	366	PRO	13.4
1	B	359	PHE	11.5

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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	C	400	1/1	0.99	0.19	0.86	44,44,44,44	0
4	ZN	A	400	1/1	0.97	0.18	-0.39	130,130,130,130	0
4	ZN	B	400	1/1	0.98	0.15	-0.39	105,105,105,105	0
5	SO4	B	2500	5/5	0.95	0.17	-0.84	68,70,70,70	0
5	SO4	A	1500	5/5	0.97	0.14	-0.90	64,65,66,67	0
4	ZN	E	400	1/1	0.57	0.06	-1.96	156,156,156,156	0
5	SO4	C	5500	5/5	0.98	0.15	-2.66	36,36,39,41	0

6.5 Other polymers (i)

There are no such residues in this entry.