wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:50 AM GMT

PDB ID	:	2IX3
Title	:	STRUCTURE OF YEAST ELONGATION FACTOR 3
Authors	:	Andersen, C.B.F.; Becker, T.; Blau, M.; Anand, M.; Halic, M.; Balar, B.; Mielke, T.; Boesen, T.; Pedersen, J.S.; Spahn, C.M.T.; Kinzy, T.G.; Andersen, G.R.; Beckmann, R.
Deposited on	:	2006-07-06
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:

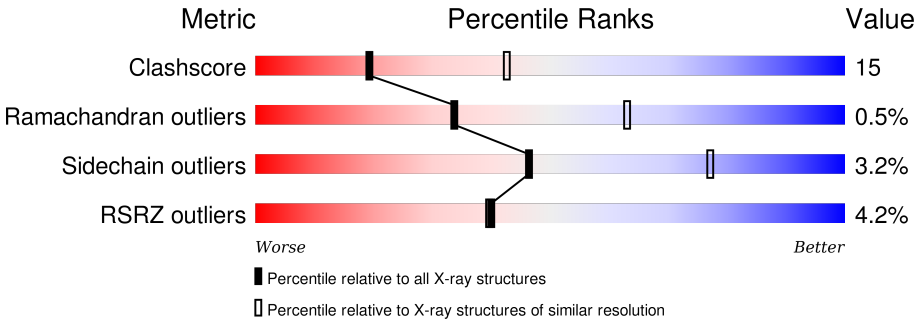
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
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	986	3% 73% 24%
1	B	986	5% 66% 32%

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
2	SO4	A	2976	-	-	-	X
2	SO4	A	2978	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	2974	-	X	X	X
2	SO4	B	2975	-	X	-	X

2 Entry composition (i)

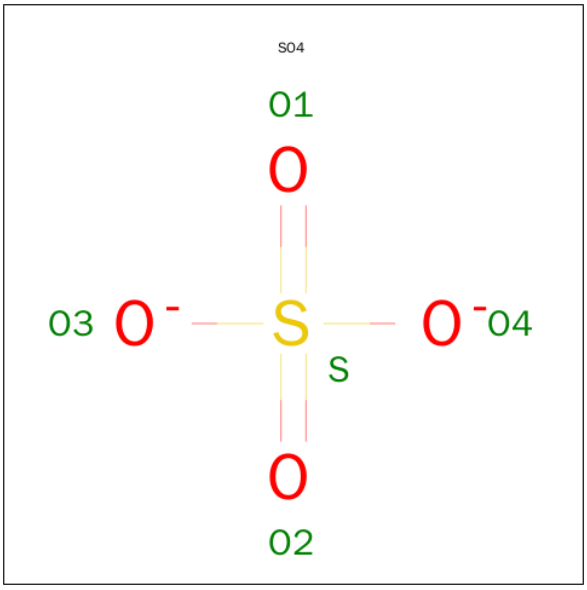
There are 2 unique types of molecules in this entry. The entry contains 15213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ELONGATION FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	0	0	1
			7579	4790	1297	1455	37			
1	B	973	Total	C	N	O	S	0	0	1
			7579	4790	1297	1455	37			

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



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

Continued on next page...

Continued from previous page...

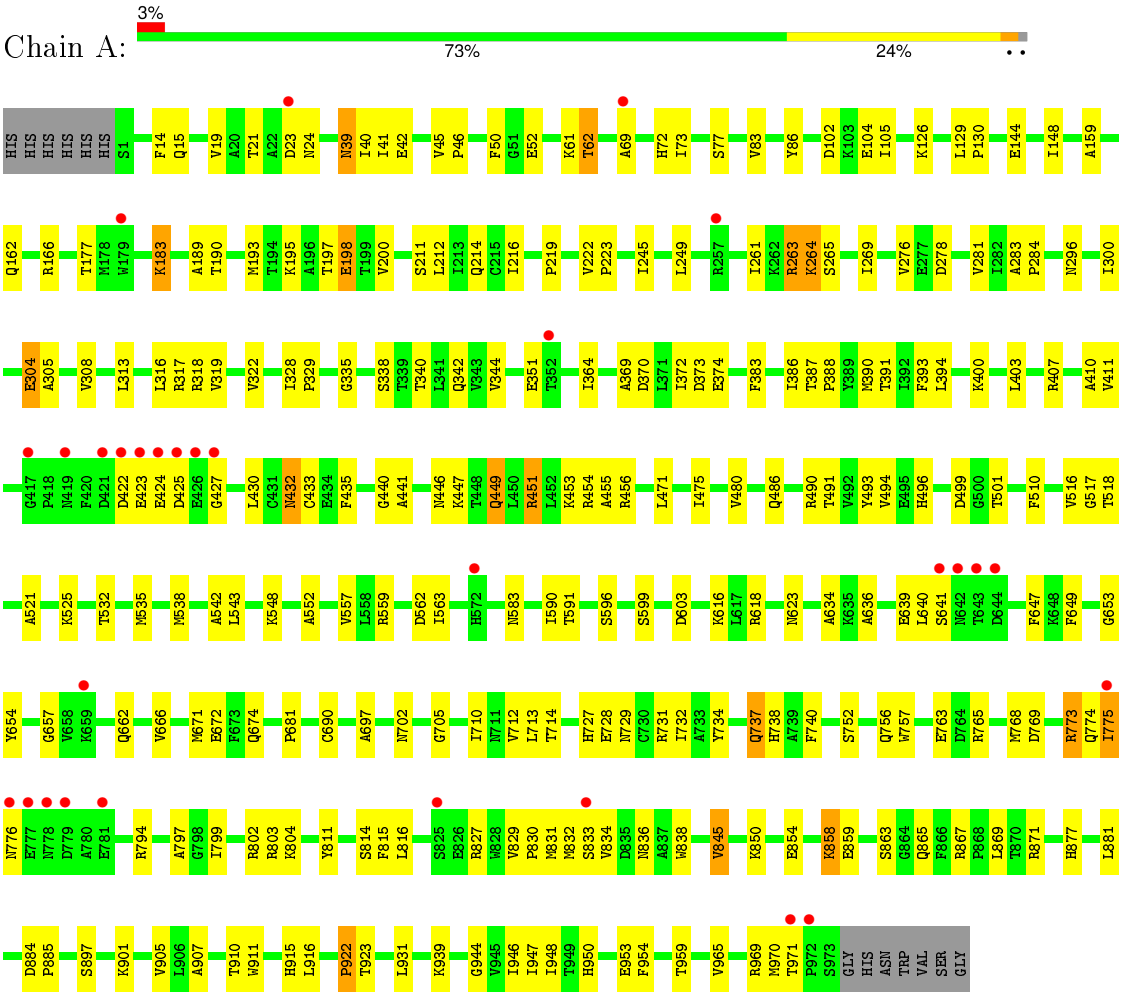
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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.

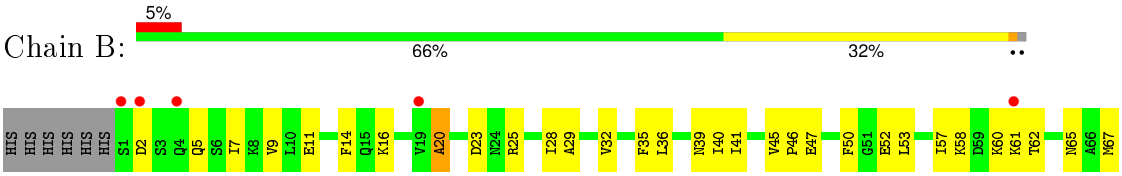
- Molecule 1: ELONGATION FACTOR 3

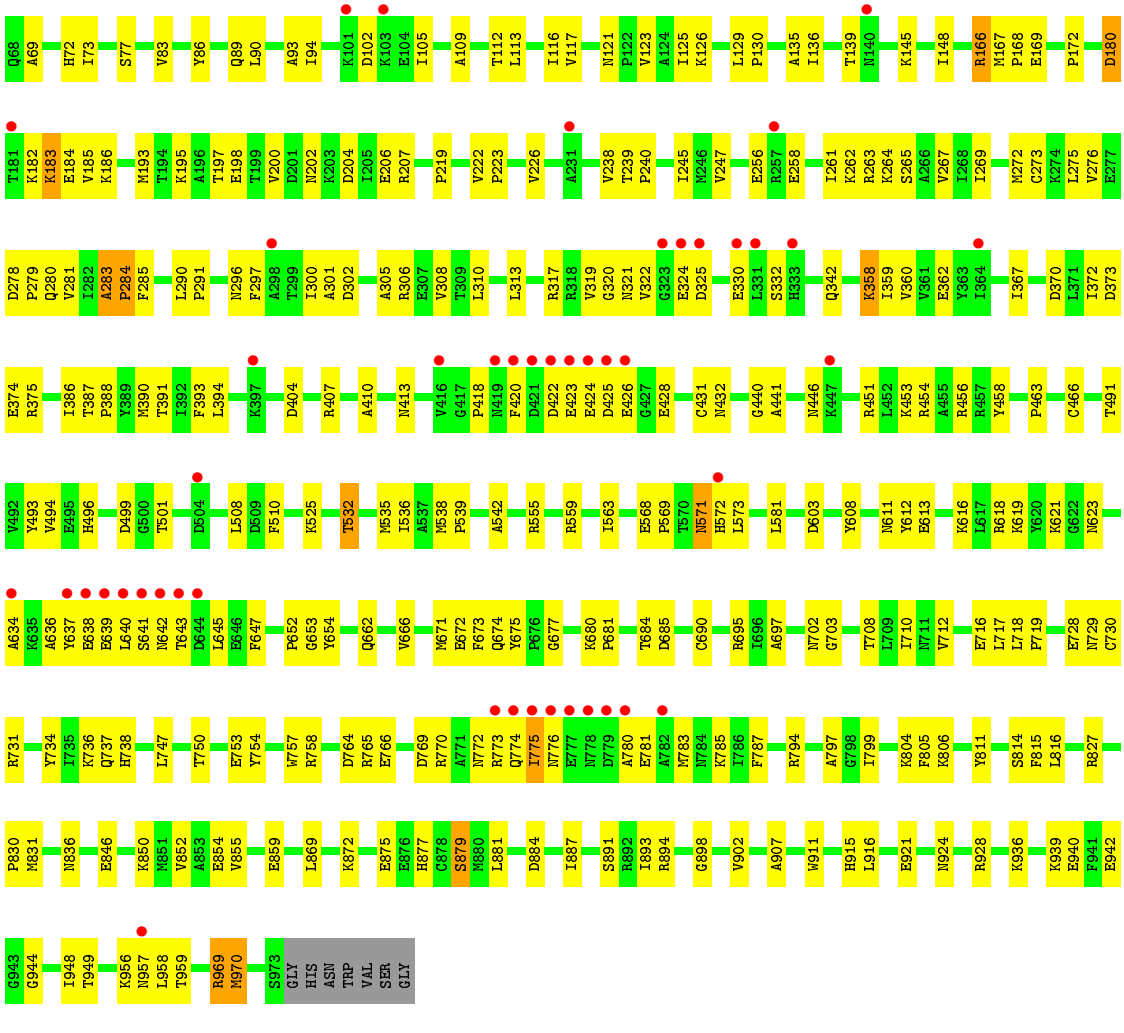
Chain A:



- Molecule 1: ELONGATION FACTOR 3

Chain B:




Q68 A69 H72 I73 S77 V83 Y86 Q89 L90 A93 I94 K101 D102 K103 E104 I105 A109 T112 L113 I116 V117 N121 P122 V123 A124 I125 K126 L129 P130 A135 I136 T139 N140 K145 I148 R166 M167 P168 E169 P172 D180
T181 K182 K183 E184 V185 K186 M193 T194 K195 A196 T197 E198 T199 V200 D201 N202 K203 D204 I205 E206 R207 P219 V222 P223 V226 A231 V238 T239 P240 I245 M246 V247 E256 R257 E258 I261 K262 R263 K264 S265 A266 V267 I268 I269 M272 C273 K274 L275 V276 E277
D278 P279 Q280 V281 I282 A283 P284 F285 L290 P291 N296 F297 A298 T299 I300 A301 D302 A305 R306 E307 V308 T309 L310 L313 R317 R318 V319 G320 N321 V322 G323 E324 D325 E330 L331 S332 H333 Q342 K358 I359 V360 V361 E362 Y363 I364 I367 D370 L371 I372 D373
E374 R375 I386 T387 P388 Y389 M390 T391 I392 F393 L394 K397 D404 R407 A410 N413 V416 G417 P418 N419 F420 D421 D422 E423 E424 D425 E426 G427 E428 C431 N432 G440 A441 N446 K447 R451 L452 K453 R454 A455 R456 R457 Y458 P463 C466 T491
V492 Y493 V494 E495 H496 D499 G500 T501 D504 L508 D509 F510 K525 T532 M535 I536 A537 M538 P539 A542 R555 R559 I563 E568 P569 T570 N571 H572 L573 L581 D603 Y608 N611 Y612 E613 K616 L617 R618 K619 Y620 K621 G622 N623
A634 K635 A636 Y637 E638 E639 L640 S641 N642 T643 D644 L645 E646 F647 P652 G653 Y654 Q662 V666 M671 E672 F673 Q674 Y675 P676 G677 K680 P681 T684 D685 C690 R695 I696 A697 N702 G703 T708 L709 I710 N711 V712 E716 L717 L718 P719 E728 N729 C730
R731 Y734 I735 K736 Q737 H738 L747 T750 E753 Y754 W757 R758 D764 R765 E766 D769 R770 A771 N772 R773 Q774 I775 N776 E777 N778 D779 A780 E781 A782 M783 N784 K785 I786 F787 R794 A797 G798 I799 K804 F805 K806 Y811 S814 F815 L816 R827
P830 M831 N836 E846 K850 M851 V852 A853 E854 V855 E859 L869 K872 E875 E876 H877 C878 S879 M880 L881 D884 I887 S891 R892 I893 R894 G898 V902 A907 W911 H915 L916 E921 N924 R928 K936 K939 E940 F941 E942
G943 G944 I948 T949 K956 N957 L958 T959 R969 M970 S973 GLY HIS ASN TRP VAL SER GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.61Å 110.66Å 212.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.63 – 2.70 20.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.63-2.70) 100.0 (20.16-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.269 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 63818 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15213	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: 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	0.41	0/7717	0.62	0/10456
1	B	0.39	0/7717	0.60	0/10456
All	All	0.40	0/15434	0.61	0/20912

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	7579	0	7627	215	0
1	B	7579	0	7627	249	0
2	A	30	0	0	3	0
2	B	25	0	0	3	0
All	All	15213	0	15254	460	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 15.

The worst 5 of 460 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:769:ASP:HB2	1:B:774:GLN:NE2	1.55	1.22
1:B:774:GLN:O	1:B:776:ASN:N	1.98	0.96
1:A:731:ARG:H	1:A:915:HIS:HD2	1.13	0.96
1:B:262:LYS:HE3	1:B:296:ASN:ND2	1.83	0.92
1:B:372:ILE:HD11	1:B:410:ALA:HB1	1.51	0.91

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	971/986 (98%)	926 (95%)	41 (4%)	4 (0%)	39	69
1	B	971/986 (98%)	907 (93%)	59 (6%)	5 (0%)	34	63
All	All	1942/1972 (98%)	1833 (94%)	100 (5%)	9 (0%)	34	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	640	LEU
1	A	833	SER
1	B	640	LEU
1	B	775	ILE
1	A	775	ILE

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	831/843 (99%)	802 (96%)	29 (4%)	43 74
1	B	831/843 (99%)	807 (97%)	24 (3%)	50 80
All	All	1662/1686 (99%)	1609 (97%)	53 (3%)	46 77

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	804	LYS
1	B	23	ASP
1	B	872	LYS
1	A	827	ARG
1	A	867	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	915	HIS
1	B	97	ASN
1	B	784	ASN
1	B	24	ASN
1	B	76	GLN

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)

11 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	A	2973	-	4,4,4	3.22	2 (50%)	6,6,6	0.51	0
2	SO4	A	2974	-	4,4,4	3.24	2 (50%)	6,6,6	0.49	0
2	SO4	A	2975	-	4,4,4	3.15	2 (50%)	6,6,6	0.50	0
2	SO4	A	2976	-	4,4,4	3.21	2 (50%)	6,6,6	0.49	0
2	SO4	A	2977	-	4,4,4	3.18	2 (50%)	6,6,6	0.51	0
2	SO4	A	2978	-	4,4,4	3.10	2 (50%)	6,6,6	0.50	0
2	SO4	B	2973	-	4,4,4	3.33	2 (50%)	6,6,6	0.51	0
2	SO4	B	2974	-	4,4,4	3.16	2 (50%)	6,6,6	3.20	3 (50%)
2	SO4	B	2975	-	4,4,4	3.24	2 (50%)	6,6,6	3.20	4 (66%)
2	SO4	B	2976	-	4,4,4	3.21	2 (50%)	6,6,6	0.51	0
2	SO4	B	2977	-	4,4,4	3.20	2 (50%)	6,6,6	0.51	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
2	SO4	A	2973	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2974	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2975	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2976	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2977	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2978	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2973	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2974	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2975	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2976	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2977	-	-	0/0/0/0	0/0/0/0

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2973	SO4	O2-S	-4.78	1.30	1.47
2	B	2973	SO4	O2-S	-4.73	1.31	1.47
2	B	2975	SO4	O2-S	-4.71	1.31	1.47
2	A	2977	SO4	O2-S	-4.71	1.31	1.47
2	B	2977	SO4	O2-S	-4.55	1.31	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2974	SO4	O4-S-O3	-5.93	84.85	108.98
2	B	2975	SO4	O4-S-O3	-5.90	85.00	108.98
2	B	2974	SO4	O3-S-O1	-3.44	78.21	110.19
2	B	2975	SO4	O3-S-O1	-3.36	78.90	110.19
2	B	2975	SO4	O3-S-O2	-2.03	91.28	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2976	SO4	1	0
2	A	2978	SO4	2	0
2	B	2974	SO4	2	0
2	B	2977	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	973/986 (98%)	-0.06	30 (3%)	52	52	20, 41, 70, 120	0
1	B	973/986 (98%)	0.13	51 (5%)	31	30	24, 49, 79, 114	0
All	All	1946/1972 (98%)	0.04	81 (4%)	40	39	20, 44, 77, 120	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	LEU	11.4
1	A	778	ASN	9.4
1	B	642	ASN	7.4
1	B	641	SER	7.4
1	A	776	ASN	7.1

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
2	SO4	B	2974	5/5	0.89	0.39	5.80	80,82,82,83	0
2	SO4	B	2975	5/5	0.93	0.29	3.64	85,85,85,86	0
2	SO4	A	2976	5/5	0.95	0.23	2.01	75,75,76,76	0
2	SO4	A	2978	5/5	0.82	0.34	1.40	94,94,95,96	0
2	SO4	B	2977	5/5	0.96	0.29	1.04	91,92,93,93	0
2	SO4	A	2973	5/5	0.97	0.19	-0.11	48,50,50,53	0
2	SO4	B	2973	5/5	0.96	0.19	-0.55	74,75,76,76	0
2	SO4	A	2977	5/5	0.98	0.11	-0.61	53,53,54,55	0
2	SO4	B	2976	5/5	0.98	0.09	-1.31	50,50,52,53	0
2	SO4	A	2975	5/5	0.89	0.26	-	93,93,94,94	0
2	SO4	A	2974	5/5	0.91	0.36	-	96,96,96,98	0

6.5 Other polymers (i)

There are no such residues in this entry.