



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:52 PM UTC

PDB ID : 2XK1 / pdb_00002xk1
Title : Crystal structure of a complex between Actinomadura R39 DD-peptidase and a boronate inhibitor
Authors : Sauvage, E.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.
Deposited on : 2010-07-07
Resolution : 2.80 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

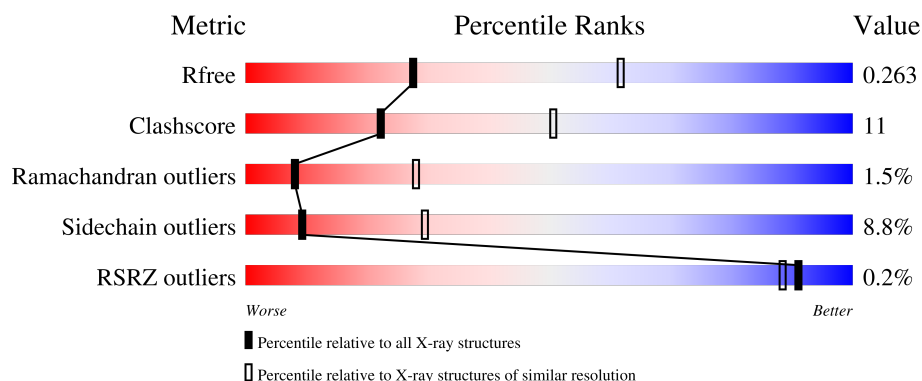
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	69% 29% .
1	B	466	75% 23% .
1	C	466	72% 25% .
1	D	466	78% 19% .

2 Entry composition [i](#)

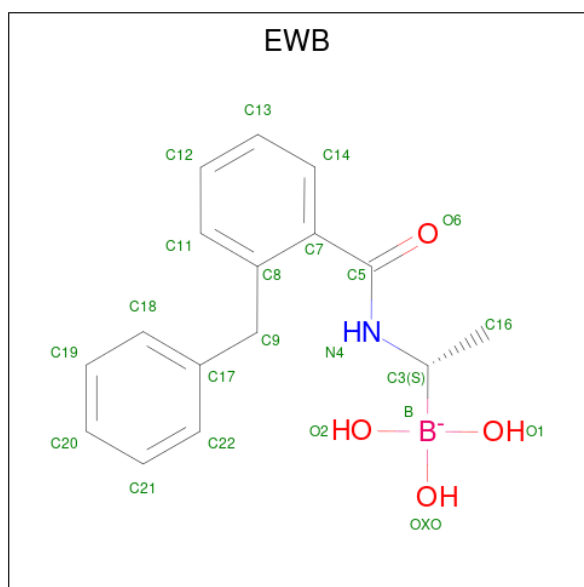
There are 5 unique types of molecules in this entry. The entry contains 13724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3352	2076	564	706	6			
1	B	465	Total	C	N	O	S	0	0	0
			3343	2071	563	703	6			
1	C	465	Total	C	N	O	S	0	0	0
			3343	2071	563	703	6			
1	D	466	Total	C	N	O	S	0	0	0
			3352	2076	564	706	6			

- Molecule 2 is [(1S)-1-{[(2-benzylphenyl)carbonyl]amino}ethyl](trihydroxy)borate(1-) (CCD ID: EWB) (formula: C₁₆H₁₉BNO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			21	1	16	1	3		
2	B	1	Total	B	C	N	O	0	0
			21	1	16	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	B	C	N	O	0	0
			21	1	16	1	3		
2	D	1	Total	B	C	N	O	0	0
			21	1	16	1	3		

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



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

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

- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Co 2 2	0	0
4	D	2	Total Co 2 2	0	0

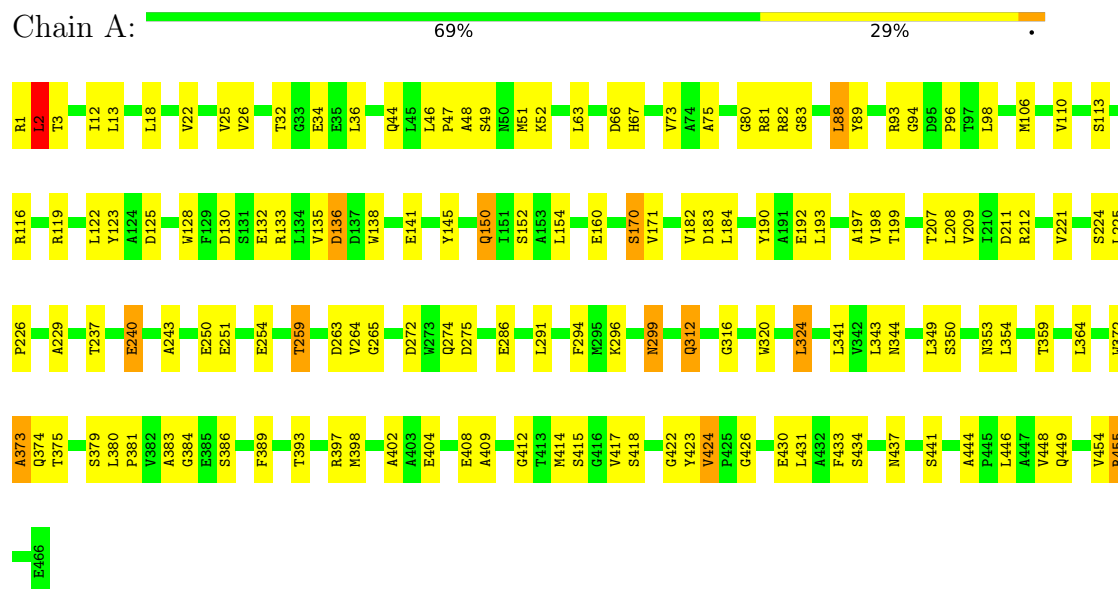
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	B	39	Total O 39 39	0	0
5	C	41	Total O 41 41	0	0
5	D	28	Total O 28 28	0	0

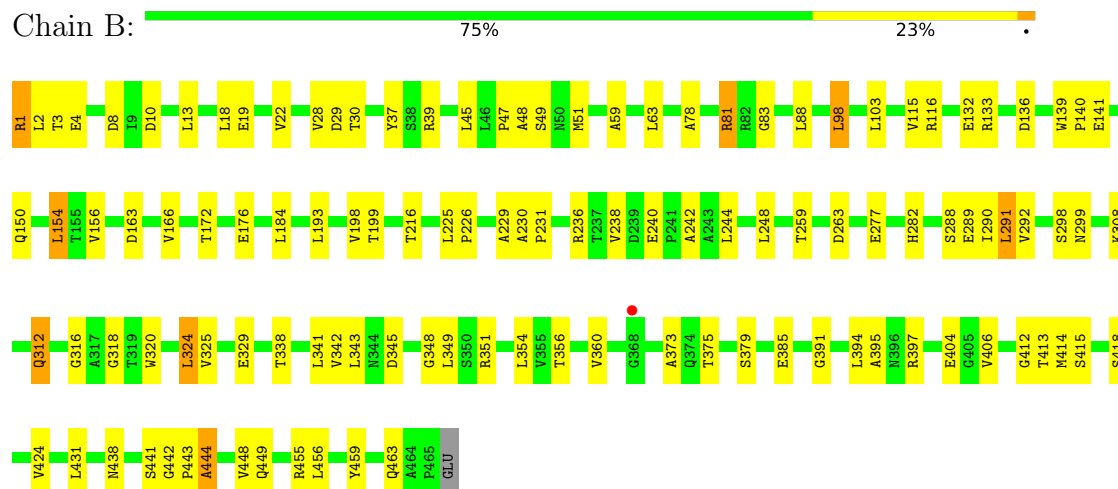
3 Residue-property plots

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: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

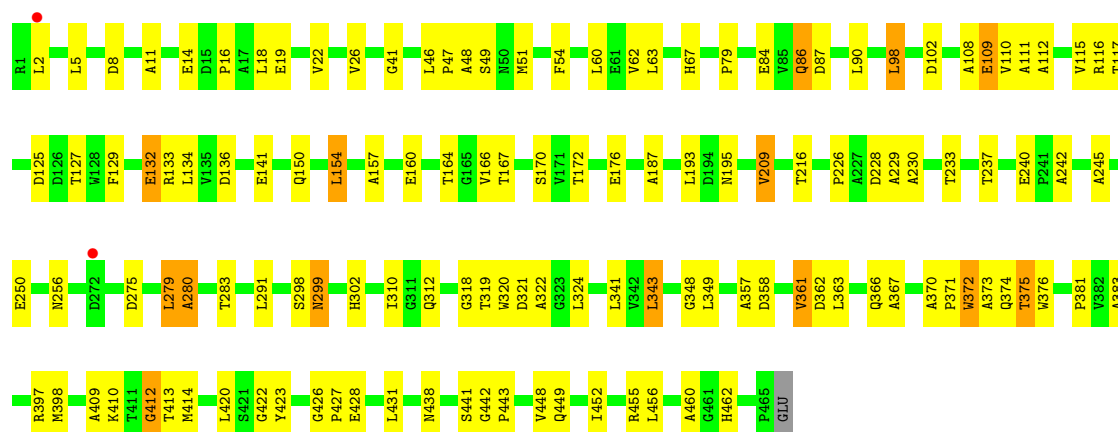


• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



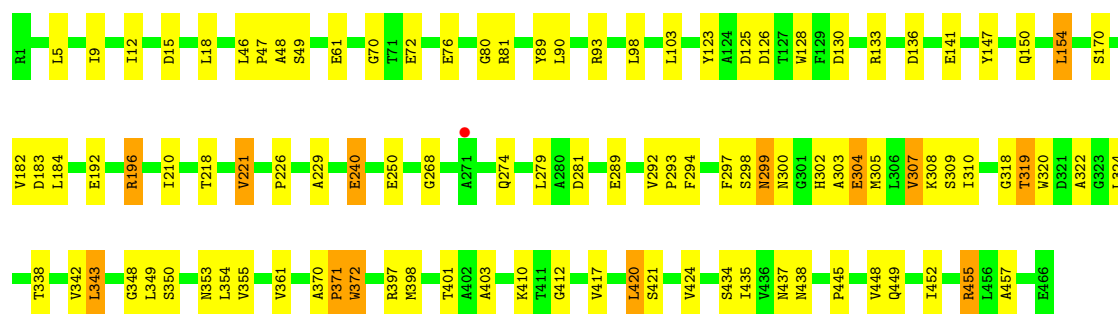
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:  72% 25% .



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain D:  78% 19% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.90Å 92.35Å 143.83Å 90.00° 92.25° 90.00°	Depositor
Resolution (Å)	27.53 – 2.80 27.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.53-2.80) 99.2 (27.53-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.264 0.216 , 0.263	Depositor DCC
R_{free} test set	2527 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.004 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13724	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.83% 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: CO, SO4, EWB

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	0.65	0/3411	0.97	4/4666 (0.1%)
1	B	0.50	0/3402	0.84	0/4654
1	C	0.51	0/3402	0.86	0/4654
1	D	0.46	0/3411	0.84	4/4666 (0.1%)
All	All	0.54	0/13626	0.88	8/18640 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	GLU	CA-C-N	6.43	126.65	119.32
1	A	240	GLU	C-N-CA	6.43	126.65	119.32
1	A	426	GLY	CA-C-N	5.79	127.07	119.84
1	A	426	GLY	C-N-CA	5.79	127.07	119.84
1	D	15	ASP	CA-C-N	5.66	126.03	119.47

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	3352	0	3200	92	0
1	B	3343	0	3194	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3343	0	3194	69	0
1	D	3352	0	3200	64	0
2	A	21	0	18	2	0
2	B	21	0	18	1	0
2	C	21	0	18	0	0
2	D	21	0	18	0	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	58	0	0	1	0
5	B	39	0	0	3	0
5	C	41	0	0	4	0
5	D	28	0	0	2	0
All	All	13724	0	12860	280	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 11.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:O	1:A:354:LEU:HD23	1.68	0.93
1:A:133:ARG:HB3	1:A:150:GLN:HG2	1.59	0.84
1:A:254:GLU:OE2	1:A:259:THR:HA	1.78	0.83
1:A:132:GLU:HG2	1:A:320:TRP:HZ3	1.47	0.79
1:A:226:PRO:HG2	1:A:229:ALA:HB2	1.69	0.74

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	464/466 (100%)	416 (90%)	43 (9%)	5 (1%)	11	36
1	B	463/466 (99%)	422 (91%)	34 (7%)	7 (2%)	8	28
1	C	463/466 (99%)	425 (92%)	28 (6%)	10 (2%)	5	19
1	D	464/466 (100%)	421 (91%)	37 (8%)	6 (1%)	9	31
All	All	1854/1864 (100%)	1684 (91%)	142 (8%)	28 (2%)	8	28

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	373	ALA
1	C	79	PRO
1	C	373	ALA
1	A	136	ASP

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	339/339 (100%)	304 (90%)	35 (10%)	7	23
1	B	338/339 (100%)	307 (91%)	31 (9%)	8	27
1	C	338/339 (100%)	306 (90%)	32 (10%)	8	26
1	D	339/339 (100%)	318 (94%)	21 (6%)	16	45
All	All	1354/1356 (100%)	1235 (91%)	119 (9%)	9	29

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	GLN
1	D	307	VAL
1	C	134	LEU

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Mol	Chain	Res	Type
1	D	304	GLU
1	D	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	ASN
1	C	437	ASN
1	D	437	ASN
1	C	366	GLN
1	C	449	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	603	-	4,4,4	0.31	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	602	-	4,4,4	0.30	0	6,6,6	0.21	0
3	SO4	A	601	-	4,4,4	0.28	0	6,6,6	0.25	0
3	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.08	0
2	EWB	B	500	1	19,22,23	0.62	0	24,29,32	0.71	0
2	EWB	D	500	1	19,22,23	0.59	0	24,29,32	0.87	0
3	SO4	A	603	-	4,4,4	0.32	0	6,6,6	0.58	0
3	SO4	C	603	-	4,4,4	0.24	0	6,6,6	0.29	0
3	SO4	A	602	-	4,4,4	0.28	0	6,6,6	0.08	0
3	SO4	B	602	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.38	0
3	SO4	D	604	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	D	601	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	C	601	-	4,4,4	0.27	0	6,6,6	0.35	0
3	SO4	C	604	-	4,4,4	0.24	0	6,6,6	0.21	0
2	EWB	C	500	1	19,22,23	0.51	0	24,29,32	0.64	0
3	SO4	D	602	-	4,4,4	0.28	0	6,6,6	0.13	0
2	EWB	A	500	1	19,22,23	0.52	0	24,29,32	0.88	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	EWB	D	500	1	-	0/11/16/18	0/2/2/2
2	EWB	B	500	1	-	0/11/16/18	0/2/2/2
2	EWB	A	500	1	-	0/11/16/18	0/2/2/2
2	EWB	C	500	1	-	0/11/16/18	0/2/2/2

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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	EWB	1	0
3	B	601	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	EWB	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/466 (100%)	-0.48	0 100 100	13, 45, 82, 107	0
1	B	465/466 (99%)	-0.28	1 (0%) 91 88	39, 66, 97, 118	0
1	C	465/466 (99%)	-0.16	2 (0%) 88 84	32, 71, 109, 144	0
1	D	466/466 (100%)	0.08	1 (0%) 91 88	69, 87, 118, 140	0
All	All	1862/1864 (99%)	-0.21	4 (0%) 91 88	13, 70, 108, 144	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	ASP	2.9
1	C	2	LEU	2.5
1	D	271	ALA	2.5
1	B	368	GLY	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	601	5/5	0.63	0.16	107,107,108,108	0
3	SO4	D	604	5/5	0.63	0.11	132,132,132,132	0
3	SO4	D	602	5/5	0.68	0.08	106,106,106,106	0
3	SO4	D	603	5/5	0.69	0.12	133,133,134,134	0
3	SO4	B	604	5/5	0.72	0.08	135,135,135,135	0
3	SO4	C	604	5/5	0.81	0.11	93,93,94,94	0
3	SO4	B	601	5/5	0.84	0.20	64,64,65,66	0
3	SO4	A	604	5/5	0.87	0.11	88,88,88,88	0
3	SO4	C	601	5/5	0.88	0.12	60,60,62,63	0
2	EWB	D	500	21/22	0.89	0.14	67,70,73,73	0
3	SO4	A	602	5/5	0.91	0.09	78,78,79,79	0
3	SO4	C	602	5/5	0.92	0.12	55,55,55,56	0
3	SO4	A	601	5/5	0.92	0.10	60,60,61,62	0
3	SO4	C	603	5/5	0.93	0.12	62,62,63,63	0
2	EWB	B	500	21/22	0.93	0.08	50,56,61,62	0
2	EWB	C	500	21/22	0.93	0.10	62,64,66,66	0
2	EWB	A	500	21/22	0.94	0.08	30,39,40,41	0
4	CO	D	611	1/1	0.94	0.07	110,110,110,110	0
4	CO	D	610	1/1	0.95	0.04	95,95,95,95	0
3	SO4	B	603	5/5	0.96	0.09	53,54,54,55	0
3	SO4	B	602	5/5	0.96	0.07	71,71,71,72	0
3	SO4	A	603	5/5	0.97	0.11	40,40,41,41	0
4	CO	A	611	1/1	0.97	0.08	48,48,48,48	0
4	CO	A	610	1/1	0.99	0.02	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.