



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 08:54 am GMT

PDB ID : 1PWQ
Title : Crystal structure of Anthrax Lethal Factor complexed with Thioacetyl-Tyr-Pro-Met-Amide, a metal-chelating peptidyl small molecule inhibitor
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.
Deposited on : 2003-07-02
Resolution : 3.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

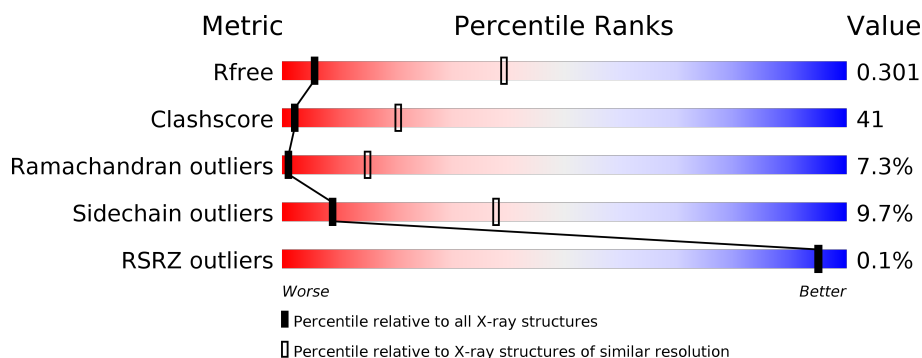
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	111664	1052 (3.62-3.42)
Clashscore	122126	1048 (3.60-3.44)
Ramachandran outliers	120053	1014 (3.60-3.44)
Sidechain outliers	120020	1015 (3.60-3.44)
RSRZ outliers	108989	1353 (3.64-3.40)

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 $\leq 5\%$. 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	776	<div> <div>31%</div> <div>54%</div> <div>9%</div> <div>6%</div> </div>
1	B	776	<div> <div>33%</div> <div>52%</div> <div>9%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12120 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.

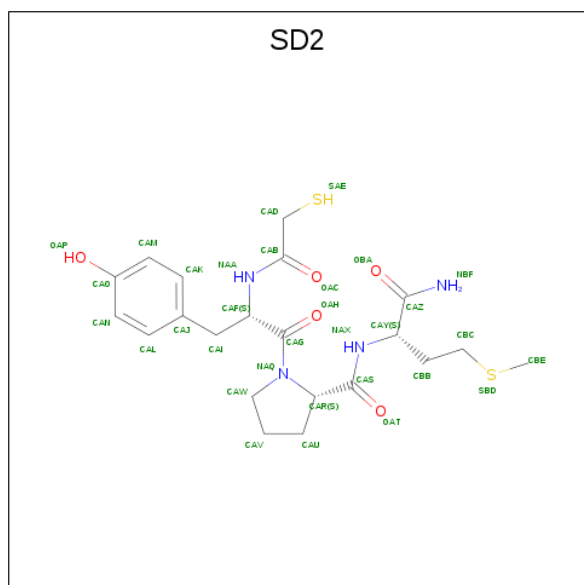
- Molecule 1 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			6020	3827	1015	1171	7			
1	B	734	Total	C	N	O	S	0	0	0
			6034	3834	1017	1176	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-(SULFANYLACETYL)TYROSYLPROLYLMETHIONINAMIDE (three-letter code: SD2) (formula: C₂₁H₃₀N₄O₅S₂).

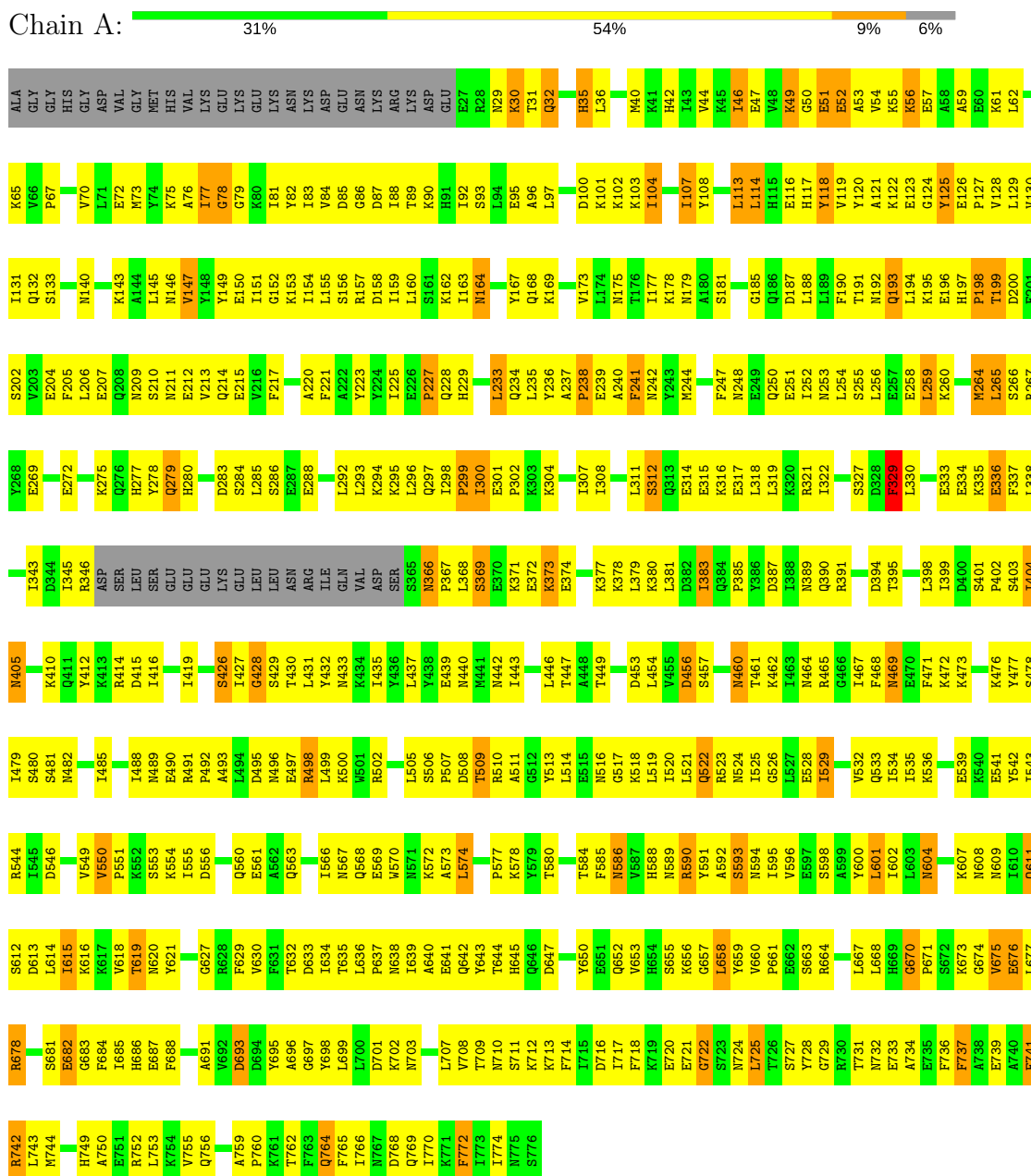


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	4	5	2		
3	B	1	Total	C	N	O	S	0	0
			32	21	4	5	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Lethal factor



● Molecule 1: Lethal factor

Chain B: 33% 52% 9% 5%

ALA	GLY	GLY	GLY	ASP	VAL	GLY	MET	HIS	VAL	LYS	GLU	LYS	GLU	LYS	ASN	LYS	ASP	GLU	E27	E27	R28	N29	N29	K30	Q32	E33	E34	R35	L36	I39	M40	R41	R42	I43	V44	K45	I46	E47	V48	K49	G50	E51	E52	A53	K56	E57	E58	A59	E60	R61	L62																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
L63	E64	R65	V66	P67	S68	D69	V70	L71	E72	M73	Y74	K75	A76	I77	G78	G79	R80	I81	Y82	A83	Y84	D85	G86	D87	I88	T89	R90	H91	I92	S93	L94	E95	A96	L97	K101	K102	K105	D106	I107	I108	E109	K110	D111	A112	L113	L114	H115	E116	H117	Y118	V119	Y120	A121	K122	E123	G124	Y125	E126																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
P127	V128	L129	V130	I131	Q132	S133	D136	N140	T141	E142	K143	A144	N146	L147	Y148	Y149	E150	I151	L155	S156	R157	D158	I159	K162	Q165	P166	Y167	Q168	K169	F170	L171	L174	N175	T176	I177	K178	N179	A180	Q186	D187	L188	L189	F190	T191	N192	Q193	L194	K195	E196	P198																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
T199	D200	F201	S202	V203	E204	F205	L206	N209	S210	N211	E212	V213	Q214	E215	V216	A220	F221	A222	Y223	Y224	I225	E226	P227	Q228	H229	V232	L233	Q234	L235	Y236	A237	P238	E239	A240	F241	N242	Y243	N244	D245	K246	F247	Q250	I252	L256	E257	E258	K259	L261	M264	L265	S266																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
R267	Y268	E269	K273	I274	G275	Q276	Q277	Q278	Y279	H280	Y281	S282	L292	L293	K294	K295	L296	Q297	I300	K303	K304	D305	I308	H309	S310	L311	L312	Q313	E314	E315	L319	I322	Q323	I324	D325	S326	L330	S331	E334	K335	L338	K339	L341	Q342	I343	I344	I345	R346																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
D347	S348	LEU	SER	GLU	GLU	GLU	LYS	LYS	LEU	ASN	ARG	ILE	GLN	VAL	ASP	SER	N366	N367	L368	S369	E370	K371	N430	E372	L376	K377	L378	L379	K380	L381	L382	L383	Q384	N385	Y386	L388	S401	P402	S403	I404	D407	V408	R409	K410	Q411	Y412	K413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 137.40Å 98.30Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.86 – 3.52 24.86 – 3.51	Depositor EDS
% Data completeness (in resolution range)	86.7 (24.86-3.52) 82.4 (24.86-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.311 0.226 , 0.301	Depositor DCC
R_{free} test set	1331 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -3.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12120	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SD2

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	0/6128	0.70	0/8253
1	B	0.50	0/6142	0.72	0/8272
All	All	0.49	0/12270	0.71	0/16525

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 [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	6020	0	6008	498	0
1	B	6034	0	6017	501	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	32	0	28	9	0
3	B	32	0	29	9	0
All	All	12120	0	12082	1000	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 41.

The worst 5 of 1000 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:91:HIS:CD2	1:B:93:SER:HB3	1.69	1.27
1:A:635:THR:HG22	1:A:637:PRO:HD2	1.21	1.16
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.16	1.12
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.32	1.10
1:B:91:HIS:HD2	1:B:93:SER:HB3	0.92	1.09

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	728/776 (94%)	529 (73%)	144 (20%)	55 (8%)	1	13
1	B	730/776 (94%)	536 (73%)	143 (20%)	51 (7%)	1	16
All	All	1458/1552 (94%)	1065 (73%)	287 (20%)	106 (7%)	1	15

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	92	ILE
1	A	227	PRO
1	A	238	PRO
1	A	405	ASN

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	671/710 (94%)	607 (90%)	64 (10%)	9	39
1	B	673/710 (95%)	607 (90%)	66 (10%)	9	37
All	All	1344/1420 (95%)	1214 (90%)	130 (10%)	9	38

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	716	ASP
1	B	111	ASP
1	B	586	ASN
1	A	727	SER
1	B	36	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	HIS
1	B	228	GLN
1	B	645	HIS
1	B	186	GLN
1	B	242	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	SD2	A	9002	2	33,33,33	0.96	1 (3%)	43,44,44	1.88	5 (11%)
3	SD2	B	9003	2	33,33,33	1.12	3 (9%)	43,44,44	2.25	8 (18%)

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
3	SD2	A	9002	2	-	0/32/44/44	0/2/2/2
3	SD2	B	9003	2	-	0/32/44/44	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	SD2	CBB-CBC	-3.53	1.37	1.51
3	B	9003	SD2	CBB-CBC	-3.33	1.38	1.51
3	B	9003	SD2	CBB-CAY	-2.02	1.48	1.53
3	B	9003	SD2	CAR-NAQ	2.21	1.51	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9002	SD2	CBB-CAY-NAX	-5.41	99.87	110.88
3	A	9002	SD2	CAR-CAS-NAX	-4.64	106.44	116.62
3	B	9003	SD2	OAT-CAS-NAX	-4.04	115.39	122.91
3	B	9003	SD2	CAS-CAR-NAQ	-2.71	105.42	112.61
3	B	9003	SD2	OAT-CAS-CAR	-2.04	115.94	120.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	SD2	9	0
3	B	9003	SD2	9	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	732/776 (94%)	-0.41	0 100 100	13, 39, 88, 93	0
1	B	734/776 (94%)	-0.42	1 (0%) 95 95	11, 38, 84, 96	0
All	All	1466/1552 (94%)	-0.41	1 (0%) 95 95	11, 38, 86, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LYS	2.3

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 carbohydrates 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
3	SD2	A	9002	32/32	0.96	0.25	21,23,30,41	0
3	SD2	B	9003	32/32	0.96	0.23	16,23,32,37	0
2	ZN	A	9001	1/1	0.99	0.12	21,21,21,21	0
2	ZN	B	9002	1/1	0.99	0.12	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.