



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:08 PM UTC

PDB ID : 9KP3 / pdb_00009kp3
Title : Ligand binding domain of Pseudomonas Aeruginosa PAO1 chemoreceptor
TlpQ in complex with MHF
Authors : Songying, O.; Yanbo, Z.; Lei, Z.; Xinyu, Q.
Deposited on : 2024-11-22
Resolution : 2.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

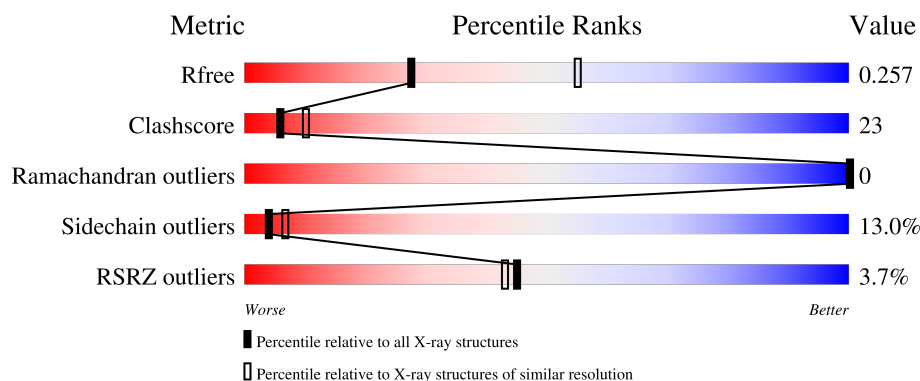
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	360	
1	B	360	

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
3	4XX	B	401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4568 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 Chemotaxis transducer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2206	1397	380	423	6			
1	B	286	Total	C	N	O	S	0	0	0
			2207	1400	381	420	6			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	HIS	-	expression tag	UNP A0A2U2Y0U1
A	5	HIS	-	expression tag	UNP A0A2U2Y0U1
A	6	HIS	-	expression tag	UNP A0A2U2Y0U1
A	7	HIS	-	expression tag	UNP A0A2U2Y0U1
A	8	HIS	-	expression tag	UNP A0A2U2Y0U1
A	9	HIS	-	expression tag	UNP A0A2U2Y0U1
A	10	SER	-	expression tag	UNP A0A2U2Y0U1
A	11	SER	-	expression tag	UNP A0A2U2Y0U1
A	12	GLY	-	expression tag	UNP A0A2U2Y0U1
A	13	LEU	-	expression tag	UNP A0A2U2Y0U1
A	14	VAL	-	expression tag	UNP A0A2U2Y0U1
A	15	PRO	-	expression tag	UNP A0A2U2Y0U1
A	16	ARG	-	expression tag	UNP A0A2U2Y0U1
A	17	GLY	-	expression tag	UNP A0A2U2Y0U1
A	18	SER	-	expression tag	UNP A0A2U2Y0U1
A	19	HIS	-	expression tag	UNP A0A2U2Y0U1
A	20	MET	-	expression tag	UNP A0A2U2Y0U1
A	21	ALA	-	expression tag	UNP A0A2U2Y0U1
A	22	SER	-	expression tag	UNP A0A2U2Y0U1
A	23	MET	-	expression tag	UNP A0A2U2Y0U1
A	24	THR	-	expression tag	UNP A0A2U2Y0U1
A	25	GLY	-	expression tag	UNP A0A2U2Y0U1
A	26	GLY	-	expression tag	UNP A0A2U2Y0U1
A	27	GLN	-	expression tag	UNP A0A2U2Y0U1
A	28	GLN	-	expression tag	UNP A0A2U2Y0U1

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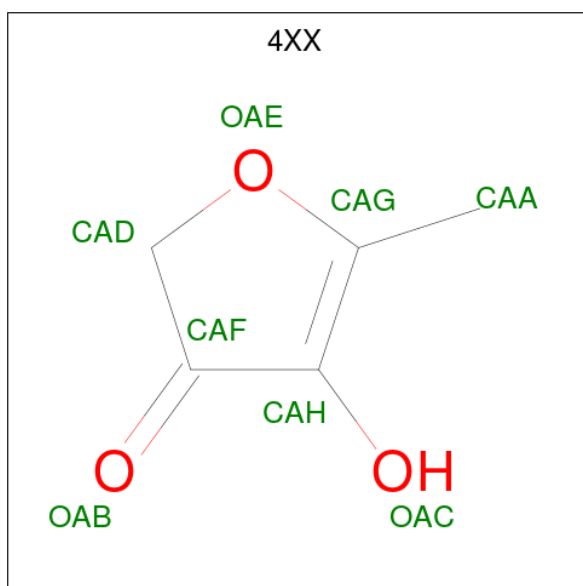
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	expression tag	UNP A0A2U2Y0U1
A	30	GLY	-	expression tag	UNP A0A2U2Y0U1
A	31	ARG	-	expression tag	UNP A0A2U2Y0U1
A	32	GLY	-	expression tag	UNP A0A2U2Y0U1
B	4	HIS	-	expression tag	UNP A0A2U2Y0U1
B	5	HIS	-	expression tag	UNP A0A2U2Y0U1
B	6	HIS	-	expression tag	UNP A0A2U2Y0U1
B	7	HIS	-	expression tag	UNP A0A2U2Y0U1
B	8	HIS	-	expression tag	UNP A0A2U2Y0U1
B	9	HIS	-	expression tag	UNP A0A2U2Y0U1
B	10	SER	-	expression tag	UNP A0A2U2Y0U1
B	11	SER	-	expression tag	UNP A0A2U2Y0U1
B	12	GLY	-	expression tag	UNP A0A2U2Y0U1
B	13	LEU	-	expression tag	UNP A0A2U2Y0U1
B	14	VAL	-	expression tag	UNP A0A2U2Y0U1
B	15	PRO	-	expression tag	UNP A0A2U2Y0U1
B	16	ARG	-	expression tag	UNP A0A2U2Y0U1
B	17	GLY	-	expression tag	UNP A0A2U2Y0U1
B	18	SER	-	expression tag	UNP A0A2U2Y0U1
B	19	HIS	-	expression tag	UNP A0A2U2Y0U1
B	20	MET	-	expression tag	UNP A0A2U2Y0U1
B	21	ALA	-	expression tag	UNP A0A2U2Y0U1
B	22	SER	-	expression tag	UNP A0A2U2Y0U1
B	23	MET	-	expression tag	UNP A0A2U2Y0U1
B	24	THR	-	expression tag	UNP A0A2U2Y0U1
B	25	GLY	-	expression tag	UNP A0A2U2Y0U1
B	26	GLY	-	expression tag	UNP A0A2U2Y0U1
B	27	GLN	-	expression tag	UNP A0A2U2Y0U1
B	28	GLN	-	expression tag	UNP A0A2U2Y0U1
B	29	MET	-	expression tag	UNP A0A2U2Y0U1
B	30	GLY	-	expression tag	UNP A0A2U2Y0U1
B	31	ARG	-	expression tag	UNP A0A2U2Y0U1
B	32	GLY	-	expression tag	UNP A0A2U2Y0U1

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 4-hydroxy-5-methylfuran-3(2H)-one (CCD ID: 4XX) (formula: $C_5H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	5	3		

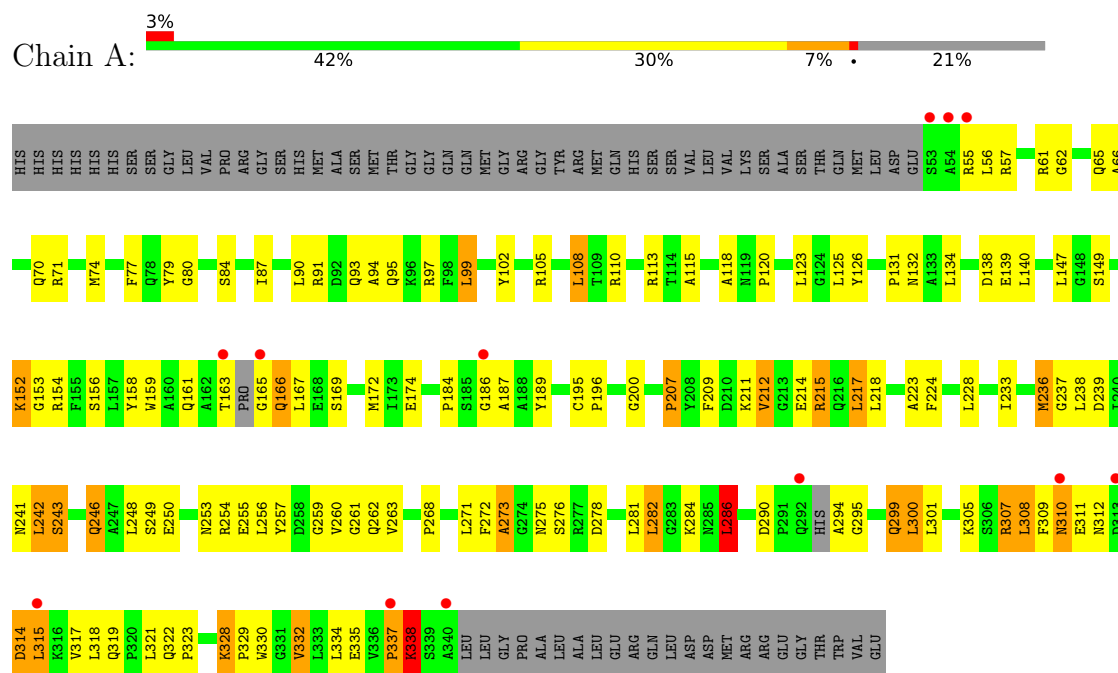
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total 67	O 67	0	0
4	B	73	Total 73	O 73	0	0

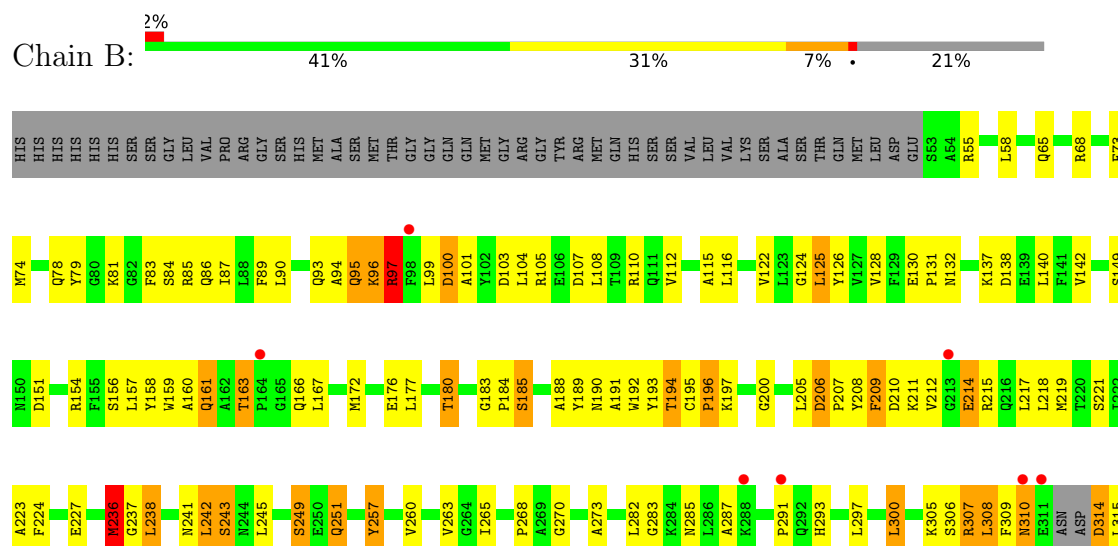
3 Residue-property plots

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: Chemotaxis transducer



• Molecule 1: Chemotaxis transducer



K316	V317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	K1000
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.80Å 124.91Å 58.34Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	40.31 – 2.74 40.31 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.31-2.74) 95.8 (40.31-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.73Å)	Xtriage
Refinement program	PHENIX v1.18.2-3874	Depositor
R, R_{free}	0.222 , 0.259 0.222 , 0.257	Depositor DCC
R_{free} test set	1818 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4568	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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: PEG, 4XX

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	1.01	3/2245 (0.1%)	1.40	16/3034 (0.5%)
1	B	1.06	8/2249 (0.4%)	1.38	15/3042 (0.5%)
All	All	1.04	11/4494 (0.2%)	1.39	31/6076 (0.5%)

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	A	0	2
1	B	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	PRO	C-O	-8.06	1.14	1.24
1	A	189	TYR	C-O	-7.70	1.14	1.24
1	B	251	GLN	C-O	-6.44	1.16	1.24
1	A	184	PRO	C-O	-6.36	1.16	1.24
1	B	196	PRO	C-O	-6.12	1.16	1.24
1	B	194	THR	C-O	-6.04	1.16	1.24
1	B	200	GLY	C-O	-5.55	1.16	1.24
1	B	257	TYR	C-O	-5.47	1.17	1.23
1	A	187	ALA	C-O	-5.34	1.17	1.23
1	B	329	PRO	C-O	-5.20	1.17	1.23
1	B	325	PRO	C-O	-5.16	1.17	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ASN	CB-CA-C	-9.73	105.35	116.54
1	A	257	TYR	CA-C-O	-8.71	110.91	121.28
1	B	97	ARG	N-CA-C	-8.29	100.79	113.89
1	B	185	SER	N-CA-C	-7.62	100.26	110.55
1	B	339	SER	N-CA-C	-7.42	104.75	113.88
1	B	273	ALA	N-CA-C	-6.57	104.89	113.17
1	B	73	PHE	CA-CB-CG	6.55	120.35	113.80
1	A	286	LEU	CA-C-N	6.48	130.97	120.60
1	A	286	LEU	C-N-CA	6.48	130.97	120.60
1	B	236	MET	CA-C-N	-6.41	114.75	121.35
1	B	236	MET	C-N-CA	-6.41	114.75	121.35
1	A	200	GLY	N-CA-C	-6.15	106.75	115.43
1	B	180	THR	N-CA-C	-5.87	105.43	112.59
1	B	163	THR	CB-CA-C	5.85	116.51	109.31
1	B	209	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	273	ALA	N-CA-C	-5.68	105.66	112.59
1	A	255	GLU	N-CA-C	-5.66	106.23	113.02
1	B	206	ASP	CA-CB-CG	5.58	118.17	112.60
1	A	338	LYS	N-CA-C	-5.48	106.43	113.01
1	A	329	PRO	N-CA-C	5.42	119.38	111.03
1	A	246	GLN	N-CA-C	-5.42	105.45	111.36
1	B	329	PRO	N-CA-C	5.41	119.36	111.03
1	B	184	PRO	CB-CA-C	5.40	121.53	112.62
1	A	207	PRO	N-CA-CB	-5.38	98.43	103.27
1	B	328	LYS	N-CA-C	-5.33	103.06	109.83
1	A	186	GLY	CA-C-N	5.27	130.14	121.39
1	A	186	GLY	C-N-CA	5.27	130.14	121.39
1	A	207	PRO	CB-CA-C	5.26	118.27	111.64
1	A	248	LEU	N-CA-CB	-5.24	102.41	110.12
1	B	95	GLN	N-CA-C	-5.24	103.57	110.33
1	A	243	SER	N-CA-C	-5.11	106.89	113.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	215	ARG	Sidechain

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	2206	0	2189	103	0
1	B	2207	0	2194	99	0
2	A	7	0	8	2	0
3	B	8	0	6	6	0
4	A	67	0	0	5	0
4	B	73	0	0	4	0
All	All	4568	0	4397	202	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 23.

All (202) 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:131:PRO:HD3	1:A:154:ARG:HH21	1.16	1.05
1:A:131:PRO:HD3	1:A:154:ARG:NH2	1.79	0.98
1:B:218:LEU:HD21	1:B:283:GLY:HA3	1.52	0.92
1:B:263:VAL:HG22	1:B:334:LEU:HG	1.53	0.86
1:A:212:VAL:HG13	1:A:217:LEU:HD22	1.55	0.85
1:A:139:GLU:HG3	1:A:140:LEU:HD22	1.59	0.82
1:B:126:TYR:CZ	1:B:237:GLY:HA3	2.19	0.78
1:B:205:LEU:HD12	1:B:221:SER:HB2	1.65	0.78
1:A:132:ASN:ND2	1:A:138:ASP:H	1.83	0.77
1:A:62:GLY:HA2	1:A:334:LEU:HD11	1.66	0.76
1:A:300:LEU:HD21	1:A:307:ARG:HE	1.50	0.75
1:A:84:SER:HB3	1:A:236:MET:HE2	1.68	0.75
1:B:180:THR:HG22	1:B:190:ASN:HD21	1.51	0.74
1:A:79:TYR:HD2	1:A:238:LEU:HD21	1.53	0.74
1:B:68:ARG:NH2	4:B:501:HOH:O	2.21	0.73
1:B:242:LEU:HD23	1:B:282:LEU:HD22	1.72	0.72
1:A:214:GLU:HG3	1:A:214:GLU:O	1.89	0.71
1:B:132:ASN:ND2	1:B:138:ASP:H	1.89	0.69
1:B:112:VAL:HG11	1:B:157:LEU:CD2	2.22	0.69
1:A:123:LEU:HD21	1:A:212:VAL:HG11	1.74	0.68
1:A:242:LEU:HD21	1:A:273:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ALA:HB3	1:B:212:VAL:HG13	1.76	0.67
1:A:315:LEU:HD21	1:A:338:LYS:HE2	1.76	0.66
1:B:128:VAL:HG22	1:B:156:SER:CB	2.26	0.66
1:B:160:ALA:CB	1:B:212:VAL:HG13	2.26	0.66
1:B:211:LYS:HD2	1:B:214:GLU:HA	1.77	0.66
1:A:62:GLY:CA	1:A:334:LEU:HD11	2.25	0.65
1:A:253:ASN:ND2	1:A:262:GLN:HA	2.11	0.65
1:B:65:GLN:HG3	1:B:332:VAL:HG21	1.77	0.65
1:A:132:ASN:HD21	1:A:138:ASP:H	1.44	0.65
1:B:172:MET:HG2	3:B:401:4XX:H1	1.79	0.64
1:A:301:LEU:HD13	1:A:318:LEU:HD11	1.80	0.64
1:B:209:PHE:CD1	1:B:218:LEU:HD13	2.33	0.63
1:B:112:VAL:HG11	1:B:157:LEU:HD21	1.80	0.63
1:A:260:VAL:HG22	1:A:337:PRO:HG2	1.80	0.63
1:A:323:PRO:HG3	1:A:330:TRP:CD1	2.34	0.62
1:B:137:LYS:HB3	1:B:140:LEU:HD13	1.82	0.62
1:A:242:LEU:HD23	1:A:282:LEU:HG	1.82	0.62
1:A:91:ARG:HG2	1:A:91:ARG:HH11	1.65	0.61
1:B:74:MET:O	1:B:78:GLN:HG2	2.00	0.61
1:B:328:LYS:HB3	4:B:565:HOH:O	2.00	0.61
1:A:272:PHE:HB2	1:A:281:LEU:O	2.01	0.60
1:A:218:LEU:HD23	1:A:242:LEU:HD22	1.83	0.59
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.17	0.59
1:B:94:ALA:O	1:B:97:ARG:HB3	2.02	0.59
1:A:262:GLN:HG3	1:A:335:GLU:HB3	1.83	0.59
1:A:91:ARG:HD2	1:A:134:LEU:HD12	1.84	0.58
1:B:89:PHE:O	1:B:93:GLN:HG2	2.05	0.57
1:B:189:TYR:O	1:B:192:TRP:CD1	2.57	0.57
1:A:310:ASN:HA	1:A:315:LEU:HD22	1.86	0.57
1:B:55:ARG:HH21	1:B:308:LEU:HD13	1.69	0.57
1:B:319:GLN:HB3	1:B:332:VAL:HG12	1.87	0.57
1:A:163:THR:HG1	1:A:166:GLN:H	1.52	0.57
1:B:125:LEU:HD12	1:B:238:LEU:HD22	1.87	0.56
1:A:196:PRO:HG3	1:A:223:ALA:HB1	1.87	0.56
1:A:207:PRO:HD2	1:A:271:LEU:HD12	1.86	0.56
1:B:188:ALA:HB1	1:B:190:ASN:OD1	2.05	0.56
1:A:161:GLN:NE2	4:A:506:HOH:O	2.38	0.56
1:A:93:GLN:NE2	4:A:505:HOH:O	2.38	0.56
1:A:163:THR:HG1	1:A:165:GLY:N	2.04	0.56
1:A:126:TYR:HB3	1:A:158:TYR:HD1	1.70	0.55
1:A:113:ARG:HD3	4:A:524:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HG22	1:A:334:LEU:HD23	1.87	0.55
1:B:180:THR:HG22	1:B:190:ASN:ND2	2.20	0.55
1:B:112:VAL:HG11	1:B:157:LEU:HD23	1.88	0.55
1:B:210:ASP:OD1	3:B:401:4XX:CAD	2.55	0.55
1:B:268:PRO:HD3	1:B:330:TRP:CD1	2.41	0.55
1:A:195:CYS:HB3	1:A:196:PRO:CD	2.37	0.55
1:B:192:TRP:HA	1:B:205:LEU:HD11	1.88	0.55
1:B:142:VAL:HG13	1:B:151:ASP:O	2.08	0.54
1:A:295:GLY:O	1:A:299:GLN:HB2	2.08	0.54
1:B:149:SER:HA	1:B:154:ARG:O	2.08	0.53
1:B:210:ASP:OD1	3:B:401:4XX:OAE	2.26	0.53
1:A:224:PHE:HE1	1:A:238:LEU:HD13	1.74	0.53
1:A:290:ASP:O	1:A:294:ALA:HB2	2.08	0.53
1:A:113:ARG:HB2	1:A:159:TRP:CE2	2.42	0.53
1:A:300:LEU:HD23	1:A:305:LYS:CB	2.37	0.53
1:A:102:TYR:CE1	1:A:147:LEU:HD11	2.44	0.52
1:A:300:LEU:HD23	1:A:305:LYS:HB2	1.91	0.52
1:A:253:ASN:HD21	1:A:262:GLN:HA	1.73	0.52
1:B:130:GLU:OE1	1:B:197:LYS:HE3	2.08	0.52
1:B:209:PHE:CE1	1:B:218:LEU:HD13	2.45	0.52
1:B:126:TYR:CE2	1:B:237:GLY:HA3	2.44	0.52
1:A:268:PRO:HB3	1:A:328:LYS:HD3	1.91	0.52
1:A:79:TYR:CD2	1:A:238:LEU:HD21	2.40	0.52
1:B:84:SER:HB3	1:B:236:MET:HE2	1.92	0.52
1:B:218:LEU:CD2	1:B:283:GLY:HA3	2.35	0.52
1:B:151:ASP:N	1:B:151:ASP:OD1	2.43	0.52
1:B:125:LEU:CD1	1:B:238:LEU:HD22	2.40	0.51
1:A:118:ALA:O	1:A:120:PRO:HD3	2.09	0.51
1:A:125:LEU:HD21	1:A:238:LEU:HG	1.92	0.51
1:B:122:VAL:HG21	1:B:238:LEU:CD1	2.41	0.51
1:B:122:VAL:HG11	1:B:238:LEU:HD13	1.93	0.51
1:B:124:GLY:HA3	1:B:158:TYR:CE1	2.46	0.51
1:A:87:ILE:HG23	1:A:108:LEU:HD21	1.92	0.51
1:A:228:LEU:HA	4:A:513:HOH:O	2.10	0.50
1:B:65:GLN:HG2	1:B:334:LEU:HD11	1.92	0.50
1:A:66:ALA:HA	1:A:332:VAL:HG11	1.92	0.50
1:B:176:GLU:OE2	3:B:401:4XX:H2	2.11	0.50
1:B:314:ASP:HB3	1:B:337:PRO:HA	1.94	0.50
1:A:55:ARG:HB2	1:A:308:LEU:HD13	1.94	0.50
1:A:126:TYR:CZ	1:A:237:GLY:HA3	2.47	0.50
1:A:139:GLU:HG3	1:A:140:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:O	1:A:61:ARG:HG2	2.12	0.49
1:B:130:GLU:CD	1:B:197:LYS:HE3	2.37	0.49
1:A:152:LYS:HD3	1:A:174:GLU:HG3	1.94	0.49
1:B:287:ALA:O	1:B:291:PRO:HB3	2.11	0.49
1:B:86:GLN:O	1:B:90:LEU:HG	2.13	0.49
1:A:65:GLN:NE2	1:A:256:LEU:HB2	2.28	0.48
1:B:326:GLY:N	4:B:503:HOH:O	2.28	0.48
1:B:95:GLN:C	1:B:97:ARG:H	2.21	0.48
1:B:95:GLN:O	1:B:96:LYS:HB2	2.12	0.48
1:B:158:TYR:CZ	1:B:160:ALA:HB2	2.48	0.48
1:A:272:PHE:CZ	1:A:286:LEU:HD23	2.49	0.48
1:B:97:ARG:HH21	1:B:97:ARG:HB2	1.78	0.48
1:B:310:ASN:ND2	1:B:315:LEU:HD11	2.28	0.48
1:B:257:TYR:O	1:B:260:VAL:HG13	2.13	0.48
1:A:308:LEU:HG	1:A:317:VAL:HG22	1.94	0.48
1:A:172:MET:SD	2:A:401:PEG:H31	2.53	0.47
1:A:241:ASN:C	1:A:243:SER:H	2.22	0.47
1:B:268:PRO:HD3	1:B:330:TRP:CG	2.50	0.47
1:B:249:SER:OG	1:B:265:ILE:HG13	2.15	0.47
1:B:125:LEU:CD1	1:B:238:LEU:CD2	2.93	0.47
1:B:55:ARG:HD3	1:B:308:LEU:HD22	1.96	0.47
1:A:163:THR:O	1:A:165:GLY:N	2.47	0.47
1:A:254:ARG:HD2	1:A:254:ARG:N	2.30	0.47
1:B:310:ASN:O	1:B:314:ASP:O	2.33	0.47
1:A:253:ASN:HB3	1:A:254:ARG:NH2	2.30	0.46
1:A:271:LEU:HA	1:A:284:LYS:O	2.16	0.46
1:B:191:ALA:C	1:B:193:TYR:H	2.23	0.46
1:B:128:VAL:HG22	1:B:156:SER:HA	1.97	0.46
1:A:275:ASN:HB3	1:A:278:ASP:O	2.16	0.46
1:B:128:VAL:HG22	1:B:156:SER:HB2	1.97	0.46
1:A:212:VAL:HG13	1:A:217:LEU:CD2	2.36	0.45
1:B:160:ALA:CB	1:B:212:VAL:CG1	2.93	0.45
1:A:80:GLY:HA3	1:A:238:LEU:HD11	1.98	0.45
1:B:195:CYS:SG	4:B:554:HOH:O	2.61	0.45
1:B:241:ASN:OD1	1:B:243:SER:HB2	2.16	0.45
1:A:139:GLU:CG	1:A:140:LEU:HD22	2.39	0.45
1:A:246:GLN:O	1:A:250:GLU:HG3	2.15	0.45
1:B:196:PRO:HG3	1:B:223:ALA:HB1	1.97	0.45
1:A:94:ALA:HA	1:A:99:LEU:HD22	1.99	0.45
1:A:250:GLU:O	1:A:254:ARG:HD2	2.17	0.45
1:A:308:LEU:HG	1:A:317:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:O	1:B:194:THR:HG23	2.16	0.45
1:B:227:GLU:H	1:B:227:GLU:HG2	1.62	0.45
1:A:138:ASP:O	1:A:153:GLY:HA3	2.17	0.45
1:B:160:ALA:HB1	1:B:212:VAL:CG1	2.47	0.44
1:B:224:PHE:CD2	1:B:236:MET:CE	3.01	0.44
1:B:300:LEU:HD23	1:B:305:LYS:HB2	1.99	0.44
1:A:268:PRO:HD3	1:A:330:TRP:CE2	2.53	0.44
1:A:253:ASN:OD1	1:A:259:GLY:HA2	2.17	0.44
1:B:108:LEU:O	1:B:112:VAL:HG12	2.18	0.44
1:B:128:VAL:HG21	1:B:177:LEU:HD21	2.00	0.44
1:B:210:ASP:OD1	3:B:401:4XX:H5	2.17	0.44
1:A:79:TYR:OH	1:A:115:ALA:O	2.30	0.44
1:A:250:GLU:O	1:A:254:ARG:CD	2.66	0.43
1:B:83:PHE:CE2	1:B:87:ILE:HD11	2.53	0.43
1:A:212:VAL:HG22	1:A:212:VAL:O	2.18	0.43
1:B:339:SER:O	1:B:340:ALA:HB2	2.18	0.43
1:B:209:PHE:CG	1:B:218:LEU:HD13	2.54	0.43
1:A:77:PHE:HA	1:A:224:PHE:HZ	1.83	0.43
1:B:94:ALA:HB1	1:B:99:LEU:HD23	2.00	0.43
1:B:125:LEU:HD11	1:B:238:LEU:HD21	2.01	0.43
1:A:322:GLN:HA	1:A:323:PRO:HD2	1.83	0.43
1:B:112:VAL:HG13	1:B:159:TRP:CD1	2.53	0.43
1:A:97:ARG:HB2	1:A:99:LEU:HD22	2.00	0.43
1:B:307:ARG:HG3	1:B:308:LEU:H	1.83	0.42
1:A:159:TRP:CE3	1:A:169:SER:HB3	2.54	0.42
1:A:105:ARG:NH1	1:A:149:SER:OG	2.45	0.42
1:A:239:ASP:OD2	2:A:401:PEG:H11	2.20	0.42
1:B:297:LEU:HD21	1:B:309:PHE:CZ	2.54	0.42
1:B:270:GLY:O	1:B:285:ASN:HA	2.19	0.42
1:A:246:GLN:O	1:A:249:SER:HB2	2.20	0.42
1:B:101:ALA:O	1:B:105:ARG:HG3	2.20	0.42
1:B:183:GLY:O	1:B:185:SER:O	2.37	0.42
1:A:195:CYS:HB3	1:A:196:PRO:HD2	2.00	0.42
1:A:209:PHE:CE2	1:A:218:LEU:HD13	2.54	0.42
1:B:100:ASP:HB3	1:B:103:ASP:H	1.85	0.41
1:B:172:MET:HG2	3:B:401:4XX:CAA	2.48	0.41
1:A:253:ASN:HB3	1:A:254:ARG:HH21	1.84	0.41
1:B:116:LEU:HD21	1:B:161:GLN:HG2	2.02	0.41
1:B:125:LEU:HD11	1:B:238:LEU:CD2	2.50	0.41
1:B:206:ASP:O	1:B:207:PRO:C	2.62	0.41
1:A:91:ARG:O	1:A:95:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:O	1:A:97:ARG:HB2	2.20	0.41
1:A:123:LEU:HD11	1:A:212:VAL:HG21	2.02	0.41
1:A:307:ARG:HB3	1:A:309:PHE:CE2	2.55	0.41
1:A:311:GLU:O	1:A:314:ASP:O	2.38	0.41
1:A:161:GLN:HE21	1:A:167:LEU:HD11	1.86	0.41
1:A:218:LEU:N	4:A:507:HOH:O	2.46	0.41
1:A:228:LEU:HB2	1:A:233:ILE:HD13	2.02	0.41
1:B:81:LYS:O	1:B:84:SER:OG	2.36	0.41
1:A:261:GLY:HA2	1:A:337:PRO:HD3	2.03	0.41
1:A:126:TYR:HB3	1:A:158:TYR:CD1	2.54	0.41
1:B:208:TYR:CE1	1:B:219:MET:HG3	2.55	0.40
1:B:314:ASP:OD1	1:B:314:ASP:N	2.53	0.40
1:A:55:ARG:CG	1:A:56:LEU:N	2.85	0.40
1:A:70:GLN:O	1:A:74:MET:HG2	2.20	0.40
1:B:58:LEU:HD12	1:B:58:LEU:HA	1.88	0.40
1:A:90:LEU:N	1:A:90:LEU:HD23	2.36	0.40
1:B:79:TYR:OH	1:B:115:ALA:O	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	280/360 (78%)	262 (94%)	18 (6%)	0	100	100
1	B	282/360 (78%)	268 (95%)	14 (5%)	0	100	100
All	All	562/720 (78%)	530 (94%)	32 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	230/292 (79%)	202 (88%)	28 (12%)	5	8
1	B	230/292 (79%)	198 (86%)	32 (14%)	3	5
All	All	460/584 (79%)	400 (87%)	60 (13%)	4	7

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	108	LEU
1	A	110	ARG
1	A	152	LYS
1	A	156	SER
1	A	166	GLN
1	A	211	LYS
1	A	212	VAL
1	A	215	ARG
1	A	217	LEU
1	A	236	MET
1	A	242	LEU
1	A	276	SER
1	A	282	LEU
1	A	286	LEU
1	A	299	GLN
1	A	300	LEU
1	A	307	ARG
1	A	308	LEU
1	A	310	ASN
1	A	314	ASP
1	A	315	LEU
1	A	319	GLN
1	A	321	LEU
1	A	328	LYS
1	A	332	VAL
1	A	337	PRO

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Mol	Chain	Res	Type
1	A	338	LYS
1	B	85	ARG
1	B	96	LYS
1	B	97	ARG
1	B	100	ASP
1	B	104	LEU
1	B	107	ASP
1	B	110	ARG
1	B	125	LEU
1	B	131	PRO
1	B	161	GLN
1	B	163	THR
1	B	166	GLN
1	B	167	LEU
1	B	214	GLU
1	B	217	LEU
1	B	236	MET
1	B	238	LEU
1	B	242	LEU
1	B	243	SER
1	B	245	LEU
1	B	249	SER
1	B	251	GLN
1	B	293	HIS
1	B	300	LEU
1	B	306	SER
1	B	307	ARG
1	B	308	LEU
1	B	310	ASN
1	B	314	ASP
1	B	317	VAL
1	B	321	LEU
1	B	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	132	ASN
1	A	161	GLN
1	A	253	ASN
1	A	292	GLN

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	319	GLN
1	B	132	ASN
1	B	161	GLN
1	B	166	GLN
1	B	292	GLN
1	B	310	ASN
1	B	319	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](#)

2 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	$\# Z > 2$
3	4XX	B	401	-	7,8,8	3.77	4 (57%)	8,11,11	3.74	6 (75%)
2	PEG	A	401	-	6,6,6	1.16	0	5,5,5	1.27	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
3	4XX	B	401	-	-	-	0/1/1/1
2	PEG	A	401	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	4XX	OAE-CAD	7.67	1.57	1.44
3	B	401	4XX	CAH-CAG	4.30	1.45	1.35
3	B	401	4XX	OAB-CAF	-3.02	1.17	1.23
3	B	401	4XX	CAH-CAF	-2.83	1.41	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	4XX	CAA-CAG-CAH	-8.33	119.92	133.18
3	B	401	4XX	OAE-CAG-CAA	3.73	118.25	113.57
3	B	401	4XX	OAC-CAH-CAG	-3.01	119.62	128.59
3	B	401	4XX	OAB-CAF-CAH	2.80	128.04	125.42
3	B	401	4XX	OAC-CAH-CAF	-2.18	119.02	122.68
3	B	401	4XX	OAE-CAG-CAH	-2.09	110.97	113.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PEG	C4-C3-O2-C2
2	A	401	PEG	O1-C1-C2-O2

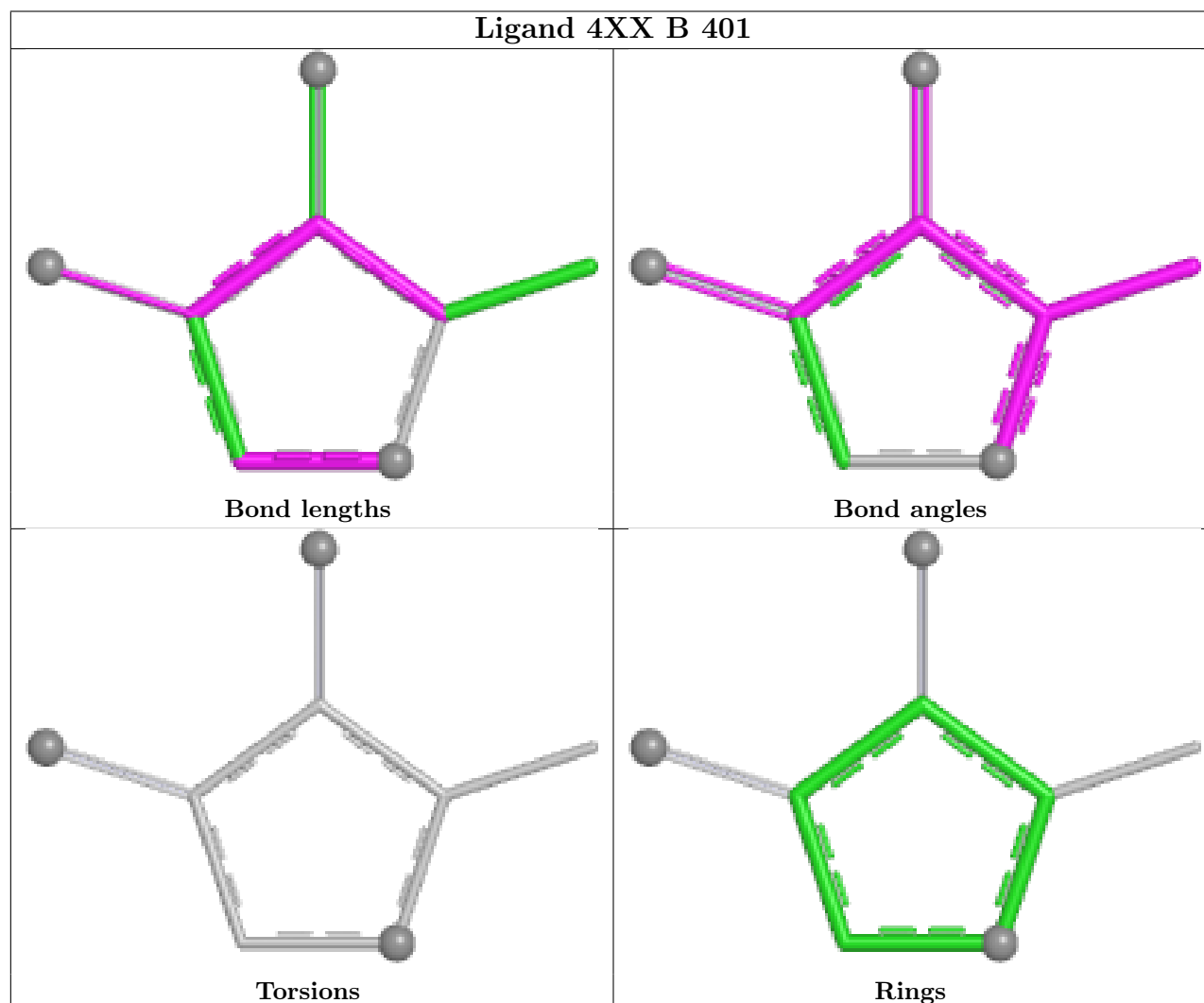
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	4XX	6	0
2	A	401	PEG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	286/360 (79%)	0.43	12 (4%) 40 39	11, 25, 55, 80	0
1	B	286/360 (79%)	0.31	9 (3%) 51 49	10, 24, 57, 81	0
All	All	572/720 (79%)	0.37	21 (3%) 45 43	10, 25, 57, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	ALA	3.7
1	A	340	ALA	3.2
1	A	54	ALA	3.1
1	A	310	ASN	3.1
1	A	53	SER	3.1
1	A	163	THR	3.0
1	A	292	GLN	3.0
1	B	310	ASN	3.0
1	A	313	ASP	2.9
1	B	288	LYS	2.8
1	B	98	PHE	2.8
1	B	213	GLY	2.6
1	A	165	GLY	2.5
1	A	186	GLY	2.5
1	A	55	ARG	2.4
1	A	315	LEU	2.4
1	A	337	PRO	2.3
1	B	291	PRO	2.2
1	B	164	PRO	2.2
1	B	339	SER	2.1
1	B	311	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

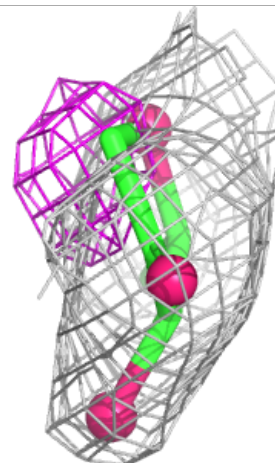
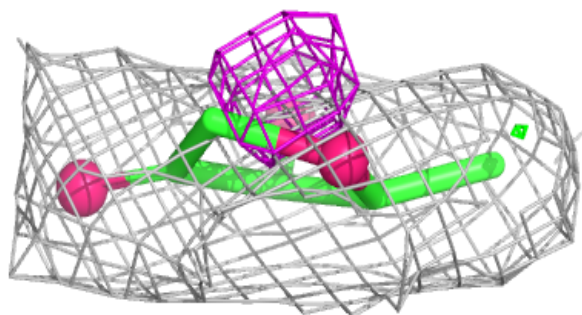
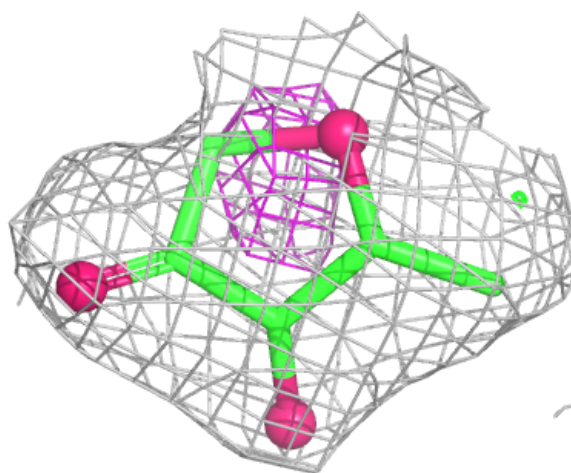
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	4XX	B	401	8/8	0.84	0.20	21,23,33,41	0
2	PEG	A	401	7/7	0.88	0.13	27,29,36,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4XX B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.