



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:47 AM GMT

PDB ID : 2ECP
Title : THE CRYSTAL STRUCTURE OF THE E. COLI MALTODEXTRIN PHOSPHORYLASE COMPLEX
Authors : O'Reilly, M.; Watson, K.A.; Johnson, L.N.
Deposited on : 1998-10-27
Resolution : 2.95 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 ⓘ 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 (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

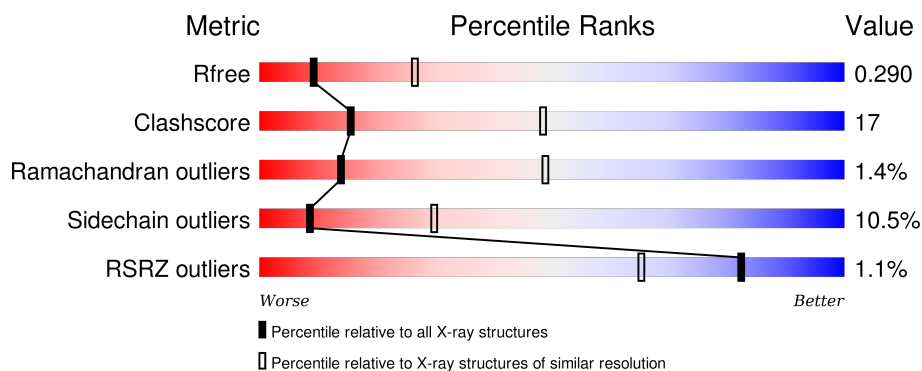
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	796	<div> <div>53%</div> <div>36%</div> <div>10%</div> <div>.</div> </div>
1	B	796	<div> <div>51%</div> <div>39%</div> <div>7%</div> <div>.</div> </div>

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	ACR	A	992	X	-	-	X
2	ACR	B	992	X	-	-	X
4	GOL	A	998	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12961 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.

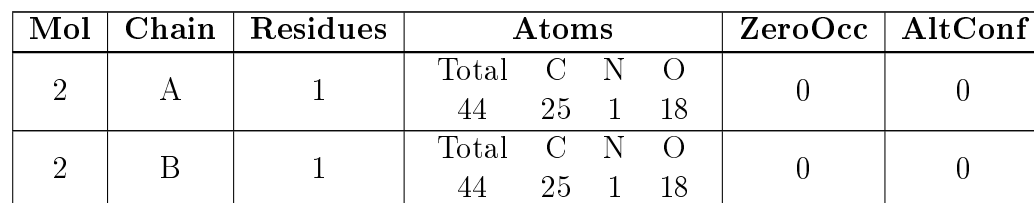
- Molecule 1 is a protein called MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6369	4065	1127	1157	20			
1	B	796	Total	C	N	O	S	0	0	0
			6369	4065	1127	1157	20			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	LYS	CONFLICT	UNP P00490
A	532	ASP	GLN	CONFLICT	UNP P00490
A	582	ARG	HIS	CONFLICT	UNP P00490
A	716	LYS	GLU	CONFLICT	UNP P00490
A	828	ALA	LYS	CONFLICT	UNP P00490
B	205	ALA	LYS	CONFLICT	UNP P00490
B	532	ASP	GLN	CONFLICT	UNP P00490
B	582	ARG	HIS	CONFLICT	UNP P00490
B	716	LYS	GLU	CONFLICT	UNP P00490
B	828	ALA	LYS	CONFLICT	UNP P00490

- Molecule 2 is SUGAR (ACARBOSE) (three-letter code: ACR) (formula: C₂₅H₄₃NO₁₈).



- PLP
-
- The diagram shows the chemical structure of Pyridoxal Phosphate (PLP). It consists of a pyridine ring substituted at the 2-position with a hydroxyl group (-OH), at the 3-position with a phosphate group (-O-PO₃H₂), and at the 4-position with an aldehyde group (-CHO). The atoms are color-coded: Nitrogen (N1) is blue; Carbon atoms (C2, C3, C4, C5, C6) are green; Oxygen atoms (O3, O4A, O4P, O2P, O3P) are red; Hydrogen atoms (H) are black; and the Phosphorus atom (P) is purple. Bond orders are indicated by single or double lines.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

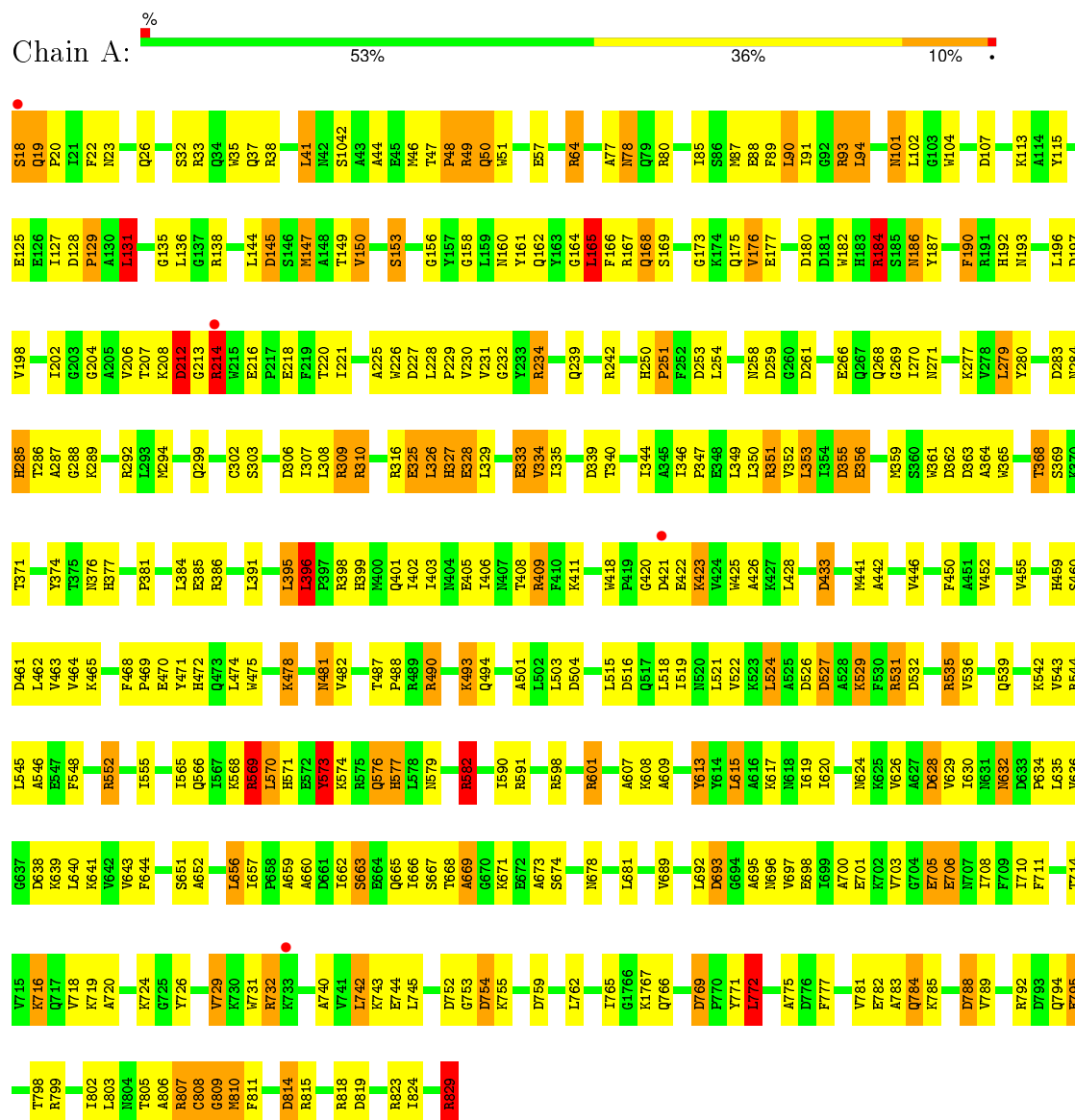
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	39	Total	O	0	0
			39	39		

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 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: MALTODEXTRIN PHOSPHORYLASE



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A783	Q784	Q785	Q786	Q787	Q788	R792	D793	Q794	E795	R799	A800	A801	L802	L803	N804	T805	A806	R807	N810	F811	S812	S813	D814	R815	S816	I817	R818	D819	Y820	Q821	R823	I824	A828	R829	D828	V629	V630	N631	N632	D633	P634	L635	D638	K641	V642	V643	F644	L645	V650	A653	E654	K655	L656	I657	P658	A659	A660	D661	I662	S663	E664	Q665	I666	Y667	T668	S667	A669	G670	K671	S674	N678	K679	L681	G690	T691	L692	D693	E698	I699	A700	E701	K702	V703	G704	E705	E706	H707	I708	F711	T714	V715	K716	Q717	K718	K719	A720	A723	K724	D727	F728	V729	K730	W731	R732	D735	D739	A740	V741	L742	K743	E744	L745	E746	Y750	S751	D752	Q753	D754	K755	L762	I765	G1766	K1767	Q766	D769	F770	Y771	L772	A775	D776	F777	Y780	V781	E782	S18	Q19	P20	I21	L126	G137	R138	N23	Q26	S32	R33	Q34	Q35	Q37	R38	L41	N42	E45	F46	T47	P48	R49	Q50	A73	A77	N78	Q79	R80	M87	E88	F89	L90	R93	L94	N101	L102	G103	W104	Y105	Q106	D107	D110	S111	L112	K113	D116	D121	D128	L131	G135	L136	G137	R138	L139	F143	L144	D145	S146	K147	A148	T149	V150	S153	Y157	G158	Q162	I165	F166	R167	S169	V176	D181	R184	S185	M186	Y187	F190	R191	H192	N193	E194	A195	D197	G204	A205	V206	T207	K208	D212	G213	R214	V215	E216	P217	E218	F219	T220	I221	T222	G223	Q224	R225	A226	W226	D227	L228	P229	R230	V231	Q232	G233	R234	Q239	R242	H248	A249	H250	P251	L254	N258	D261	F262	L263	R264	A265	E266	Q267	Q268	G269	L270	N271	A272	T276	K277	V278	L279	Y280	D283	R284	P285	G288	K289	R292	L293	M294	R297	F298	Q299	C300	D306	R309	R310	R316	E325	L326	R327	E328	L329	E333	V334	L335	Q336	L337	T340	R341	F342	T343	L344	A345	L346	P347	E348	L349	R351	V352	L353	T354	D355	E356	N359	S360	R361	D362	R363	A364	R365	A366	T367	T368	S369	K370	T371	F372	A373	Y374	T375	R376	R377	T378	L379	P381	L384	E385	R386	L391	L395	L396	P397	R398	R399	L402	L403	N404	E405	T406	T408	R409	F410	K411	V414	E415	K416	W417	W418	P419	G420	D421	E422	K423	W424	L425	V426	K427	L428	A429	R432	D433	M441	V446	V447	F450	A451	V452	N453	G454	A456	L457	L458	H459	V463	V464	K465	F468	P469	E470	Y471	H472	Q473	L474	W475	K478	N481	V482	T483	N484	T487	P488	R489	R490	W491	A500	L503	D516	Q517	L518	I519	R520	L521	V522	K523	L524	A525	D526	D527	A528	K529	F530	R531	R535	Q539	V543	R544	L545	A546	E547	P548	V549	R552	L555	D556	L557	D564	L565	Q566	L567	K568	R569	L570	H571	E572	Y573	K574	R575	Q576	H577	L578	R579	L580	L581	R582	K588	R591	P594	Q595	R598	R601	V602	F603	L604	A607	R608	A609	Y613	V614	L615	A616	K617	I618	L619	E701	K702	V703	G704	E705	E706	I707	I708	F711	T714	V715	K716	Q717	K718	K719	A720	A723	K724	D727	F728	V729	K730	W731	R732	D735	D739	A740	V741	L742	K743	E744	L745	E746	Y750	S751	D752	Q753	D754	K755	L762	I765	G1766	K1767	Q766	D769	F770	Y771	L772	A775	D776	F777	Y780	V781	E782	S18	Q19	P20	I21	L126	G137	R138	N23	Q26	S32	R33	Q34	Q35	Q37	R38	L41	N42	E45	F46	T47	P48	R49	Q50	A73	A77	N78	Q79	R80	M87	E88	F89	L90	R93	L94	N101	L102	G103	W104	Y105	Q106	D107	D110	S111	L112	K113	D116	D121	D128	L131	G135	L136	G137	R138	L139	F143	L144	D145	S146	K147	A148	T149	V150	S153	Y157	G158	Q162	I165	F166	R167	S169	V176	D181	R184	S185	M186	Y187	F190	R191	H192	N193	E194	A195	D197	G204	A205	V206	T207	K208	D212	G213	R214	V215	E216	P217	E218	F219	T220	I221	T222	G223	Q224	R225	A226	W226	D227	L228	P229	R230	V231	Q232	G233	R234	Q239	R242	H248	A249	H250	P251	L254	N258	D261	F262	L263	R264	A265	E266	Q267	Q268	G269	L270	N271	A272	T276	K277	V278	L279	Y280	D283	R284	P285	G288	K289	R292	L293	M294	R297	F298	Q299	C300	D306	R309	R310	R316	E325	L326	R327	E328	L329	E333	V334	L335	Q336	L337	T340	R341	F342	T343	L344	A345	L346	P347	E348	L349	R351	V352	L353	T354	D355	E356	N359	S360	R361	D362	R363	A364	R365	A366	T367	T368	S369	K370	T371	F372	A373	Y374	T375	R376	R377	T378	L379	P381	L384	E385	R386	L391	L395	L396	P397	R398	R399	L402	L403	N404	E405	T406	T408	R409	F410	K411	V414	E415	K416	W417	W418	P419	G420	D421	E422	K423	W424	L425	V426	K427	L428	A429	R432	D433	M441	V446	V447	F450	A451	V452	N453	G454	A456	L457	L458	H459	V463	V464	K465	F468	P469	E470	Y471	H472	Q473	L474	W475	K478	N481	V482	T483	N484	T487	P488	R489	R490	W491	A500	L503	D516	Q517	L518	I519	R520	L521	V522	K523	L524	A525	D526	D527	A528	K529	F530	R531	R535	Q539	V543	R544	L545	A546	E547	P548	V549	R552	L555	D556	L557	D564	L565	Q566	L567	K568	R569	L570	H571	E572	Y573	K574	R575	Q576	H577	L578	R579	L580	L581	R582	K588	R591	P594	Q595	R598	R601	V602	F603	L604	A607	R608	A609	Y613	V614	L615	A616	K617	I618	L619	E701	K702	V703	G704	E705	E706	I707	I708	F711	T714	V715	K716	Q717	K718	K719	A720	A723	K724	D727	F728	V729	K730	W731	R732	D735	D739	A740	V741	L742	K743	E744	L745	E746	Y750	S751	D752	Q753	D754	K755	L762	I765	G1766	K1767	Q766	D769	F770	Y771	L772	A775	D776	F777	Y780	V781	E782	S18	Q19	P20	I21	L126	G137	R138	N23	Q26	S32	R33	Q34	Q35	Q37	R38	L41	N42	E45	F46	T47	P48	R49	Q50	A73	A77	N78	Q79	R80	M87	E88	F89	L90	R93	L94	N101	L102	G103	W104	Y105	Q106	D107	D110	S111	L112	K113	D116	D121	D128	L131	G135	L136	G137	R138	L139	F143	L144	D145	S146	K147	A148	T149	V150	S153	Y157	G158	Q162	I165	F166	R167	S169	V176	D181	R184	S185	M186	Y187	F190	R191	H192	N193	E194	A195	D197	G204	A205	V206	T207	K208	D212	G213	R214	V215	E216	P217	E218	F219	T220	I221	T222	G223	Q224	R225	A226	W226	D227	L228	P229	R230	V231	Q232	G233	R234	Q239	R242	H248	A249	H250	P251	L254	N258	D261	F262	L263	R264	A265	E266	Q267	Q268	G269	L270	N271	A272	T276	K277	V278	L279	Y280	D283	R284	P285	G288	K289	R292	L293	M294	R297	F298	Q299	C300	D306	R309	R310	R316	E325	L326	R327	E328	L329	E333	V334	L335	Q336	L337	T340	R341	F342	T343	L344	A345	L346	P347	E348	L349	R351	V352	L353	T354	D355	E356	N359	S360	R361	D362	R363	A364	R365	A366	T367	T368	S369	K370	T371	F372	A373	Y374	T375	R376	R377	T378	L379	P381	L384	E385	R386	L391	L395	L396	P397	R398	R399	L402	L403	N404	E405	T406	T408	R409	F410	K411	V414	E415	K416	W417	W418	P419	G420	D421	E422	K423	W424	L425	V426	K427	L428	A429	R432	D433	M441	V446	V447	F450	A451	V452	N453	G454	A456	L457	L458	H459	V463	V464	K465	F468	P469	E470	Y471	H472	Q473	L474	W475	K478	N481	V482	T483	N484	T487	P488	R489	R490	W491	A500	L503	D516	Q517	L518	I519	R520	L521	V522	K523	L524	A525	D526	D527	A528	K529	F530	R531	R535	Q539	V543	R544	L545	A546	E547	P548	V549	R552	L555	D556	L557	D564	L565	Q566	L567	K568	R569	L570	H571	E572	Y573	K574	R575	Q576	H577	L578	R579	L580	L581	R582	K588	R591	P594	Q595	R598	R601	V602	F603	L604	A607	R608	A609	Y613	V614	L615	A616	K617	I618	L619	E701	K702	V703	G704	E705	E706	I707	I708	F711	T714	V715	K716	Q717	K718	K719	A720	A723	K724	D727	F728	V729	K730	W731	R732	D735	D739	A740	V741	L742	K743	E744	L745	E746	Y750	S751	D752	Q753	D754	K755	L762	I765	G1766	K1767	Q766	D769	F770	Y771	L772	A775	D776	F777	Y780	V781	E782	S18	Q19	P20	I21	L126	G137	R138	N23	Q26	S32	R33	Q34	Q35	Q37	R38	L41	N42	E45	F46	T47	P48	R49	Q50	A73	A77	N78	Q79	R80	M87	E88	F89	L90	R93	L94	N101	L102	G103	W104	Y105	Q106	D107	D110	S111	L112	K113	D116	D121	D128	L131	G135	L136	G137	R138	L139	F143	L144	D145	S146	K147	A148	T149	V150	S153	Y157	G158	Q162	I165	F166	R167	S169	V176	D181	R184	S185	M186	Y187	F190	R191	H192	N193	E194	A195	D197	G204	A205	V206	T207	K208	D212	G213	R214	V215	E216	P217	E218	F219	T220	I221	T222	G223	Q224	R225	A226	W226	D227	L228	P229	R230	V231	Q232	G233	R234	Q239	R242	H248	A249	H250	P251	L254	N258	D261	F262	L263	R264	A265	E266	Q267	Q268	G269	L270	N271	A272	T276	K277	V278	L279	Y280	D283	R284	P285	G288	K289	R292	L293	M294	R297	F298	Q299	C300	D306	R309	R310	R316	E325	L326	R327	E328	L329	E333	V334	L335	Q336	L337	T340	R341	F342	T343	L344	A345	L346	P347	E348	L349	R351	V352	L353	T354	D355	E356	N359	S360	R361	D362	R363	A364	R365	A366	T367	T368	S369	K370	T371	F372	A373	Y374	T375	R376	R377	T378	L379	P381	L384	E385	R386	L391	L395	L396	P397	R398	R399
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.49Å 105.84Å 217.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 15.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.00-2.95) 88.5 (15.00-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.293 0.242 , 0.290	Depositor DCC
R_{free} test set	852 reflections (2.62%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 33376 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12961	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 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: GOL, PLP, ACR

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	0.77	1/6517 (0.0%)	1.99	165/8841 (1.9%)
1	B	0.75	1/6517 (0.0%)	2.12	163/8841 (1.8%)
All	All	0.76	2/13034 (0.0%)	2.05	328/17682 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	ARG	NE-CZ	-5.76	1.25	1.33
1	B	292	ARG	CD-NE	-5.03	1.38	1.46

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH2	65.00	152.80	120.30
1	A	292	ARG	NE-CZ-NH2	46.98	143.79	120.30
1	B	569	ARG	NE-CZ-NH2	44.11	142.35	120.30
1	A	569	ARG	NE-CZ-NH1	32.74	136.67	120.30
1	B	292	ARG	NE-CZ-NH1	-32.15	104.22	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	516	ASP	Mainchain

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	6369	0	6324	223	0
1	B	6369	0	6324	220	0
2	A	44	0	43	3	0
2	B	44	0	43	5	0
3	A	15	0	6	1	0
3	B	15	0	6	3	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
5	A	54	0	0	11	0
5	B	39	0	0	9	0
All	All	12961	0	12762	440	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 17.

The worst 5 of 440 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:716:LYS:HE2	1:A:719:LYS:HD2	1.42	0.99
1:A:522:VAL:HG11	5:A:1777:HOH:O	1.61	0.97
1:B:310:ARG:HD2	5:B:1804:HOH:O	1.71	0.88
1:A:266:GLU:HG3	1:B:270:ILE:HD13	1.55	0.87
1:B:292:ARG:NH2	2:B:992:ACR:O2B	2.09	0.85

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	794/796 (100%)	729 (92%)	54 (7%)	11 (1%)	14	49
1	B	794/796 (100%)	725 (91%)	58 (7%)	11 (1%)	14	49
All	All	1588/1592 (100%)	1454 (92%)	112 (7%)	22 (1%)	14	49

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
1	B	423	LYS
1	A	285	HIS
1	A	421	ASP
1	B	207	THR

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	665/665 (100%)	594 (89%)	71 (11%)	8	29
1	B	665/665 (100%)	596 (90%)	69 (10%)	9	30
All	All	1330/1330 (100%)	1190 (90%)	140 (10%)	8	30

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	742	LEU

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Mol	Chain	Res	Type
1	B	165	LEU
1	B	716	LYS
1	A	766	GLN
1	B	18	SER

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	784	GLN
1	B	183	HIS
1	B	579	ASN
1	B	26	GLN
1	B	109	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](#)

6 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	ACR	A	992	-	46,47,47	1.05	1 (2%)	58,70,70	2.07	14 (24%)
4	GOL	A	998	-	5,5,5	0.70	0	5,5,5	0.77	0
3	PLP	A	999	1	15,15,16	2.14	2 (13%)	21,22,23	1.97	5 (23%)
2	ACR	B	992	-	46,47,47	1.23	5 (10%)	58,70,70	1.84	17 (29%)
4	GOL	B	998	-	5,5,5	0.43	0	5,5,5	0.56	0
3	PLP	B	999	1	15,15,16	3.43	2 (13%)	21,22,23	2.07	7 (33%)

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	ACR	A	992	-	1/1/20/22	0/18/98/98	0/4/4/4
4	GOL	A	998	-	-	0/4/4/4	0/0/0/0
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
2	ACR	B	992	-	1/1/20/22	0/18/98/98	0/4/4/4
4	GOL	B	998	-	-	0/4/4/4	0/0/0/0
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	PLP	C3-C2	-12.15	1.32	1.40
3	A	999	PLP	C3-C2	-6.27	1.36	1.40
3	B	999	PLP	P-O3P	-3.43	1.42	1.54
3	A	999	PLP	P-O3P	-3.33	1.42	1.54
2	B	992	ACR	C2A-C1A	2.09	1.56	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	992	ACR	C1C-O4D-C4D	-5.49	103.66	118.01
2	A	992	ACR	C1C-O4D-C4D	-5.43	103.81	118.01
3	A	999	PLP	C2A-C2-C3	-5.28	114.68	121.04
2	A	992	ACR	O2A-C2A-C3A	-4.32	100.62	110.34
2	B	992	ACR	O4A-C4A-C3A	-4.10	101.59	109.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	992	ACR	C1D
2	B	992	ACR	C1D

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	992	ACR	3	0
4	A	998	GOL	2	0
3	A	999	PLP	1	0
2	B	992	ACR	5	0
3	B	999	PLP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	796/796 (100%)	-0.17	4 (0%) 91 81	41, 50, 76, 114	0
1	B	796/796 (100%)	-0.28	13 (1%) 74 55	41, 50, 76, 114	0
All	All	1592/1592 (100%)	-0.23	17 (1%) 82 65	41, 50, 76, 114	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	SER	5.5
1	B	207	THR	4.2
1	B	723	ALA	3.7
1	B	208	LYS	3.3
1	B	421	ASP	3.0

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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	998	6/6	0.91	0.27	3.88	58,58,59,59	0
2	ACR	A	992	44/44	0.88	0.23	2.06	58,58,59,60	0
2	ACR	B	992	44/44	0.89	0.21	2.03	58,58,59,60	0
4	GOL	B	998	6/6	0.90	0.20	0.94	58,58,59,59	0
3	PLP	A	999	15/16	0.94	0.17	0.05	37,42,47,51	0
3	PLP	B	999	15/16	0.97	0.12	-1.07	41,43,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.