



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 03:53 PM EDT

PDB ID : 3PVM
Title : Structure of Complement C5 in Complex with CVF
Authors : Laursen, N.S.; Andersen, K.R.; Braren, I.; Sottrup-Jensen, L.; Spillner, E.; Andersen, G.R.
Deposited on : 2010-12-07
Resolution : 4.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

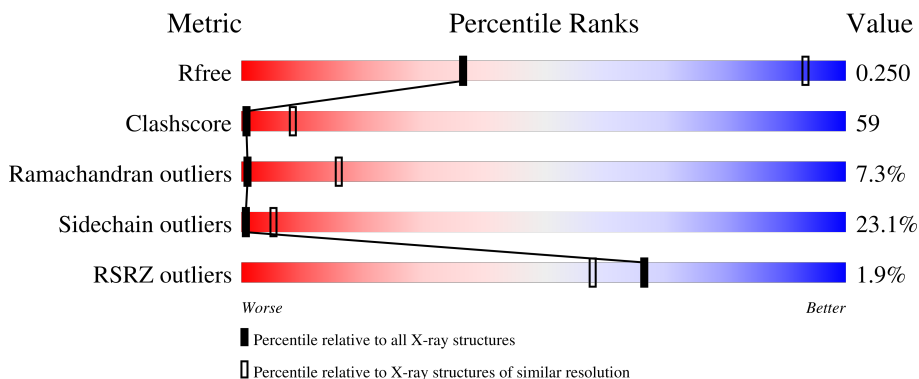
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1676	 2% 24% 52% 20% . .
1	C	1676	 2% 24% 52% 20% . .
2	B	1642	 2% 23% 38% 13% . 25%
2	D	1642	 2% 23% 38% 13% . 25%

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	NAG	B	2002	-	-	-	X
3	NAG	D	2002	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45268 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.

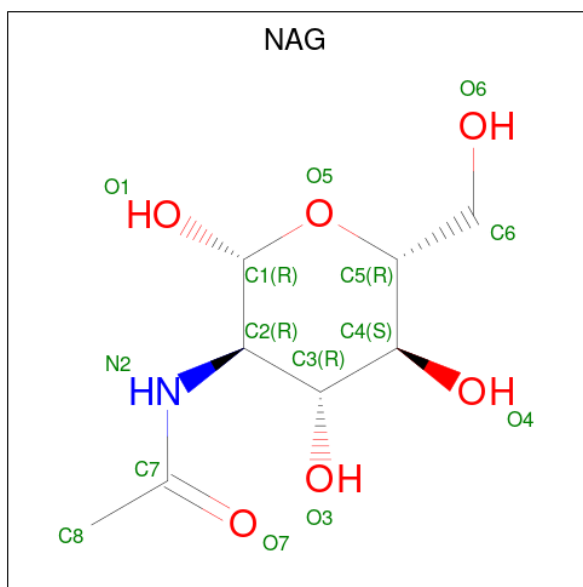
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1627	12881	8246	2114	2469	52	0	0	0
1	C	1627	12881	8246	2114	2469	52	0	0	0

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1225	9711	6187	1633	1851	40	0	0	0
2	D	1225	9711	6187	1633	1851	40	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

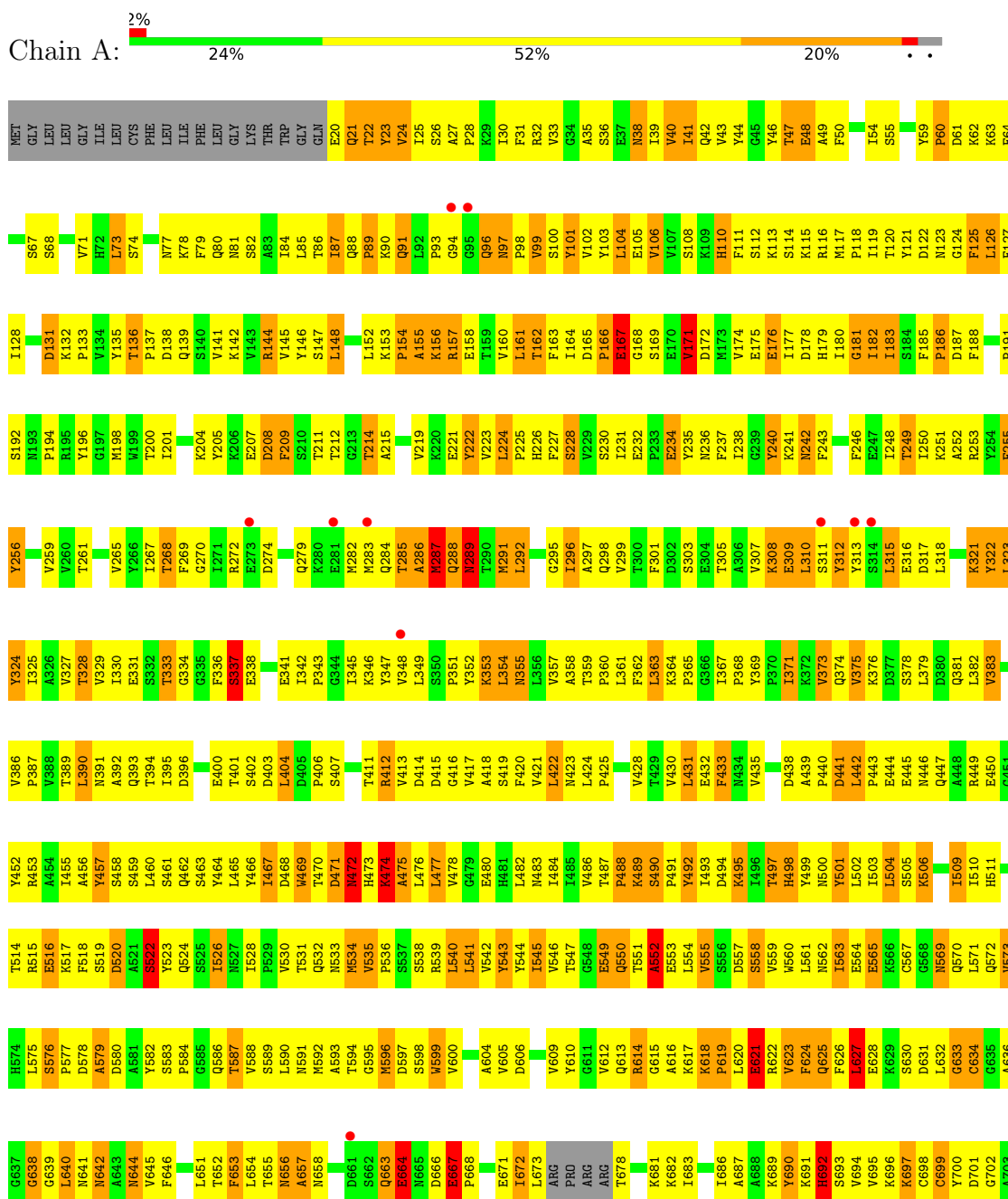


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

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.

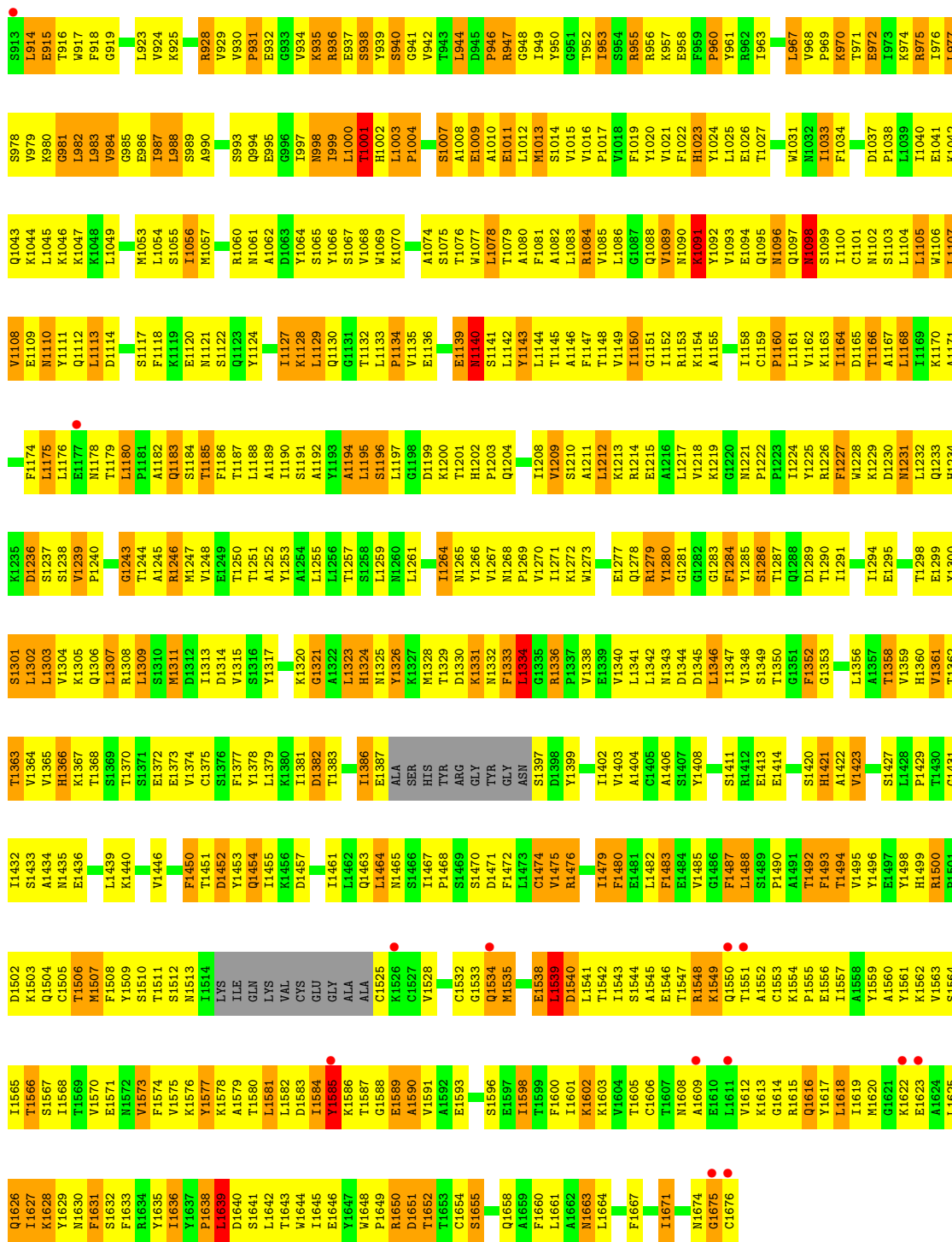
• Molecule 1: Complement C5



● Molecule 1: Complement C5



MET	GLY	LEU	LEU	GLY	ILE	LEU	CYS	PHE	LEU	ILE	PHE	LEU	GLY	GLN	E20	Q21	Q22	T22	Y22	Y23	Y24	T25	S26	A27	P28	K29	F30	F31	R32	V33	G34	A35	S36	E37	R38	V40	V40	I41	Q42	E43	V44	Y44	G45	T46	E48	A49	F50	F54	F64																																																																																																																																																																																																																																																																																																																																																																																
S87	S88	V71	V72	L73	S74	N77	K78	Y205	F80	Q80	N81	S82	A83	I84	L85	T86	I87	Q88	P89	K90	Q91	L92	P93	G94	G95	Q96	N97	F98	P98	Y99	S100	Y101	Y102	S36	S169	L104	E105	V106	H110	F111	E175	S112	I177	S114	D178	H179	I180	M117	I182	I183	T120	Y121	D122	P186	N123	K251	A252	R253	F254	Y255	P256	I128	N193																																																																																																																																																																																																																																																																																																																																																																		
D131	K132	P133	V134	V135	T136	P137	D138	Q139	K204	Y205	K206	E207	D208	F209	S210	Y211	T212	G213	T214	A215	K153	P154	A155	K156	R157	E158	L159	V160	L161	T162	F163	N164	D165	P166	E167	G168	S169	E170	V171	D172	M173	V174	E175	E176	I177	D178	H179	I180	M117	I182	I183	S184	F185	P186	D187	K251	A252	R253	F254	Y255	P256	I128	N193																																																																																																																																																																																																																																																																																																																																																																		
P194	R195	Y196	G197	M198	Y199	T200	L201	K204	Y205	K206	E207	D208	F209	S210	Y211	T212	G213	T214	A215	K153	P154	A155	K156	R157	E158	L159	V160	L161	T162	F163	N164	D165	P166	E167	G168	S169	E170	V171	D172	M173	V174	E175	E176	I177	D178	H179	I180	M117	I182	I183	S184	F185	P186	D187	K251	A252	R253	F254	Y255	P256	I128	N193																																																																																																																																																																																																																																																																																																																																																																			
V259	Y260	T261	V265	Y266	L267	T268	T269	F336	S337	G338	E341	I342	P343	G344	T345	K346	Y347	V348	S350	P351	Y352	K353	L354	M355	L356	V357	A358	T359	P360	L361	F362	T363	F301	B302	S303	E304	T305	A306	V307	I238	G239	K308	E309	L310	S311	Y312	Y313	S314	L315	E316	D317	L318	K321	L323	Y324	I325	T326	V386	P387	Y388	S392	T389																																																																																																																																																																																																																																																																																																																																																																			
T328	V329	I330	E331	S332	Y333	G334	G335	F336	S337	G338	E341	I342	P343	G344	T345	K346	Y347	V348	S350	P351	Y352	K353	L354	M355	L356	V357	A358	T359	P360	L361	F362	T363	F301	B302	S303	E304	T305	A306	V307	I238	G239	K308	E309	L310	S311	Y312	Y313	S314	L315	E316	D317	L318	K321	L323	Y324	I325	T326	V386	P387	Y388	S392	T389																																																																																																																																																																																																																																																																																																																																																																			
L390	N391	A392	Q393	T394	I395	D396	Y397	N398	Q399	E400	T401	D403	L404	D405	P406	S407	T411	R412	L349	S350	P351	Y352	K353	L354	M355	L356	V357	A358	T359	P360	L361	F362	T363	F301	B302	S303	E304	T305	A306	V307	I238	G239	K308	E309	L310	S311	Y312	Y313	S314	L315	E316	D317	L318	K321	L323	Y324	I325	T326	V386	P387	Y388	S392	T389																																																																																																																																																																																																																																																																																																																																																																		
R453	A454	L455	A456	Y457	S458	S459	L460	S461	Q462	S463	Y464	L465	L466	L467	W468	T470	D471	M472	H473	K474	A475	L476	L477	V478	G479	H481	L482	Y483	V484	K485	S486	L487	K488	K489	P491	Y492	E493	D494	M494	V495	K496	T497	H498	Y499	N500	N501	L502	L503	L504	S505	E506	K507	L508	N509	H511	F512	G513	T514																																																																																																																																																																																																																																																																																																																																																																							
R515	E516	K517	F518	S519	D520	A521	S522	Y523	Q524	S525	Y526	L527	S528	F529	M530	T531	Y532	N533	M534	V535	P536	S537	S538	R539	L540	L541	V542	Y543	Y544	L545	V546	G547	Q548	H481	K489	P491	Y492	E493	D494	M494	V495	K496	T497	H498	Y499	N500	N501	L502	L503	L504	S505	E506	K507	L508	N509	H511	F512	G513	T514																																																																																																																																																																																																																																																																																																																																																																						
P577	S578	D580	A581	Y582	S583	F584	G585	Y586	Q587	S588	T589	L590	N591	M592	D593	Y594	G595	M596	D597	S598	Y599	V600	A604	V605	D606	V609	V610	G611	V612	Q613	R614	G615	A616	K617	K618	L619	L620	E621	R622	V623	F624	G625	F626	L627	E628	K629	S630	D631	L632	G633	C634	G635	L636	V637	E638	F639	G640	V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V663	V664	V665	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681	V682	V683	V684	V685	V686	V687	V688	V689	V690	V691	V692	V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V708	V709	V710	V711	V712	V713	V714	V715	V716	V717	V718	V719	V720	V721	V722	V723	V724	V725	V726	V727	V728	V729	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000



ASX	V1339	L1278	ALA	GLN	ALA	ASN	GLN	ALA	SER	K912	E842	D782	LEU	L587	R519	I454	S886	S317
GLY	V1340	I1279	LEU	PRO	LEU	TYR	PRO	LEU	ILE	L913	D843	S783	LEU	M588	F520	K454	M367	V316
GLY	V1341	E1280	LEU	ASP	LEU	LEU	ASP	LEU	ASP	K914	I844	T784	LEU	M589	V521	K455	M368	V319
GLY	V1342	L1281	ALA	GLN	ALA	LEU	GLN	ALA	GLY	V915	T845	T785	ASP	I583	A522	D458	T369	V320
GLY	V1343	P1282	LEU	VAL	LEU	LYS	VAL	LEU	SER	V916	V846	T786	SER	S594	Y523	N459	T390	M321
GLY	V1344	D1283	LEU	PHE	LEU	LYS	PHE	LEU	ASN	V917	R847	T787	ASN	O595	Y524	N460	D383	K322
GLY	V1345	R1284	LYS	LYS	LEU	ASN	LYS	LEU	ASN	E918	V848	V788	ALA	A596	Q525	R461	D394	E323
GLY	V1346	E1285	MET	LYS	ASN	ASN	LYS	LEU	ASN	G919	E849	V789	SER	K597	Q526	V462	C394	
GLY	V1347	V1286	LYS	ASN	HIS	HIS	ASN	LEU	HIS	L790	L850	L790	LYS	M598	G527	V463	T395	S326
GLY	V1348	P1287	LYS	ALA	ASP	LEU	ALA	LEU	SER	Q921	L851	V791	ALA	F464	N528	F464	L398	D327
GLY	V1349	I1288	PHE	HIS	ASP	LEU	HIS	LEU	ASP	V792	V852	V792	ALA	N465	N529	N465	L399	M328
GLY	V1350	R1289	ASP	SER	ARG	LEU	VAL	LEU	GLY	S923	R853	S793	GLU	E530	E530	V466	I399	V329
GLY	V1351	L1290	GLN	THR	THR	THR	THR	LEU	THR	I924	M853	S794	PHE	I531	I531	K467	L401	V330
GLY	V1352	R1291	THR	ALA	PRO	PRO	ALA	LEU	PRO	V925	F856	T795	LEU	K604	V522	G468	N401	
GLY	V1353	I1292	GLY	GLY	SER	THR	GLY	LEU	SER	T926	C857	T796	ALA	S605	A533	M463	L402	Q333
GLY	V1354	M1293	PRO	THR	THR	THR	PHE	THR	GLY	T927	S858	T797	ALA	D606	A533	M463	L402	
GLY	V1355	L1294	ILE	THR	THR	THR	THR	THR	GLY	T928	A859	V798	ASP	F607	S535	F464	P403	
GLY	V1356	M1295	VAL	GLN	ASN	GLY	GLN	ASN	GLY	K929	S860	G799	ASP	G608	V536	N404	L404	
GLY	V1357	A1296	ARG	ARG	ARG	ALA	ARG	ALA	GLU	L930	T861	I800	ARG	M537	W537	L473	N406	
GLY	V1358	A1297	TRP	ALA	ALA	ALA	ALA	ALA	GLU	V937	K862	C801	LYS	S643	W538	L473	A406	
GLY	V1359	L1298	LEU	SER	LEU	TYR	ILE	LEU	ASN	T937	K863	R802	LYS	G614	V538	I476	S407	
GLY	V1360	L1299	LEU	SER	LEU	TYR	ILE	LEU	ASN	G938	K864	A803	CYS	G614	Q407	K477	S408	
GLY	V1361	A1300	ASP	SER	LEU	LEU	GLY	LEU	ILE	G939	K865	E804	GLU	N616	L409	K477	L409	
GLY	V1362	R1301	GLN	TRP	ALA	ALA	ALA	ALA	MET	T940	R866	P805	VAL	N617	P410	F479	P410	
GLY	V1363	L1302	ASN	THR	ALA	ALA	THR	THR	MET	Q941	R867	Y806	VAL	L618	R414	F479	R414	
GLY	V1364	V1303	PHE	THR	ALA	ALA	THR	THR	ALA	L942	K868	E807	MET	M619	M445	Y481	T415	
GLY	V1365	E1304	THR	GLU	ALA	ALA	ALA	ALA	ALA	E943	K869	I808	HIS	V620	M445	Y481	T415	
GLY	V1366	L1305	GLY	GLU	ALA	ALA	ALA	ALA	ALA	E944	R870	I809	GLU	F621	G546	L482	M416	
GLY	V1367	K1306	GLU	VAL	VAL	VAL	VAL	VAL	ILE	V944	R871	I810	GLU	F621	G546	L482	M416	
GLY	V1368	L1307	THR	VAL	VAL	VAL	VAL	VAL	ILE	V945	P871	V811	ASN	E622	T547	I483	H417	
GLY	V1369	M1308	THR	VAL	VAL	VAL	VAL	VAL	ILE	K946	R872	M811	PRO	E622	L548	L484	G418	
GLY	V1370	Q1309	TYR	LYS	VAL	VAL	VAL	VAL	ILE	A947	K873	K812	PRO	E622	V549	M485	D419	
GLY	V1371	D1310	GLY	VAL	VAL	VAL	VAL	VAL	ILE	R948	K873	R748	MET	G625	V550	K486	L420	
GLY	V1372	L1310	GLN	PHE	VAL	VAL	VAL	VAL	THR	R949	R878	S749	GLY	L626	V550	K486	L420	
GLY	V1373	I1311	THR	ALA	ALA	VAL	ALA	ALA	TYR	R949	R878	D750	TYR	A627	D553	K487	R421	
GLY	V1374	T1312	GLN	LEU	ALA	VAL	LEU	LEU	TYR	L950	P881	F751	THR	G627	E423	K488	R422	
GLY	V1375	V1313	ALA	VAL	ALA	VAL	LEU	LEU	LEU	D951	P882	F752	CYS	L628	E423	K488	R422	
GLY	V1376	T1314	THR	ALA	ALA	VAL	VAL	VAL	LEU	D952	F882	F753	THR	L628	E423	K488	R422	
GLY	V1377	A1315	VAL	VAL	VAL	VAL	VAL	VAL	THR	R953	V883	S754	GLY	T630	K491	F490	E423	
GLY	V1378	S1316	MET	LEU	VAL	VAL	VAL	VAL	THR	V954	I884	V755	ARG	S631	K492	F490	E423	
GLY	V1379	G1317	THR	GLU	VAL	VAL	VAL	VAL	GLU	P955	V885	M820	ARG	S631	K492	F490	E423	
GLY	V1380	D1318	ALA	GLY	VAL	VAL	VAL	VAL	GLU	P956	V886	M821	ARG	S631	K492	F490	E423	
GLY	V1381	G1319	PHE	GLY	VAL	VAL	VAL	VAL	GLU	P957	V887	Y822	LYS	T630	K492	F490	E423	
GLY	V1382	K1320	GLN	GLY	VAL	VAL	VAL	VAL	GLU	P958	V888	S823	LYS	T630	K492	F490	E423	
GLY	V1383	A1321	ALA	ILE	VAL	VAL	VAL	VAL	THR	P959	V889	V824	ILE	T630	K492	F490	E423	
GLY	V1384	L1322	ALA	SER	VAL	VAL	VAL	VAL	THR	E960	V890	V825	GLN	T630	K492	F490	E423	
GLY	V1385	M1323	ALA	HIS	VAL	VAL	VAL	VAL	GLY	P961	L891	K826	GLY	T630	K492	F490	E423	
GLY	V1386	T1324	GLU	GLY	VAL	VAL	VAL	VAL	ILE	R962	V891	K826	GLY	T630	K492	F490	E423	
GLY	V1387	L1325	TYR	ASP	VAL	VAL	VAL	VAL	ILE	R963	E895	E827	ASP	T630	K492	F490	E423	
GLY	V1388	I1326	TYR	ASP	VAL	VAL	VAL	VAL	ILE	R964	E896	E828	ASP	T630	K492	F490	E423	
GLY	V1389	L1327	ILE	VAL	VAL	VAL	VAL	VAL	ARG	P965	V892	Q829	CYS	T630	K492	F490	E423	
GLY	V1390	F1328	GLN	ASN	VAL	VAL	VAL	VAL	ARG	P966	V893	Q831	LYS	T630	K492	F490	E423	
GLY	V1391	F1329	GLN	ASN	VAL	VAL	VAL	VAL	THR	G967	V894	E831	ALA	T630	K492	F490	E423	
GLY	V1392	F1330	MET	GLY	VAL	VAL	VAL	VAL	GLU	G968	V895	I832	ALA	T630	K492	F490	E423	
GLY	V1393	Y1329	PRO	THR	VAL	VAL	VAL	VAL	GLU	D988	Q901	I833	ALA	T630	K492	F490	E423	
GLY	V1394	M1330	THR	THR	VAL	VAL	VAL	VAL	ALA	E902	E902	I834	PHE	T630	K492	F490	E423	
GLY	V1395	L1331	HIS	ASP	ARG	VAL	VAL	VAL	VAL	A834	E903	I835	LEU	T630	K492	F490	E423	
GLY	V1396	I1332	ASN	SER	TRP	TRP	TRP	TRP	ASN	S772	A903	I836	GLU	T630	K492	F490	E423	
GLY	V1397	L1333	ILE	SER	LEU	LEU	LEU	LEU	GLN	S773	L904	L836	CYS	T630	K492	F490	E423	
GLY	V1398	I1334	ILE	SER	LEU	LEU	LEU	LEU	GLN	S774	W905	H837	ARG	T630	K492	F490	E423	
GLY	V1399	Q1332	GLY	VAL	VAL	VAL	VAL	VAL	ILE	S775	W906	H838	ARG	T630	K492	F490	E423	
GLY	V1400	L1400	GLY	ASN	VAL	VAL	VAL	VAL	THR	F778	W907	H839	ARG	T630	K492	F490	E423	
GLY	V1401	K1401	THR	THR	THR	THR	THR	THR	THR	F779	W908	H840	TYR	T630	K492	F490	E423	
GLY	V1402	L1402	ALA	ARG	ALA	ALA	ALA	ALA	ILE	F780	W909	H841	ILE	T630	K492	F490	E423	
GLY	V1403	L1403	ALA	ARG	ALA	ALA	ALA	ALA	VAL	R781	R910	H842	VAL	T630	K492	F490	E423	
GLY	V1404	L1404	ALA	ARG	ALA	ALA	ALA	ALA	VAL	R781	R911	H843	VAL	T630	K492	F490	E423	

R1406	L1481	C1490	D1553	K1623
Y1407	M1482	R1491	P1556	L1624
I1408	K1483	Q1492	R1557	C1625
E1412	I1484	A1493	A1558	D1626
M1417	C1485	G1494	K1559	D1627
A1418	C1490	E1495	T1560	F1628
Q1419	R1491	T1496	H1561	A1629
K1420	Q1492	C1497	Q1562	Q1630
V1421	A1493	Q1497	Y1563	S1632
A1422	G1494	Q1566	Q1566	L1635
V1423	E1495	Q1570	Q1570	T1636
I1424	T1496	E1571	E1571	E1637
I1425	C1497	A1572	A1572	T1642
Y1426	L1500	L1573	L1573	
L1427	M1501	N1574	N1574	
N1428	H1502	L1575	L1575	
K1429	Q1503	K1576	K1576	
V1430	E1504	V1577	V1577	
S1431	R1505	N1578	N1578	
H1432	I1506	Y1581	Y1581	
S1433	D1507	L1582	L1582	
C1437	V1508	I1583	I1583	
L1438	P1509	W1584	W1584	
H1439	L1510	L1590	L1590	
I1442	Q1511	L1591	L1591	
L1443	I1512	P1592	P1592	
K1444	E1513	T1593	T1593	
H1445	A1515	K1594	K1594	
F1446	C1516	I1597	I1597	
F1447	E1517	S1598	S1598	
E1447	T1518	Y1599	Y1599	
V1448	M1519	I1600	I1600	
G1449	M1520	I1601	I1601	
F1450	D1521	T1602	T1602	
I1451	Y1522	K1603	K1603	
S1455	V1523	N1604	N1604	
V1456	Y1524	T1605	T1605	
K1457	K1525	Y1606	Y1606	
V1458	T1526	I1607	I1607	
Y1459	K1527	E1608	E1608	
S1460	L1528	R1609	R1609	
L1464	L1529	W1610	W1610	
D1465	R1530	P1611	P1611	
E1466	I1531	H1612	H1612	
K1467	I1531	E1613	E1613	
C1468	Q1534	D1614	D1614	
T1469	D1535	E1615	E1615	
T1470	D1535	C1616	C1616	
K1471	I1539	Q1617	Q1617	
F1471	Y1540	E1618	E1618	
Y1472	V1541	E1619	E1619	
H1473	M1542	E1620	E1620	
P1474	L1545	F1621	F1621	
D1475	I1548	Q1622	Q1622	
L1480	I1548			

4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	176.52Å 179.20Å 389.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 4.30 49.47 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.47-4.30) 94.3 (49.47-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.233 , 0.262 0.225 , 0.250	Depositor DCC
R_{free} test set	1734 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtrriage
Anisotropy	0.503	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 172.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45268	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: NAG

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	0.57	1/13158 (0.0%)	0.77	6/17851 (0.0%)
1	C	0.58	0/13158	0.76	5/17851 (0.0%)
2	B	0.55	0/9912	0.74	1/13454 (0.0%)
2	D	0.55	0/9912	0.74	2/13454 (0.0%)
All	All	0.57	1/46140 (0.0%)	0.75	14/62610 (0.0%)

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	3
1	C	0	3
2	B	0	1
2	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	CYS	CB-SG	-5.27	1.73	1.81

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1539	LEU	CA-CB-CG	6.88	131.12	115.30
1	A	1539	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	1195	LEU	CA-CB-CG	-6.42	100.53	115.30
1	C	1195	LEU	CA-CB-CG	-6.27	100.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1346	ASN	CA-CB-CG	5.54	125.58	113.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	ASN	Peptide
1	A	552	ALA	Peptide
1	A	667	GLU	Peptide
2	B	1351	ASN	Peptide
1	C	472	ASN	Peptide

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	12881	0	12821	1676	0
1	C	12881	0	12821	1666	0
2	B	9711	0	9702	1046	0
2	D	9711	0	9702	1061	0
3	A	14	0	13	2	0
3	B	28	0	26	1	0
3	C	14	0	13	2	0
3	D	28	0	26	1	0
All	All	45268	0	45124	5374	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 59.

The worst 5 of 5374 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)
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.24	1.15
2:D:380:VAL:HG12	2:D:387:MET:HB3	1.26	1.15
2:D:1609:ARG:HG2	2:D:1609:ARG:HH11	1.12	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:H	1:A:411:THR:HG22	1.02	1.12
1:C:386:VAL:H	1:C:411:THR:HG22	1.00	1.11

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	1617/1676 (96%)	1173 (72%)	292 (18%)	152 (9%)	0	12
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	0	12
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	2	24
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	2	23
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	16

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	97	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	1446/1484 (97%)	1108 (77%)	338 (23%)	1	5
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1	5
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1	6
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1	6
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1	5

5 of 1171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	54	LEU
2	D	1497	CYS
2	D	191	LEU
2	D	43	VAL
2	D	588	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	344	GLN
2	D	528	ASN
2	D	1330	ASN
2	B	469	ASN
2	B	417	HIS

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 monosaccharides 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
3	NAG	B	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
3	NAG	B	2001	2	14,14,15	0.81	1 (7%)	17,19,21	2.07	3 (17%)
3	NAG	C	2003	1	14,14,15	0.58	0	17,19,21	2.21	4 (23%)
3	NAG	A	2003	1	14,14,15	0.60	0	17,19,21	2.19	4 (23%)
3	NAG	D	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
3	NAG	D	2001	2	14,14,15	0.74	0	17,19,21	2.16	4 (23%)

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	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NAG	C1-C2	2.16	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NAG	C1-O5-C5	6.57	121.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	NAG	C1-O5-C5	6.17	120.56	112.19
3	A	2003	NAG	C1-O5-C5	5.70	119.91	112.19
3	C	2003	NAG	C1-O5-C5	5.67	119.87	112.19
3	C	2003	NAG	C4-C3-C2	4.36	117.41	111.02

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2003	NAG	C3-C2-N2-C7
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	B	2001	NAG	C8-C7-N2-C2
3	B	2001	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	NAG	1	0
3	C	2003	NAG	2	0
3	A	2003	NAG	2	0
3	D	2001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1627/1676 (97%)	0.03	37 (2%) 60 51	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.01	31 (1%) 66 58	97, 186, 299, 486	0
2	B	1225/1642 (74%)	-0.01	25 (2%) 65 56	107, 174, 261, 395	0
2	D	1225/1642 (74%)	-0.01	18 (1%) 73 64	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.01	111 (1%) 66 58	90, 183, 291, 486	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1355	ASN	5.3
1	A	1650	ARG	5.2
1	A	1622	LYS	4.9
2	B	155	SER	4.8
1	C	1676	CYS	4.8

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 monosaccharides 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(\AA^2)	Q<0.9
3	NAG	B	2002	14/15	0.45	0.44	321,327,336,339	0
3	NAG	A	2003	14/15	0.64	0.38	284,286,289,289	0
3	NAG	C	2003	14/15	0.72	0.34	260,272,284,287	0
3	NAG	D	2002	14/15	0.74	0.47	289,293,305,308	0
3	NAG	B	2001	14/15	0.78	0.26	275,285,305,313	0
3	NAG	D	2001	14/15	0.80	0.31	285,296,309,310	0

6.5 Other polymers [i](#)

There are no such residues in this entry.