



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:46 AM GMT

PDB ID : 3PRX
Title : Structure of Complement C5 in Complex with CVF and SSL7
Authors : Laursen, N.S.; Andersen, G.R.; Sottrup-Jensen, L.; Andersen, K.R.; Spillner, E.; Braren, I.
Deposited on : 2010-11-30
Resolution : 4.30 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

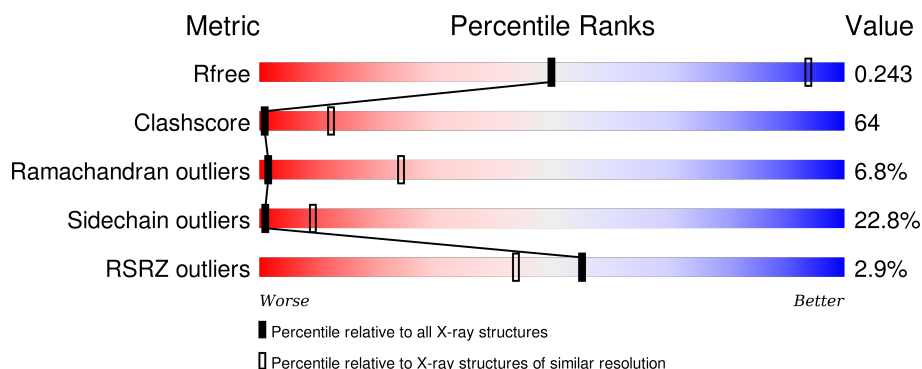
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	1676	<div> <div>24%</div> <div>50%</div> <div>21%</div> <div>• •</div> </div>
1	C	1676	<div> <div>3%</div> <div>23%</div> <div>51%</div> <div>21%</div> <div>• •</div> </div>
2	B	1642	<div> <div>23%</div> <div>38%</div> <div>13%</div> <div>26%</div> </div>
2	D	1642	<div> <div>2%</div> <div>22%</div> <div>39%</div> <div>12%</div> <div>26%</div> </div>
3	X	231	<div> <div>13%</div> <div>26%</div> <div>44%</div> <div>11%</div> <div>•</div> <div>17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Y	231	<div><div></div><div></div><div></div><div></div><div></div></div> <div>7%24%45%13%17%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 48236 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
1	A	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			
1	C	1626	Total	C	N	O	S	0	0	0
			12874	8242	2113	2467	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			
2	D	1215	Total	C	N	O	S	0	0	0
			9635	6143	1617	1836	39			

- Molecule 3 is a protein called Superantigen-like protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
3	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

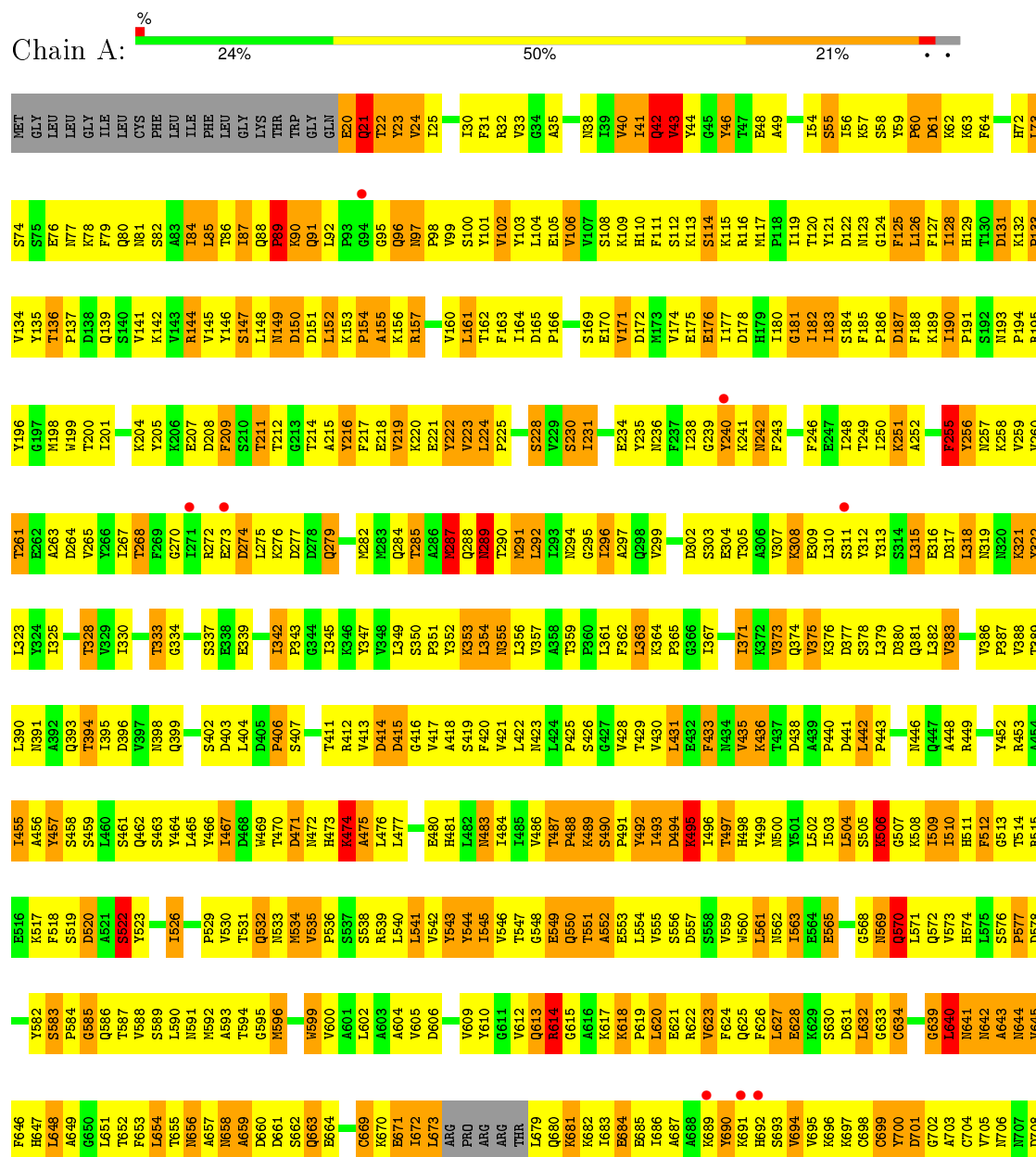
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		

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 ($\text{RSRZ} > 2$). 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

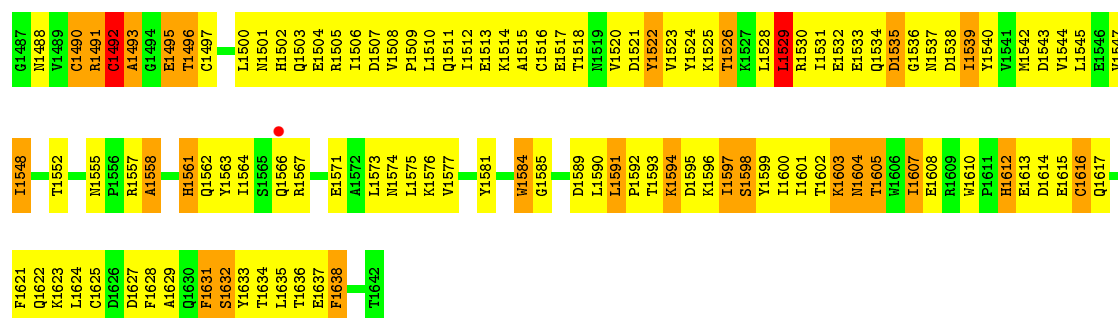




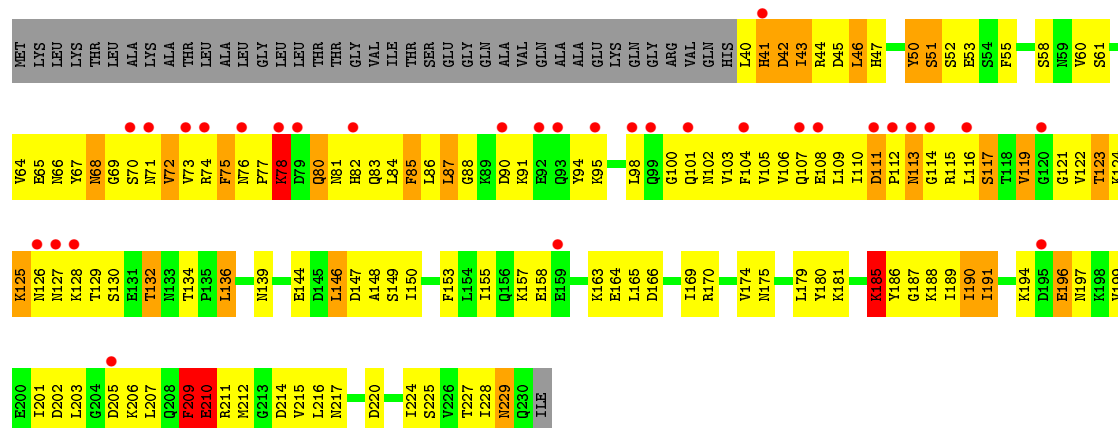




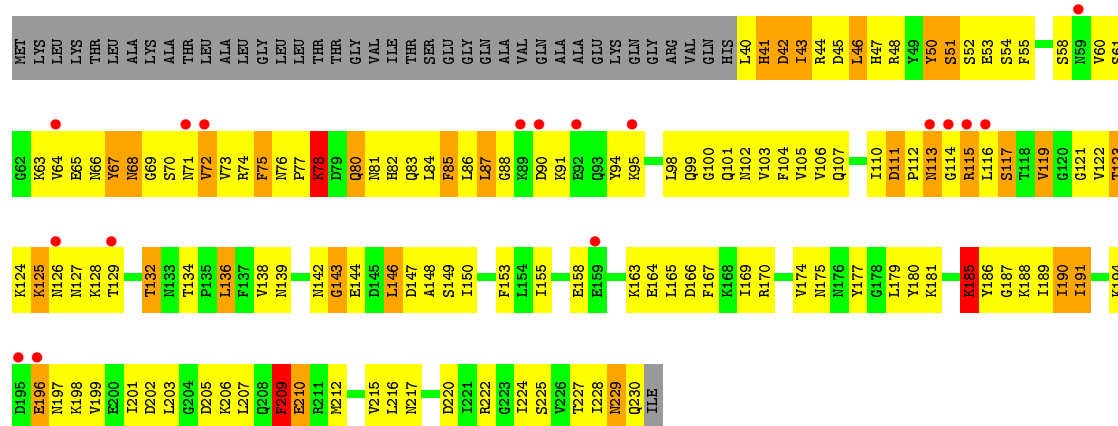
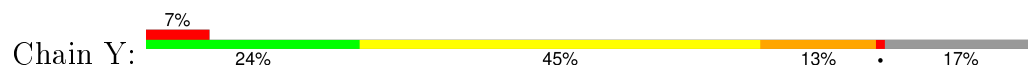
V1421	V1348	E1285	LYS	ASN	ALA	ALA	HIS	S923	S860	I800	ARG	GLN	V538	V1471
A1422	V1349	V1286	LYS	ALA	ASP	ASP	LEU	I924	T861	I801	ASP	ASP	V539	S472
V1423	E1350	P1287	PHE	PRO	HIS	HIS	ILE	V925	R862	C801	ASN	LEU	K541	Q475
I1424	N1351	I1288	ASP	VAL	SER	SER	ILE	T926	R863	V802	ASN	ARG	D542	I476
I1425	I1352	R1289	THR	LEU	TYR	TYR	THR	I927	Q864	A803	D737	LYS	T543	K477
I1426	H1353	Y1290	GLN	SER	ALA	ALA	PRO	R928	R865	P805	G738	CYS	C544	Y478
Y1426	R1291	R1291	GLY	GLY	ALA	ALA	SER	K929	R866	R806	G739	GLY	K545	Y479
L1427	I1292	I1292	PRO	THR	PHE	PHE	GLY	L930	R867	Y807	I740	ASP	G546	F479
N1428	ALA	ALA	ILE	MET	THR	THR	CYS	D931	Q868	R808	I741	VAL	T547	Y480
V1430	E1294	Y1294	VAL	GLN	ASN	ASN	GLY	P932	R869	I808	D742	MET	L548	L482
S1431	E1295	E1295	ARG	GLY	ARG	ARG	GLY	R933	R870	R809	R743	GLY	V550	L483
H1432	N1296	N1296	THR	GLY	ALA	ALA	GLN	V937	R871	V810	D744	HIS	K551	L484
S1433	A1297	A1297	ILE	ASN	SER	SER	ASN	G938	R872	M811	G745	GLY	G552	
E1434	L1298	L1298	THR	MET	SER	SER	MET	G939	R873	K812	I746	ASN	D553	K488
D1435	L1299	L1299	ASP	GLY	SER	SER	ILE	G940	R874	R813	I747	PRO	D554	F490
E1436	A1300	A1300	ALA	GLN	TRP	TRP	ARG	T940	L875	F814	S747	THR	L555	
E1437	R1301	R1301	ASN	GLY	LEU	LEU	MET	Q941	S876	F815	R748	GLY	I556	K491
L1438	K1366	K1366	PHE	ALA	THR	THR	ALA	L942	S877	I816	S749	TYR	Q557	Y492
H1439	I1367	V1303	TYR	GLY	ALA	ALA	ALA	E943	R878	L817	D750	THR	L628	
	C1368	E1304	GLY	VAL	THR	THR	PRO	T944	R879	L818	F751	CYS	T629	G493
	T1369	T1305	GLY	TYR	VAL	VAL	VAL	I945	R880	Q819	P752	GLY	T630	R494
	R1370	ALA	THR	LEU	VAL	VAL	ILE	K946	P881	M820	R753	LYS	G560	
	Y1371	ALA	TYR	THR	LYS	LYS	ALA	A947	R882	P821		ARG	A561	R497
L1372	ALA	ALA	GLY	ALA	VAL	VAL	THR	R948	V883	R822	L756	ALA	A562	R498
	GLY	GLN	THR	PHE	PHE	PHE	TYR	K949	T884	S823	L757	LYS	M563	
D1376	GLN	THR	ILE	ILE	ALA	ALA	TYR	L950	V885	R824	L758	TYR	K564	
S1377	THR	THR	THR	VAL	ALA	ALA	LEU	D951	P886	R825	L759	ILE	K565	Q501
T1378	ALA	V1313	ALA	VAL	MET	VAL	LEU	R952	R887	K826	K760	GLN	K566	I502
M1379	ALA	T1314	ALA	ALA	ALA	ALA	THR	R953	P888	R827	D761	GLY	S640	I503
V1450	ALA	A1315	ALA	LEU	LYS	LYS	THR	R954	Q889	R828	L762	GLY	E568	V504
I1451	I1381	GLY	MET	LEU	MET	MET	GLY	P955	Q890	Q829	T763	ASP	E569	T505
	I1382	D1318	ALA	GLY	VAL	VAL	GLN	D956	L891	V830	E764	ALA	G569	I506
	D1383	G1319	PHE	SER	ALA	ALA	TRP	T957	P895	E831	E765	CYS	D570	I507
S1384	GLN	T1322	ALA	LYS	GLY	GLY	GLY	E958	R896	R832	Q769	LYS	A573	L508
M1385	ALA	M1323	THR	THR	ILE	ILE	THR	I959	K960	I833		ALA	A574	H509
L1387	LEU	T1324	THR	ILE	SER	SER	LEU	E960	K961	A834		ALA	V575	T511
	ALA	L1325	CYS	CYS	HIS	HIS	GLY	T961	A898	I835	S772	PHE	V880	P512
	GLY	L1326	ASN	ASN	GLY	GLY	ILE	K962		L836	S773	LEU	D581	D513
F1390	TYR	T1327	ASP	ASP	ILE	ILE	ASN	I963	Q901	R837	R774	GLY	D582	L514
L1391	GLY	T1327	TYR	TYR	ILE	ILE	ARG	E964	E902	N838	T775	CYS	K582	T515
P1392	ILE	T1328	ASN	VAL	ILE	ILE	ARG	I965	A903	R839	S776	ARG	A583	
D1393	GLN	Y1329	ALA	ASN	GLY	GLY	THR	Q966	L904	V840	S777	ARG	V584	F518
A1394	MET	M1330	MET	SER	GLY	GLY	THR	Q967	Q905	N841	T778	ARG	V585	R519
E1395	PRO	A1331	PRO	LEU	VAL	VAL	ALA	P968	S906	E842	V779	ILE	Y585	F520
	THR	Q1332	THR	ASP	ARG	ARG	VAL	P969	D907	D843	L780	SER	N888	V521
	HIS	L1333	HIS	ASP	THR	THR	GLY	VAL	G908	I844	R781	LYS	V522	
R1399	ASN	V1339	ASN	SER	TRP	TRP	ASN	VAL	Y909	Y845	D782	GLY	I593	Y523
K1400	ILE	L1400	ILE	SER	LEU	LEU	GLN	ALA	R910	V846	S783	VAL	S594	Y524
Y1401	GLY	LYS	GLY	ILE	ILE	ILE	ILE	GLN	K911	R847	I784	ARG	Q595	Q525
V1404	ALA	ALA	LYS	LYS	ASN	ASN	THR	ILE	K912		T785	GLY	ASP	V526
D1405	ASN	ASN	LYS	LYS	ALA	ALA	GLY	ILE	L913	L850	T786	ASN	I598	G527
R1406	THR	T1275	THR	THR	GLN	GLN	TYR	ASN	R914	L851	R787	GLN	M599	N527
G1407	ALA	D1276	ALA	SER	GLN	GLN	THR	SER	V915	Y852	V788	ARG	M529	N528
I1408	LEU	T1277	LEU	TYR	PRO	PRO	ALA	ILE	V916	N853	V789	GLY	T601	E530
S1409	LEU	I1279	LEU	GLN	ASP	ASP	GLN	GLY	P917	P854		SER	I602	V531
F1410	ALA	F1343	ALA	LEU	GLY	GLY	MET	GLY	E918	A855		GLY	E603	V532
L1480	LEU	H1344	LEU	LYS	ALA	ALA	VAL	SER	G919	R856	S793	LEU	K604	A533
L1481	LEU	H1345	LEU	LYS	PHE	PHE	TYR	LYS	V920	C857	F794	PHE	S605	L534
N1482	LYS	N1346	LYS	TYR	LYS	LYS	LYS	LEU	Q921	S858	T795	LEU	D606	S535
	M1417	V1347	MET	GLY	GLY	GLY	LYS	ASN	K922	A859	P796	ALA	F607	



• Molecule 3: Superantigen-like protein 7



• Molecule 3: Superantigen-like protein 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	163.65Å 181.96Å 392.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 4.30 49.21 – 4.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.21-4.30) 96.9 (49.21-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.208 , 0.261 0.191 , 0.243	Depositor DCC
R_{free} test set	1815 reflections (2.33%)	DCC
Wilson B-factor (Å ²)	116.2	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 160.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77966 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48236	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [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	0.60	1/13151 (0.0%)	0.80	3/17841 (0.0%)
1	C	0.60	0/13151	0.80	5/17841 (0.0%)
2	B	0.53	1/9833 (0.0%)	0.73	2/13345 (0.0%)
2	D	0.54	0/9833	0.74	3/13345 (0.0%)
3	X	0.47	1/1560 (0.1%)	0.67	1/2096 (0.0%)
3	Y	0.49	0/1560	0.69	1/2096 (0.0%)
All	All	0.57	3/49088 (0.0%)	0.77	15/66564 (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	2
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	210	GLU	C-N	5.35	1.46	1.34
2	B	347	PHE	CB-CG	-5.29	1.42	1.51
1	A	42	GLN	CB-CG	5.16	1.66	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	PHE	CB-CA-C	-7.26	95.88	110.40
2	D	347	PHE	CB-CA-C	-6.90	96.60	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	640	LEU	CA-CB-CG	6.49	130.23	115.30
1	C	640	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	871	PRO	CA-N-CD	-6.16	102.87	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1504	GLN	Peptide
1	A	98	PRO	Peptide
1	C	1504	GLN	Peptide

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	12874	0	12814	1855	0
1	C	12874	0	12814	1901	0
2	B	9635	0	9630	1082	0
2	D	9635	0	9630	1079	0
3	X	1539	0	1530	166	0
3	Y	1539	0	1530	194	0
4	A	14	0	13	1	0
4	C	14	0	13	2	0
5	B	56	0	50	6	0
5	D	56	0	50	7	0
All	All	48236	0	48074	6152	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 64.

The worst 5 of 6152 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:1525:CYS:O	1:A:1528:VAL:HG22	1.34	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:207:LEU:O	3:X:207:LEU:HD12	1.32	1.24
3:Y:207:LEU:HD12	3:Y:207:LEU:O	1.32	1.23
1:C:386:VAL:H	1:C:411:THR:HG22	1.03	1.17
1:A:500:ASN:HB2	1:A:543:TYR:CE1	1.79	1.17

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	1616/1676 (96%)	1165 (72%)	300 (19%)	151 (9%)	1	16
1	C	1616/1676 (96%)	1179 (73%)	290 (18%)	147 (9%)	1	16
2	B	1203/1642 (73%)	981 (82%)	176 (15%)	46 (4%)	4	39
2	D	1203/1642 (73%)	982 (82%)	177 (15%)	44 (4%)	4	40
3	X	189/231 (82%)	148 (78%)	31 (16%)	10 (5%)	2	30
3	Y	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	2	28
All	All	6016/7098 (85%)	4605 (76%)	1002 (17%)	409 (7%)	1	24

5 of 409 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	150	ASP

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	1445/1484 (97%)	1090 (75%)	355 (25%)	1	7
1	C	1445/1484 (97%)	1098 (76%)	347 (24%)	1	7
2	B	1084/1435 (76%)	849 (78%)	235 (22%)	1	10
2	D	1084/1435 (76%)	855 (79%)	229 (21%)	1	11
3	X	175/205 (85%)	143 (82%)	32 (18%)	2	16
3	Y	175/205 (85%)	142 (81%)	33 (19%)	2	14
All	All	5408/6248 (87%)	4177 (77%)	1231 (23%)	1	9

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1480	LEU
1	C	435	VAL
2	D	1480	LEU
2	B	1539	ILE
1	C	161	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	77	ASN
1	C	658	ASN
3	X	113	ASN
1	C	97	ASN
1	C	294	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 carbohydrates 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
5	NAG	B	2001	2,5	14,14,15	0.97	1 (7%)	15,19,21	1.67	3 (20%)
5	NAG	B	2002	5	14,14,15	0.99	1 (7%)	15,19,21	2.48	5 (33%)
5	NAG	B	2003	2,5	14,14,15	2.03	7 (50%)	15,19,21	3.44	5 (33%)
5	NAG	B	2004	5	14,14,15	1.69	1 (7%)	15,19,21	1.68	4 (26%)
5	NAG	D	2001	2,5	14,14,15	0.88	1 (7%)	15,19,21	1.70	4 (26%)
5	NAG	D	2002	5	14,14,15	1.05	1 (7%)	15,19,21	1.74	3 (20%)
5	NAG	D	2003	2,5	14,14,15	1.95	6 (42%)	15,19,21	3.68	6 (40%)
5	NAG	D	2004	5	14,14,15	1.57	1 (7%)	15,19,21	1.81	4 (26%)

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
5	NAG	B	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2002	5	-	0/6/23/26	0/1/1/1
5	NAG	D	2003	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2004	5	-	0/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2003	NAG	C3-C2	2.02	1.57	1.52
5	B	2003	NAG	C2-N2	2.11	1.50	1.46
5	B	2002	NAG	C3-C2	2.13	1.57	1.52
5	D	2003	NAG	C3-C2	2.25	1.57	1.52
5	D	2003	NAG	C4-C5	2.43	1.58	1.53

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2001	NAG	O3-C3-C2	-2.78	103.61	109.11
5	D	2004	NAG	O7-C7-C8	-2.49	117.50	122.06
5	D	2003	NAG	O3-C3-C2	-2.31	104.54	109.11
5	B	2004	NAG	O7-C7-C8	-2.26	117.91	122.06
5	D	2001	NAG	C3-C4-C5	-2.19	106.39	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	3	0
5	B	2002	NAG	3	0
5	B	2003	NAG	3	0
5	D	2001	NAG	4	0
5	D	2002	NAG	4	0
5	D	2003	NAG	3	0

5.6 Ligand geometry

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
4	NAG	A	2003	1	14,14,15	1.79	4 (28%)	15,19,21	3.50	11 (73%)
4	NAG	C	2003	1	14,14,15	2.01	4 (28%)	15,19,21	2.62	8 (53%)

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
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2003	NAG	O4-C4	2.13	1.48	1.43
4	A	2003	NAG	C4-C3	2.14	1.58	1.52
4	A	2003	NAG	C4-C5	2.14	1.57	1.53
4	A	2003	NAG	O4-C4	2.39	1.48	1.43
4	C	2003	NAG	C4-C5	3.06	1.59	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	NAG	O7-C7-C8	-5.17	112.57	122.06
4	C	2003	NAG	O7-C7-C8	-3.58	115.49	122.06
4	A	2003	NAG	C3-C4-C5	-3.57	103.97	110.20
4	A	2003	NAG	O3-C3-C4	-3.23	103.06	110.34
4	C	2003	NAG	C4-C3-C2	2.03	114.38	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	NAG	1	0
4	C	2003	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1626/1676 (97%)	0.00	20 (1%) 81 73	72, 150, 260, 469	0
1	C	1626/1676 (97%)	0.08	58 (3%) 46 37	60, 153, 277, 515	0
2	B	1215/1642 (73%)	0.06	23 (1%) 70 61	73, 160, 235, 335	0
2	D	1215/1642 (73%)	0.01	26 (2%) 67 57	85, 155, 241, 362	0
3	X	191/231 (82%)	0.75	31 (16%) 3 4	99, 230, 333, 437	0
3	Y	191/231 (82%)	0.46	17 (8%) 12 9	95, 195, 300, 385	0
All	All	6064/7098 (85%)	0.07	175 (2%) 55 44	60, 157, 264, 515	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	112	PRO	12.0
3	Y	114	GLY	7.0
1	C	1651	ASP	5.9
3	X	114	GLY	5.8
3	X	113	ASN	5.7

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](#)

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
5	NAG	B	2002	14/15	0.72	0.69	-	228,239,253,257	0
5	NAG	D	2001	14/15	0.88	0.41	-	228,253,282,288	0
5	NAG	D	2002	14/15	0.66	0.60	-	228,239,251,252	0
5	NAG	B	2001	14/15	0.73	0.55	-	278,305,319,322	0
5	NAG	D	2004	14/15	0.72	0.83	-	271,274,277,278	0
5	NAG	D	2003	14/15	0.54	0.53	-	246,253,258,265	0
5	NAG	B	2003	14/15	0.24	0.78	-	225,233,240,245	0
5	NAG	B	2004	14/15	0.56	0.78	-	297,301,307,310	0

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	NAG	C	2003	14/15	0.74	0.40	0.85	177,180,183,183	0
4	NAG	A	2003	14/15	0.77	0.29	0.34	166,169,171,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.