



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:35 am GMT

PDB ID : 1Z68
Title : Crystal Structure Of Human Fibroblast Activation Protein alpha
Authors : Aertgeerts, K.; Levin, I.; Shi, L.; Prasad, G.S.; Zhang, Y.; Kraus, M.L.;
Salakian, S.; Snell, G.P.; Sridhar, V.; Wijnands, R.; Tennant, M.G.
Deposited on : 2005-03-21
Resolution : 2.60 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

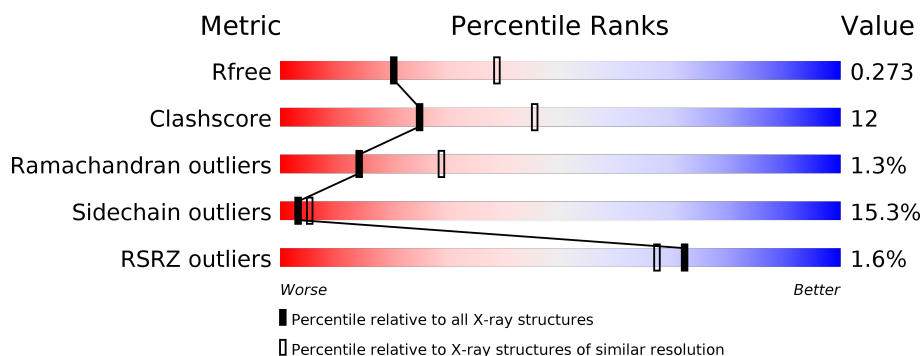
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	719	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>7%</div> </div> </div>
1	B	719	<div> <div></div> <div> <div>63%</div> <div>30%</div> <div>6%</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
3	NAG	A	9201	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12600 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 fibroblast activation protein, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5889	3812	961	1094	22			
1	B	719	Total	C	N	O	S	0	6	0
			5915	3825	965	1103	22			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

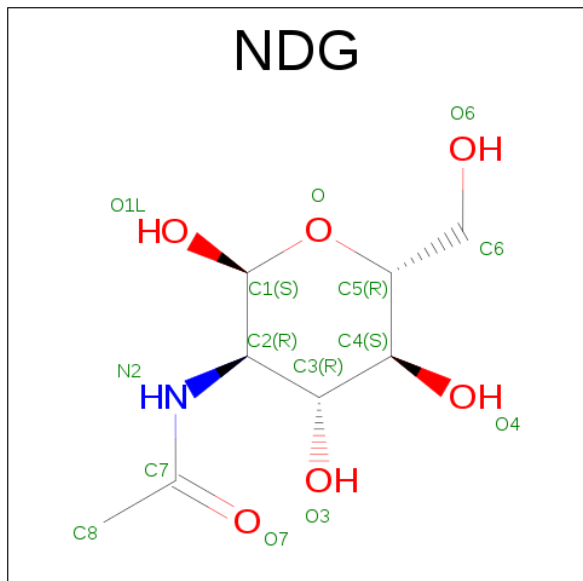
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

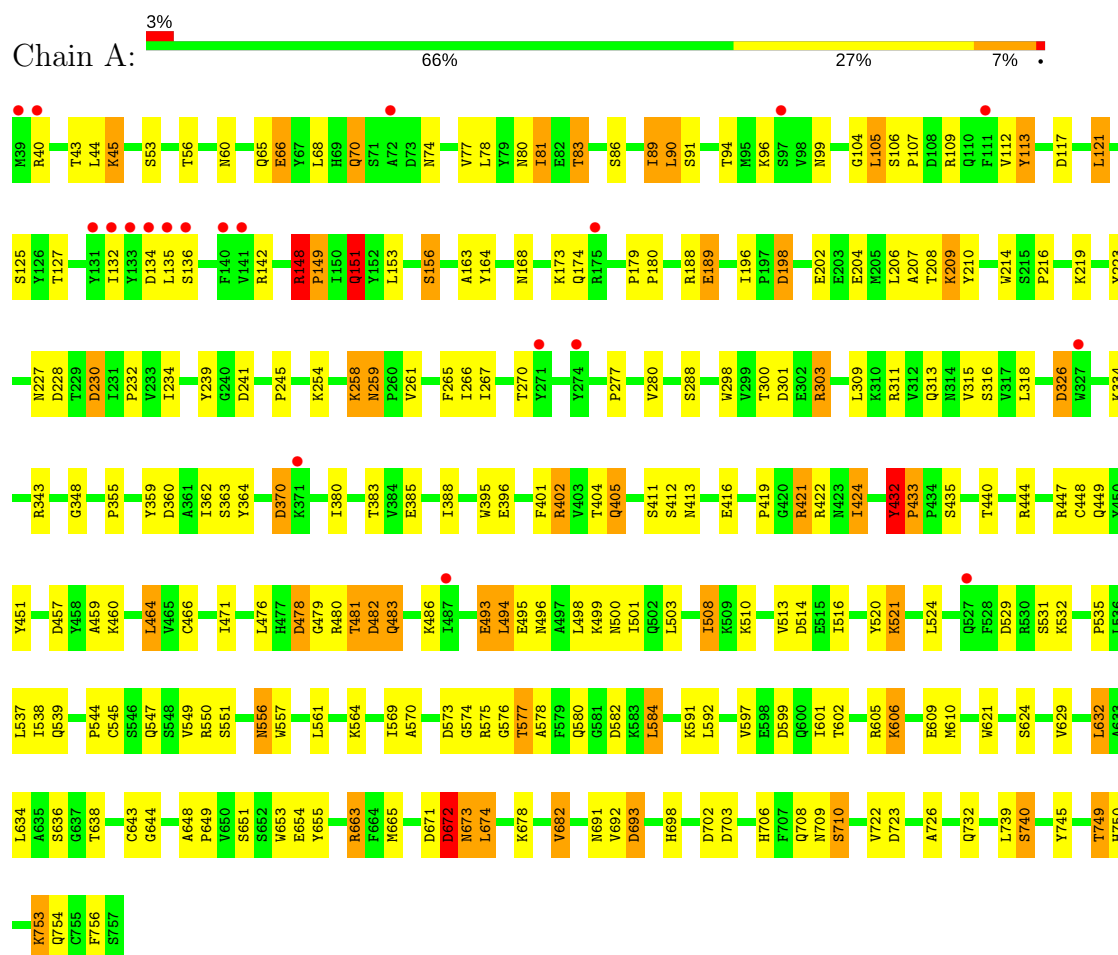
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total 208	O 208	0	0
6	B	420	Total 420	O 420	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: fibroblast activation protein, alpha subunit



Y729	S730	D731	Q732	N733	H734	G738	L739	S740	H743	T746	H747	M748	F751	L752	K753	Q754	C755	F756	S757																																	
Y625	F628	V629	L632			S636	G637	T638	G639	L640	F641	K642	C643	G644	I645	A648	P649	V650	S651	S652	W653	E654	Y655	Y656	V659	V660	T661	L667	K670	D671	D672	T681	R685	A686	F689	D693	N704	V705	H706	F707	Q708	N709	I713	V722	D723	W728						
L524	P525			F528	F529	R530	S531	K532	K533	Y534	P535	C545	S546	Q547	R550	S551	V552	N556	S559	Y560		V568		D573	G574	R575	G576	T577	A578	F579	Q580	K583	L584	L585	R590	K591	L592	D599	G600	I601	R605	F612	K616	R617	I620	W621	G622	W623	S624			
T440	L443			R447	C448	Q449	Y450	Y451		F455	S456		Y462	A463	L464	V465	C466		T471		S474	H477	D478	G479	R480	T481	D482	Q483	E484	T485	K486	E490	N491	K492	E493	L494	E495	N496	A497	L498	K499		L503	E506	K509	K510	D514	T517	L518	K521	M522	I523
H338	F350			S353		V356	Y359	D360	T247	A361	I362	S363	Y364	D370	K371	D372	K375	H376	T380	K381	D382	T383	V384	T391	W395	E396	F401	R402	V403	D406	S411	S412	N413	E414	R421	R422	N423	I424	Y425	R426	I427	S431	Y432	P433	P434	S435	C438	V439				
A235	D241	E242	Q243	Y244	P245	R246	T247	I248	K254	K258	V262	T266	T267	D268	T269	T270	Y271	P272		P277		V280	P281	V282	D290	Y291	Y292	D301	E302	R303	L306	R311	L318	D322	F323	R324	E325	B326	W330	D331	C332	P333	K334	T335	Q336	E337						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.30Å 152.58Å 214.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.60) 97.7 (49.49-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.283 0.220 , 0.273	Depositor DCC
R_{free} test set	3550 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.0	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	0.93	EDS
Total number of atoms	12600	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

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

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	0.43	0/6065	0.73	20/8250 (0.2%)
1	B	0.53	0/6119	0.81	24/8322 (0.3%)
All	All	0.48	0/12184	0.77	44/16572 (0.3%)

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	2
3	A	1	0
All	All	1	4

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ASP	CB-CG-OD2	7.81	125.33	118.30
1	B	301	ASP	CB-CG-OD2	7.50	125.05	118.30
1	B	108	ASP	CB-CG-OD2	7.06	124.65	118.30
1	B	78	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	117	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	228	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	582	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	290	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	702	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	149	PRO	N-CD-CG	-6.17	93.94	103.20
1	B	117	ASP	CB-CG-OD2	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	360	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	372	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	46	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	42	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	693	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	723	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	599	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	723	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	331	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	573	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	671	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	703	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	198	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	482	ASP	CB-CG-OD2	5.39	123.16	118.30
1	B	514	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	478	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	326	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	134	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	370	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	672	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	241	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	478	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	360	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	529	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	457	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	514	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	230[A]	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	230[B]	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	326	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	482	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	241	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	672	ASP	CB-CG-OD2	5.03	122.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	9201	NAG	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Peptide
1	A	432	TYR	Peptide
1	B	148	ARG	Peptide
1	B	432	TYR	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	5889	0	5660	128	0
1	B	5915	0	5674	165	0
2	A	28	0	26	0	0
2	B	42	0	39	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	28	0	25	1	0
5	B	14	0	13	0	0
6	A	208	0	0	4	0
6	B	420	0	0	6	0
All	All	12600	0	11487	287	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 12.

All (287) 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:148:ARG:HB3	1:A:149:PRO:HD2	1.34	1.07
1:B:376:HIS:ND1	1:B:391:THR:HG22	1.72	1.05
1:B:254:LYS:NZ	1:B:706:HIS:HD2	1.65	0.93
1:B:651:SER:H	1:B:709:ASN:HD22	1.14	0.93
1:A:651:SER:H	1:A:709:ASN:HD22	0.97	0.92
1:B:151:GLN:HE22	1:B:168:ASN:H	1.22	0.88
1:A:651:SER:H	1:A:709:ASN:ND2	1.70	0.88
1:B:396:GLU:H	1:B:413:ASN:HD21	1.23	0.86
1:A:421:ARG:HB2	1:A:449:GLN:O	1.78	0.82
1:A:745:TYR:O	1:A:749:THR:CG2	2.30	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD13	1:B:48:LEU:HD11	1.64	0.79
1:A:574:GLY:O	1:A:577:THR:HB	1.82	0.79
1:A:43:THR:HG22	1:A:45:LYS:NZ	1.96	0.79
1:A:148:ARG:HB3	1:A:149:PRO:CD	2.13	0.78
1:B:132:ILE:HD11	1:B:176:PRO:HB3	1.66	0.77
1:A:43:THR:HG22	1:A:45:LYS:HZ2	1.48	0.76
1:B:55:LYS:H	1:B:491:ASN:HD21	1.34	0.76
1:B:197:PRO:HA	1:B:226:PHE:CE2	2.23	0.74
1:B:254:LYS:HZ3	1:B:706:HIS:HD2	1.32	0.74
1:B:218:GLY:O	1:B:269:THR:HG21	1.87	0.74
1:A:651:SER:N	1:A:709:ASN:HD22	1.79	0.73
1:B:173:LYS:HE3	1:B:178:ASP:O	1.88	0.73
1:B:638:THR:HG23	1:B:640:LEU:H	1.53	0.73
1:B:421:ARG:HD3	1:B:449:GLN:HE21	1.54	0.72
1:A:254:LYS:NZ	1:A:706:HIS:HD2	1.88	0.72
1:B:254:LYS:HZ1	1:B:706:HIS:HD2	1.38	0.70
1:A:539:GLN:HE21	1:A:621:TRP:HE1	1.41	0.68
1:A:745:TYR:O	1:A:749:THR:HG23	1.92	0.68
1:A:521:LYS:NZ	1:A:550:ARG:O	2.27	0.67
1:B:391:THR:HG23	1:B:395:TRP:CH2	2.29	0.67
1:B:432:TYR:CD2	1:B:433:PRO:HD3	2.29	0.66
1:B:254:LYS:HZ3	1:B:706:HIS:CD2	2.11	0.66
1:B:704:ASN:C	1:B:704:ASN:HD22	1.97	0.66
1:A:597:VAL:HG21	1:A:632:LEU:HB3	1.78	0.66
1:B:732:GLN:HG3	1:B:740:SER:OG	1.95	0.66
1:B:573:ASP:HB3	1:B:577:THR:HG21	1.77	0.65
1:B:175:ARG:HG2	1:B:176:PRO:HD2	1.78	0.65
1:A:254:LYS:HE3	1:A:655:TYR:HA	1.79	0.65
1:B:734:HIS:CD2	6:B:9595:HOH:O	2.50	0.64
1:B:254:LYS:NZ	1:B:706:HIS:CD2	2.57	0.64
1:A:404:THR:HG22	1:A:405:GLN:H	1.62	0.64
1:B:132:ILE:CD1	1:B:176:PRO:HB3	2.26	0.64
1:B:254:LYS:HZ2	1:B:708:GLN:HE22	1.45	0.64
1:A:481:THR:CG2	1:A:483:GLN:HB2	2.28	0.63
1:B:208:THR:CG2	1:B:210:TYR:O	2.47	0.63
1:A:575:ARG:HA	1:A:584:LEU:HD22	1.80	0.63
1:B:422:ARG:HH12	1:B:547:GLN:NE2	1.97	0.63
1:A:105:LEU:HD11	1:A:109:ARG:HG2	1.81	0.62
1:B:651:SER:HB3	1:B:713:ILE:HD11	1.81	0.62
1:B:208:THR:HG23	1:B:210:TYR:H	1.64	0.62
1:A:513:VAL:HG11	1:A:606:LYS:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:TYR:O	1:A:749:THR:HG22	1.98	0.61
1:B:221:LEU:HB3	1:B:267:ILE:HD11	1.82	0.61
1:B:396:GLU:H	1:B:413:ASN:ND2	1.96	0.61
1:A:245:PRO:HD3	1:B:708:GLN:OE1	2.01	0.60
1:B:221:LEU:HB3	1:B:267:ILE:CD1	2.33	0.59
1:B:652:SER:HB2	1:B:681:THR:HG22	1.85	0.59
1:B:208:THR:HG23	1:B:210:TYR:O	2.02	0.59
1:B:55:LYS:H	1:B:491:ASN:ND2	2.01	0.58
1:B:254:LYS:NZ	1:B:708:GLN:HE22	2.01	0.58
1:A:148:ARG:CB	1:A:149:PRO:HD2	2.23	0.58
1:A:223:TYR:CZ	1:A:265:PHE:HB2	2.39	0.58
1:B:292:TYR:CZ	1:B:659:VAL:HG22	2.39	0.58
1:A:422:ARG:NH2	1:A:547:GLN:OE1	2.33	0.57
1:B:432:TYR:CD2	1:B:433:PRO:CD	2.87	0.57
1:A:498:LEU:HD22	1:A:503:LEU:HD11	1.85	0.57
1:B:80:ASN:ND2	1:B:83:THR:H	2.02	0.57
1:B:75:ASN:ND2	1:B:92:ASN:H	2.02	0.57
1:A:577:THR:CG2	6:A:9281:HOH:O	2.52	0.57
1:B:324:ARG:NH2	1:B:326:ASP:OD1	2.38	0.57
1:B:547:GLN:O	1:B:550:ARG:NH2	2.37	0.56
1:A:544:PRO:HA	1:A:576:GLY:O	2.06	0.56
1:B:651:SER:H	1:B:709:ASN:ND2	1.94	0.56
1:A:254:LYS:NZ	1:A:708:GLN:HE22	2.04	0.56
1:B:535:PRO:HB3	1:B:617:ARG:HB3	1.88	0.56
1:B:161:LYS:HE2	1:B:174:GLN:HE21	1.71	0.55
1:B:574:GLY:O	1:B:577:THR:HB	2.06	0.55
1:B:423:ASN:HD21	1:B:449:GLN:NE2	2.04	0.55
1:B:620:ILE:O	1:B:644:GLY:HA2	2.07	0.55
1:B:733:ASN:HD22	1:B:733:ASN:H	1.53	0.55
1:A:634:LEU:HG	1:A:692:VAL:HG21	1.88	0.55
1:A:81:ILE:HD12	1:A:476:LEU:HD21	1.88	0.55
1:B:148:ARG:HB3	1:B:149:PRO:HD2	1.88	0.55
1:A:478:ASP:HB3	1:A:481:THR:HG22	1.88	0.55
1:B:290:ASP:OD1	1:B:311:ARG:NH2	2.39	0.55
1:A:107:PRO:HG2	1:A:156:SER:O	2.07	0.55
1:A:481:THR:HG23	1:A:483:GLN:HB2	1.89	0.54
1:B:217:ASN:HB2	1:B:301:ASP:OD1	2.07	0.54
1:A:227:ASN:HB3	1:A:261:VAL:HG22	1.90	0.54
1:A:508:ILE:HG13	1:A:508:ILE:O	2.06	0.54
1:B:303:ARG:HD2	1:B:322:ASP:OD1	2.08	0.54
1:A:538:ILE:HD13	1:A:570:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:THR:O	1:A:753:LYS:HB2	2.08	0.54
1:A:592:LEU:HD22	1:A:665:MET:HG2	1.89	0.53
1:B:111:PHE:CE1	1:B:176:PRO:HG2	2.43	0.53
1:A:45:LYS:H	1:A:45:LYS:HZ2	1.56	0.53
1:A:654:GLU:HG2	1:B:243:GLN:HG3	1.89	0.53
1:B:645:ILE:HD13	1:B:748:MET:HE2	1.89	0.53
1:A:432:TYR:O	1:A:433:PRO:C	2.45	0.53
1:A:70:GLN:HE22	1:A:74:ASN:HD22	1.56	0.52
1:A:267:ILE:HD12	1:A:277:PRO:HG3	1.91	0.52
1:B:447:ARG:HD3	1:B:471:ILE:O	2.09	0.52
1:B:111:PHE:CD1	1:B:176:PRO:HG2	2.44	0.52
1:B:651:SER:N	1:B:709:ASN:HD22	1.96	0.52
1:B:375:LYS:H	1:B:396:GLU:HG2	1.75	0.52
1:A:722:VAL:O	1:B:743:HIS:HE1	1.93	0.51
1:B:401:PHE:HE1	1:B:411:SER:HB3	1.74	0.51
1:B:601:ILE:HG23	1:B:640:LEU:HD11	1.91	0.51
1:A:70:GLN:NE2	1:A:74:ASN:HD22	2.08	0.51
1:A:479:GLY:H	1:A:482:ASP:H	1.59	0.51
1:B:592:LEU:HG	1:B:625:TYR:OH	2.11	0.51
1:A:580:GLN:HB2	1:A:584:LEU:HD12	1.93	0.51
1:B:643:CYS:HB3	1:B:693:ASP:HB2	1.92	0.51
1:A:557:TRP:CE2	1:A:561:LEU:HD11	2.46	0.50
1:B:226:PHE:CD1	1:B:262:VAL:HG12	2.47	0.50
1:B:380:ILE:HD13	1:B:384:VAL:HG23	1.93	0.50
1:B:421:ARG:HD3	1:B:449:GLN:HB3	1.94	0.50
1:B:212:LEU:HD13	1:B:221:LEU:HD11	1.92	0.50
1:B:455:PHE:CD1	1:B:462:TYR:HB3	2.47	0.50
1:B:625:TYR:O	1:B:629:VAL:HG23	2.11	0.50
1:A:643:CYS:HB3	1:A:693:ASP:HB2	1.94	0.50
1:B:656:TYR:CE2	1:B:704:ASN:ND2	2.80	0.50
1:B:280:VAL:HG11	1:B:306:LEU:HD13	1.93	0.50
1:B:292:TYR:CE2	1:B:659:VAL:HG22	2.47	0.50
1:A:636:SER:HB3	1:A:638:THR:HG23	1.93	0.50
1:B:167:GLN:NE2	6:B:9351:HOH:O	2.44	0.50
1:A:309:LEU:HD22	1:A:313:GLN:HG2	1.94	0.50
1:A:601:ILE:HD13	1:A:638:THR:HG21	1.94	0.49
1:B:545:CYS:HB3	6:B:9224:HOH:O	2.11	0.49
1:A:432:TYR:CD2	1:A:433:PRO:HD3	2.47	0.49
1:A:148:ARG:CB	1:A:149:PRO:CD	2.88	0.49
1:A:395:TRP:HB2	1:A:413:ASN:HB3	1.94	0.49
1:B:391:THR:CG2	1:B:395:TRP:CH2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ASN:O	1:A:674:LEU:C	2.51	0.49
1:B:68:LEU:HD23	1:B:78:LEU:HB2	1.93	0.49
1:A:216:PRO:HD3	1:A:298:TRP:HB3	1.95	0.49
1:A:401:PHE:CE2	1:A:424:ILE:HD11	2.48	0.49
1:A:254:LYS:HG2	1:A:655:TYR:O	2.11	0.48
1:B:427:ILE:HA	1:B:435:SER:O	2.13	0.48
1:B:61:TRP:CE3	1:B:456:SER:HB3	2.48	0.48
1:A:89:ILE:HG13	1:A:135:LEU:HD21	1.96	0.48
1:A:230:ASP:HB2	4:A:2271:NDG:H8C3	1.95	0.48
1:B:623:TRP:HZ2	1:B:734:HIS:O	1.96	0.48
1:B:47:ILE:HD13	1:B:560:TYR:HB2	1.94	0.48
1:B:556:ASN:ND2	1:B:559:SER:OG	2.47	0.48
1:A:43:THR:HG22	1:A:45:LYS:HZ3	1.77	0.48
1:B:391:THR:HG23	1:B:395:TRP:HH2	1.77	0.48
1:A:448:CYS:HB3	1:A:451:TYR:CE2	2.49	0.47
1:A:732:GLN:HG3	1:A:740:SER:OG	2.14	0.47
1:B:267:ILE:HG23	1:B:277:PRO:HA	1.96	0.47
1:B:590:ARG:NH2	1:B:672:ASP:OD2	2.45	0.47
1:A:239:TYR:HA	1:A:245:PRO:HB3	1.97	0.47
1:B:425:TYR:CE2	1:B:438:CYS:HB2	2.49	0.47
1:B:481:THR:HG23	1:B:483:GLN:H	1.80	0.47
1:A:364:TYR:CE2	1:A:380:ILE:HD12	2.50	0.47
1:B:356:VAL:CG2	1:B:403:VAL:HG23	2.45	0.47
1:A:66:GLU:HG2	1:A:78:LEU:HD21	1.96	0.47
1:B:311:ARG:HG2	6:B:9604:HOH:O	2.15	0.47
1:A:556:ASN:H	1:A:556:ASN:HD22	1.62	0.47
1:A:81:ILE:HG21	1:A:476:LEU:HD21	1.96	0.46
1:B:656:TYR:HE2	1:B:704:ASN:ND2	2.13	0.46
1:A:402:ARG:HG2	1:A:459:ALA:HB2	1.96	0.46
1:A:90:LEU:HG	1:A:112:VAL:HG11	1.97	0.46
1:B:155:TRP:CE3	1:B:162:LEU:HD13	2.50	0.46
1:B:254:LYS:HZ1	1:B:706:HIS:CD2	2.26	0.46
1:B:302[A]:GLU:HG2	1:B:323:PHE:HB3	1.98	0.46
1:A:60:ASN:HB3	1:A:68:LEU:O	2.15	0.46
1:B:413:ASN:ND2	1:B:413:ASN:H	2.13	0.46
1:A:151:GLN:O	1:A:209:LYS:NZ	2.41	0.46
1:A:202:GLU:O	1:A:207:ALA:HA	2.16	0.46
1:B:376:HIS:ND1	1:B:391:THR:CG2	2.61	0.46
1:B:506:GLU:HG2	1:B:523:ILE:HD13	1.98	0.46
1:A:573:ASP:HB3	1:A:577:THR:HG21	1.97	0.46
1:A:501:ILE:HG22	1:A:503:LEU:HG	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:HB3	1:B:481:THR:HG22	1.98	0.45
1:A:396:GLU:H	1:A:413:ASN:HB3	1.81	0.45
1:A:80:ASN:HB3	1:A:83:THR:HG22	1.98	0.45
1:B:80:ASN:HD22	1:B:83:THR:H	1.61	0.45
1:A:125:SER:HA	1:A:209:LYS:HB2	1.98	0.45
1:A:496:ASN:O	1:A:499:LYS:HB2	2.16	0.45
1:B:439:VAL:HG13	1:B:440:THR:HG23	1.98	0.45
1:B:55:LYS:N	1:B:491:ASN:HD21	2.08	0.45
1:B:751:PHE:O	1:B:754:GLN:HB3	2.16	0.45
1:A:313:GLN:OE1	1:A:663:ARG:HD2	2.16	0.45
1:A:698:HIS:CD2	1:A:710:SER:HB2	2.52	0.45
1:A:153:LEU:HD12	1:A:164:TYR:HB3	1.99	0.45
1:A:168:ASN:HD22	1:A:168:ASN:N	2.14	0.45
1:B:545:CYS:HA	1:B:578:ALA:HB2	1.98	0.45
1:B:638:THR:HG23	1:B:640:LEU:N	2.27	0.45
1:A:513:VAL:CG1	1:A:606:LYS:HD3	2.45	0.45
1:B:490:GLU:HB3	1:B:492:LYS:HE3	1.99	0.45
1:B:318:LEU:HB3	1:B:338:HIS:HB2	1.98	0.44
1:B:61:TRP:CZ3	1:B:456:SER:HB3	2.52	0.44
1:B:576:GLY:HA2	1:B:585:LEU:O	2.17	0.44
1:A:259:ASN:HD22	1:A:259:ASN:HA	1.60	0.44
1:B:533:LYS:HA	1:B:612:PHE:O	2.17	0.44
1:A:440:THR:HG22	1:A:464:LEU:HD21	1.99	0.44
1:B:580:GLN:HB2	1:B:584:LEU:HD23	2.00	0.44
1:B:75:ASN:HD22	1:B:92:ASN:H	1.63	0.44
1:B:85:GLN:HB3	1:B:87:TYR:CZ	2.52	0.44
1:A:535:PRO:HB2	1:A:756:PHE:CE2	2.52	0.44
1:B:280:VAL:HG11	1:B:306:LEU:CD1	2.47	0.44
1:A:104:GLY:HA3	1:A:113:TYR:CE1	2.53	0.44
1:A:547:GLN:HB3	1:A:550:ARG:HE	1.82	0.44
1:B:413:ASN:HD22	1:B:413:ASN:H	1.66	0.44
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.50	0.44
1:A:198:ASP:HB2	1:A:228:ASP:OD2	2.17	0.44
1:A:471:ILE:HG12	1:A:494:LEU:HD13	1.99	0.44
1:B:364:TYR:CE1	1:B:380:ILE:HD12	2.53	0.43
1:B:424:ILE:O	1:B:439:VAL:HG12	2.18	0.43
1:A:401:PHE:HE2	1:A:411:SER:HB3	1.82	0.43
1:B:181:PHE:CE1	1:B:272:PRO:HB2	2.53	0.43
1:B:704:ASN:ND2	1:B:704:ASN:C	2.69	0.43
1:A:520:TYR:HA	1:A:549:VAL:HG21	1.98	0.43
1:A:651:SER:HA	1:A:682:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:HIS:NE2	1:B:484:GLU:HB3	2.32	0.43
1:B:481:THR:CG2	1:B:483:GLN:H	2.32	0.43
1:B:524:LEU:HD23	1:B:568:VAL:HG22	2.01	0.43
1:B:648:ALA:N	1:B:649:PRO:CD	2.82	0.43
1:A:230:ASP:HB3	1:A:258:LYS:HD2	2.00	0.43
1:B:203:GLU:HB2	6:B:9286:HOH:O	2.17	0.43
1:A:232:PRO:HB2	1:B:244:TYR:CZ	2.53	0.43
1:B:689:PHE:HB2	1:B:722:VAL:HG11	2.00	0.43
1:A:78:LEU:O	1:A:86:SER:HA	2.19	0.43
1:B:125:SER:HA	1:B:209:LYS:HB2	2.00	0.43
1:B:440:THR:HB	1:B:451:TYR:CE1	2.54	0.43
1:B:636:SER:OG	1:B:638:THR:HB	2.18	0.43
1:B:422:ARG:HH22	1:B:547:GLN:HE22	1.67	0.43
1:A:254:LYS:NZ	1:A:706:HIS:CD2	2.77	0.43
1:A:577:THR:HG21	6:A:9281:HOH:O	2.19	0.43
1:B:103:TYR:HA	1:B:113:TYR:O	2.18	0.43
1:B:190:ASN:HA	1:B:193:PHE:CZ	2.54	0.43
1:B:199:TRP:CZ2	1:B:704:ASN:HA	2.53	0.42
1:A:545:CYS:HA	1:A:578:ALA:HB2	2.00	0.42
1:A:592:LEU:HD23	1:A:653:TRP:CE2	2.54	0.42
1:A:300:THR:OG1	1:A:303:ARG:HB2	2.19	0.42
1:B:266:ILE:HD12	1:B:330:TRP:CE2	2.55	0.42
1:A:348:GLY:HA2	6:A:9260:HOH:O	2.18	0.42
1:A:643:CYS:CB	1:A:693:ASP:HB2	2.50	0.42
1:A:556:ASN:N	1:A:556:ASN:HD22	2.16	0.42
1:B:494:LEU:HG	1:B:498:LEU:HD22	2.01	0.42
1:B:653:TRP:HB3	1:B:661:THR:CG2	2.49	0.42
1:A:537:LEU:HD23	1:A:569:ILE:HD12	2.01	0.42
1:A:148:ARG:HA	1:A:148:ARG:HD3	1.83	0.42
1:A:206:LEU:HB3	1:A:208:THR:HG22	2.00	0.42
1:A:404:THR:HG22	6:A:9262:HOH:O	2.19	0.42
1:B:254:LYS:NZ	1:B:708:GLN:NE2	2.68	0.42
1:A:726:ALA:HB1	1:B:728:TRP:CZ3	2.55	0.42
1:B:271:TYR:N	1:B:272:PRO:CD	2.83	0.42
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.55	0.42
1:B:267:ILE:HG23	1:B:277:PRO:CA	2.50	0.42
1:A:188:ARG:O	1:A:189:GLU:C	2.58	0.42
1:A:413:ASN:OD1	1:A:419:PRO:HA	2.20	0.42
1:A:493:GLU:CD	1:A:493:GLU:N	2.73	0.41
1:A:208:THR:HG23	1:A:210:TYR:O	2.20	0.41
1:A:648:ALA:N	1:A:649:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:PRO:O	6:B:9346:HOH:O	2.22	0.41
1:B:494:LEU:O	1:B:495:GLU:C	2.57	0.41
1:B:685:ARG:O	1:B:686:ALA:C	2.57	0.41
1:A:634:LEU:HD22	1:A:644:GLY:HA3	2.03	0.41
1:B:152:TYR:HD2	1:B:209:LYS:HE2	1.85	0.41
1:B:656:TYR:HE2	1:B:704:ASN:HD22	1.68	0.41
1:A:318:LEU:HD11	1:A:355:PRO:HG3	2.02	0.41
1:B:68:LEU:CD2	1:B:78:LEU:HB2	2.49	0.41
1:A:416:GLU:OE2	1:A:421:ARG:NH2	2.54	0.41
1:B:235:ALA:HA	1:B:248:ILE:O	2.20	0.41
1:B:395:TRP:CD2	1:B:414:GLU:HB2	2.56	0.41
1:B:423:ASN:HD21	1:B:449:GLN:HE22	1.66	0.41
1:B:592:LEU:HA	1:B:592:LEU:HD12	1.77	0.41
1:B:605:ARG:CG	1:B:605:ARG:HH21	2.34	0.41
1:B:617:ARG:HG2	1:B:756:PHE:CD2	2.56	0.41
1:A:493:GLU:CD	1:A:493:GLU:H	2.24	0.41
1:B:148:ARG:HB3	1:B:149:PRO:CD	2.49	0.41
1:B:464:LEU:HA	1:B:464:LEU:HD23	1.86	0.41
1:B:98:VAL:O	1:B:99:ASN:C	2.58	0.41
1:B:280:VAL:HA	1:B:281:PRO:HD3	1.93	0.41
1:A:179:PRO:HA	1:A:180:PRO:HD3	1.89	0.40
1:A:750:HIS:CD2	1:B:723:ASP:OD1	2.75	0.40
1:B:333:PRO:HG2	1:B:336:GLN:HG3	2.03	0.40
1:B:628:TYR:CE1	1:B:632:LEU:HD11	2.56	0.40
1:B:350:PHE:HD2	1:B:545:CYS:HB2	1.86	0.40
1:A:362:ILE:HG23	1:A:363:SER:N	2.36	0.40
1:A:672:ASP:HB3	1:A:673:ASN:H	1.65	0.40
1:B:524:LEU:HA	1:B:525:PRO:HD3	1.94	0.40
1:B:62:ILE:HG21	1:B:105:LEU:HD12	2.04	0.40
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.98	0.40
1:B:161:LYS:HZ3	1:B:269:THR:HG23	1.86	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	717/719 (100%)	652 (91%)	58 (8%)	7 (1%)	18	37
1	B	723/719 (101%)	656 (91%)	56 (8%)	11 (2%)	12	24
All	All	1440/1438 (100%)	1308 (91%)	114 (8%)	18 (1%)	14	29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	432	TYR
1	B	149	PRO
1	B	433	PRO
1	A	99	ASN
1	A	433	PRO
1	B	99	ASN
1	B	144	ASN
1	B	190	ASN
1	A	151	GLN
1	B	335	THR
1	B	382	ASP
1	A	674	LEU
1	B	76	ILE
1	B	528	PHE
1	B	686	ALA
1	A	370	ASP
1	B	738	GLY

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	634/634 (100%)	528 (83%)	106 (17%)	2	4
1	B	640/634 (101%)	550 (86%)	90 (14%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1274/1268 (100%)	1078 (85%)	196 (15%)	3 5

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	44	LEU
1	A	45	LYS
1	A	53	SER
1	A	56	THR
1	A	65	GLN
1	A	66	GLU
1	A	70	GLN
1	A	77	VAL
1	A	81	ILE
1	A	83	THR
1	A	89	ILE
1	A	90	LEU
1	A	91	SER
1	A	94	THR
1	A	96	LYS
1	A	105	LEU
1	A	106	SER
1	A	113	TYR
1	A	121	LEU
1	A	127	THR
1	A	132	ILE
1	A	136	SER
1	A	142	ARG
1	A	148	ARG
1	A	151	GLN
1	A	156	SER
1	A	173	LYS
1	A	174	GLN
1	A	189	GLU
1	A	196	ILE
1	A	204	GLU
1	A	209	LYS
1	A	219	LYS
1	A	230	ASP
1	A	234	ILE
1	A	258	LYS

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Mol	Chain	Res	Type
1	A	259	ASN
1	A	266	ILE
1	A	270	THR
1	A	280	VAL
1	A	288	SER
1	A	301	ASP
1	A	303	ARG
1	A	311	ARG
1	A	315	VAL
1	A	316	SER
1	A	326	ASP
1	A	334	LYS
1	A	343	ARG
1	A	359	TYR
1	A	383	THR
1	A	385	GLU
1	A	388	ILE
1	A	402	ARG
1	A	405	GLN
1	A	412	SER
1	A	421	ARG
1	A	424	ILE
1	A	435	SER
1	A	444	ARG
1	A	447	ARG
1	A	460	LYS
1	A	464	LEU
1	A	466	CYS
1	A	480	ARG
1	A	481	THR
1	A	483	GLN
1	A	486	LYS
1	A	493	GLU
1	A	494	LEU
1	A	495	GLU
1	A	500	ASN
1	A	508	ILE
1	A	510	LYS
1	A	516	ILE
1	A	521	LYS
1	A	524	LEU
1	A	531	SER

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Mol	Chain	Res	Type
1	A	532	LYS
1	A	551	SER
1	A	556	ASN
1	A	564	LYS
1	A	577	THR
1	A	584	LEU
1	A	591	LYS
1	A	602	THR
1	A	605	ARG
1	A	606	LYS
1	A	609	GLU
1	A	610	MET
1	A	624	SER
1	A	629	VAL
1	A	632	LEU
1	A	663	ARG
1	A	672	ASP
1	A	673	ASN
1	A	678	LYS
1	A	682	VAL
1	A	691	ASN
1	A	710	SER
1	A	739	LEU
1	A	740	SER
1	A	749	THR
1	A	753	LYS
1	A	754	GLN
1	B	42	LEU
1	B	44	LEU
1	B	45	LYS
1	B	48	LEU
1	B	56	THR
1	B	78	LEU
1	B	80	ASN
1	B	87	TYR
1	B	88	THR
1	B	90	LEU
1	B	93	ARG
1	B	96	LYS
1	B	99	ASN
1	B	101	SER
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	105	LEU
1	B	109	ARG
1	B	116	SER
1	B	121	LEU
1	B	132	ILE
1	B	142	ARG
1	B	144	ASN
1	B	153	LEU
1	B	162	LEU
1	B	174	GLN
1	B	176	PRO
1	B	208	THR
1	B	231	ILE
1	B	246[A]	ARG
1	B	246[B]	ARG
1	B	258	LYS
1	B	267	ILE
1	B	269	THR
1	B	282	VAL
1	B	306	LEU
1	B	326	ASP
1	B	334	LYS
1	B	353	SER
1	B	359	TYR
1	B	362	ILE
1	B	406	ASP
1	B	412	SER
1	B	413	ASN
1	B	424	ILE
1	B	431	SER
1	B	435	SER
1	B	443	LEU
1	B	447	ARG
1	B	466	CYS
1	B	474	SER
1	B	480	ARG
1	B	481	THR
1	B	486	LYS
1	B	492	LYS
1	B	495	GLU
1	B	498	LEU
1	B	499	LYS

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Mol	Chain	Res	Type
1	B	503	LEU
1	B	509	LYS
1	B	510	LYS
1	B	514	ASP
1	B	517	THR
1	B	518	LEU
1	B	521	LYS
1	B	523	ILE
1	B	530	ARG
1	B	532	LYS
1	B	552	VAL
1	B	556	ASN
1	B	559	SER
1	B	560	TYR
1	B	577	THR
1	B	583	LYS
1	B	592	LEU
1	B	605	ARG
1	B	616	LYS
1	B	617	ARG
1	B	621	TRP
1	B	642	LYS
1	B	652	SER
1	B	654[A]	GLU
1	B	654[B]	GLU
1	B	667	LEU
1	B	670	LYS
1	B	671	ASP
1	B	704	ASN
1	B	730	SER
1	B	733	ASN
1	B	746	THR
1	B	753	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	70	GLN
1	A	151	GLN
1	A	168	ASN
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	243	GLN
1	A	259	ASN
1	A	423	ASN
1	A	449	GLN
1	A	500	ASN
1	A	539	GLN
1	A	556	ASN
1	A	673	ASN
1	A	676	HIS
1	A	691	ASN
1	A	698	HIS
1	A	704	ASN
1	A	706	HIS
1	A	708	GLN
1	A	709	ASN
1	A	719	ASN
1	A	742	ASN
1	A	750	HIS
1	A	754	GLN
1	B	60	ASN
1	B	69	HIS
1	B	75	ASN
1	B	80	ASN
1	B	102	ASN
1	B	151	GLN
1	B	167	GLN
1	B	168	ASN
1	B	174	GLN
1	B	182	GLN
1	B	243	GLN
1	B	313	GLN
1	B	378	HIS
1	B	413	ASN
1	B	449	GLN
1	B	477	HIS
1	B	491	ASN
1	B	547	GLN
1	B	556	ASN
1	B	704	ASN
1	B	706	HIS
1	B	708	GLN
1	B	709	ASN

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Mol	Chain	Res	Type
1	B	719	ASN
1	B	733	ASN
1	B	743	HIS
1	B	747	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	$\# Z > 2$
4	NDG	A	2271	1,4	14,14,15	0.66	0	15,19,21	1.41	2 (13%)
4	NAG	A	2272	4	14,14,15	0.62	0	15,19,21	0.76	0
3	NAG	A	9201	1,3	14,14,15	0.46	0	15,19,21	0.95	1 (6%)
3	NAG	A	9202	3	14,14,15	0.49	0	15,19,21	0.85	0
3	NAG	B	9201	1,3	14,14,15	1.18	1 (7%)	15,19,21	1.60	3 (20%)
3	NAG	B	9202	3	14,14,15	0.75	1 (7%)	15,19,21	1.20	1 (6%)

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	NDG	A	2271	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2272	4	-	0/6/23/26	0/1/1/1
3	NAG	A	9201	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	9202	3	-	0/6/23/26	0/1/1/1
3	NAG	B	9201	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	9202	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	9201	NAG	O5-C1	-3.88	1.37	1.43
3	B	9202	NAG	C1-C2	2.21	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9201	NAG	O5-C1-C2	-2.91	107.42	111.47
3	A	9201	NAG	C1-O5-C5	2.47	115.57	112.17
4	A	2271	NDG	C2-N2-C7	2.87	127.14	122.94
4	A	2271	NDG	O3-C3-C4	2.90	116.66	110.36
3	B	9202	NAG	C4-C3-C2	3.08	115.53	111.02
3	B	9201	NAG	C1-O5-C5	3.17	116.53	112.17
3	B	9201	NAG	C1-C2-N2	3.52	116.50	110.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	9201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2271	NDG	1	0

5.6 Ligand geometry ⓘ

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	NAG	A	3141	1	14,14,15	0.62	0	15,19,21	1.37	1 (6%)
2	NAG	A	4901	1	14,14,15	0.84	1 (7%)	15,19,21	1.62	4 (26%)
2	NAG	B	2271	1	14,14,15	0.57	0	15,19,21	1.41	2 (13%)
5	NDG	B	3141	1	14,14,15	0.61	0	15,19,21	1.38	3 (20%)
2	NAG	B	4901	1	14,14,15	0.59	0	15,19,21	2.05	3 (20%)
2	NAG	B	6791	1	14,14,15	0.46	0	15,19,21	1.87	1 (6%)

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	NAG	A	3141	1	-	1/6/23/26	0/1/1/1
2	NAG	A	4901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2271	1	-	0/6/23/26	0/1/1/1
5	NDG	B	3141	1	-	0/6/23/26	0/1/1/1
2	NAG	B	4901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	6791	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4901	NAG	C1-C2	2.49	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4901	NAG	O5-C1-C2	-3.08	107.18	111.47
2	B	2271	NAG	O5-C1-C2	-3.04	107.24	111.47
5	B	3141	NDG	O-C1-C2	-2.09	108.56	111.47
5	B	3141	NDG	C1-O-C5	-2.05	109.34	112.17
2	A	4901	NAG	C1-O5-C5	2.40	115.48	112.17
2	B	4901	NAG	C1-C2-N2	2.44	114.66	110.49
5	B	3141	NDG	C2-N2-C7	2.55	126.66	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4901	NAG	C1-C2-N2	2.55	114.84	110.49
2	B	4901	NAG	C2-N2-C7	2.72	126.91	122.94
2	B	2271	NAG	C1-O5-C5	3.43	116.90	112.17
2	A	4901	NAG	C2-N2-C7	3.55	128.13	122.94
2	A	3141	NAG	C4-C3-C2	3.97	116.83	111.02
2	B	4901	NAG	C1-O5-C5	6.16	120.66	112.17
2	B	6791	NAG	C1-O5-C5	6.41	121.00	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3141	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	719/719 (100%)	-0.13	20 (2%) 53 46	7, 27, 40, 67	0
1	B	719/719 (100%)	-0.34	3 (0%) 92 91	9, 23, 35, 47	0
All	All	1438/1438 (100%)	-0.24	23 (1%) 72 67	7, 25, 39, 67	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	4.7
1	A	133	TYR	4.7
1	A	274	TYR	4.5
1	A	141	VAL	4.5
1	A	135	LEU	4.0
1	A	72	ALA	3.1
1	A	131	TYR	3.0
1	A	39	MET	3.0
1	A	111	PHE	2.9
1	A	134	ASP	2.8
1	A	527	GLN	2.5
1	A	40	ARG	2.4
1	A	271	TYR	2.4
1	B	499	LYS	2.4
1	A	140	PHE	2.4
1	A	371	LYS	2.4
1	A	136	SER	2.3
1	A	487	ILE	2.3
1	A	97	SER	2.2
1	A	327	TRP	2.2
1	B	69	HIS	2.1
1	B	496	ASN	2.1
1	A	175	ARG	2.1

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
4	NDG	A	2271	14/15	0.86	0.24	1.37	44,47,48,48	0
3	NAG	A	9201	14/15	0.85	0.26	-	55,56,57,57	0
3	NAG	B	9201	14/15	0.88	0.19	-	43,45,46,48	0
3	NAG	B	9202	14/15	0.88	0.30	-	50,51,51,52	0
3	NAG	A	9202	14/15	0.81	0.26	-	57,57,57,57	0
4	NAG	A	2272	14/15	0.82	0.43	-	50,51,52,52	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
2	NAG	A	3141	14/15	0.75	0.27	0.97	105,115,121,121	0
5	NDG	B	3141	14/15	0.90	0.17	0.77	47,51,53,53	0
2	NAG	B	2271	14/15	0.91	0.15	0.15	38,42,44,44	0
2	NAG	B	6791	14/15	0.81	0.42	-	53,56,59,59	0
2	NAG	A	4901	14/15	0.82	0.31	-	49,51,52,52	0
2	NAG	B	4901	14/15	0.86	0.28	-	36,38,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.