



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:00 AM UTC

PDB ID : 5E6S / pdb_00005e6s
Title : Structures of leukocyte integrin α LB2: The α I domain, the headpiece, and the pocket for the internal ligand
Authors : Springer, T.A.; Sen, M.
Deposited on : 2015-10-10
Resolution : 2.15 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

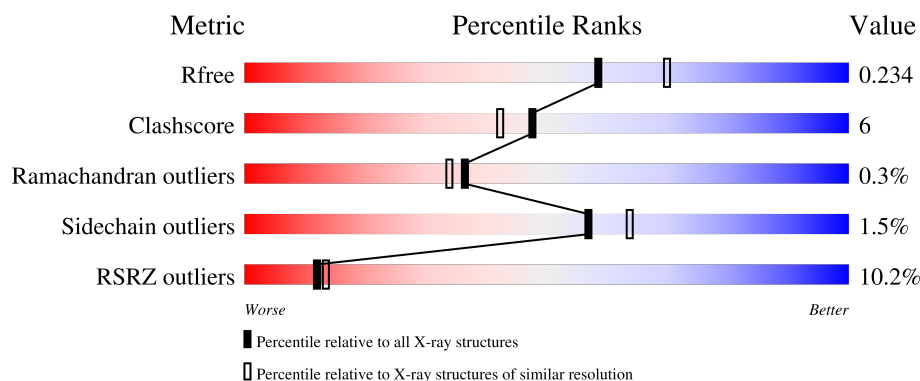
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	795	4% 64% 9% 27%
1	C	795	5% 62% 10% 27%
1	E	795	4% 62% 11% 27%
2	B	510	13% 78% 10% 11%
2	D	510	15% 77% 12% 11%

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Mol	Chain	Length	Quality of chain
2	F	510	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (15%), green (75%), yellow (13%), and grey (11%). The percentages are labeled above each segment.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26342 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 Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	13	0
			4512	2859	768	869	16			
1	C	578	Total	C	N	O	S	0	9	0
			4483	2841	768	858	16			
1	E	580	Total	C	N	O	S	0	5	0
			4479	2838	766	859	16			

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	TRP	ARG	variant	UNP P20701
A	645	ARG	ASN	engineered mutation	UNP P20701
A	701	ARG	ASN	engineered mutation	UNP P20701
A	746	PRO	-	expression tag	UNP P20701
A	747	ALA	-	expression tag	UNP P20701
A	748	ALA	-	expression tag	UNP P20701
A	749	LEU	-	expression tag	UNP P20701
A	750	GLN	-	expression tag	UNP P20701
A	751	THR	-	expression tag	UNP P20701
A	752	LEU	-	expression tag	UNP P20701
A	753	PHE	-	expression tag	UNP P20701
A	754	GLN	-	expression tag	UNP P20701
A	755	GLY	-	expression tag	UNP P20701
A	756	PRO	-	expression tag	UNP P20701
A	757	LEU	-	expression tag	UNP P20701
A	758	GLY	-	expression tag	UNP P20701
A	759	ALA	-	expression tag	UNP P20701
A	760	GLN	-	expression tag	UNP P20701
A	761	GLY	-	expression tag	UNP P20701
A	762	GLU	-	expression tag	UNP P20701
A	763	LYS	-	expression tag	UNP P20701
A	764	GLU	-	expression tag	UNP P20701
A	765	LEU	-	expression tag	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
A	766	GLN	-	expression tag	UNP P20701
A	767	ALA	-	expression tag	UNP P20701
A	768	LEU	-	expression tag	UNP P20701
A	769	GLU	-	expression tag	UNP P20701
A	770	LYS	-	expression tag	UNP P20701
A	771	GLU	-	expression tag	UNP P20701
A	772	ASN	-	expression tag	UNP P20701
A	773	ALA	-	expression tag	UNP P20701
A	774	GLN	-	expression tag	UNP P20701
A	775	LEU	-	expression tag	UNP P20701
A	776	GLU	-	expression tag	UNP P20701
A	777	TRP	-	expression tag	UNP P20701
A	778	GLU	-	expression tag	UNP P20701
A	779	LEU	-	expression tag	UNP P20701
A	780	GLN	-	expression tag	UNP P20701
A	781	ALA	-	expression tag	UNP P20701
A	782	LEU	-	expression tag	UNP P20701
A	783	GLU	-	expression tag	UNP P20701
A	784	LYS	-	expression tag	UNP P20701
A	785	GLU	-	expression tag	UNP P20701
A	786	LEU	-	expression tag	UNP P20701
A	787	ALA	-	expression tag	UNP P20701
A	788	GLN	-	expression tag	UNP P20701
A	789	HIS	-	expression tag	UNP P20701
A	790	HIS	-	expression tag	UNP P20701
A	791	HIS	-	expression tag	UNP P20701
A	792	HIS	-	expression tag	UNP P20701
A	793	HIS	-	expression tag	UNP P20701
A	794	HIS	-	expression tag	UNP P20701
A	795	ALA	-	expression tag	UNP P20701
C	189	TRP	ARG	variant	UNP P20701
C	645	ARG	ASN	engineered mutation	UNP P20701
C	701	ARG	ASN	engineered mutation	UNP P20701
C	746	PRO	-	expression tag	UNP P20701
C	747	ALA	-	expression tag	UNP P20701
C	748	ALA	-	expression tag	UNP P20701
C	749	LEU	-	expression tag	UNP P20701
C	750	GLN	-	expression tag	UNP P20701
C	751	THR	-	expression tag	UNP P20701
C	752	LEU	-	expression tag	UNP P20701
C	753	PHE	-	expression tag	UNP P20701
C	754	GLN	-	expression tag	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
C	755	GLY	-	expression tag	UNP P20701
C	756	PRO	-	expression tag	UNP P20701
C	757	LEU	-	expression tag	UNP P20701
C	758	GLY	-	expression tag	UNP P20701
C	759	ALA	-	expression tag	UNP P20701
C	760	GLN	-	expression tag	UNP P20701
C	761	GLY	-	expression tag	UNP P20701
C	762	GLU	-	expression tag	UNP P20701
C	763	LYS	-	expression tag	UNP P20701
C	764	GLU	-	expression tag	UNP P20701
C	765	LEU	-	expression tag	UNP P20701
C	766	GLN	-	expression tag	UNP P20701
C	767	ALA	-	expression tag	UNP P20701
C	768	LEU	-	expression tag	UNP P20701
C	769	GLU	-	expression tag	UNP P20701
C	770	LYS	-	expression tag	UNP P20701
C	771	GLU	-	expression tag	UNP P20701
C	772	ASN	-	expression tag	UNP P20701
C	773	ALA	-	expression tag	UNP P20701
C	774	GLN	-	expression tag	UNP P20701
C	775	LEU	-	expression tag	UNP P20701
C	776	GLU	-	expression tag	UNP P20701
C	777	TRP	-	expression tag	UNP P20701
C	778	GLU	-	expression tag	UNP P20701
C	779	LEU	-	expression tag	UNP P20701
C	780	GLN	-	expression tag	UNP P20701
C	781	ALA	-	expression tag	UNP P20701
C	782	LEU	-	expression tag	UNP P20701
C	783	GLU	-	expression tag	UNP P20701
C	784	LYS	-	expression tag	UNP P20701
C	785	GLU	-	expression tag	UNP P20701
C	786	LEU	-	expression tag	UNP P20701
C	787	ALA	-	expression tag	UNP P20701
C	788	GLN	-	expression tag	UNP P20701
C	789	HIS	-	expression tag	UNP P20701
C	790	HIS	-	expression tag	UNP P20701
C	791	HIS	-	expression tag	UNP P20701
C	792	HIS	-	expression tag	UNP P20701
C	793	HIS	-	expression tag	UNP P20701
C	794	HIS	-	expression tag	UNP P20701
C	795	ALA	-	expression tag	UNP P20701
E	189	TRP	ARG	variant	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
E	645	ARG	ASN	engineered mutation	UNP P20701
E	701	ARG	ASN	engineered mutation	UNP P20701
E	746	PRO	-	expression tag	UNP P20701
E	747	ALA	-	expression tag	UNP P20701
E	748	ALA	-	expression tag	UNP P20701
E	749	LEU	-	expression tag	UNP P20701
E	750	GLN	-	expression tag	UNP P20701
E	751	THR	-	expression tag	UNP P20701
E	752	LEU	-	expression tag	UNP P20701
E	753	PHE	-	expression tag	UNP P20701
E	754	GLN	-	expression tag	UNP P20701
E	755	GLY	-	expression tag	UNP P20701
E	756	PRO	-	expression tag	UNP P20701
E	757	LEU	-	expression tag	UNP P20701
E	758	GLY	-	expression tag	UNP P20701
E	759	ALA	-	expression tag	UNP P20701
E	760	GLN	-	expression tag	UNP P20701
E	761	GLY	-	expression tag	UNP P20701
E	762	GLU	-	expression tag	UNP P20701
E	763	LYS	-	expression tag	UNP P20701
E	764	GLU	-	expression tag	UNP P20701
E	765	LEU	-	expression tag	UNP P20701
E	766	GLN	-	expression tag	UNP P20701
E	767	ALA	-	expression tag	UNP P20701
E	768	LEU	-	expression tag	UNP P20701
E	769	GLU	-	expression tag	UNP P20701
E	770	LYS	-	expression tag	UNP P20701
E	771	GLU	-	expression tag	UNP P20701
E	772	ASN	-	expression tag	UNP P20701
E	773	ALA	-	expression tag	UNP P20701
E	774	GLN	-	expression tag	UNP P20701
E	775	LEU	-	expression tag	UNP P20701
E	776	GLU	-	expression tag	UNP P20701
E	777	TRP	-	expression tag	UNP P20701
E	778	GLU	-	expression tag	UNP P20701
E	779	LEU	-	expression tag	UNP P20701
E	780	GLN	-	expression tag	UNP P20701
E	781	ALA	-	expression tag	UNP P20701
E	782	LEU	-	expression tag	UNP P20701
E	783	GLU	-	expression tag	UNP P20701
E	784	LYS	-	expression tag	UNP P20701
E	785	GLU	-	expression tag	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
E	786	LEU	-	expression tag	UNP P20701
E	787	ALA	-	expression tag	UNP P20701
E	788	GLN	-	expression tag	UNP P20701
E	789	HIS	-	expression tag	UNP P20701
E	790	HIS	-	expression tag	UNP P20701
E	791	HIS	-	expression tag	UNP P20701
E	792	HIS	-	expression tag	UNP P20701
E	793	HIS	-	expression tag	UNP P20701
E	794	HIS	-	expression tag	UNP P20701
E	795	ALA	-	expression tag	UNP P20701

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	455	Total	C	N	O	S	0	6	0
			3557	2218	627	683	29			
2	D	455	Total	C	N	O	S	0	5	0
			3547	2210	626	682	29			
2	F	455	Total	C	N	O	S	0	9	0
			3568	2220	632	687	29			

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	232	LYS	ASN	engineered mutation	UNP P05107
B	461	PRO	-	expression tag	UNP P05107
B	462	ALA	-	expression tag	UNP P05107
B	463	ALA	-	expression tag	UNP P05107
B	464	LEU	-	expression tag	UNP P05107
B	465	GLN	-	expression tag	UNP P05107
B	466	THR	-	expression tag	UNP P05107
B	467	LEU	-	expression tag	UNP P05107
B	468	PHE	-	expression tag	UNP P05107
B	469	GLN	-	expression tag	UNP P05107
B	470	GLY	-	expression tag	UNP P05107
B	471	PRO	-	expression tag	UNP P05107
B	472	LEU	-	expression tag	UNP P05107
B	473	GLY	-	expression tag	UNP P05107
B	474	ALA	-	expression tag	UNP P05107
B	475	GLN	-	expression tag	UNP P05107
B	476	GLY	-	expression tag	UNP P05107
B	477	LYS	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	-	expression tag	UNP P05107
B	479	LYS	-	expression tag	UNP P05107
B	480	LEU	-	expression tag	UNP P05107
B	481	GLN	-	expression tag	UNP P05107
B	482	ALA	-	expression tag	UNP P05107
B	483	LEU	-	expression tag	UNP P05107
B	484	LYS	-	expression tag	UNP P05107
B	485	LYS	-	expression tag	UNP P05107
B	486	LYS	-	expression tag	UNP P05107
B	487	ASN	-	expression tag	UNP P05107
B	488	ALA	-	expression tag	UNP P05107
B	489	GLN	-	expression tag	UNP P05107
B	490	LEU	-	expression tag	UNP P05107
B	491	LYS	-	expression tag	UNP P05107
B	492	TRP	-	expression tag	UNP P05107
B	493	LYS	-	expression tag	UNP P05107
B	494	LEU	-	expression tag	UNP P05107
B	495	GLN	-	expression tag	UNP P05107
B	496	ALA	-	expression tag	UNP P05107
B	497	LEU	-	expression tag	UNP P05107
B	498	LYS	-	expression tag	UNP P05107
B	499	LYS	-	expression tag	UNP P05107
B	500	LYS	-	expression tag	UNP P05107
B	501	LEU	-	expression tag	UNP P05107
B	502	ALA	-	expression tag	UNP P05107
B	503	GLN	-	expression tag	UNP P05107
B	504	HIS	-	expression tag	UNP P05107
B	505	HIS	-	expression tag	UNP P05107
B	506	HIS	-	expression tag	UNP P05107
B	507	HIS	-	expression tag	UNP P05107
B	508	HIS	-	expression tag	UNP P05107
B	509	HIS	-	expression tag	UNP P05107
B	510	ALA	-	expression tag	UNP P05107
D	232	LYS	ASN	engineered mutation	UNP P05107
D	461	PRO	-	expression tag	UNP P05107
D	462	ALA	-	expression tag	UNP P05107
D	463	ALA	-	expression tag	UNP P05107
D	464	LEU	-	expression tag	UNP P05107
D	465	GLN	-	expression tag	UNP P05107
D	466	THR	-	expression tag	UNP P05107
D	467	LEU	-	expression tag	UNP P05107
D	468	PHE	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
D	469	GLN	-	expression tag	UNP P05107
D	470	GLY	-	expression tag	UNP P05107
D	471	PRO	-	expression tag	UNP P05107
D	472	LEU	-	expression tag	UNP P05107
D	473	GLY	-	expression tag	UNP P05107
D	474	ALA	-	expression tag	UNP P05107
D	475	GLN	-	expression tag	UNP P05107
D	476	GLY	-	expression tag	UNP P05107
D	477	LYS	-	expression tag	UNP P05107
D	478	LYS	-	expression tag	UNP P05107
D	479	LYS	-	expression tag	UNP P05107
D	480	LEU	-	expression tag	UNP P05107
D	481	GLN	-	expression tag	UNP P05107
D	482	ALA	-	expression tag	UNP P05107
D	483	LEU	-	expression tag	UNP P05107
D	484	LYS	-	expression tag	UNP P05107
D	485	LYS	-	expression tag	UNP P05107
D	486	LYS	-	expression tag	UNP P05107
D	487	ASN	-	expression tag	UNP P05107
D	488	ALA	-	expression tag	UNP P05107
D	489	GLN	-	expression tag	UNP P05107
D	490	LEU	-	expression tag	UNP P05107
D	491	LYS	-	expression tag	UNP P05107
D	492	TRP	-	expression tag	UNP P05107
D	493	LYS	-	expression tag	UNP P05107
D	494	LEU	-	expression tag	UNP P05107
D	495	GLN	-	expression tag	UNP P05107
D	496	ALA	-	expression tag	UNP P05107
D	497	LEU	-	expression tag	UNP P05107
D	498	LYS	-	expression tag	UNP P05107
D	499	LYS	-	expression tag	UNP P05107
D	500	LYS	-	expression tag	UNP P05107
D	501	LEU	-	expression tag	UNP P05107
D	502	ALA	-	expression tag	UNP P05107
D	503	GLN	-	expression tag	UNP P05107
D	504	HIS	-	expression tag	UNP P05107
D	505	HIS	-	expression tag	UNP P05107
D	506	HIS	-	expression tag	UNP P05107
D	507	HIS	-	expression tag	UNP P05107
D	508	HIS	-	expression tag	UNP P05107
D	509	HIS	-	expression tag	UNP P05107
D	510	ALA	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
F	232	LYS	ASN	engineered mutation	UNP P05107
F	461	PRO	-	expression tag	UNP P05107
F	462	ALA	-	expression tag	UNP P05107
F	463	ALA	-	expression tag	UNP P05107
F	464	LEU	-	expression tag	UNP P05107
F	465	GLN	-	expression tag	UNP P05107
F	466	THR	-	expression tag	UNP P05107
F	467	LEU	-	expression tag	UNP P05107
F	468	PHE	-	expression tag	UNP P05107
F	469	GLN	-	expression tag	UNP P05107
F	470	GLY	-	expression tag	UNP P05107
F	471	PRO	-	expression tag	UNP P05107
F	472	LEU	-	expression tag	UNP P05107
F	473	GLY	-	expression tag	UNP P05107
F	474	ALA	-	expression tag	UNP P05107
F	475	GLN	-	expression tag	UNP P05107
F	476	GLY	-	expression tag	UNP P05107
F	477	LYS	-	expression tag	UNP P05107
F	478	LYS	-	expression tag	UNP P05107
F	479	LYS	-	expression tag	UNP P05107
F	480	LEU	-	expression tag	UNP P05107
F	481	GLN	-	expression tag	UNP P05107
F	482	ALA	-	expression tag	UNP P05107
F	483	LEU	-	expression tag	UNP P05107
F	484	LYS	-	expression tag	UNP P05107
F	485	LYS	-	expression tag	UNP P05107
F	486	LYS	-	expression tag	UNP P05107
F	487	ASN	-	expression tag	UNP P05107
F	488	ALA	-	expression tag	UNP P05107
F	489	GLN	-	expression tag	UNP P05107
F	490	LEU	-	expression tag	UNP P05107
F	491	LYS	-	expression tag	UNP P05107
F	492	TRP	-	expression tag	UNP P05107
F	493	LYS	-	expression tag	UNP P05107
F	494	LEU	-	expression tag	UNP P05107
F	495	GLN	-	expression tag	UNP P05107
F	496	ALA	-	expression tag	UNP P05107
F	497	LEU	-	expression tag	UNP P05107
F	498	LYS	-	expression tag	UNP P05107
F	499	LYS	-	expression tag	UNP P05107
F	500	LYS	-	expression tag	UNP P05107
F	501	LEU	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
F	502	ALA	-	expression tag	UNP P05107
F	503	GLN	-	expression tag	UNP P05107
F	504	HIS	-	expression tag	UNP P05107
F	505	HIS	-	expression tag	UNP P05107
F	506	HIS	-	expression tag	UNP P05107
F	507	HIS	-	expression tag	UNP P05107
F	508	HIS	-	expression tag	UNP P05107
F	509	HIS	-	expression tag	UNP P05107
F	510	ALA	-	expression tag	UNP P05107

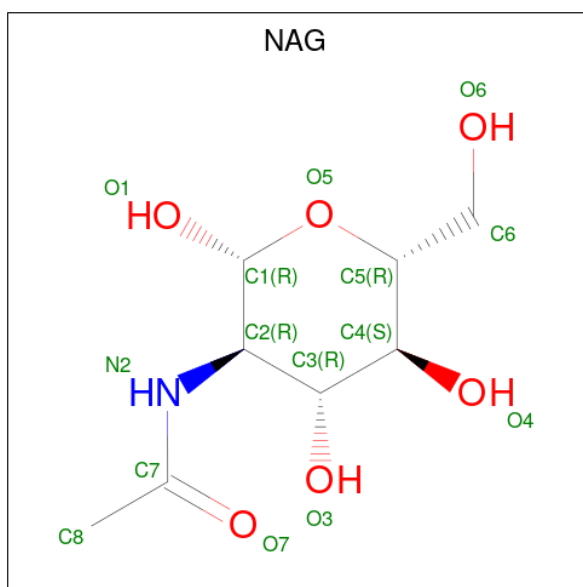
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	B	2	Total Ca 2 2	0	0
4	C	3	Total Ca 3 3	0	0
4	D	2	Total Ca 2 2	0	0
4	E	3	Total Ca 3 3	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	433	Total	O	0	0
			433	433		
6	B	267	Total	O	0	0
			267	267		
6	C	375	Total	O	0	0
			375	375		

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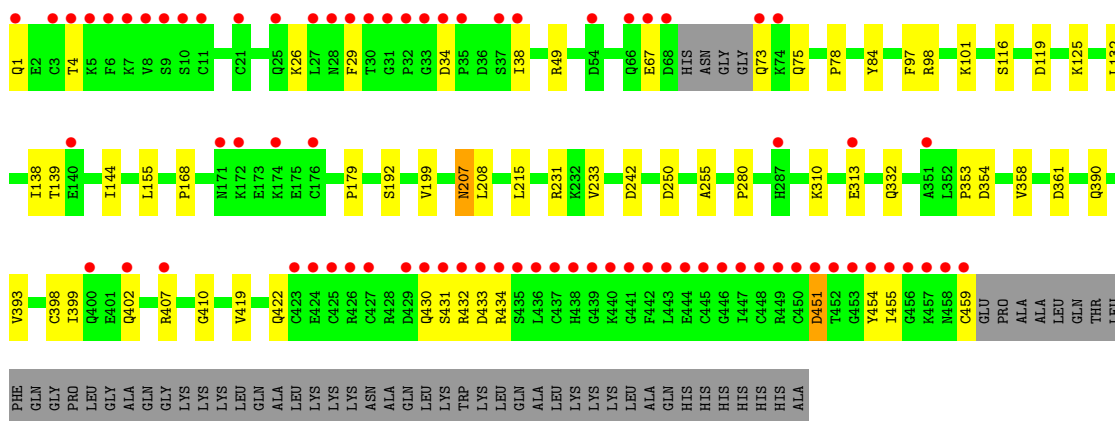
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	265	Total 265	O 265	0	0
6	E	430	Total 430	O 430	0	0
6	F	282	Total 282	O 282	0	0



LYS
TRP
LYS
LEU
GLN
ALA
LEU
LYS
LYS
LYS
LEU
GLN
HIS
HIS
HIS
HIS
HIS
HIS
ALA

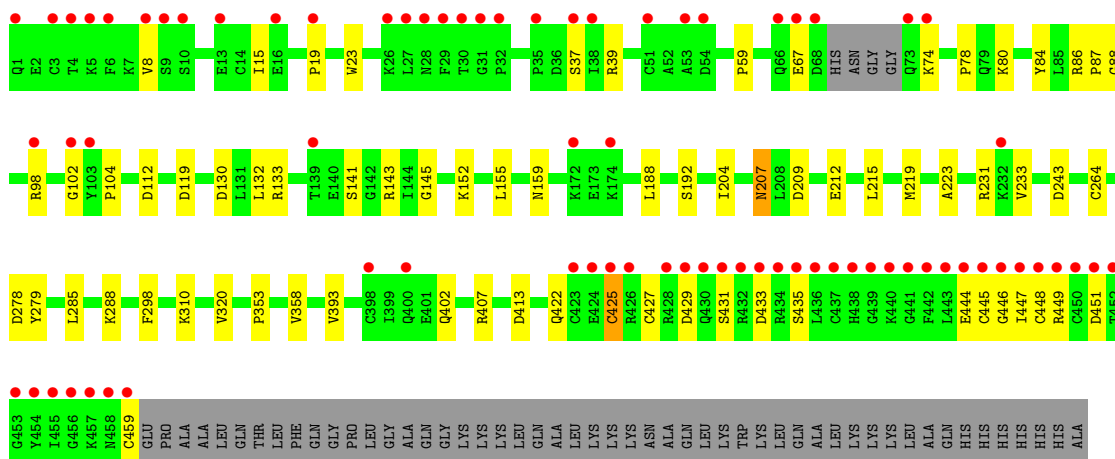
● Molecule 2: Integrin beta-2

Chain D: 15% 77% 12% 11%



● Molecule 2: Integrin beta-2

Chain F: 15% 75% 13% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 118.88Å 150.97Å 90.00° 118.52° 90.00°	Depositor
Resolution (Å)	49.45 – 2.15 49.45 – 2.15	Depositor EDS
% Data completeness (in resolution range)	70.5 (49.45-2.15) 70.6 (49.45-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.194 , 0.234 0.195 , 0.234	Depositor DCC
R_{free} test set	9078 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for l,k,-h-l 0.027 for -h-l,k,h 0.025 for -h-l,-k,l 0.016 for h,-k,-h-l 0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26342	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: MG, CA, 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	0.21	0/4645	0.46	0/6283
1	C	0.20	0/4604	0.43	0/6228
1	E	0.20	0/4589	0.44	0/6208
2	B	0.21	0/3641	0.45	0/4926
2	D	0.20	0/3627	0.44	0/4907
2	F	0.21	0/3658	0.44	0/4948
All	All	0.20	0/24764	0.44	0/33500

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
2	B	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	434	ARG	Peptide
2	B	458	ASN	Peptide
2	D	434	ARG	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	4512	0	4429	49	0
1	C	4483	0	4406	53	0
1	E	4479	0	4389	54	0
2	B	3557	0	3476	35	1
2	D	3547	0	3458	38	0
2	F	3568	0	3488	47	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	14	0	13	0	0
5	B	28	0	26	1	0
5	C	14	0	13	1	0
5	D	28	0	26	1	0
5	E	14	0	13	1	0
5	F	28	0	26	1	0
6	A	433	0	0	12	3
6	B	267	0	0	9	1
6	C	375	0	0	12	0
6	D	265	0	0	8	0
6	E	430	0	0	14	0
6	F	282	0	0	9	1
All	All	26342	0	23763	271	3

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 6.

All (271) 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:293:GLU:OE2	6:A:4001:HOH:O	1.84	0.95
1:A:145[A]:ASP:OD2	6:A:4002:HOH:O	2.02	0.77
2:F:130:ASP:OD2	6:F:4001:HOH:O	2.05	0.74
1:A:588:ARG:NH2	6:A:4008:HOH:O	2.21	0.72
1:C:13:PRO:HD2	1:C:16:ALA:HB2	1.73	0.71
1:E:300:THR:O	1:E:304:LYS:N	2.17	0.71
1:C:473:GLN:NE2	6:C:4004:HOH:O	2.23	0.70
1:E:503:LEU:HD11	1:E:515:ALA:HB2	1.74	0.70
2:B:48:MET:O	6:B:4001:HOH:O	2.11	0.68
2:B:84:TYR:HB3	2:B:422:GLN:HG3	1.74	0.68
1:A:503:LEU:HD11	1:A:515:ALA:HB2	1.76	0.68
1:A:1:TYR:HA	1:A:542:GLN:HB2	1.77	0.67
1:E:200:LYS:NZ	6:E:4008:HOH:O	2.28	0.67
2:F:74:LYS:NZ	2:F:98:ARG:HH21	1.93	0.66
1:E:1:TYR:HA	1:E:542:GLN:HB2	1.76	0.66
1:A:554[B]:GLN:OE1	6:A:4003:HOH:O	2.13	0.66
1:A:409:LEU:HD22	1:A:425:THR:HG22	1.77	0.65
1:A:301:GLU:O	1:A:305:LYS:HB2	1.95	0.65
2:B:372:ASN:ND2	6:B:4005:HOH:O	2.28	0.65
1:C:427:HIS:ND1	6:C:4013:HOH:O	2.29	0.65
1:E:253:ASP:OD1	6:E:4001:HOH:O	2.15	0.65
1:C:446:GLN:NE2	6:C:4015:HOH:O	2.30	0.64
1:E:569:ASP:OD2	6:E:4002:HOH:O	2.15	0.64
1:E:4:ASP:HB2	1:E:588:ARG:HG3	1.81	0.63
2:F:407[A]:ARG:NH2	6:F:4015:HOH:O	2.32	0.63
2:D:34:ASP:HB3	2:D:38:ILE:HG13	1.80	0.62
1:E:299:PHE:O	1:E:303:GLN:HB3	1.99	0.62
1:A:163:ASN:O	1:A:163:ASN:ND2	2.32	0.62
1:C:409:LEU:HD22	1:C:425:THR:HG22	1.79	0.62
2:D:84:TYR:HB3	2:D:422:GLN:HG3	1.80	0.62
1:A:293:GLU:N	1:A:293:GLU:OE1	2.32	0.62
1:E:158:MET:HE2	1:E:192:PRO:HG3	1.82	0.61
1:A:50:SER:HB3	1:A:567:GLU:OE2	2.01	0.61
1:E:495:ARG:HD3	6:E:4014:HOH:O	2.01	0.60
1:E:249:ASP:OD1	6:E:4004:HOH:O	2.17	0.60
1:C:495:ARG:NH1	6:C:4005:HOH:O	2.24	0.60
2:F:209:ASP:OD2	6:F:4002:HOH:O	2.16	0.60
1:C:503:LEU:HD11	1:C:515:ALA:HB2	1.83	0.60
1:E:112:GLN:NE2	6:E:4012:HOH:O	2.34	0.59
1:E:167:GLN:OE1	6:E:4003:HOH:O	2.16	0.59
2:F:132:LEU:HD12	2:F:192:SER:HB3	1.83	0.59
2:B:65:THR:HG22	2:B:81:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:GLU:HG2	2:D:78:PRO:HB3	1.83	0.59
1:E:289:LEU:HD11	1:E:298:LEU:HD22	1.84	0.59
1:E:551[A]:SER:OG	6:E:4005:HOH:O	2.17	0.59
1:C:464:GLN:NE2	6:C:4019:HOH:O	2.35	0.59
1:C:1:TYR:HA	1:C:542:GLN:HB2	1.84	0.59
1:C:565:ASP:OD2	1:C:569:ASP:N	2.35	0.58
2:D:454:TYR:O	2:D:455:ILE:HG13	2.04	0.58
1:A:137:ASP:HB2	1:A:238:THR:HA	1.84	0.58
2:B:313:GLU:OE1	6:B:4002:HOH:O	2.17	0.58
1:E:549:VAL:HG11	1:E:583:ILE:HD13	1.86	0.58
2:F:353:PRO:HG3	2:F:402:GLN:OE1	2.03	0.58
2:D:119:ASP:N	2:D:119:ASP:OD1	2.36	0.58
2:D:353:PRO:HG3	2:D:402:GLN:NE2	2.18	0.57
1:E:532[B]:ARG:NH2	6:E:4018:HOH:O	2.38	0.57
2:D:75:GLN:O	2:D:97:PHE:HA	2.05	0.57
1:E:405:MET:SD	2:F:310:LYS:NZ	2.78	0.57
2:F:84:TYR:HB3	2:F:422:GLN:HG3	1.87	0.57
2:B:441:GLY:HA2	2:B:451:ASP:H	1.70	0.57
2:F:15:ILE:HD13	2:F:59:PRO:HG3	1.85	0.57
1:A:549:VAL:HG11	1:A:583:ILE:HD13	1.86	0.56
1:A:550:LEU:HB2	1:A:553:ILE:HB	1.85	0.56
1:A:532[C]:ARG:NH2	6:A:4022:HOH:O	2.35	0.56
2:B:206:GLY:HA2	6:B:4003:HOH:O	2.04	0.56
2:B:441:GLY:HA3	2:B:450:CYS:HA	1.87	0.56
1:C:163:ASN:H	1:C:190:LYS:NZ	2.03	0.56
2:F:133:ARG:NH2	6:F:4019:HOH:O	2.39	0.56
1:C:360:GLN:N	6:C:4002:HOH:O	2.37	0.56
2:B:332:GLN:NE2	1:C:12:SER:OG	2.38	0.56
2:D:313:GLU:OE1	6:D:4001:HOH:O	2.18	0.56
1:A:4:ASP:HB2	1:A:588:ARG:HG3	1.88	0.55
1:E:197:LYS:HE3	1:E:198:HIS:NE2	2.22	0.55
1:C:249:ASP:HA	1:C:252[B]:LYS:HG2	1.88	0.55
2:F:74:LYS:HZ3	2:F:98:ARG:HH21	1.52	0.55
1:C:356:LYS:HB3	6:C:4002:HOH:O	2.05	0.55
2:F:445:CYS:C	2:F:447:ILE:H	2.15	0.55
1:C:64:ASN:HD22	5:C:3064:NAG:H83	1.72	0.54
2:D:4:THR:OG1	6:D:4002:HOH:O	2.19	0.54
1:E:27:VAL:HG11	1:E:83:ILE:HD11	1.89	0.54
1:C:335[A]:ARG:NH2	1:C:413:GLU:OE1	2.41	0.54
1:E:13:PRO:HD2	1:E:16:ALA:HB2	1.88	0.54
1:E:137:ASP:HB2	1:E:238:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:ILE:HG22	2:D:139:THR:HG23	1.89	0.53
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.90	0.53
2:F:86:ARG:HD2	2:F:87:PRO:HD2	1.89	0.53
1:E:221:ARG:HD3	1:E:223:GLU:OE2	2.09	0.53
2:B:207:ASN:HD22	2:B:207:ASN:N	2.07	0.53
1:C:25:LEU:HD21	1:C:76:THR:HB	1.90	0.52
2:D:132:LEU:HD12	2:D:192:SER:HB3	1.91	0.52
2:F:112:ASP:OD2	6:F:4003:HOH:O	2.19	0.52
2:B:287[A]:HIS:CE1	2:B:291:GLU:OE2	2.62	0.52
2:F:67:GLU:HG2	2:F:78:PRO:HB3	1.92	0.52
1:C:27:VAL:HG21	1:C:83:ILE:HD11	1.91	0.51
5:B:3094:NAG:O7	5:B:3094:NAG:O3	2.23	0.51
1:E:97:ASN:HA	2:F:159:ASN:HD21	1.75	0.51
1:A:145[B]:ASP:OD2	6:A:4004:HOH:O	2.19	0.51
1:C:98:THR:HG21	2:D:155:LEU:HD11	1.93	0.51
1:E:149:LYS:NZ	1:E:293:GLU:OE2	2.43	0.51
2:F:207:ASN:N	2:F:207:ASN:HD22	2.09	0.51
2:F:80:LYS:HE3	6:F:4096:HOH:O	2.10	0.51
2:D:75:GLN:HA	2:D:98:ARG:O	2.10	0.51
2:F:358:VAL:HG22	2:F:393:VAL:HG22	1.92	0.51
1:E:346:LYS:NZ	6:E:4027:HOH:O	2.44	0.51
2:D:358:VAL:HG22	2:D:393:VAL:HG22	1.93	0.50
2:F:133:ARG:NE	6:F:4018:HOH:O	2.39	0.50
1:A:281:PRO:HB2	1:A:361:ASP:OD1	2.12	0.50
1:A:2:ASN:HB2	1:A:588:ARG:O	2.11	0.50
1:C:137:ASP:HB2	1:C:238:THR:HA	1.94	0.50
2:D:1:GLN:OE1	6:D:4003:HOH:O	2.19	0.50
2:B:5:LYS:HD3	2:B:40:CYS:O	2.12	0.49
1:E:28:GLY:C	1:E:30:GLY:H	2.20	0.49
1:E:58:VAL:HG21	1:E:111:LEU:HD13	1.93	0.49
1:E:290:ASP:OD1	1:E:294:LYS:NZ	2.37	0.49
1:A:66:THR:OG1	6:A:4005:HOH:O	2.20	0.49
1:A:28:GLY:HA2	1:A:564:LYS:HZ1	1.78	0.49
1:C:27:VAL:HG12	1:C:32:ILE:HG12	1.95	0.49
1:E:344:GLY:HA2	1:E:348:TRP:CD1	2.48	0.49
5:E:3064:NAG:H82	6:E:4015:HOH:O	2.13	0.49
1:C:344:GLY:HA2	1:C:348:TRP:CD1	2.48	0.48
1:E:136:PHE:CZ	1:E:172:GLN:HB2	2.47	0.48
1:E:550:LEU:HB2	1:E:553:ILE:HB	1.95	0.48
1:A:259:ILE:HD11	1:A:302:LEU:HD22	1.96	0.48
2:D:207:ASN:N	2:D:207:ASN:HD22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:VAL:HA	1:C:512:VAL:HB	1.95	0.48
2:D:255:ALA:O	6:D:4004:HOH:O	2.20	0.47
2:F:74:LYS:NZ	2:F:98:ARG:NH2	2.61	0.47
1:A:215:VAL:HG11	1:A:234:LEU:HD13	1.96	0.47
2:D:332:GLN:HG3	6:E:4007:HOH:O	2.14	0.47
2:F:445:CYS:O	2:F:447:ILE:N	2.46	0.47
2:D:407[A]:ARG:HH21	2:D:410:GLY:H	1.62	0.47
1:E:9:ARG:NH1	1:E:50:SER:O	2.45	0.47
1:E:171:VAL:HG21	1:E:219:VAL:HG21	1.96	0.47
2:F:141:SER:HG	2:F:231:ARG:HH12	1.61	0.47
2:D:38:ILE:O	2:D:49:ARG:NH2	2.48	0.47
1:A:18:ARG:NH2	6:A:4003:HOH:O	2.29	0.47
2:B:332:GLN:HG3	6:C:4317:HOH:O	2.14	0.47
1:A:136:PHE:CZ	1:A:172:GLN:HB2	2.50	0.47
1:E:301:GLU:HG3	1:E:305:LYS:HG3	1.97	0.47
2:F:74:LYS:HB2	6:F:4198:HOH:O	2.14	0.47
2:B:41:ASP:OD2	2:B:49:ARG:NH1	2.48	0.47
1:C:124:GLU:HG3	6:C:4158:HOH:O	2.15	0.47
2:B:353:PRO:HG3	2:B:402:GLN:NE2	2.30	0.47
1:C:149:LYS:NZ	1:C:293:GLU:OE2	2.48	0.47
2:D:132:LEU:HG	2:D:144:ILE:HD13	1.97	0.46
2:B:431:SER:C	2:B:433:ASP:H	2.23	0.46
1:E:98:THR:HG21	2:F:155:LEU:HD11	1.97	0.46
1:A:258:ILE:HG22	1:A:278:ALA:HB2	1.98	0.46
1:C:4:ASP:HA	1:C:588[B]:ARG:NH1	2.30	0.46
1:A:458:PRO:O	1:A:495:ARG:HA	2.15	0.46
2:D:451:ASP:N	2:D:451:ASP:OD1	2.49	0.46
2:F:143:ARG:NH1	5:F:3190:NAG:O6	2.48	0.46
1:A:28:GLY:HA2	1:A:564:LYS:NZ	2.31	0.46
2:B:9:SER:OG	2:B:13:GLU:OE1	2.28	0.46
1:C:425:THR:OG1	6:C:4001:HOH:O	2.21	0.46
1:E:332:ASP:C	1:E:333:LEU:HD12	2.40	0.46
1:C:163:ASN:H	1:C:190:LYS:HZ3	1.61	0.46
1:E:61:ARG:NH1	1:E:114:PRO:HA	2.31	0.46
2:B:115:TYR:HE1	2:B:173:GLU:HG2	1.80	0.46
2:F:449:ARG:HD2	2:F:449:ARG:HA	1.60	0.46
1:A:106:LEU:HB2	1:A:359:LEU:HD11	1.97	0.45
1:C:291:THR:OG1	1:C:294:LYS:HG3	2.16	0.45
2:B:371:ARG:NH1	6:B:4023:HOH:O	2.48	0.45
1:C:26:GLN:HE22	1:C:573:ASP:C	2.25	0.45
1:E:368:GLU:HA	1:E:369:PRO:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:TYR:OH	2:B:459:CYS:HB3	2.16	0.45
2:D:407[A]:ARG:NH2	2:D:410:GLY:H	2.14	0.45
1:E:103:LEU:HD12	1:E:118:GLY:O	2.17	0.45
2:F:119:ASP:N	2:F:119:ASP:OD1	2.50	0.45
2:F:215:LEU:HG	2:F:285:LEU:HD22	1.98	0.45
2:F:451:ASP:OD1	2:F:451:ASP:N	2.49	0.45
1:C:215:VAL:HG11	1:C:234:LEU:HD13	1.99	0.45
1:E:458:PRO:O	1:E:495:ARG:HA	2.17	0.45
2:F:223:ALA:O	2:F:264:CYS:HB2	2.17	0.45
1:C:458:PRO:O	1:C:495:ARG:HA	2.17	0.45
2:D:101:LYS:NZ	6:D:4033:HOH:O	2.49	0.45
1:C:141:SER:OG	1:C:239:ASP:OD2	2.35	0.44
1:C:263:LYS:NZ	6:C:4052:HOH:O	2.49	0.44
1:E:133:VAL:HG22	1:E:169:ALA:HB3	1.99	0.44
2:F:19:PRO:HG3	2:F:88:GLY:HA3	1.98	0.44
1:A:11:PHE:HB3	1:A:55:CYS:SG	2.58	0.44
2:D:431:SER:C	2:D:433:ASP:H	2.26	0.44
1:A:124[A]:GLU:OE2	6:A:4006:HOH:O	2.21	0.44
1:A:344:GLY:HA2	1:A:348:TRP:CD1	2.53	0.44
2:B:449:ARG:HD2	2:B:449:ARG:HA	1.35	0.44
1:A:465:ARG:NH2	6:A:4051:HOH:O	2.50	0.44
1:A:465:ARG:HB3	1:A:489:PRO:HA	2.00	0.44
2:F:104:PRO:HB2	2:F:233:VAL:HG11	1.99	0.44
1:E:25:LEU:HD21	1:E:76:THR:HB	1.98	0.44
1:A:404:HIS:HB3	1:A:431:ILE:HG13	2.00	0.43
2:B:231:ARG:HB2	2:B:233:VAL:HG22	2.00	0.43
2:B:98:ARG:NH1	6:B:4019:HOH:O	2.46	0.43
2:B:407[B]:ARG:NH1	6:B:4028:HOH:O	2.50	0.43
1:E:258:ILE:HG22	1:E:278:ALA:HB2	2.00	0.43
1:C:401:ARG:HD2	2:D:250:ASP:OD2	2.19	0.43
5:D:3190:NAG:O7	5:D:3190:NAG:C3	2.66	0.43
2:F:152:LYS:HE2	2:F:279:TYR:CE1	2.53	0.43
1:C:136:PHE:CZ	1:C:172:GLN:HB2	2.53	0.43
1:C:153:PHE:CD1	1:C:299:PHE:HE1	2.36	0.43
2:F:444:GLU:HG3	2:F:444:GLU:O	2.19	0.43
1:A:235:ILE:HD13	1:A:302:LEU:HD23	2.01	0.43
2:F:448:CYS:O	6:F:4004:HOH:O	2.21	0.43
2:B:398:CYS:SG	6:B:4043:HOH:O	2.62	0.43
2:D:242:ASP:OD1	6:D:4005:HOH:O	2.21	0.43
1:E:38:GLU:HG2	6:E:4245:HOH:O	2.18	0.43
1:E:158:MET:HE3	1:E:186:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:407[B]:ARG:HG3	2:F:413:ASP:O	2.19	0.43
2:B:132:LEU:HD12	2:B:192:SER:HB3	2.01	0.42
1:C:2:ASN:ND2	1:C:506:ILE:O	2.44	0.42
1:A:13:PRO:HD2	1:A:16:ALA:HB2	2.01	0.42
1:A:324:LEU:O	1:A:344:GLY:HA3	2.19	0.42
2:B:407[B]:ARG:HG2	2:B:414:ILE:HG22	2.00	0.42
1:C:483:SER:OG	1:C:484:GLU:N	2.52	0.42
2:F:204:ILE:HD12	2:F:204:ILE:HA	1.94	0.42
2:F:425:CYS:HB2	2:F:427:CYS:SG	2.59	0.42
2:D:231:ARG:HB2	2:D:233:VAL:HG22	2.00	0.42
1:A:298:LEU:HA	1:A:298:LEU:HD23	1.87	0.42
2:D:168:PRO:HG3	2:D:179:PRO:HD3	2.01	0.42
1:E:178:LYS:NZ	6:E:4054:HOH:O	2.53	0.42
2:B:445:CYS:C	2:B:447:ILE:H	2.28	0.42
1:C:153:PHE:HZ	1:C:302:LEU:HD12	1.85	0.42
1:A:465:ARG:NH1	6:A:4007:HOH:O	2.21	0.42
2:F:145:GLY:N	2:F:188:LEU:HD23	2.35	0.42
1:E:442:VAL:HB	1:E:452:LEU:HB2	2.02	0.41
1:C:69:TYR:CD1	1:C:89:GLY:HA3	2.55	0.41
1:A:1:TYR:HB3	1:A:541:SER:HB2	2.02	0.41
1:C:26:GLN:HG2	1:C:31:VAL:HG22	2.01	0.41
1:C:134:PHE:CD1	1:C:154:MET:HG2	2.55	0.41
1:E:156:ASP:OD2	1:E:299:PHE:CZ	2.73	0.41
1:A:132:LEU:HD21	1:A:235:ILE:HD12	2.03	0.41
1:C:86:CYS:HA	1:C:104:CYS:HA	2.02	0.41
1:C:181:PHE:CD2	1:C:195:LEU:HB3	2.55	0.41
1:C:324:LEU:O	1:C:344:GLY:HA3	2.21	0.41
1:C:498:GLU:OE1	6:C:4003:HOH:O	2.22	0.41
2:D:399:ILE:HD11	2:D:419:VAL:HG12	2.03	0.41
1:A:1:TYR:N	6:A:4032:HOH:O	2.41	0.41
2:D:208:LEU:HG	6:D:4011:HOH:O	2.20	0.41
1:A:122:PHE:HE2	1:A:124[A]:GLU:HG2	1.85	0.41
1:C:588[A]:ARG:HD2	1:C:588[A]:ARG:HA	1.90	0.41
2:D:26:LYS:HB3	2:D:29:PHE:HB2	2.03	0.41
2:F:298:PHE:HB2	2:F:320:VAL:HG22	2.02	0.41
2:F:431:SER:C	2:F:433:ASP:H	2.28	0.41
1:A:98:THR:CG2	2:B:155:LEU:HD11	2.51	0.41
1:A:399:ALA:O	1:A:406:GLY:HA2	2.21	0.41
2:B:457:LYS:HG3	2:B:458:ASN:H	1.86	0.41
2:D:125:LYS:HG2	2:D:199:VAL:HG12	2.03	0.41
2:D:215:LEU:HB3	2:D:280:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ARG:HH11	1:E:114:PRO:HA	1.85	0.41
2:F:278:ASP:OD1	2:F:279:TYR:N	2.54	0.41
1:C:507:ASN:C	1:C:590:VAL:HG21	2.46	0.41
2:D:116:SER:OG	2:D:242:ASP:OD2	2.23	0.41
2:F:402:GLN:HE21	2:F:402:GLN:HB2	1.69	0.41
2:B:406:ILE:HB	2:B:415:VAL:HB	2.04	0.40
2:D:431:SER:O	2:D:432:ARG:HB2	2.21	0.40
1:E:2:ASN:HB2	1:E:588:ARG:O	2.21	0.40
1:E:98:THR:CG2	2:F:155:LEU:HD11	2.51	0.40
2:F:219:MET:SD	2:F:288:LYS:HG2	2.61	0.40
1:A:483:SER:OG	1:A:484:GLU:N	2.54	0.40
2:F:23:TRP:HA	2:F:39:ARG:O	2.21	0.40
2:B:122:ARG:HD2	6:B:4128:HOH:O	2.20	0.40
2:B:358:VAL:HG22	2:B:393:VAL:HG22	2.04	0.40
1:E:137:ASP:CB	1:E:238:THR:HA	2.52	0.40
1:E:216:ALA:HB2	1:E:251:ALA:HB2	2.04	0.40
1:A:69:TYR:CD1	1:A:89:GLY:HA3	2.56	0.40
1:A:132:LEU:HD11	1:A:235:ILE:HD11	2.04	0.40
2:B:431:SER:O	2:B:432:ARG:HB2	2.22	0.40
1:C:25:LEU:HD11	1:C:76:THR:HG22	2.02	0.40
1:C:368:GLU:HA	1:C:369:PRO:HA	1.82	0.40
2:D:361:ASP:HB2	2:D:390:GLN:HB3	2.04	0.40
1:C:129:ASN:OD1	1:C:165:SER:HB3	2.21	0.40
2:D:310:LYS:NZ	6:D:4020:HOH:O	2.41	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:4028:HOH:O	6:F:4129:HOH:O[2_545]	2.17	0.03
2:B:369:THR:O	6:A:4002:HOH:O[2_445]	2.18	0.02
6:A:4053:HOH:O	6:B:4023:HOH:O[2_455]	2.18	0.02

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	588/795 (74%)	568 (97%)	19 (3%)	1 (0%)	43	44
1	C	583/795 (73%)	557 (96%)	25 (4%)	1 (0%)	43	44
1	E	581/795 (73%)	557 (96%)	22 (4%)	2 (0%)	36	34
2	B	457/510 (90%)	434 (95%)	22 (5%)	1 (0%)	43	44
2	D	456/510 (89%)	435 (95%)	21 (5%)	0	100	100
2	F	460/510 (90%)	439 (95%)	17 (4%)	4 (1%)	14	9
All	All	3125/3915 (80%)	2990 (96%)	126 (4%)	9 (0%)	36	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
2	F	8	VAL
2	B	455	ILE
1	C	29	ASN
1	E	28	GLY
2	F	102	GLY
2	F	446	GLY
2	F	435	SER
1	E	174	SER

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	485/666 (73%)	477 (98%)	8 (2%)	55	61
1	C	480/666 (72%)	476 (99%)	4 (1%)	73	79
1	E	479/666 (72%)	472 (98%)	7 (2%)	57	64
2	B	398/440 (90%)	391 (98%)	7 (2%)	51	58
2	D	396/440 (90%)	389 (98%)	7 (2%)	51	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	399/440 (91%)	390 (98%)	9 (2%)	44	49
All	All	2637/3318 (80%)	2595 (98%)	42 (2%)	57	61

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	177	TYR
1	A	302	LEU
1	A	368[A]	GLU
1	A	368[B]	GLU
1	A	389	ARG
1	A	434	TYR
1	A	579	GLU
2	B	133	ARG
2	B	207	ASN
2	B	384	ASN
2	B	422	GLN
2	B	425	CYS
2	B	449	ARG
2	B	454	TYR
1	C	177	TYR
1	C	302	LEU
1	C	434	TYR
1	C	554	GLN
2	D	73	GLN
2	D	207	ASN
2	D	354	ASP
2	D	398	CYS
2	D	430	GLN
2	D	451	ASP
2	D	459	CYS
1	E	29	ASN
1	E	177	TYR
1	E	302	LEU
1	E	303	GLN
1	E	368	GLU
1	E	434	TYR
1	E	590	VAL
2	F	37	SER
2	F	207	ASN
2	F	212[A]	GLU

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Mol	Chain	Res	Type
2	F	212[B]	GLU
2	F	243[A]	ASP
2	F	243[B]	ASP
2	F	425	CYS
2	F	429	ASP
2	F	459	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	HIS
1	A	427	HIS
2	B	295	GLN
2	B	332	GLN
2	B	373	GLN
1	C	26	GLN
1	C	47	GLN
1	C	117	GLN
1	C	554	GLN
2	D	370	HIS
1	E	49	GLN
1	E	213	ASN
1	E	264	HIS
2	F	284	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 18 are monoatomic - leaving 9 for Mogul analysis.

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	C	3064	1	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	A	3064	1	14,14,15	0.41	0	17,19,21	0.63	0
5	NAG	D	3190	2	14,14,15	0.58	0	17,19,21	1.25	1 (5%)
5	NAG	E	3064	1	14,14,15	0.55	0	17,19,21	0.66	0
5	NAG	B	3094	2	14,14,15	1.12	1 (7%)	17,19,21	0.85	1 (5%)
5	NAG	F	3190	2	14,14,15	0.35	0	17,19,21	0.48	0
5	NAG	F	3094	2	14,14,15	0.45	0	17,19,21	0.48	0
5	NAG	D	3094	2	14,14,15	0.42	0	17,19,21	0.39	0
5	NAG	B	3190	2	14,14,15	0.54	0	17,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	3064	1	-	3/6/23/26	0/1/1/1
5	NAG	A	3064	1	-	2/6/23/26	0/1/1/1
5	NAG	D	3190	2	-	1/6/23/26	0/1/1/1
5	NAG	E	3064	1	-	2/6/23/26	0/1/1/1
5	NAG	B	3094	2	-	2/6/23/26	0/1/1/1
5	NAG	F	3190	2	-	2/6/23/26	0/1/1/1
5	NAG	F	3094	2	-	2/6/23/26	0/1/1/1
5	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3190	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)
5	B	3094	NAG	O5-C1	-3.93	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3190	NAG	C2-N2-C7	4.37	128.76	122.90
5	B	3094	NAG	C1-O5-C5	-2.55	108.77	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	3190	NAG	C3-C2-N2-C7
5	F	3094	NAG	O5-C5-C6-O6
5	A	3064	NAG	O5-C5-C6-O6
5	A	3064	NAG	C4-C5-C6-O6
5	F	3094	NAG	C4-C5-C6-O6
5	B	3190	NAG	O5-C5-C6-O6
5	B	3190	NAG	C4-C5-C6-O6
5	F	3190	NAG	C4-C5-C6-O6
5	C	3064	NAG	C8-C7-N2-C2
5	C	3064	NAG	O7-C7-N2-C2
5	F	3190	NAG	O5-C5-C6-O6
5	E	3064	NAG	C4-C5-C6-O6
5	C	3064	NAG	O5-C5-C6-O6
5	E	3064	NAG	O5-C5-C6-O6
5	B	3094	NAG	C3-C2-N2-C7
5	B	3094	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3064	NAG	1	0
5	D	3190	NAG	1	0
5	E	3064	NAG	1	0
5	B	3094	NAG	1	0
5	F	3190	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 ⓘ

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	579/795 (72%)	-0.12	29 (5%)	34 38	11, 27, 63, 204	13 (2%)
1	C	578/795 (72%)	-0.02	37 (6%)	25 28	13, 28, 64, 174	9 (1%)
1	E	580/795 (72%)	-0.13	35 (6%)	27 31	13, 27, 66, 209	5 (0%)
2	B	455/510 (89%)	0.31	64 (14%)	6 7	12, 30, 125, 293	6 (1%)
2	D	455/510 (89%)	0.51	76 (16%)	4 5	14, 33, 140, 313	5 (1%)
2	F	455/510 (89%)	0.50	74 (16%)	4 5	11, 31, 137, 247	9 (1%)
All	All	3102/3915 (79%)	0.14	315 (10%)	12 13	11, 29, 94, 313	47 (1%)

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	443	LEU	8.8
2	B	448	CYS	8.2
1	C	299	PHE	8.0
2	F	446	GLY	7.9
1	C	300	THR	7.8
2	F	448	CYS	7.7
2	F	447	ILE	7.3
1	E	302	LEU	7.2
2	D	6	PHE	7.1
2	B	443	LEU	6.9
2	F	450	CYS	6.5
1	C	568	GLY	6.3
1	A	299	PHE	6.3
2	F	6	PHE	6.3
2	F	445	CYS	6.2
2	D	446	GLY	6.2
2	F	433	ASP	6.2
2	B	437	CYS	6.0
1	A	303	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
2	D	438	HIS	6.0
2	F	454	TYR	6.0
2	D	455	ILE	6.0
2	F	455	ILE	6.0
2	F	436	LEU	5.9
1	C	304	LYS	5.9
2	D	437	CYS	5.9
2	F	431	SER	5.9
2	D	431	SER	5.8
2	D	435	SER	5.7
2	F	453	GLY	5.7
2	F	438	HIS	5.7
2	D	442	PHE	5.7
1	E	301	GLU	5.6
1	E	300	THR	5.6
2	F	430	GLN	5.5
2	B	441	GLY	5.5
1	A	306	ILE	5.5
2	D	436	LEU	5.5
2	B	436	LEU	5.5
1	C	28	GLY	5.4
1	C	302	LEU	5.4
2	D	448	CYS	5.3
2	B	452	THR	5.3
2	D	452	THR	5.3
2	B	438	HIS	5.3
2	B	6	PHE	5.3
2	F	435	SER	5.3
2	D	433	ASP	5.1
2	F	437	CYS	5.0
2	B	440	LYS	5.0
1	A	317	LEU	5.0
1	E	567	GLU	4.9
2	B	433	ASP	4.9
2	D	441	GLY	4.9
2	B	455	ILE	4.9
2	D	447	ILE	4.9
1	C	301	GLU	4.9
2	D	73	GLN	4.8
1	E	317	LEU	4.8
2	B	74	LYS	4.8
2	F	459	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	300	THR	4.8
2	B	431	SER	4.8
2	D	453	GLY	4.8
2	B	450	CYS	4.7
2	D	449	ARG	4.7
1	E	306	ILE	4.7
1	C	51	GLY	4.7
2	B	442	PHE	4.6
1	E	303	GLN	4.6
2	F	452	THR	4.6
2	D	457	LYS	4.6
2	B	458	ASN	4.6
2	D	445	CYS	4.6
2	B	439	GLY	4.6
1	E	299	PHE	4.6
2	D	429	ASP	4.6
2	F	38	ILE	4.6
2	D	74	LYS	4.6
1	A	189	TRP	4.5
2	B	429	ASP	4.5
2	F	32	PRO	4.5
2	F	8	VAL	4.5
2	D	443	LEU	4.5
2	D	454	TYR	4.5
2	F	442	PHE	4.5
1	C	318	THR	4.5
2	F	449	ARG	4.5
2	F	74	LYS	4.5
1	E	189	TRP	4.4
2	F	439	GLY	4.4
1	E	318	THR	4.4
1	A	28	GLY	4.3
1	A	302	LEU	4.3
2	B	445	CYS	4.3
2	B	12	ARG	4.3
2	F	1	GLN	4.3
1	E	305	LYS	4.3
2	D	459	CYS	4.3
2	D	30	THR	4.3
2	D	430	GLN	4.3
2	F	424	GLU	4.3
2	F	172	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	429	ASP	4.2
1	A	301	GLU	4.2
2	F	456	GLY	4.1
2	B	3	CYS	4.1
1	C	303	GLN	4.1
1	E	61	ARG	4.1
1	A	61[A]	ARG	4.1
2	D	35	PRO	4.1
1	C	590	VAL	4.0
2	B	35	PRO	4.0
2	B	447	ILE	4.0
2	B	73	GLN	3.9
2	B	33	GLY	3.9
2	D	456	GLY	3.9
1	C	163	ASN	3.9
1	A	305	LYS	3.8
1	C	29	ASN	3.8
2	B	454	TYR	3.8
2	D	432	ARG	3.8
1	C	368	GLU	3.8
2	D	7	LYS	3.8
2	F	432	ARG	3.8
2	D	450	CYS	3.8
2	D	444	GLU	3.8
1	E	564	LYS	3.7
1	E	569	ASP	3.7
1	A	229	ASP	3.7
2	B	34	ASP	3.7
1	A	318	THR	3.7
2	D	37	SER	3.6
2	D	67	GLU	3.6
2	F	232	LYS	3.6
1	E	29	ASN	3.6
2	D	31	GLY	3.6
2	F	440	LYS	3.6
2	F	73	GLN	3.6
1	C	504	THR	3.5
1	C	564	LYS	3.5
1	E	188	LYS	3.5
2	D	440	LYS	3.5
1	E	590	VAL	3.5
2	B	32	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	451	ASP	3.5
2	D	21	CYS	3.5
2	F	3	CYS	3.5
2	B	4	THR	3.5
2	B	435	SER	3.5
2	B	423	CYS	3.5
1	E	304	LYS	3.4
2	D	38	ILE	3.4
1	E	566	LEU	3.4
2	B	2	GLU	3.4
1	A	304	LYS	3.4
2	B	68	ASP	3.4
1	E	368	GLU	3.4
2	B	427	CYS	3.3
2	D	423	CYS	3.3
2	F	444	GLU	3.3
2	D	451	ASP	3.3
2	F	441	GLY	3.3
2	B	430	GLN	3.3
1	E	504	THR	3.3
2	F	4	THR	3.3
2	D	66	GLN	3.3
2	D	27	LEU	3.3
2	F	66	GLN	3.3
2	D	426	ARG	3.3
2	F	5	LYS	3.3
2	D	434	ARG	3.2
2	D	424	GLU	3.2
2	D	10	SER	3.2
2	F	35	PRO	3.2
2	D	4	THR	3.2
2	F	434	ARG	3.2
2	B	434	ARG	3.2
2	B	457	LYS	3.2
2	F	398	CYS	3.2
2	F	458	ASN	3.2
2	B	1	GLN	3.2
2	B	172	LYS	3.1
2	F	457	LYS	3.1
1	C	189	TRP	3.1
2	B	449	ARG	3.1
2	F	27	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	399	ILE	3.1
1	C	551	SER	3.1
2	D	1	GLN	3.1
2	D	28	ASN	3.0
2	D	407[A]	ARG	3.0
2	B	459	CYS	3.0
2	B	36	ASP	3.0
2	F	451	ASP	3.0
1	A	55	CYS	3.0
2	D	458	ASN	2.9
1	C	570	GLY	2.9
2	F	102	GLY	2.9
1	E	298	LEU	2.8
2	F	428	ARG	2.8
2	F	30	THR	2.8
1	C	50	SER	2.8
2	D	439	GLY	2.8
1	C	571	LEU	2.8
2	D	172	LYS	2.8
2	F	28	ASN	2.8
1	A	368[A]	GLU	2.8
2	D	351	ALA	2.8
1	C	547	THR	2.8
1	E	163	ASN	2.8
2	D	171	ASN	2.8
1	C	565	ASP	2.8
1	C	569	ASP	2.8
2	D	68	ASP	2.8
1	C	296	LYS	2.8
1	C	160	LYS	2.7
2	B	174	LYS	2.7
1	A	369	PRO	2.7
2	F	26	LYS	2.7
1	C	317	LEU	2.7
1	A	29	ASN	2.7
1	E	1	TYR	2.7
2	B	28	ASN	2.7
2	B	432	ARG	2.7
2	F	67	GLU	2.6
2	F	68	ASP	2.6
2	F	103	TYR	2.6
1	A	190	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	8	VAL	2.6
1	C	64	ASN	2.6
2	F	426	ARG	2.6
2	D	33	GLY	2.6
2	B	67	GLU	2.6
2	D	29	PHE	2.6
1	A	1	TYR	2.6
2	B	7	LYS	2.6
1	A	253	ASP	2.6
2	D	313	GLU	2.5
2	D	3	CYS	2.5
2	B	426	ARG	2.5
2	F	13	GLU	2.5
2	B	287[A]	HIS	2.5
1	C	252[A]	LYS	2.5
1	C	40	ASN	2.5
1	C	162	SER	2.5
1	C	27	VAL	2.5
2	F	423	CYS	2.5
2	F	425	CYS	2.5
2	F	400	GLN	2.5
1	A	296	LYS	2.5
1	E	27	VAL	2.4
2	D	11	CYS	2.4
2	F	16	GLU	2.4
2	D	427	CYS	2.4
2	B	5	LYS	2.4
1	A	477	LEU	2.4
1	C	298	LEU	2.4
2	B	456	GLY	2.4
1	A	64	ASN	2.4
2	B	66	GLN	2.4
2	D	32	PRO	2.4
1	C	198	HIS	2.4
2	B	16	GLU	2.3
2	B	428	ARG	2.3
2	D	174	LYS	2.3
2	D	5	LYS	2.3
1	A	476	GLN	2.3
1	E	570	GLY	2.3
2	D	9	SER	2.3
2	F	9	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	38	ILE	2.3
1	C	563	VAL	2.3
2	B	8	VAL	2.3
1	A	297	ASP	2.3
2	D	34	ASP	2.3
1	C	533	HIS	2.2
1	C	548	GLN	2.2
2	D	54	ASP	2.2
1	E	568	GLY	2.2
2	F	53	ALA	2.2
1	E	571	LEU	2.2
2	F	174	LYS	2.2
2	B	354	ASP	2.2
2	F	37	SER	2.2
1	E	297	ASP	2.2
1	A	298	LEU	2.2
1	E	370	LEU	2.2
2	D	176	CYS	2.2
1	A	504	THR	2.2
2	D	140[A]	GLU	2.1
2	F	29	PHE	2.1
2	D	425	CYS	2.1
1	E	40	ASN	2.1
2	B	30	THR	2.1
2	B	31	GLY	2.1
2	B	453	GLY	2.1
1	A	266	GLN	2.1
1	E	369	PRO	2.1
2	D	25	GLN	2.1
2	D	402	GLN	2.1
2	F	98	ARG	2.1
1	E	197	LYS	2.1
1	E	296	LYS	2.1
2	F	19	PRO	2.1
2	F	139	THR	2.1
1	E	28	GLY	2.1
2	F	10	SER	2.1
2	F	51	CYS	2.0
2	F	54	ASP	2.0
2	D	287[A]	HIS	2.0
2	F	31	GLY	2.0
2	B	444	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	351	ALA	2.0
2	D	400	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	NAG	F	3190	14/15	0.51	0.20	84,96,100,101	0
5	NAG	C	3064	14/15	0.52	0.27	113,122,127,127	0
5	NAG	A	3064	14/15	0.63	0.25	114,124,126,127	0
5	NAG	B	3190	14/15	0.67	0.21	82,97,104,107	0
5	NAG	D	3190	14/15	0.69	0.18	84,95,97,97	0
4	CA	C	2004	1/1	0.73	0.21	88,88,88,88	0
5	NAG	E	3064	14/15	0.77	0.25	108,117,128,128	0
5	NAG	B	3094	14/15	0.77	0.19	41,50,60,63	0
4	CA	A	2004	1/1	0.80	0.22	114,114,114,114	0
5	NAG	F	3094	14/15	0.81	0.15	34,49,58,63	0
4	CA	E	2004	1/1	0.90	0.16	104,104,104,104	0
5	NAG	D	3094	14/15	0.91	0.09	38,45,50,52	0
4	CA	E	2002	1/1	0.98	0.03	48,48,48,48	0
4	CA	E	2003	1/1	0.98	0.10	47,47,47,47	0
3	MG	A	2001	1/1	0.98	0.03	22,22,22,22	0
4	CA	F	2002	1/1	0.98	0.05	40,40,40,40	0
4	CA	F	2003	1/1	0.98	0.07	41,41,41,41	0
4	CA	C	2002	1/1	0.98	0.06	44,44,44,44	0
4	CA	A	2002	1/1	0.98	0.06	48,48,48,48	0
3	MG	E	2001	1/1	0.99	0.03	26,26,26,26	0
4	CA	B	2002	1/1	0.99	0.02	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	2003	1/1	0.99	0.06	48,48,48,48	0
3	MG	C	2001	1/1	0.99	0.02	22,22,22,22	0
4	CA	C	2003	1/1	0.99	0.03	36,36,36,36	0
4	CA	A	2003	1/1	0.99	0.02	27,27,27,27	0
4	CA	D	2002	1/1	0.99	0.02	36,36,36,36	0
4	CA	D	2003	1/1	1.00	0.04	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.