



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:09 PM GMT

PDB ID : 1SDD
Title : Crystal Structure of Bovine Factor Vai
Authors : Adams, T.E.; Hockin, M.F.; Mann, K.G.; Everse, S.J.
Deposited on : 2004-02-13
Resolution : 2.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

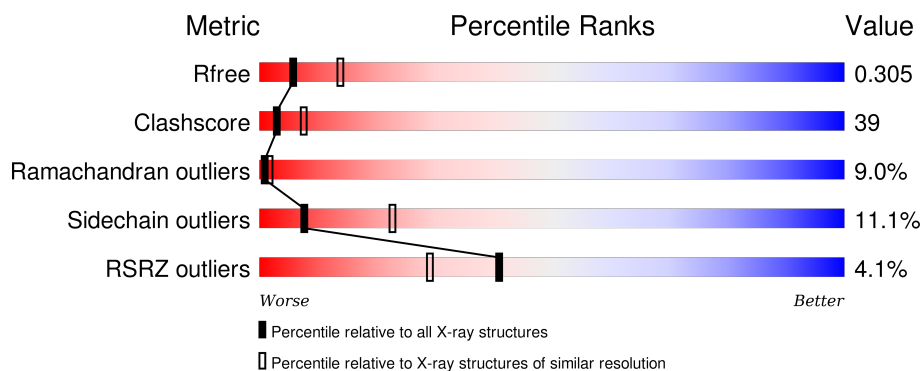
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	306	
2	B	647	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7271 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 Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2132	1366	356	398	12			

- Molecule 2 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	601	Total	C	N	O	S	0	0	0
			4878	3127	840	888	23			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



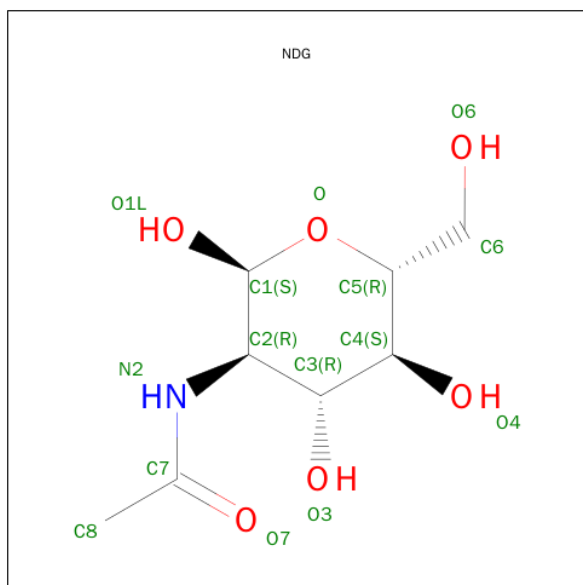
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cu	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

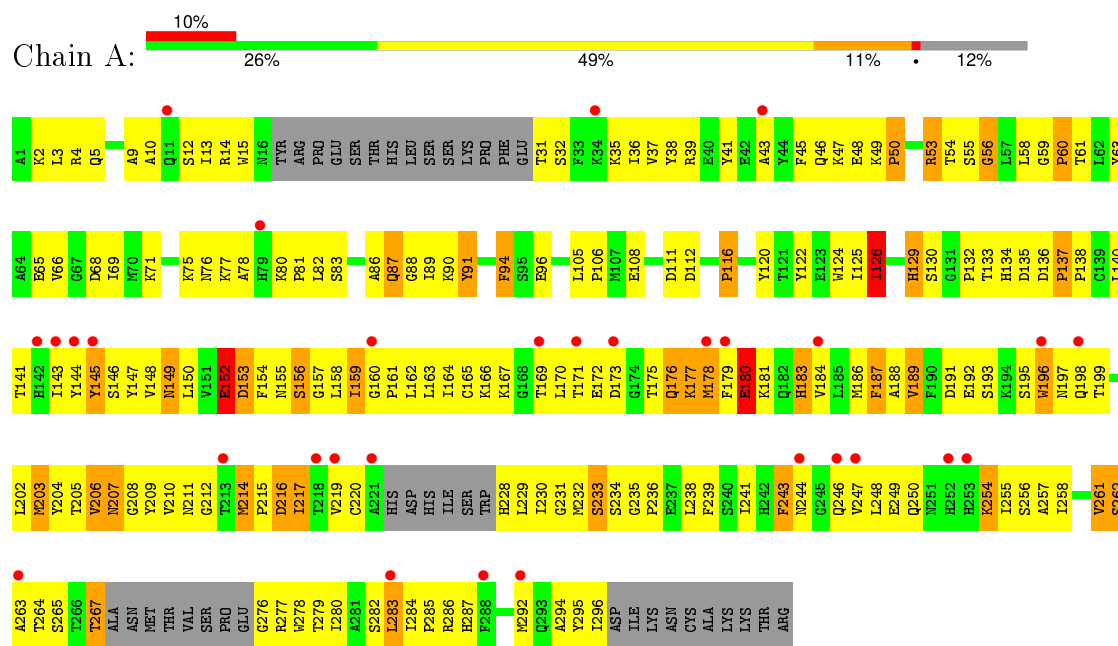
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total 47	O 47	0	0
7	B	142	Total 142	O 142	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Coagulation factor V



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.37Å 86.56Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 28.63 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.80) 90.7 (28.63-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.296 0.248 , 0.305	Depositor DCC
R_{free} test set	918 reflections (3.19%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28745 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NDG, CU, 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	0.35	0/2188	0.60	0/2960
2	B	0.46	0/5012	0.70	2/6792 (0.0%)
All	All	0.43	0/7200	0.67	2/9752 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1847	VAL	N-CA-C	-6.63	93.11	111.00
2	B	2014	ARG	N-CA-C	-6.47	93.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1890	TYR	Sidechain

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	2132	0	2074	198	0
2	B	4878	0	4767	357	0
3	A	28	0	26	3	0
3	B	14	0	13	4	0
4	B	28	0	26	6	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	47	0	0	1	0
7	B	142	0	0	3	0
All	All	7271	0	6906	548	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 39.

All (548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1992:ASP:HB3	2:B:1993:PRO:HD3	1.13	1.13
2:B:2152:ASN:HB2	2:B:2153:PRO:HD3	1.22	1.10
2:B:1721:MET:HG3	2:B:1786:ARG:HH22	1.01	1.08
2:B:1914:THR:HB	2:B:1920:PRO:HD2	1.38	1.05
1:A:264:THR:HG21	2:B:1822:PRO:HG3	1.44	0.98
2:B:1597:GLU:HB2	2:B:1600:LEU:HD22	1.46	0.97
2:B:1542:ARG:CZ	2:B:1542:ARG:H	1.78	0.96
2:B:1992:ASP:CB	2:B:1993:PRO:HD3	1.93	0.95
2:B:1721:MET:HG3	2:B:1786:ARG:NH2	1.81	0.94
1:A:229:LEU:HD23	1:A:241:ILE:HD12	1.51	0.92
2:B:1542:ARG:NE	2:B:1542:ARG:H	1.69	0.91
2:B:1580:ARG:HH11	2:B:1580:ARG:HG2	1.30	0.91
2:B:2067:ARG:HA	2:B:2067:ARG:HH11	1.33	0.90
2:B:1894:LYS:H	2:B:1894:LYS:HE2	1.40	0.85
2:B:1628:SER:O	2:B:1691:SER:HA	1.77	0.84
2:B:1893:PRO:HD2	2:B:1894:LYS:NZ	1.92	0.84
2:B:2152:ASN:HB2	2:B:2153:PRO:CD	2.08	0.83
1:A:198:GLN:HB2	3:A:2185:NAG:H81	1.59	0.82
1:A:140:LEU:HA	1:A:267:THR:HG21	1.62	0.82
2:B:2030:GLY:HA3	2:B:2036:ILE:HG13	1.61	0.82
1:A:4:ARG:HH22	1:A:170:LEU:HD23	1.45	0.81
1:A:91:TYR:CE1	1:A:96:GLU:HG3	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1721:MET:CG	2:B:1786:ARG:HH22	1.91	0.80
2:B:1911:LYS:O	2:B:1911:LYS:HD2	1.83	0.79
2:B:2096:VAL:HG23	2:B:2178:PHE:HE1	1.48	0.79
2:B:1992:ASP:HB3	2:B:1993:PRO:CD	2.07	0.79
2:B:2111:SER:HB2	2:B:2166:THR:HG22	1.63	0.78
2:B:2162:ILE:N	2:B:2162:ILE:HD12	1.99	0.78
2:B:1721:MET:HE1	2:B:1723:VAL:HB	1.66	0.77
2:B:1905:ASN:H	2:B:1905:ASN:HD22	1.32	0.77
2:B:1893:PRO:HD2	2:B:1894:LYS:HZ1	1.50	0.76
2:B:2083:GLN:HB3	2:B:2161:ARG:HG2	1.67	0.76
1:A:197:ASN:HD21	3:A:2185:NAG:H4	1.50	0.76
2:B:1808:LEU:HB3	2:B:1831:LEU:HD12	1.68	0.76
2:B:2168:ASN:C	2:B:2168:ASN:HD22	1.90	0.75
2:B:2096:VAL:HG23	2:B:2178:PHE:CE1	2.21	0.75
1:A:232:MET:HA	1:A:262:SER:O	1.87	0.75
2:B:1917:ASN:HD21	2:B:1919:GLU:HB2	1.52	0.75
1:A:167:LYS:H	1:A:167:LYS:HD2	1.51	0.75
2:B:1593:GLN:HG3	2:B:1597:GLU:HG3	1.70	0.73
1:A:279:THR:HA	1:A:295:TYR:HA	1.69	0.73
2:B:2152:ASN:CB	2:B:2153:PRO:HD3	2.11	0.73
2:B:1680:PRO:HG2	2:B:1813:THR:HA	1.70	0.73
1:A:161:PRO:HG2	1:A:184:VAL:HG11	1.69	0.73
2:B:1580:ARG:HG2	2:B:1580:ARG:NH1	1.95	0.73
2:B:2071:TRP:O	2:B:2172:ALA:HA	1.88	0.73
2:B:1692:ALA:O	2:B:1695:PRO:HD3	1.89	0.72
1:A:141:THR:OG1	1:A:267:THR:HB	1.89	0.72
2:B:1685:ARG:HD2	2:B:1686:ALA:H	1.55	0.71
1:A:133:THR:HG22	1:A:134:HIS:H	1.55	0.71
2:B:2126:TYR:OH	2:B:2153:PRO:HD2	1.91	0.71
1:A:162:LEU:O	1:A:163:LEU:HD23	1.91	0.70
2:B:1706:PRO:HB3	2:B:1729:VAL:HG11	1.73	0.70
1:A:202:LEU:HD23	1:A:203:MET:H	1.57	0.70
2:B:2101:LYS:HD3	2:B:2144:ARG:NH2	2.07	0.69
2:B:2055:TRP:HB2	2:B:2072:GLN:HB2	1.73	0.69
1:A:159:ILE:HD13	1:A:186:MET:SD	2.32	0.68
2:B:1915:GLU:C	2:B:1917:ASN:H	1.95	0.68
1:A:80:LYS:NZ	1:A:152:GLU:HG2	2.08	0.68
1:A:264:THR:CG2	2:B:1822:PRO:HG3	2.21	0.68
1:A:146:SER:HB3	1:A:153:ASP:OD1	1.93	0.68
2:B:1577:VAL:HG22	2:B:1703:LEU:HD21	1.75	0.67
2:B:1680:PRO:O	3:B:2188:NAG:H62	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1725:MET:HG2	2:B:1726:ARG:N	2.10	0.67
2:B:2168:ASN:HD22	2:B:2169:GLN:N	1.93	0.66
1:A:37:VAL:HG11	1:A:39:ARG:NH1	2.10	0.66
2:B:1742:TYR:C	2:B:1744:ASP:H	1.98	0.65
2:B:1541:ASN:HA	2:B:1542:ARG:HH21	1.61	0.65
2:B:2101:LYS:NZ	2:B:2144:ARG:HH22	1.94	0.65
2:B:2110:LYS:HB2	2:B:2166:THR:HG23	1.78	0.65
1:A:37:VAL:HG11	1:A:39:ARG:HH11	1.60	0.65
2:B:1542:ARG:NE	2:B:1542:ARG:N	2.44	0.65
2:B:2111:SER:CB	2:B:2166:THR:HG22	2.26	0.65
1:A:71:LYS:HB2	1:A:71:LYS:NZ	2.12	0.65
2:B:1998:ARG:HD3	2:B:1999:TYR:CE1	2.32	0.65
1:A:206:VAL:O	1:A:207:ASN:HB2	1.96	0.65
2:B:1543:LYS:HD2	7:B:2358:HOH:O	1.97	0.65
2:B:2092:ILE:HG22	2:B:2151:PHE:HE2	1.62	0.64
2:B:1724:ASP:O	2:B:1725:MET:O	2.15	0.64
2:B:1664:THR:HG22	2:B:1665:TYR:H	1.63	0.64
2:B:1821:TRP:HZ3	2:B:1823:LEU:HD23	1.62	0.63
2:B:2002:ILE:HD12	2:B:2015:LEU:HD22	1.80	0.63
2:B:1927:GLN:C	2:B:1998:ARG:HE	2.01	0.63
2:B:1890:TYR:HB3	2:B:1904:TYR:CE2	2.34	0.63
2:B:1721:MET:CE	2:B:1723:VAL:HB	2.28	0.63
2:B:1803:PHE:CD2	2:B:1808:LEU:HD11	2.34	0.63
2:B:1969:ASN:OD1	4:B:2189:NDG:N2	2.30	0.63
2:B:1541:ASN:OD1	2:B:1542:ARG:NH2	2.31	0.63
1:A:132:PRO:HA	1:A:140:LEU:HD11	1.79	0.63
2:B:1931:LEU:HD12	2:B:2022:VAL:HA	1.80	0.63
1:A:255:ILE:HD11	1:A:258:ILE:HG12	1.79	0.63
2:B:2091:LYS:O	2:B:2179:GLY:HA3	1.99	0.62
1:A:4:ARG:NH2	1:A:170:LEU:HD23	2.13	0.62
1:A:38:TYR:O	1:A:39:ARG:HD2	2.00	0.62
2:B:2090:LYS:HE2	2:B:2181:ASP:OD2	1.98	0.62
2:B:1963:TRP:CZ3	2:B:2001:ARG:HB2	2.34	0.62
2:B:1894:LYS:H	2:B:1894:LYS:CE	2.11	0.62
2:B:1898:LEU:HD22	2:B:1938:GLN:OE1	1.99	0.62
1:A:76:ASN:ND2	1:A:116:PRO:HA	2.14	0.61
1:A:161:PRO:HG3	1:A:230:ILE:CD1	2.30	0.61
2:B:1727:GLU:CD	2:B:1786:ARG:HH21	2.04	0.61
1:A:231:GLY:O	1:A:239:PHE:HE2	1.84	0.61
2:B:1662:ASN:HB2	4:B:2187:NDG:H5	1.81	0.61
2:B:2110:LYS:HD3	2:B:2167:TRP:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:HG3	1:A:50:PRO:HD3	1.82	0.61
2:B:1765:HIS:HD2	2:B:1850:ILE:HG23	1.66	0.61
2:B:2076:ASN:OD1	2:B:2170:SER:HA	2.00	0.61
2:B:1610:GLU:O	2:B:1613:ASP:HB2	2.01	0.61
2:B:2049:SER:HB2	2:B:2051:TRP:CE3	2.35	0.61
2:B:1543:LYS:HD2	2:B:1719:THR:HG21	1.83	0.60
2:B:1725:MET:HG2	2:B:1726:ARG:H	1.65	0.60
1:A:203:MET:O	1:A:205:THR:HG23	2.01	0.60
2:B:1803:PHE:CE1	2:B:1843:LEU:HD13	2.35	0.60
2:B:2109:VAL:HG21	2:B:2173:LEU:HG	1.83	0.60
2:B:1629:LEU:HD22	2:B:1669:TRP:HH2	1.64	0.60
2:B:1681:GLY:HA2	3:B:2188:NAG:H62	1.81	0.60
2:B:1662:ASN:HB2	4:B:2187:NDG:C5	2.32	0.60
2:B:1844:ASP:HB2	2:B:1851:GLN:HG3	1.84	0.60
1:A:90:LYS:NZ	2:B:1807:THR:HB	2.17	0.59
2:B:1780:TYR:O	2:B:1783:GLU:HB3	2.03	0.59
2:B:1685:ARG:HD2	2:B:1686:ALA:N	2.17	0.59
1:A:87:GLN:O	1:A:87:GLN:HG3	2.03	0.59
2:B:2092:ILE:HB	2:B:2155:ILE:HB	1.84	0.59
2:B:2008:TYR:O	2:B:2009:ASN:HB2	2.01	0.59
1:A:278:TRP:O	1:A:296:ILE:N	2.34	0.59
2:B:2037:GLU:O	2:B:2040:GLN:HB2	2.03	0.59
1:A:80:LYS:HZ1	1:A:152:GLU:HG2	1.66	0.59
2:B:1631:ALA:HB2	2:B:1669:TRP:CH2	2.38	0.59
1:A:236:PRO:HG3	2:B:1850:ILE:HD11	1.83	0.59
1:A:206:VAL:HG11	1:A:294:ALA:HB2	1.83	0.59
2:B:1731:LEU:HD12	2:B:1790:LEU:O	2.03	0.59
2:B:2055:TRP:CB	2:B:2072:GLN:HB2	2.31	0.58
2:B:1680:PRO:HG2	2:B:1813:THR:CA	2.33	0.58
2:B:1551:GLU:OE2	2:B:1741:TRP:CH2	2.56	0.58
2:B:1620:LYS:O	2:B:1621:ASN:HB3	2.03	0.58
1:A:206:VAL:O	1:A:206:VAL:HG12	2.03	0.58
1:A:158:LEU:O	1:A:159:ILE:HB	2.03	0.58
2:B:1912:LEU:HD23	2:B:2011:PRO:HG3	1.86	0.58
2:B:1988:GLU:H	2:B:1988:GLU:CD	2.07	0.58
2:B:2167:TRP:CZ3	2:B:2171:ILE:HD11	2.39	0.58
1:A:14:ARG:HG3	1:A:32:SER:HB3	1.86	0.58
1:A:167:LYS:N	1:A:167:LYS:HD2	2.19	0.57
2:B:1765:HIS:CD2	2:B:1850:ILE:HG23	2.39	0.57
2:B:1634:LEU:HD23	2:B:1635:SER:N	2.19	0.57
2:B:1803:PHE:HD2	2:B:1808:LEU:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:HD21	3:A:2185:NAG:C4	2.16	0.57
2:B:1942:HIS:HD1	2:B:1943:TYR:HD1	1.51	0.57
1:A:186:MET:HG2	1:A:186:MET:O	2.03	0.57
1:A:229:LEU:N	1:A:229:LEU:HD12	2.20	0.57
2:B:1887:PHE:N	2:B:1887:PHE:CD1	2.73	0.56
2:B:2081:TRP:CZ3	2:B:2083:GLN:HG2	2.39	0.56
1:A:143:ILE:CG2	1:A:265:SER:HB3	2.35	0.56
2:B:1596:TYR:HD2	2:B:1596:TYR:N	2.04	0.56
1:A:132:PRO:HG3	1:A:140:LEU:HG	1.87	0.56
1:A:90:LYS:HZ1	2:B:1807:THR:HB	1.69	0.56
1:A:186:MET:O	1:A:188:ALA:N	2.38	0.56
2:B:1959:ASP:O	2:B:1960:ARG:CB	2.54	0.56
2:B:1629:LEU:HD22	2:B:1669:TRP:CH2	2.39	0.56
1:A:145:TYR:CD1	1:A:145:TYR:N	2.73	0.56
2:B:1911:LYS:C	2:B:1911:LYS:HD2	2.26	0.56
1:A:133:THR:HG22	1:A:134:HIS:N	2.21	0.56
1:A:60:PRO:HD2	1:A:144:TYR:OH	2.05	0.56
2:B:1704:ILE:CD1	2:B:1792:LEU:HD12	2.36	0.56
1:A:75:LYS:HE3	1:A:77:LYS:HE3	1.86	0.56
1:A:212:GLY:HA2	1:A:214:MET:SD	2.46	0.56
1:A:171:THR:HG22	1:A:173:ASP:H	1.70	0.56
2:B:1992:ASP:CB	2:B:1993:PRO:CD	2.75	0.55
2:B:1912:LEU:O	2:B:1914:THR:N	2.38	0.55
1:A:9:ALA:HB1	1:A:75:LYS:O	2.06	0.55
2:B:1596:TYR:CD2	2:B:1596:TYR:N	2.74	0.55
2:B:1892:GLU:O	2:B:1895:LEU:HB2	2.06	0.55
2:B:2110:LYS:HD3	2:B:2167:TRP:C	2.26	0.55
1:A:284:ILE:O	1:A:286:ARG:N	2.39	0.55
2:B:1596:TYR:CE2	2:B:1597:GLU:HG2	2.41	0.55
2:B:1657:ASN:C	2:B:1657:ASN:HD22	2.10	0.55
1:A:238:LEU:H	1:A:238:LEU:HD23	1.71	0.55
1:A:248:LEU:HD11	1:A:256:SER:O	2.06	0.55
1:A:86:ALA:HB2	1:A:124:TRP:CH2	2.41	0.55
1:A:71:LYS:HZ2	1:A:71:LYS:HB2	1.72	0.55
1:A:189:VAL:HB	1:A:204:TYR:HD1	1.72	0.55
2:B:1543:LYS:HA	2:B:1543:LYS:HE2	1.87	0.55
2:B:1543:LYS:CD	2:B:1719:THR:HG21	2.37	0.55
1:A:66:VAL:HG21	1:A:167:LYS:HE3	1.89	0.55
1:A:249:GLU:OE2	1:A:254:LYS:HB3	2.07	0.55
1:A:138:PRO:HG2	1:A:179:PHE:CE2	2.41	0.55
1:A:250:GLN:OE1	1:A:255:ILE:HD13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2025:CYS:SG	2:B:2091:LYS:HD3	2.47	0.55
2:B:2048:LYS:HG2	2:B:2054:TYR:HD2	1.70	0.55
2:B:2112:TYR:CD2	2:B:2112:TYR:N	2.74	0.55
1:A:261:VAL:O	1:A:263:ALA:N	2.41	0.54
1:A:91:TYR:CZ	1:A:96:GLU:HG3	2.40	0.54
1:A:278:TRP:HB2	1:A:296:ILE:HD12	1.89	0.54
2:B:1681:GLY:HA3	2:B:1811:ASN:OD1	2.08	0.54
2:B:1704:ILE:HD13	2:B:1731:LEU:HD22	1.88	0.54
2:B:1782:GLN:NE2	2:B:1834:LYS:HE2	2.23	0.54
2:B:1906:ALA:HB2	2:B:2014:ARG:HG3	1.89	0.54
2:B:2071:TRP:HE3	2:B:2173:LEU:HB2	1.72	0.54
2:B:1606:VAL:O	2:B:1606:VAL:HG22	2.08	0.54
1:A:38:TYR:C	1:A:39:ARG:HD2	2.28	0.54
2:B:1596:TYR:HD2	2:B:1596:TYR:H	1.55	0.54
2:B:2039:LYS:HZ3	2:B:2039:LYS:H	1.55	0.54
2:B:2121:THR:HB	7:B:2267:HOH:O	2.08	0.53
2:B:1817:GLN:HE21	2:B:1817:GLN:HA	1.73	0.53
2:B:2077:ASN:O	2:B:2167:TRP:HH2	1.90	0.53
2:B:1577:VAL:HG13	2:B:1703:LEU:HG	1.90	0.53
1:A:214:MET:SD	1:A:214:MET:N	2.80	0.53
1:A:177:LYS:HE3	1:A:178:MET:HE3	1.88	0.53
2:B:1810:GLU:O	2:B:1815:GLN:HA	2.08	0.53
1:A:13:ILE:O	1:A:13:ILE:HG13	2.06	0.53
2:B:1870:MET:HG2	2:B:1926:MET:HE1	1.91	0.53
1:A:232:MET:O	1:A:233:SER:HB2	2.08	0.53
2:B:2062:LEU:O	2:B:2063:ASN:HB2	2.09	0.53
1:A:69:ILE:HG22	1:A:69:ILE:O	2.09	0.53
1:A:261:VAL:HG23	1:A:264:THR:CG2	2.38	0.53
1:A:183:HIS:O	1:A:228:HIS:HB2	2.09	0.53
2:B:1912:LEU:HB3	2:B:2011:PRO:HG2	1.91	0.53
1:A:233:SER:HB2	1:A:239:PHE:HZ	1.74	0.52
2:B:2038:ASN:C	2:B:2040:GLN:H	2.12	0.52
2:B:2086:LEU:CD1	2:B:2092:ILE:HD11	2.39	0.52
2:B:2054:TYR:CD1	2:B:2054:TYR:N	2.77	0.52
1:A:36:ILE:HG12	1:A:156:SER:OG	2.08	0.52
2:B:2109:VAL:CG2	2:B:2173:LEU:HG	2.39	0.52
2:B:1809:LEU:O	2:B:1831:LEU:HB2	2.10	0.52
1:A:47:LYS:HG2	1:A:48:GLU:N	2.25	0.52
2:B:1887:PHE:CE2	2:B:1892:GLU:HG2	2.44	0.52
2:B:1835:ALA:HB1	2:B:1861:ILE:HD13	1.92	0.52
1:A:37:VAL:HG12	1:A:38:TYR:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1742:TYR:C	2:B:1744:ASP:N	2.63	0.52
1:A:56:GLY:HA3	1:A:207:ASN:O	2.10	0.52
2:B:2039:LYS:N	2:B:2039:LYS:HZ3	2.08	0.52
2:B:1551:GLU:OE2	2:B:1741:TRP:HH2	1.92	0.52
2:B:1959:ASP:O	2:B:1960:ARG:HB2	2.09	0.52
1:A:212:GLY:O	1:A:214:MET:HG3	2.09	0.52
1:A:196:TRP:HA	1:A:196:TRP:HE3	1.75	0.52
2:B:2101:LYS:HZ3	2:B:2144:ARG:HH22	1.57	0.52
2:B:1610:GLU:HA	2:B:1710:CYS:O	2.10	0.52
1:A:87:GLN:HG2	1:A:143:ILE:HG13	1.91	0.52
1:A:177:LYS:C	1:A:179:PHE:H	2.13	0.52
1:A:132:PRO:HB2	1:A:166:LYS:HE2	1.90	0.51
2:B:1905:ASN:O	2:B:2014:ARG:HD3	2.10	0.51
2:B:2125:PRO:O	2:B:2127:ARG:HG3	2.10	0.51
2:B:1912:LEU:C	2:B:1914:THR:H	2.13	0.51
1:A:49:LYS:O	1:A:50:PRO:O	2.29	0.51
2:B:1921:TRP:C	2:B:1921:TRP:CD1	2.84	0.51
1:A:58:LEU:HD11	1:A:161:PRO:HD3	1.92	0.51
1:A:196:TRP:HA	1:A:196:TRP:CE3	2.45	0.51
2:B:2086:LEU:HD13	2:B:2092:ILE:HD11	1.92	0.51
1:A:206:VAL:O	1:A:207:ASN:CB	2.58	0.51
1:A:187:PHE:CE2	1:A:241:ILE:HG12	2.45	0.51
2:B:2069:ASN:O	2:B:2070:ALA:HB2	2.11	0.51
2:B:1714:THR:O	2:B:1722:PRO:CD	2.59	0.51
2:B:1960:ARG:HD2	2:B:1960:ARG:O	2.10	0.51
1:A:155:ASN:C	1:A:157:GLY:H	2.12	0.51
2:B:1991:ILE:O	2:B:1991:ILE:HG22	2.11	0.51
2:B:2083:GLN:HB3	2:B:2161:ARG:CG	2.38	0.51
2:B:1664:THR:HG22	2:B:1665:TYR:N	2.24	0.51
2:B:2075:ALA:C	2:B:2076:ASN:HD22	2.14	0.51
2:B:1781:GLU:OE2	2:B:1864:ARG:HB2	2.10	0.51
1:A:167:LYS:H	1:A:167:LYS:CD	2.21	0.51
2:B:1679:ASN:HB2	2:B:1680:PRO:HD3	1.93	0.51
1:A:177:LYS:HG2	1:A:178:MET:N	2.26	0.51
2:B:1818:LEU:HD22	2:B:1818:LEU:N	2.25	0.51
1:A:90:LYS:HD2	1:A:130:SER:HB3	1.92	0.50
2:B:2038:ASN:O	2:B:2040:GLN:N	2.41	0.50
2:B:1812:GLY:C	2:B:1814:GLN:H	2.13	0.50
2:B:2086:LEU:O	2:B:2088:LYS:N	2.44	0.50
2:B:1618:ARG:HH11	2:B:1664:THR:HG21	1.77	0.50
2:B:1789:LEU:HD12	2:B:1831:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1694:ASN:C	2:B:1694:ASN:HD22	2.14	0.50
2:B:1731:LEU:HB2	2:B:1790:LEU:CD1	2.42	0.50
2:B:1965:ILE:HG21	2:B:1974:VAL:HG11	1.93	0.50
2:B:2086:LEU:C	2:B:2088:LYS:H	2.14	0.50
1:A:165:CYS:SG	1:A:170:LEU:HD13	2.51	0.50
2:B:1789:LEU:CD1	2:B:1831:LEU:HD21	2.42	0.50
2:B:1721:MET:HE2	2:B:1786:ARG:HH12	1.77	0.50
2:B:1917:ASN:ND2	2:B:1919:GLU:HB2	2.24	0.50
1:A:177:LYS:O	1:A:179:PHE:N	2.44	0.50
2:B:2168:ASN:C	2:B:2168:ASN:ND2	2.63	0.50
2:B:1784:TRP:CD2	3:B:2188:NAG:H81	2.46	0.50
1:A:105:LEU:HB3	1:A:106:PRO:HD2	1.94	0.50
2:B:2048:LYS:HG2	2:B:2054:TYR:CD2	2.47	0.49
2:B:1931:LEU:O	2:B:2019:GLY:HA3	2.12	0.49
1:A:180:GLU:OE1	1:A:181:LYS:HB2	2.12	0.49
1:A:3:LEU:C	1:A:3:LEU:HD23	2.32	0.49
2:B:1575:LYS:HE2	2:B:1741:TRP:CE3	2.48	0.49
1:A:254:LYS:HD3	1:A:254:LYS:C	2.32	0.49
2:B:1730:LEU:HD22	2:B:1730:LEU:N	2.27	0.49
2:B:1723:VAL:HG12	2:B:1724:ASP:N	2.28	0.49
1:A:149:ASN:C	1:A:149:ASN:HD22	2.16	0.49
2:B:1740:SER:OG	2:B:1741:TRP:CD1	2.66	0.49
2:B:1657:ASN:HD22	2:B:1658:ALA:N	2.11	0.49
1:A:83:SER:HB3	1:A:112:ASP:O	2.13	0.49
1:A:247:VAL:O	1:A:247:VAL:HG22	2.12	0.49
2:B:1870:MET:HG2	2:B:1926:MET:CE	2.43	0.49
2:B:1935:ILE:HD11	2:B:2002:ILE:HD13	1.95	0.49
2:B:1617:VAL:HG21	2:B:1629:LEU:HD13	1.94	0.49
2:B:1550:GLU:OE2	2:B:1582:TYR:HE1	1.96	0.49
2:B:1919:GLU:HB3	2:B:1920:PRO:HD3	1.95	0.48
1:A:37:VAL:CG1	1:A:39:ARG:HH11	2.24	0.48
1:A:126:ILE:O	1:A:126:ILE:HG13	2.12	0.48
2:B:1723:VAL:O	2:B:1724:ASP:C	2.51	0.48
1:A:229:LEU:HD23	1:A:241:ILE:CD1	2.32	0.48
1:A:36:ILE:N	1:A:156:SER:O	2.39	0.48
2:B:1554:TRP:O	2:B:1573:VAL:HA	2.13	0.48
1:A:189:VAL:HB	1:A:204:TYR:CD1	2.48	0.48
1:A:147:TYR:O	1:A:149:ASN:N	2.47	0.48
2:B:1590:LEU:O	2:B:1592:PRO:HD3	2.14	0.48
2:B:1914:THR:CB	2:B:1920:PRO:HD2	2.27	0.48
2:B:1843:LEU:O	2:B:1856:GLN:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1742:TYR:O	2:B:1744:ASP:N	2.46	0.48
2:B:1574:TYR:CD1	2:B:1737:GLU:HG3	2.48	0.48
1:A:125:ILE:O	1:A:125:ILE:HG22	2.12	0.48
2:B:1540:GLY:HA2	2:B:1612:ASP:O	2.13	0.48
2:B:1915:GLU:C	2:B:1917:ASN:N	2.65	0.48
1:A:233:SER:O	1:A:235:GLY:N	2.43	0.48
1:A:179:PHE:O	1:A:180:GLU:O	2.32	0.48
2:B:1914:THR:HB	2:B:1920:PRO:CD	2.27	0.48
1:A:161:PRO:HG3	1:A:230:ILE:HD12	1.94	0.48
2:B:1821:TRP:CZ3	2:B:1823:LEU:HA	2.49	0.48
2:B:2099:GLY:HA3	2:B:2108:TYR:HB3	1.96	0.48
2:B:1716:ASP:O	2:B:1719:THR:N	2.47	0.48
1:A:248:LEU:HD23	1:A:248:LEU:H	1.78	0.48
1:A:145:TYR:HE2	1:A:150:LEU:HD22	1.79	0.48
1:A:282:SER:O	1:A:284:ILE:N	2.47	0.48
2:B:1550:GLU:OE2	2:B:1582:TYR:CE1	2.67	0.47
1:A:212:GLY:C	1:A:214:MET:SD	2.93	0.47
2:B:1898:LEU:O	2:B:1899:ASN:HB2	2.14	0.47
1:A:47:LYS:HG2	1:A:48:GLU:H	1.78	0.47
2:B:1612:ASP:HB2	2:B:1712:LYS:HZ3	1.78	0.47
2:B:1804:HIS:O	2:B:1806:GLN:HG2	2.15	0.47
2:B:1721:MET:CE	2:B:1786:ARG:HH12	2.28	0.47
2:B:1831:LEU:N	2:B:1831:LEU:HD23	2.29	0.47
1:A:250:GLN:CD	1:A:255:ILE:HD13	2.34	0.47
2:B:2049:SER:HB2	2:B:2051:TRP:CZ3	2.49	0.47
1:A:143:ILE:HD12	1:A:143:ILE:C	2.34	0.47
2:B:2076:ASN:HD22	2:B:2076:ASN:N	2.12	0.47
2:B:1557:SER:O	2:B:1558:LYS:C	2.53	0.47
2:B:1787:LEU:HD21	2:B:1833:MET:HB3	1.95	0.47
2:B:1868:MET:HE1	2:B:2027:THR:HA	1.95	0.47
2:B:1854:GLY:O	2:B:1856:GLN:N	2.46	0.47
2:B:1926:MET:C	2:B:1928:LYS:H	2.16	0.47
2:B:1710:CYS:SG	2:B:1715:LEU:HD21	2.54	0.47
1:A:53:ARG:HH22	1:A:217:ILE:HG12	1.78	0.47
2:B:1770:MET:HE3	2:B:1774:LEU:HD12	1.96	0.47
2:B:2162:ILE:N	2:B:2162:ILE:CD1	2.69	0.47
2:B:1899:ASN:O	2:B:1900:ASN:C	2.53	0.47
2:B:1844:ASP:HB2	2:B:1851:GLN:CG	2.45	0.47
1:A:87:GLN:O	1:A:87:GLN:CG	2.62	0.47
1:A:149:ASN:HD22	1:A:150:LEU:N	2.12	0.47
2:B:2121:THR:O	2:B:2122:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1576:LYS:HD2	2:B:1701:SER:O	2.14	0.47
2:B:1797:ASP:O	2:B:1798:ILE:O	2.33	0.47
2:B:2106:GLU:CD	2:B:2143:VAL:HG21	2.36	0.47
2:B:1618:ARG:HD2	2:B:1664:THR:CG2	2.45	0.47
2:B:1629:LEU:CD2	2:B:1669:TRP:HH2	2.27	0.47
2:B:1905:ASN:HD22	2:B:1905:ASN:N	1.99	0.47
1:A:147:TYR:CD1	1:A:150:LEU:HD21	2.50	0.47
2:B:1771:ILE:O	2:B:1771:ILE:HG13	2.15	0.47
1:A:65:GLU:HB2	1:A:68:ASP:OD1	2.14	0.47
2:B:2044:SER:HB3	2:B:2081:TRP:CE2	2.50	0.46
2:B:1802:HIS:HB3	2:B:1844:ASP:OD1	2.14	0.46
2:B:2110:LYS:CB	2:B:2166:THR:HG23	2.44	0.46
1:A:161:PRO:HG3	1:A:230:ILE:HD11	1.98	0.46
1:A:177:LYS:HG2	1:A:178:MET:HE2	1.97	0.46
2:B:1812:GLY:C	2:B:1814:GLN:N	2.69	0.46
1:A:81:PRO:O	1:A:82:LEU:HD23	2.15	0.46
2:B:2047:LYS:O	2:B:2048:LYS:HG3	2.15	0.46
2:B:2046:PHE:HA	2:B:2072:GLN:O	2.15	0.46
2:B:1714:THR:O	2:B:1722:PRO:HD2	2.14	0.46
2:B:1722:PRO:HG2	2:B:1723:VAL:H	1.80	0.46
2:B:1912:LEU:C	2:B:1914:THR:N	2.69	0.46
2:B:1539:THR:O	2:B:1541:ASN:N	2.48	0.46
2:B:1599:HIS:NE2	2:B:1728:PHE:HD1	2.14	0.46
1:A:136:ASP:HB2	1:A:137:PRO:HD2	1.97	0.46
2:B:2068:VAL:O	2:B:2068:VAL:HG23	2.16	0.46
2:B:1814:GLN:HG2	2:B:1816:HIS:NE2	2.31	0.46
2:B:1557:SER:O	2:B:1560:VAL:HG12	2.15	0.46
1:A:205:THR:O	1:A:206:VAL:HG23	2.16	0.46
2:B:1770:MET:CE	2:B:1774:LEU:HD12	2.46	0.46
2:B:1893:PRO:HD2	2:B:1894:LYS:HZ3	1.74	0.46
1:A:36:ILE:HD12	1:A:78:ALA:HB1	1.98	0.46
2:B:1872:LEU:HG	2:B:1877:ILE:HD12	1.98	0.46
2:B:1724:ASP:OD2	2:B:1786:ARG:HB2	2.16	0.45
1:A:243:PHE:CE1	1:A:280:ILE:HD13	2.51	0.45
2:B:2055:TRP:CG	2:B:2072:GLN:HB2	2.50	0.45
1:A:71:LYS:CB	1:A:71:LYS:NZ	2.79	0.45
1:A:169:THR:O	1:A:177:LYS:HB2	2.15	0.45
2:B:2050:TRP:HE3	2:B:2050:TRP:H	1.63	0.45
2:B:1836:SER:O	2:B:1837:LYS:HB2	2.15	0.45
2:B:1583:LEU:HD21	2:B:1973:ASN:HD21	1.81	0.45
2:B:1803:PHE:CD1	2:B:1843:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HZ3	1:A:152:GLU:HG2	1.78	0.45
2:B:1942:HIS:ND1	2:B:1943:TYR:HD1	2.14	0.45
1:A:94:PHE:HE2	2:B:2182:MET:CE	2.30	0.45
1:A:187:PHE:HD1	1:A:187:PHE:H	1.65	0.45
1:A:239:PHE:HD1	1:A:287:HIS:CE1	2.34	0.45
2:B:1870:MET:HG3	7:B:2199:HOH:O	2.16	0.45
1:A:59:GLY:O	1:A:60:PRO:O	2.35	0.45
2:B:1939:GLY:O	2:B:2014:ARG:NE	2.46	0.45
2:B:1801:VAL:HG23	2:B:1801:VAL:O	2.14	0.45
2:B:1791:ASN:HB2	2:B:1823:LEU:HD13	1.98	0.45
2:B:2049:SER:OG	2:B:2053:ASN:HB2	2.16	0.45
2:B:1632:HIS:HB3	2:B:1688:ALA:O	2.16	0.45
1:A:255:ILE:HD12	1:A:257:ALA:O	2.16	0.45
2:B:1611:VAL:O	2:B:1612:ASP:HB2	2.16	0.45
2:B:2140:ASN:HA	2:B:2147:VAL:HG21	1.99	0.45
2:B:1631:ALA:HB2	2:B:1669:TRP:CZ2	2.52	0.45
1:A:238:LEU:HD23	1:A:238:LEU:N	2.32	0.45
2:B:1618:ARG:HD2	2:B:1664:THR:HG22	1.99	0.44
1:A:89:ILE:HD11	1:A:164:ILE:HD11	1.99	0.44
1:A:10:ALA:O	1:A:77:LYS:HB2	2.17	0.44
1:A:261:VAL:HG23	1:A:264:THR:HG23	2.00	0.44
1:A:229:LEU:CD1	1:A:229:LEU:N	2.80	0.44
2:B:1726:ARG:HD3	2:B:1726:ARG:HA	1.62	0.44
1:A:133:THR:HG21	2:B:1815:GLN:HB2	1.99	0.44
2:B:1716:ASP:O	2:B:1718:GLU:N	2.50	0.44
2:B:2123:TRP:CZ3	2:B:2161:ARG:HG3	2.53	0.44
2:B:1704:ILE:HD11	2:B:1792:LEU:HD12	1.99	0.44
2:B:1871:GLY:HA3	2:B:1876:LEU:HB2	2.00	0.44
2:B:2000:ILE:HG13	2:B:2017:LEU:HD13	1.99	0.44
2:B:1686:ALA:HA	2:B:1708:LEU:HD12	2.00	0.44
1:A:108:GLU:O	1:A:111:ASP:OD1	2.35	0.44
1:A:219:VAL:HG12	1:A:220:CYS:N	2.32	0.44
2:B:2067:ARG:CA	2:B:2067:ARG:HH11	2.17	0.44
2:B:1832:GLU:HG3	3:B:2188:NAG:O7	2.17	0.44
1:A:161:PRO:CG	1:A:184:VAL:HG11	2.43	0.44
1:A:35:LYS:NZ	1:A:192:GLU:OE1	2.46	0.44
2:B:2092:ILE:HG22	2:B:2151:PHE:CE2	2.48	0.44
2:B:2112:TYR:HD2	2:B:2112:TYR:N	2.16	0.44
2:B:1900:ASN:OD1	2:B:1905:ASN:HB2	2.18	0.43
2:B:1939:GLY:O	2:B:2014:ARG:NH2	2.50	0.43
1:A:204:TYR:HB3	1:A:292:MET:SD	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1790:LEU:HD12	2:B:1790:LEU:O	2.18	0.43
2:B:1657:ASN:C	2:B:1657:ASN:ND2	2.70	0.43
1:A:152:GLU:O	1:A:153:ASP:C	2.56	0.43
2:B:1926:MET:O	2:B:1927:GLN:HB2	2.18	0.43
2:B:1722:PRO:HG2	2:B:1723:VAL:N	2.32	0.43
1:A:136:ASP:OD2	1:A:140:LEU:HD21	2.18	0.43
1:A:133:THR:CG2	1:A:134:HIS:H	2.22	0.43
1:A:87:GLN:CG	1:A:143:ILE:HG13	2.49	0.43
1:A:163:LEU:HD22	1:A:228:HIS:CE1	2.53	0.43
1:A:209:TYR:CD2	1:A:214:MET:HB3	2.53	0.43
2:B:1872:LEU:HB2	2:B:2016:GLU:OE2	2.18	0.43
2:B:1950:THR:O	2:B:1951:GLU:HB2	2.18	0.43
2:B:2070:ALA:HB1	2:B:2173:LEU:O	2.18	0.43
1:A:143:ILE:HD12	1:A:144:TYR:N	2.34	0.43
2:B:1944:LEU:O	2:B:1946:PRO:HD3	2.19	0.43
2:B:1894:LYS:CD	2:B:1894:LYS:N	2.82	0.43
1:A:146:SER:CB	1:A:153:ASP:OD1	2.64	0.43
2:B:2049:SER:C	2:B:2051:TRP:H	2.22	0.43
2:B:2162:ILE:H	2:B:2162:ILE:HD12	1.79	0.43
2:B:1927:GLN:CA	2:B:1998:ARG:HE	2.32	0.43
1:A:133:THR:HB	1:A:136:ASP:OD1	2.19	0.42
2:B:1706:PRO:CB	2:B:1729:VAL:HG11	2.47	0.42
2:B:2054:TYR:O	2:B:2068:VAL:HG21	2.18	0.42
2:B:2098:GLN:HA	2:B:2140:ASN:ND2	2.34	0.42
1:A:276:GLY:O	1:A:277:ARG:HG2	2.19	0.42
2:B:1914:THR:HG21	2:B:2004:PRO:O	2.19	0.42
1:A:39:ARG:HB3	1:A:48:GLU:OE2	2.19	0.42
2:B:1868:MET:CE	2:B:2027:THR:HA	2.48	0.42
2:B:1935:ILE:HD11	2:B:2002:ILE:CD1	2.49	0.42
2:B:2016:GLU:HA	2:B:2016:GLU:OE2	2.18	0.42
1:A:154:PHE:CD1	1:A:232:MET:HG2	2.55	0.42
2:B:1876:LEU:HD22	2:B:2148:LYS:HB2	2.01	0.42
1:A:181:LYS:HA	7:A:2276:HOH:O	2.20	0.42
2:B:1967:LYS:HG2	2:B:1968:GLY:N	2.34	0.42
2:B:2155:ILE:HG21	2:B:2160:ILE:HD11	2.02	0.42
2:B:1594:GLY:H	2:B:1596:TYR:HE2	1.68	0.42
1:A:287:HIS:O	1:A:292:MET:HB2	2.19	0.42
1:A:280:ILE:HB	1:A:294:ALA:O	2.20	0.42
1:A:248:LEU:HG	1:A:248:LEU:O	2.18	0.42
1:A:191:ASP:OD2	1:A:191:ASP:C	2.57	0.42
2:B:2081:TRP:HZ3	2:B:2083:GLN:HG2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1895:LEU:O	2:B:1897:ARG:N	2.51	0.42
2:B:1784:TRP:CZ2	2:B:1834:LYS:HB2	2.55	0.42
2:B:1716:ASP:O	2:B:1717:LYS:C	2.58	0.42
2:B:1817:GLN:NE2	2:B:1817:GLN:HA	2.33	0.42
1:A:83:SER:HB2	1:A:122:TYR:OH	2.20	0.42
2:B:1557:SER:O	2:B:1560:VAL:N	2.50	0.42
2:B:2167:TRP:CE3	2:B:2171:ILE:HD11	2.55	0.42
2:B:1969:ASN:OD1	4:B:2189:NDG:H3	2.19	0.42
2:B:2037:GLU:HB3	2:B:2039:LYS:HE2	2.02	0.42
1:A:15:TRP:CH2	1:A:208:GLY:HA3	2.55	0.42
2:B:1632:HIS:HB2	2:B:1690:TYR:CE1	2.55	0.42
1:A:133:THR:H	1:A:136:ASP:CG	2.23	0.42
2:B:2044:SER:HB3	2:B:2081:TRP:NE1	2.35	0.41
2:B:1714:THR:O	2:B:1722:PRO:HD3	2.20	0.41
2:B:1913:SER:O	2:B:1915:GLU:OE2	2.38	0.41
2:B:2101:LYS:CD	2:B:2144:ARG:NH2	2.81	0.41
1:A:171:THR:HG22	1:A:172:GLU:N	2.34	0.41
2:B:1893:PRO:C	2:B:1895:LEU:H	2.23	0.41
1:A:53:ARG:O	1:A:53:ARG:HG3	2.20	0.41
1:A:153:ASP:HA	1:A:158:LEU:HD12	2.02	0.41
2:B:1618:ARG:HD3	2:B:1666:THR:OG1	2.19	0.41
2:B:1802:HIS:N	2:B:1844:ASP:O	2.47	0.41
2:B:2034:GLY:O	2:B:2035:LYS:C	2.59	0.41
2:B:2085:ASP:C	2:B:2087:LEU:H	2.22	0.41
2:B:1724:ASP:C	2:B:1725:MET:O	2.58	0.41
1:A:160:GLY:HA2	1:A:161:PRO:HD3	1.84	0.41
2:B:1662:ASN:CB	4:B:2187:NDG:H5	2.49	0.41
1:A:66:VAL:HG23	1:A:66:VAL:O	2.20	0.41
2:B:1813:THR:HG22	2:B:1813:THR:O	2.21	0.41
2:B:1692:ALA:O	2:B:1693:VAL:C	2.59	0.41
1:A:89:ILE:CG2	1:A:90:LYS:N	2.83	0.41
1:A:254:LYS:HD3	1:A:254:LYS:O	2.21	0.41
2:B:1970:SER:HG	2:B:1975:MET:HA	1.86	0.41
1:A:216:ASP:HB3	1:A:295:TYR:O	2.21	0.41
2:B:1998:ARG:NH1	2:B:1999:TYR:OH	2.54	0.41
1:A:191:ASP:OD2	1:A:193:SER:CB	2.69	0.41
2:B:1820:VAL:HG11	2:B:1846:GLU:OE2	2.20	0.41
2:B:1578:VAL:HA	2:B:1703:LEU:HD23	2.03	0.41
2:B:1740:SER:OG	2:B:1741:TRP:HD1	2.04	0.41
1:A:176:GLN:HB3	1:A:180:GLU:HA	2.02	0.41
1:A:179:PHE:CD1	1:A:179:PHE:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1557:SER:HB3	2:B:1771:ILE:HD11	2.01	0.41
2:B:1851:GLN:C	2:B:1851:GLN:HE21	2.24	0.41
2:B:1704:ILE:HG12	2:B:1705:GLY:N	2.36	0.41
2:B:1817:GLN:HE21	2:B:1817:GLN:CA	2.32	0.41
2:B:1818:LEU:CD2	2:B:1818:LEU:N	2.84	0.41
1:A:135:ASP:OD1	1:A:135:ASP:O	2.39	0.41
2:B:1914:THR:CG2	2:B:2004:PRO:O	2.69	0.41
2:B:1694:ASN:O	2:B:1695:PRO:C	2.58	0.41
1:A:12:SER:HA	1:A:35:LYS:O	2.21	0.41
2:B:2151:PHE:O	2:B:2152:ASN:C	2.58	0.40
2:B:2083:GLN:HA	2:B:2160:ILE:O	2.21	0.40
2:B:2003:SER:HA	2:B:2004:PRO:HD3	1.85	0.40
2:B:1894:LYS:H	2:B:1894:LYS:CD	2.35	0.40
2:B:1886:GLU:OE1	2:B:1911:LYS:HE3	2.20	0.40
1:A:202:LEU:HD23	1:A:203:MET:N	2.30	0.40
1:A:31:THR:HB	1:A:32:SER:H	1.67	0.40
2:B:2089:ILE:HD11	2:B:2118:ASP:OD2	2.21	0.40
1:A:133:THR:N	1:A:136:ASP:OD1	2.55	0.40
2:B:1789:LEU:HD13	2:B:1801:VAL:HG21	2.03	0.40
1:A:55:SER:O	1:A:56:GLY:O	2.40	0.40
1:A:37:VAL:CG1	1:A:38:TYR:N	2.83	0.40
2:B:1969:ASN:CG	4:B:2189:NDG:HA	2.21	0.40
1:A:36:ILE:O	1:A:156:SER:O	2.39	0.40
1:A:192:GLU:HB3	1:A:199:THR:OG1	2.22	0.40
2:B:1557:SER:O	2:B:1559:PHE:N	2.55	0.40
2:B:2045:SER:HB2	2:B:2074:LYS:HB3	2.02	0.40
1:A:15:TRP:O	1:A:32:SER:HA	2.20	0.40
1:A:175:THR:HG22	1:A:176:GLN:N	2.36	0.40
1:A:129:HIS:ND1	1:A:129:HIS:C	2.75	0.40
2:B:1721:MET:HE3	2:B:1724:ASP:HB3	2.03	0.40
1:A:244:ASN:HB3	1:A:278:TRP:CE3	2.56	0.40
1:A:155:ASN:C	1:A:157:GLY:N	2.75	0.40
2:B:1770:MET:HG2	2:B:1773:ASN:O	2.22	0.40
2:B:2058:PHE:CD1	2:B:2058:PHE:C	2.95	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	260/306 (85%)	178 (68%)	46 (18%)	36 (14%)	0	1
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	1	3
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	1	2

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	60	PRO
1	A	180	GLU
1	A	187	PHE
1	A	206	VAL
1	A	207	ASN
1	A	210	VAL
1	A	233	SER
1	A	262	SER
1	A	285	PRO
2	B	1680	PRO
2	B	1682	SER
2	B	1723	VAL
2	B	1725	MET
2	B	1867	LYS
2	B	1970	SER
2	B	2050	TRP
2	B	2067	ARG
1	A	56	GLY
1	A	61	THR
1	A	159	ILE
1	A	178	MET
1	A	246	GLN
1	A	283	LEU
2	B	1540	GLY

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Mol	Chain	Res	Type
2	B	1558	LYS
2	B	1662	ASN
2	B	1671	ALA
2	B	1695	PRO
2	B	1717	LYS
2	B	1719	THR
2	B	1848	GLY
2	B	1889	GLY
2	B	1913	SER
2	B	2039	LYS
2	B	2087	LEU
1	A	53	ARG
1	A	88	GLY
1	A	148	VAL
1	A	153	ASP
1	A	203	MET
1	A	216	ASP
2	B	1634	LEU
2	B	1665	TYR
2	B	1722	PRO
2	B	1794	GLY
2	B	1846	GLU
2	B	1896	ALA
2	B	2078	ASN
1	A	2	LYS
1	A	41	TYR
1	A	43	ALA
1	A	116	PRO
1	A	156	SER
1	A	195	SER
1	A	215	PRO
2	B	1712	LYS
2	B	1797	ASP
2	B	1798	ILE
2	B	1837	LYS
2	B	1918	PRO
2	B	1993	PRO
2	B	2122	ASP
1	A	152	GLU
1	A	177	LYS
1	A	234	SER
2	B	1557	SER

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Mol	Chain	Res	Type
2	B	1914	THR
2	B	2009	ASN
1	A	45	PHE
1	A	137	PRO
2	B	1743	TYR
2	B	1942	HIS
2	B	1960	ARG
1	A	217	ILE
2	B	1661	PRO
1	A	126	ILE

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	233/269 (87%)	208 (89%)	25 (11%)	8	24
2	B	526/570 (92%)	467 (89%)	59 (11%)	7	22
All	All	759/839 (90%)	675 (89%)	84 (11%)	8	23

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	46	GLN
1	A	54	THR
1	A	63	TYR
1	A	87	GLN
1	A	91	TYR
1	A	94	PHE
1	A	120	TYR
1	A	126	ILE
1	A	129	HIS
1	A	145	TYR
1	A	149	ASN
1	A	152	GLU

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Mol	Chain	Res	Type
1	A	176	GLN
1	A	180	GLU
1	A	183	HIS
1	A	189	VAL
1	A	196	TRP
1	A	211	ASN
1	A	214	MET
1	A	243	PHE
1	A	254	LYS
1	A	261	VAL
1	A	267	THR
1	A	283	LEU
2	B	1539	THR
2	B	1542	ARG
2	B	1580	ARG
2	B	1596	TYR
2	B	1600	LEU
2	B	1613	ASP
2	B	1617	VAL
2	B	1657	ASN
2	B	1660	GLN
2	B	1684	CYS
2	B	1694	ASN
2	B	1696	GLU
2	B	1707	LEU
2	B	1708	LEU
2	B	1711	ARG
2	B	1717	LYS
2	B	1718	GLU
2	B	1720	ASN
2	B	1721	MET
2	B	1726	ARG
2	B	1790	LEU
2	B	1797	ASP
2	B	1808	LEU
2	B	1823	LEU
2	B	1831	LEU
2	B	1832	GLU
2	B	1845	THR
2	B	1851	GLN
2	B	1852	ARG
2	B	1887	PHE

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Mol	Chain	Res	Type
2	B	1890	TYR
2	B	1894	LYS
2	B	1895	LEU
2	B	1898	LEU
2	B	1900	ASN
2	B	1905	ASN
2	B	1911	LYS
2	B	1914	THR
2	B	1915	GLU
2	B	1918	PRO
2	B	1921	TRP
2	B	1928	LYS
2	B	1931	LEU
2	B	2039	LYS
2	B	2054	TYR
2	B	2067	ARG
2	B	2079	ASN
2	B	2089	ILE
2	B	2097	THR
2	B	2112	TYR
2	B	2113	THR
2	B	2132	MET
2	B	2140	ASN
2	B	2141	ASN
2	B	2143	VAL
2	B	2146	HIS
2	B	2165	LYS
2	B	2168	ASN
2	B	2175	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	11	GLN
1	A	73	HIS
1	A	103	HIS
1	A	142	HIS
1	A	149	ASN
1	A	155	ASN
1	A	176	GLN
1	A	242	HIS

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Mol	Chain	Res	Type
2	B	1632	HIS
2	B	1657	ASN
2	B	1694	ASN
2	B	1782	GLN
2	B	1804	HIS
2	B	1814	GLN
2	B	1815	GLN
2	B	1817	GLN
2	B	1851	GLN
2	B	1905	ASN
2	B	1917	ASN
2	B	1927	GLN
2	B	2009	ASN
2	B	2023	ASN
2	B	2065	GLN
2	B	2076	ASN
2	B	2079	ASN
2	B	2083	GLN
2	B	2115	HIS
2	B	2168	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
3	NAG	A	2185	1	14,14,15	0.64	0	15,19,21	0.75	0
3	NAG	A	2186	1	14,14,15	0.51	0	15,19,21	0.73	1 (6%)
4	NDG	B	2187	2	14,14,15	0.58	0	15,19,21	0.73	0
3	NAG	B	2188	2	14,14,15	0.55	0	15,19,21	0.82	1 (6%)
4	NDG	B	2189	2	14,14,15	0.62	0	15,19,21	0.73	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
3	NAG	A	2185	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2186	1	-	0/6/23/26	0/1/1/1
4	NDG	B	2187	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2188	2	-	0/6/23/26	0/1/1/1
4	NDG	B	2189	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2188	NAG	C2-N2-C7	-2.41	119.94	123.04
3	A	2186	NAG	C2-N2-C7	-2.16	120.27	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2185	NAG	3	0
4	B	2187	NDG	3	0
3	B	2188	NAG	4	0
4	B	2189	NDG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	268/306 (87%)	0.58	30 (11%) 7 3	48, 89, 127, 136	0
2	B	601/647 (92%)	-0.19	6 (0%) 84 77	26, 54, 91, 112	0
All	All	869/953 (91%)	0.05	36 (4%) 41 29	26, 64, 116, 136	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	THR	4.6
1	A	34	LYS	3.8
1	A	247	VAL	3.7
1	A	178	MET	3.7
2	B	1760	ASN	3.7
1	A	145	TYR	3.4
1	A	196	TRP	3.4
1	A	292	MET	3.3
1	A	169	THR	3.2
1	A	219	VAL	3.1
1	A	253	HIS	2.9
1	A	288	PHE	2.9
1	A	246	GLN	2.9
1	A	252	HIS	2.7
1	A	143	ILE	2.7
1	A	283	LEU	2.7
1	A	160	GLY	2.7
1	A	179	PHE	2.5
2	B	2050	TRP	2.5
1	A	198	GLN	2.5
1	A	43	ALA	2.5
1	A	144	TYR	2.4
1	A	263	ALA	2.4
1	A	173	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	1691	SER	2.3
1	A	213	THR	2.3
2	B	1539	THR	2.2
1	A	221	ALA	2.2
2	B	2121	THR	2.2
1	A	79	HIS	2.1
1	A	142	HIS	2.1
2	B	2132	MET	2.1
1	A	244	ASN	2.1
1	A	11	GLN	2.1
1	A	171	THR	2.0
1	A	184	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NDG	B	2189	14/15	0.90	0.19	-0.19	70,72,74,76	0
5	CU	B	2190	1/1	0.97	0.20	-0.46	65,65,65,65	0
3	NAG	B	2188	14/15	0.89	0.13	-1.25	73,74,76,78	0
3	NAG	A	2186	14/15	0.90	0.16	-1.61	86,88,90,91	0
6	CA	A	2184	1/1	0.95	0.08	-1.93	68,68,68,68	0
4	NDG	B	2187	14/15	0.83	0.34	-	94,98,101,101	0
3	NAG	A	2185	14/15	0.75	0.40	-	127,128,129,130	0

6.5 Other polymers

There are no such residues in this entry.