



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID : 1KX0
Title : Rat mannose protein A (H189V I207V) complexed with man-a13-man
Authors : Ng, K.K.; Kolatkar, A.R.; Park-Snyder, S.; Feinberg, H.; Clark, D.A.; Drick-amer, K.; Weis, W.I.
Deposited on : 2002-01-30
Resolution : 2.00 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

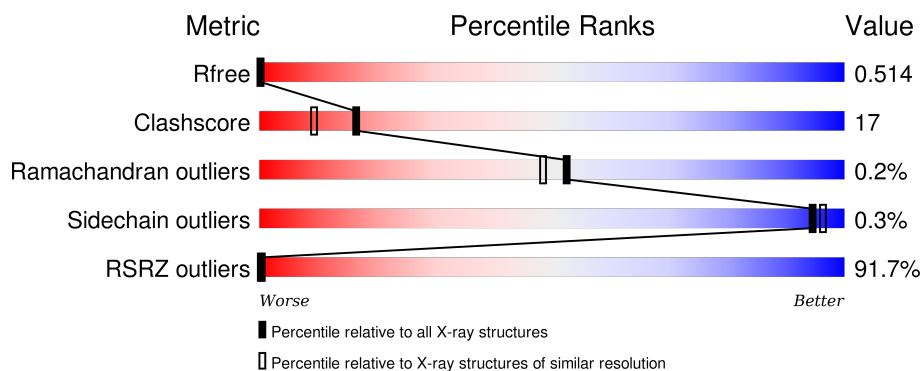
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	149	<div> <div>89%</div> <div>81%19%</div> </div>
1	B	149	<div> <div>91%</div> <div>74%26%</div> </div>
1	C	149	<div> <div>95%</div> <div>63%37%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	B	602	-	-	-	X
2	MAN	C	702[A]	-	-	-	X
2	MAN	C	702[B]	X	-	X	X
3	CA	C	705	-	-	-	X
4	CL	A	506	-	-	-	X
4	CL	C	706	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3961 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 MANNOSE-BINDING PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	3	0
			1160	725	196	230	9			
1	B	149	Total	C	N	O	S	0	4	0
			1160	725	196	231	8			
1	C	149	Total	C	N	O	S	0	3	0
			1156	723	196	229	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	VAL	HIS	ENGINEERED	UNP P19999
A	207	VAL	ILE	ENGINEERED	UNP P19999
B	189	VAL	HIS	ENGINEERED	UNP P19999
B	207	VAL	ILE	ENGINEERED	UNP P19999
C	189	VAL	HIS	ENGINEERED	UNP P19999
C	207	VAL	ILE	ENGINEERED	UNP P19999

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	2
			46	24	22		
2	B	2	Total	C	O	0	0
			23	12	11		
2	C	2	Total	C	O	0	1
			34	18	16		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0

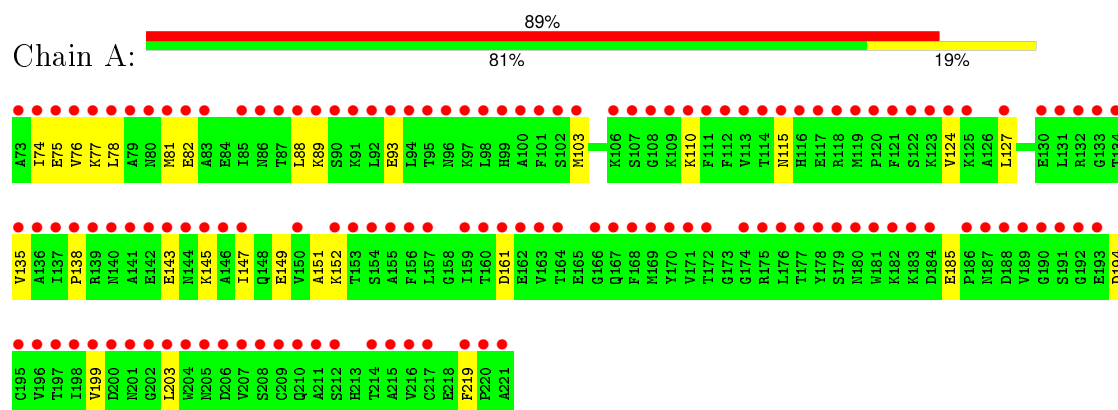
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total 163	O 163	0	0
5	B	131	Total 131	O 131	0	0
5	C	76	Total 76	O 76	0	0

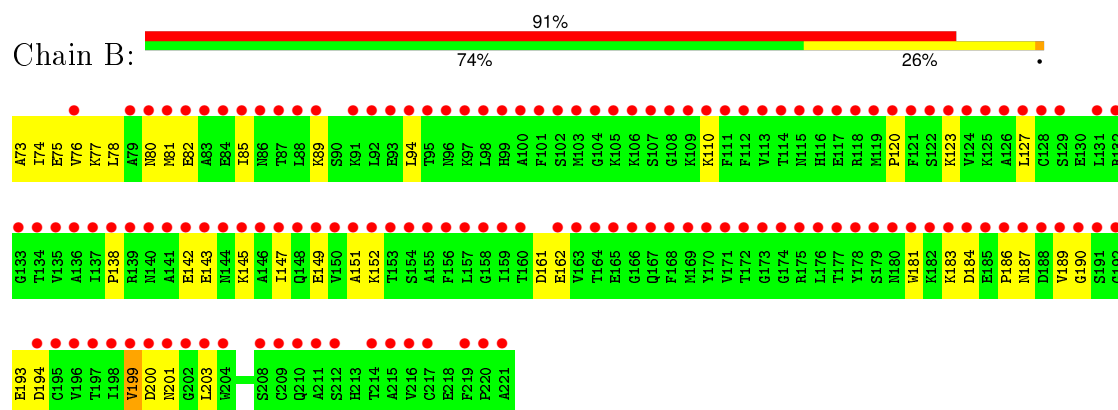
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

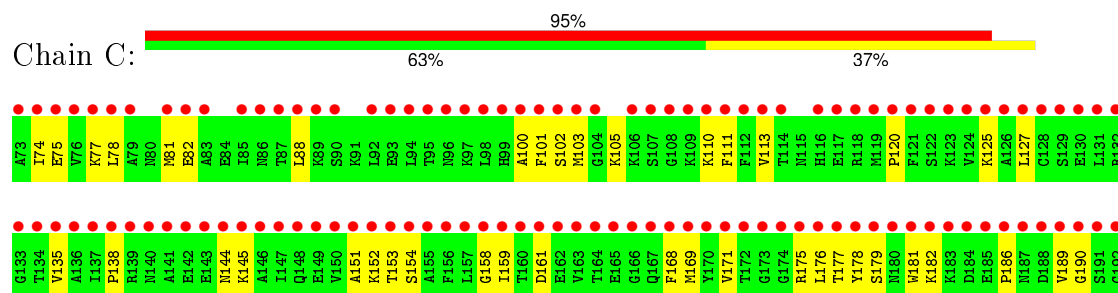
• Molecule 1: MANNOSE-BINDING PROTEIN A



• Molecule 1: MANNOSE-BINDING PROTEIN A



• Molecule 1: MANNOSE-BINDING PROTEIN A



E193	D194	C195	V196	T197	I198	V199	D200	N201	L203	H204	N205	D206	V207	S208	C209	Q210	A211	S212	H213	T214	A215	V216	C217	E218	F219	P220	A221
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.08Å 85.11Å 97.66Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 39.19 – 1.88	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 72.1 (39.19-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.232 0.501 , 0.514	Depositor DCC
R_{free} test set	3668 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39115 reflections	Xtriage
F_o, F_c correlation	0.56	EDS
Total number of atoms	3961	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1194	0.63	0/1607
1	B	0.42	0/1200	0.63	0/1616
1	C	0.38	0/1190	0.59	0/1603
All	All	0.41	0/3584	0.62	0/4826

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	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	702[B]	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1160	0	1142	42	0
1	B	1160	0	1141	46	72
1	C	1156	0	1141	48	8
2	A	46	0	39	1	0
2	B	23	0	19	0	0
2	C	34	0	28	6	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	163	0	0	3	0
5	B	131	0	0	3	3
5	C	76	0	0	0	1
All	All	3961	0	3510	118	79

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 17.

All (118) 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:82[B]:GLU:OE2	1:C:77:LYS:NZ	1.97	0.97
1:A:81[B]:MET:HE1	1:B:82:GLU:HA	1.45	0.97
2:C:701:MAN:H2	2:C:702[B]:MAN:O2	1.68	0.94
1:B:138:PRO:HG3	1:B:147:ILE:HD12	1.62	0.81
1:A:82[B]:GLU:OE2	1:C:77:LYS:CE	2.31	0.78
1:B:127[B]:LEU:CD2	1:B:127[B]:LEU:CD1	2.61	0.78
1:A:81[B]:MET:HE1	1:B:82:GLU:CA	2.13	0.78
1:C:151:ALA:O	1:C:152:LYS:HB2	1.91	0.69
1:A:75:GLU:HG2	1:C:74:ILE:HD11	1.73	0.69
1:C:159:ILE:HG23	1:C:176:LEU:HD21	1.74	0.69
2:C:701:MAN:C2	2:C:702[B]:MAN:O2	2.39	0.69
1:A:81[B]:MET:CE	1:B:82:GLU:HG2	2.24	0.68
1:A:149:GLU:O	1:A:152:LYS:HE3	1.94	0.67
1:C:168:PHE:HB2	1:C:176:LEU:HD11	1.78	0.66
1:B:110:LYS:HE3	5:B:734:HOH:O	1.95	0.66
1:A:81[B]:MET:SD	1:B:85:ILE:HD12	2.38	0.64
1:C:205:ASN:ND2	2:C:702[B]:MAN:O3	2.27	0.64
1:C:168:PHE:O	1:C:176:LEU:HG	1.99	0.62
1:A:81[B]:MET:HE2	1:B:82:GLU:CG	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HG3	1:A:147:ILE:HD12	1.80	0.62
1:C:189:VAL:HG22	1:C:190:GLY:N	2.15	0.62
1:C:189:VAL:HG22	1:C:190:GLY:H	1.65	0.61
1:A:110:LYS:HB2	1:A:219:PHE:O	2.00	0.60
1:A:161:ASP:OD1	1:A:194:ASP:HA	2.02	0.60
1:C:105:LYS:HD2	1:C:111:PHE:CD2	2.36	0.60
1:C:113[B]:VAL:CG1	1:C:219:PHE:HE2	2.15	0.59
1:B:187:ASN:CG	1:B:189:VAL:HG23	2.23	0.59
1:C:201:ASN:OD1	1:C:203:LEU:HG	2.03	0.59
1:C:138:PRO:HB3	1:C:144:ASN:HA	1.84	0.59
1:A:81[B]:MET:HE2	1:B:82:GLU:HG2	1.83	0.59
1:C:110:LYS:HE2	1:C:218:GLU:OE1	2.03	0.58
1:A:74:ILE:HD12	1:B:78:LEU:HD22	1.86	0.57
1:B:187:ASN:OD1	1:B:189:VAL:HG23	2.04	0.56
1:C:159:ILE:CG2	1:C:176:LEU:HD21	2.35	0.56
1:A:82[B]:GLU:HG3	1:C:81:MET:SD	2.45	0.55
1:A:77:LYS:HB2	1:B:78:LEU:HD21	1.88	0.55
1:A:145:LYS:O	1:A:149:GLU:HG3	2.07	0.55
1:B:145:LYS:O	1:B:149:GLU:HG2	2.07	0.54
1:B:142[B]:GLU:HG2	5:B:708:HOH:O	2.07	0.54
1:A:81[B]:MET:CE	1:B:82:GLU:CG	2.84	0.54
1:C:161:ASP:OD1	1:C:194:ASP:HA	2.07	0.54
1:C:168:PHE:HB2	1:C:176:LEU:CD1	2.38	0.53
1:C:181:TRP:CD2	1:C:186:PRO:HD3	2.44	0.53
1:A:127:LEU:HD23	1:A:127:LEU:C	2.28	0.53
1:B:151:ALA:O	1:B:152:LYS:HB2	2.08	0.53
1:A:124:VAL:HG12	1:A:135:VAL:HG22	1.91	0.52
1:B:187:ASN:ND2	1:B:189:VAL:HG23	2.24	0.52
1:C:168:PHE:CB	1:C:176:LEU:HD11	2.40	0.51
1:A:74:ILE:HG23	1:A:75:GLU:N	2.26	0.51
1:A:81[B]:MET:CE	1:B:85:ILE:HD12	2.41	0.50
1:A:138:PRO:HG3	1:A:147:ILE:CD1	2.42	0.50
1:B:161:ASP:OD1	1:B:194:ASP:HA	2.12	0.50
1:A:74:ILE:HG23	1:A:75:GLU:HG3	1.92	0.50
1:C:182:LYS:HG3	1:C:203:LEU:HD13	1.94	0.49
1:C:193:GLU:OE1	2:C:702[B]:MAN:H3	2.12	0.49
1:B:120:PRO:HD2	1:B:123:LYS:HD2	1.94	0.49
1:A:81[B]:MET:HE2	1:B:82:GLU:HG3	1.95	0.48
1:B:183:LYS:O	1:B:184:ASP:HB2	2.13	0.48
1:C:177:THR:HG22	1:C:178:TYR:N	2.29	0.48
1:A:82[B]:GLU:OE2	1:C:77:LYS:HE2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLY:HA3	5:B:679:HOH:O	2.13	0.47
1:B:199:VAL:HG22	1:B:203:LEU:O	2.14	0.47
1:C:179:SER:HA	1:C:204:TRP:CH2	2.50	0.47
2:C:701:MAN:O3	2:C:702[B]:MAN:H4	2.15	0.47
1:C:100:ALA:HA	1:C:103:MET:HE3	1.97	0.46
1:C:113[B]:VAL:HG12	1:C:219:PHE:HE2	1.80	0.46
1:A:88:LEU:HD13	1:B:89:LYS:HG2	1.97	0.46
1:C:113[B]:VAL:HG11	1:C:219:PHE:HE2	1.79	0.45
1:C:169:MET:SD	1:C:175:ARG:HG2	2.56	0.45
1:B:142[B]:GLU:OE2	1:B:142[B]:GLU:HB3	2.16	0.45
1:B:110:LYS:NZ	1:B:143:GLU:OE1	2.49	0.45
1:C:181:TRP:CE3	1:C:186:PRO:HD3	2.52	0.45
1:C:199:VAL:HG23	1:C:201:ASN:HB3	1.99	0.45
1:A:110:LYS:HE2	1:A:143:GLU:CD	2.37	0.45
1:A:81[B]:MET:SD	1:B:82:GLU:HG2	2.57	0.45
1:C:125:LYS:HG2	1:C:135:VAL:HG21	2.00	0.44
1:A:89:LYS:HG2	1:C:88:LEU:HD21	1.99	0.44
1:C:153:THR:O	1:C:154:SER:C	2.57	0.43
1:A:77:LYS:HE3	5:A:597:HOH:O	2.17	0.43
1:C:145:LYS:HB2	1:C:145:LYS:HE3	1.82	0.43
2:C:701:MAN:C2	2:C:702[B]:MAN:HO2	2.29	0.43
1:C:151:ALA:O	1:C:152:LYS:CB	2.65	0.43
1:A:151:ALA:O	1:A:152:LYS:HB2	2.18	0.43
1:C:158:GLY:C	1:C:171:VAL:HG13	2.38	0.43
1:C:195:CYS:O	1:C:206:ASP:HA	2.18	0.43
1:C:120:PRO:HA	1:C:211:ALA:O	2.19	0.43
1:B:187:ASN:ND2	1:B:189:VAL:CG2	2.81	0.42
1:B:199:VAL:HG23	1:B:200:ASP:N	2.34	0.42
1:B:181:TRP:CD2	1:B:186:PRO:HD3	2.54	0.42
1:C:199:VAL:C	1:C:201:ASN:H	2.21	0.42
1:B:200:ASP:O	1:B:201:ASN:HB2	2.20	0.42
1:A:93:GLU:HG3	5:A:638:HOH:O	2.19	0.42
1:A:74:ILE:CD1	1:B:78:LEU:HD22	2.49	0.42
1:A:115:ASN:HB3	1:C:101:PHE:CD1	2.54	0.42
1:A:103:MET:CE	1:A:103:MET:HA	2.50	0.42
1:C:189:VAL:HG12	1:C:193:GLU:CD	2.41	0.41
1:C:219:PHE:HA	1:C:220:PRO:HD3	1.84	0.41
1:A:78:LEU:HD11	1:C:74:ILE:HG23	2.02	0.41
1:A:185:GLU:OE1	2:A:502[A]:MAN:O4	2.39	0.41
1:A:76:VAL:HG23	5:A:667:HOH:O	2.21	0.41
1:B:189:VAL:HB	1:B:193:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HD23	1:C:127:LEU:C	2.41	0.41
1:A:199:VAL:HG22	1:A:203:LEU:O	2.20	0.40

All (79) 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)
1:B:75:GLU:C	1:B:76:VAL:CA[2_556]	0.39	1.81
1:B:75:GLU:CD	1:B:80:ASN:CG[2_556]	0.43	1.77
1:B:75:GLU:O	1:B:76:VAL:CA[2_556]	0.84	1.36
1:B:74:ILE:CA	1:B:77:LYS:CB[2_556]	0.87	1.33
1:B:73:ALA:C	1:B:78:LEU:N[2_556]	0.88	1.32
1:B:74:ILE:C	1:B:77:LYS:N[2_556]	0.93	1.27
1:B:74:ILE:CA	1:B:77:LYS:CA[2_556]	0.94	1.26
1:B:75:GLU:OE2	1:B:80:ASN:CG[2_556]	0.95	1.25
1:B:74:ILE:C	1:B:77:LYS:CA[2_556]	0.96	1.24
1:B:74:ILE:N	1:B:77:LYS:C[2_556]	1.00	1.20
1:B:73:ALA:C	1:B:77:LYS:C[2_556]	1.07	1.13
1:B:75:GLU:CA	1:B:76:VAL:C[2_556]	1.08	1.12
1:B:73:ALA:O	1:B:78:LEU:N[2_556]	1.08	1.12
1:B:73:ALA:CA	1:B:78:LEU:CA[2_556]	1.09	1.11
1:B:75:GLU:C	1:B:76:VAL:C[2_556]	1.17	1.03
1:B:75:GLU:OE1	1:B:80:ASN:CB[2_556]	1.22	0.98
1:C:75:GLU:OE1	1:C:82:GLU:OE2[2_556]	1.23	0.97
1:B:74:ILE:O	1:B:77:LYS:N[2_556]	1.27	0.93
1:B:75:GLU:O	1:B:76:VAL:CB[2_556]	1.27	0.93
1:B:75:GLU:N	1:B:76:VAL:C[2_556]	1.33	0.87
1:B:75:GLU:CA	1:B:76:VAL:O[2_556]	1.34	0.86
1:B:75:GLU:CD	1:B:80:ASN:CB[2_556]	1.36	0.84
1:B:75:GLU:N	1:B:77:LYS:N[2_556]	1.40	0.80
1:B:75:GLU:CD	1:B:80:ASN:ND2[2_556]	1.41	0.79
1:B:75:GLU:N	1:B:76:VAL:O[2_556]	1.42	0.78
1:C:75:GLU:CD	1:C:82:GLU:OE2[2_556]	1.43	0.77
1:B:74:ILE:N	1:B:77:LYS:O[2_556]	1.44	0.76
1:B:75:GLU:OE2	1:B:80:ASN:CB[2_556]	1.46	0.74
1:B:75:GLU:CD	1:B:80:ASN:OD1[2_556]	1.48	0.72
1:B:75:GLU:O	1:B:76:VAL:N[2_556]	1.50	0.70
1:B:75:GLU:CG	1:B:80:ASN:CG[2_556]	1.51	0.69
1:B:74:ILE:N	1:B:77:LYS:CA[2_556]	1.52	0.68
1:B:76:VAL:N	1:B:76:VAL:C[2_556]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:CG	1:B:80:ASN:ND2[2_556]	1.56	0.64
1:B:80:ASN:C	5:B:658:HOH:O[2_556]	1.56	0.64
1:B:75:GLU:CG	1:B:80:ASN:OD1[2_556]	1.57	0.63
1:B:76:VAL:N	1:B:76:VAL:CA[2_556]	1.57	0.63
1:B:75:GLU:CB	1:B:76:VAL:O[2_556]	1.59	0.61
1:B:81:MET:N	5:B:658:HOH:O[2_556]	1.60	0.60
1:B:77:LYS:CE	1:C:78:LEU:CD2[2_556]	1.60	0.60
1:B:75:GLU:C	1:B:76:VAL:N[2_556]	1.62	0.58
1:B:76:VAL:N	1:B:76:VAL:N[2_556]	1.63	0.57
1:B:73:ALA:CA	1:B:78:LEU:N[2_556]	1.65	0.55
1:B:75:GLU:N	1:B:77:LYS:CA[2_556]	1.65	0.55
1:B:75:GLU:OE1	1:B:80:ASN:CG[2_556]	1.66	0.54
1:B:73:ALA:N	1:B:77:LYS:O[2_556]	1.71	0.49
1:B:75:GLU:OE2	1:B:80:ASN:ND2[2_556]	1.72	0.48
1:C:75:GLU:OE2	1:C:82:GLU:OE1[2_556]	1.72	0.48
1:B:75:GLU:OE2	1:B:80:ASN:OD1[2_556]	1.73	0.47
1:B:75:GLU:CA	1:B:76:VAL:CA[2_556]	1.76	0.44
1:B:75:GLU:O	1:B:76:VAL:CG2[2_556]	1.76	0.44
1:B:77:LYS:NZ	5:C:769:HOH:O[2_556]	1.78	0.42
1:B:74:ILE:N	1:B:77:LYS:CB[2_556]	1.86	0.34
1:B:75:GLU:OE1	1:B:80:ASN:CA[2_556]	1.87	0.33
1:B:73:ALA:C	1:B:78:LEU:CA[2_556]	1.89	0.31
1:B:73:ALA:O	1:B:77:LYS:C[2_556]	1.90	0.30
1:B:73:ALA:C	1:B:77:LYS:O[2_556]	1.91	0.29
1:B:74:ILE:CA	1:B:77:LYS:CG[2_556]	1.91	0.29
1:B:75:GLU:OE1	1:B:80:ASN:N[2_556]	1.93	0.27
1:B:74:ILE:C	1:B:77:LYS:CB[2_556]	1.93	0.27
1:B:74:ILE:CG2	1:B:77:LYS:CG[2_556]	1.96	0.24
1:C:75:GLU:OE2	1:C:82:GLU:CD[2_556]	1.99	0.21
1:B:74:ILE:C	1:B:76:VAL:C[2_556]	2.00	0.20
1:C:75:GLU:CD	1:C:82:GLU:CD[2_556]	2.00	0.20
1:B:74:ILE:CA	1:B:77:LYS:C[2_556]	2.00	0.20
1:B:74:ILE:N	1:B:78:LEU:N[2_556]	2.02	0.18
1:B:74:ILE:O	1:B:77:LYS:CA[2_556]	2.06	0.14
1:B:75:GLU:CA	1:B:77:LYS:N[2_556]	2.06	0.14
1:B:74:ILE:CB	1:B:77:LYS:CB[2_556]	2.08	0.12
1:C:75:GLU:OE1	1:C:82:GLU:CD[2_556]	2.09	0.11
1:B:73:ALA:CA	1:B:77:LYS:C[2_556]	2.11	0.09
1:B:73:ALA:CA	1:B:78:LEU:C[2_556]	2.13	0.07
1:B:73:ALA:C	1:B:77:LYS:CA[2_556]	2.15	0.05
1:B:73:ALA:N	1:B:78:LEU:O[2_556]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:CB	5:B:658:HOH:O[2_556]	2.17	0.03
1:B:73:ALA:CA	1:B:77:LYS:O[2_556]	2.18	0.02
1:B:74:ILE:CB	1:B:77:LYS:CG[2_556]	2.18	0.02
1:B:75:GLU:C	1:B:77:LYS:N[2_556]	2.19	0.01
1:C:75:GLU:OE2	1:C:82:GLU:OE2[2_556]	2.19	0.01

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	150/149 (101%)	147 (98%)	3 (2%)	0	100	100
1	B	151/149 (101%)	145 (96%)	5 (3%)	1 (1%)	26	19
1	C	150/149 (101%)	142 (95%)	8 (5%)	0	100	100
All	All	451/447 (101%)	434 (96%)	16 (4%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/126 (102%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	130/126 (103%)	129 (99%)	1 (1%)	86	89
1	C	129/126 (102%)	129 (100%)	0	100	100
All	All	388/378 (103%)	387 (100%)	1 (0%)	94	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	96	ASN
1	A	148	GLN
1	B	80	ASN
1	B	86	ASN
1	B	96	ASN
1	B	99	HIS
1	B	148	GLN
1	B	180	ASN
1	C	96	ASN
1	C	180	ASN

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 ⓘ

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MAN	A	501[A]	2	12,12,12	0.35	0	17,17,17	0.39	0
2	MAN	A	501[B]	2	12,12,12	0.36	0	17,17,17	0.52	0
2	MAN	A	502[A]	3,2	11,11,12	0.47	0	14,15,17	0.55	0
2	MAN	A	502[B]	3,2	11,11,12	0.46	0	14,15,17	0.61	0
2	MAN	B	601	2	12,12,12	0.41	0	17,17,17	0.33	0
2	MAN	B	602	3,2	11,11,12	0.51	0	14,15,17	0.69	1 (7%)
2	MAN	C	701	2	12,12,12	0.44	0	17,17,17	0.37	0
2	MAN	C	702[A]	3,2	11,11,12	0.43	0	14,15,17	0.57	0
2	MAN	C	702[B]	3	11,11,12	0.40	0	14,15,17	0.44	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
2	MAN	A	501[A]	2	-	0/2/22/22	0/1/1/1
2	MAN	A	501[B]	2	-	0/2/22/22	0/1/1/1
2	MAN	A	502[A]	3,2	-	0/2/19/22	0/1/1/1
2	MAN	A	502[B]	3,2	-	0/2/19/22	0/1/1/1
2	MAN	B	601	2	-	0/2/22/22	0/1/1/1
2	MAN	B	602	3,2	-	0/2/19/22	0/1/1/1
2	MAN	C	701	2	-	0/2/22/22	0/1/1/1
2	MAN	C	702[A]	3,2	-	0/2/19/22	0/1/1/1
2	MAN	C	702[B]	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	MAN	C1-O5-C5	2.10	114.92	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	702[B]	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502[A]	MAN	1	0
2	C	701	MAN	4	0
2	C	702[B]	MAN	6	0

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	149/149 (100%)	4.78	133 (89%) 0 0	18, 25, 36, 42	0
1	B	149/149 (100%)	5.22	135 (90%) 0 0	21, 30, 42, 51	0
1	C	149/149 (100%)	7.25	142 (95%) 0 0	21, 39, 63, 75	0
All	All	447/447 (100%)	5.75	410 (91%) 0 0	18, 31, 58, 75	0

All (410) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	GLY	27.0
1	C	150	VAL	25.1
1	C	176	LEU	24.5
1	C	153	THR	21.2
1	C	173	GLY	21.1
1	C	181	TRP	21.0
1	C	209	CYS	20.1
1	C	163	VAL	19.8
1	C	191	SER	19.1
1	C	192	GLY	18.2
1	B	186	PRO	16.8
1	C	184	ASP	15.6
1	A	73	ALA	15.3
1	C	210	GLN	15.0
1	C	164	THR	14.8
1	B	153	THR	14.8
1	C	134	THR	14.7
1	B	113	VAL	14.5
1	B	190	GLY	14.3
1	C	100	ALA	14.0
1	B	172	THR	14.0
1	B	221	ALA	13.9
1	B	177	THR	13.9

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Mol	Chain	Res	Type	RSRZ
1	C	175	ARG	13.6
1	C	211	ALA	13.6
1	C	107	SER	13.6
1	C	147	ILE	13.1
1	A	189	VAL	13.1
1	C	169	MET	13.1
1	A	209	CYS	12.8
1	C	113[A]	VAL	12.8
1	A	118	ARG	12.2
1	A	153	THR	12.1
1	C	168	PHE	12.0
1	A	109	LYS	11.9
1	C	139	ARG	11.7
1	C	88	LEU	11.6
1	C	221	ALA	11.6
1	B	79	ALA	11.4
1	B	201	ASN	11.2
1	B	120	PRO	11.0
1	A	78	LEU	10.9
1	C	172	THR	10.8
1	C	189	VAL	10.8
1	B	127[A]	LEU	10.8
1	B	82	GLU	10.7
1	C	151	ALA	10.7
1	B	203	LEU	10.7
1	A	139	ARG	10.6
1	C	179	SER	10.5
1	C	183	LYS	10.4
1	C	73	ALA	10.1
1	C	201	ASN	10.1
1	C	131	LEU	10.1
1	C	174	GLY	9.9
1	C	171	VAL	9.9
1	C	108	GLY	9.8
1	A	130	GLU	9.6
1	A	190	GLY	9.6
1	C	202	GLY	9.6
1	A	74	ILE	9.5
1	B	184	ASP	9.5
1	B	152	LYS	9.5
1	B	141	ALA	9.4
1	B	85	ILE	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLU	9.2
1	B	194	ASP	9.1
1	B	95	THR	9.1
1	C	146	ALA	9.0
1	A	200	ASP	9.0
1	C	136	ALA	8.9
1	C	208	SER	8.9
1	C	89	LYS	8.9
1	C	200	ASP	8.8
1	C	78	LEU	8.8
1	B	189	VAL	8.7
1	A	103	MET	8.5
1	C	204	TRP	8.4
1	C	217	CYS	8.4
1	B	191	SER	8.3
1	C	109	LYS	8.3
1	B	132	ARG	8.3
1	A	75	GLU	8.2
1	B	84	GLU	8.1
1	B	216	VAL	8.1
1	B	181	TRP	8.1
1	A	121	PHE	8.0
1	C	167	GLN	8.0
1	C	123	LYS	7.9
1	A	175	ARG	7.9
1	C	199	VAL	7.9
1	A	186	PRO	7.8
1	C	180	ASN	7.8
1	C	132	ARG	7.8
1	B	210	GLN	7.6
1	C	196	VAL	7.6
1	B	183	LYS	7.4
1	B	111	PHE	7.4
1	B	142[A]	GLU	7.3
1	C	162	GLU	7.3
1	B	148	GLN	7.3
1	A	76	VAL	7.3
1	C	93[A]	GLU	7.2
1	A	98	LEU	7.2
1	A	145	LYS	7.1
1	B	187	ASN	7.1
1	B	92	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	198	ILE	7.0
1	C	182	LYS	7.0
1	A	123	LYS	7.0
1	B	99	HIS	7.0
1	C	170	TYR	6.9
1	A	212	SER	6.8
1	B	176	LEU	6.8
1	C	185	GLU	6.7
1	B	140	ASN	6.7
1	C	186	PRO	6.7
1	B	180	ASN	6.6
1	A	203	LEU	6.6
1	A	122	SER	6.6
1	B	174	GLY	6.6
1	B	131	LEU	6.5
1	B	202	GLY	6.5
1	C	157	LEU	6.5
1	B	212	SER	6.5
1	A	117	GLU	6.5
1	C	121	PHE	6.5
1	B	110	LYS	6.4
1	A	164	THR	6.4
1	A	152	LYS	6.4
1	B	211	ALA	6.4
1	C	145	LYS	6.4
1	B	199	VAL	6.4
1	C	178	TYR	6.3
1	C	216	VAL	6.3
1	A	171	VAL	6.3
1	C	142	GLU	6.2
1	A	141	ALA	6.2
1	B	114	THR	6.2
1	A	135	VAL	6.2
1	A	77	LYS	6.2
1	B	129[A]	SER	6.2
1	C	152	LYS	6.2
1	A	174	GLY	6.2
1	B	145	LYS	6.2
1	C	154	SER	6.2
1	A	196	VAL	6.1
1	B	83	ALA	6.1
1	C	161	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	197	THR	6.1
1	A	85	ILE	6.0
1	B	179	SER	6.0
1	A	207	VAL	6.0
1	B	146	ALA	6.0
1	C	103	MET	6.0
1	A	111	PHE	6.0
1	A	94	LEU	5.9
1	B	101	PHE	5.9
1	B	128	CYS	5.9
1	C	166	GLY	5.9
1	A	102	SER	5.9
1	B	173	GLY	5.9
1	B	135	VAL	5.9
1	A	92	LEU	5.8
1	B	108	GLY	5.8
1	A	115	ASN	5.8
1	B	154	SER	5.8
1	A	82[A]	GLU	5.8
1	C	159	ILE	5.8
1	B	102	SER	5.8
1	C	137	ILE	5.7
1	C	112	PHE	5.7
1	A	150	VAL	5.7
1	A	177	THR	5.6
1	B	123	LYS	5.6
1	A	133	GLY	5.6
1	C	194	ASP	5.6
1	C	74	ILE	5.5
1	C	187	ASN	5.5
1	A	114	THR	5.5
1	B	109	LYS	5.5
1	B	157	LEU	5.5
1	C	143	GLU	5.4
1	A	81[A]	MET	5.4
1	B	168	PHE	5.4
1	A	169	MET	5.4
1	B	204	TRP	5.4
1	C	101	PHE	5.4
1	A	120	PRO	5.3
1	B	208	SER	5.3
1	C	82	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	140	ASN	5.3
1	A	93	GLU	5.3
1	A	199	VAL	5.2
1	A	211	ALA	5.2
1	C	215	ALA	5.2
1	B	118	ARG	5.2
1	A	79	ALA	5.1
1	C	83	ALA	5.1
1	B	214	THR	5.1
1	A	137	ILE	5.1
1	A	112	PHE	5.1
1	C	155	ALA	5.1
1	A	99	HIS	5.1
1	A	221	ALA	5.0
1	B	126	ALA	5.0
1	A	208	SER	5.0
1	A	214	THR	5.0
1	A	97	LYS	5.0
1	A	80	ASN	4.9
1	C	177	THR	4.9
1	C	77	LYS	4.9
1	A	96	ASN	4.9
1	A	178	TYR	4.9
1	C	127	LEU	4.9
1	C	75	GLU	4.8
1	A	119	MET	4.8
1	A	172	THR	4.8
1	A	176	LEU	4.8
1	A	107	SER	4.8
1	C	220	PRO	4.8
1	B	178	TYR	4.7
1	A	167	GLN	4.7
1	B	220	PRO	4.7
1	B	165	GLU	4.7
1	A	210	GLN	4.6
1	C	219	PHE	4.6
1	C	99	HIS	4.6
1	C	118	ARG	4.6
1	B	94	LEU	4.6
1	A	159	ILE	4.5
1	C	119	MET	4.5
1	A	184	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	219	PHE	4.5
1	C	92	LEU	4.4
1	C	94	LEU	4.4
1	A	204	TRP	4.3
1	B	134	THR	4.3
1	B	209	CYS	4.3
1	B	151	ALA	4.3
1	B	125	LYS	4.3
1	B	164	THR	4.3
1	C	203	LEU	4.3
1	A	192	GLY	4.3
1	A	220	PRO	4.3
1	A	216	VAL	4.3
1	C	148	GLN	4.2
1	C	141	ALA	4.2
1	A	113	VAL	4.2
1	C	79	ALA	4.2
1	A	108	GLY	4.2
1	A	198	ILE	4.2
1	B	171	VAL	4.2
1	A	138	PRO	4.2
1	A	219	PHE	4.2
1	B	170	TYR	4.2
1	B	185	GLU	4.2
1	B	169	MET	4.1
1	B	200	ASP	4.1
1	B	155	ALA	4.1
1	C	205	ASN	4.1
1	B	182	LYS	4.1
1	C	95	THR	4.1
1	C	195	CYS	4.1
1	C	87	THR	4.1
1	C	149	GLU	4.1
1	A	101	PHE	4.0
1	B	150	VAL	4.0
1	B	197	THR	4.0
1	A	147	ILE	4.0
1	B	137	ILE	4.0
1	A	95	THR	4.0
1	A	110	LYS	4.0
1	B	149	GLU	4.0
1	C	207	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	201	ASN	4.0
1	A	83	ALA	4.0
1	B	138	PRO	4.0
1	B	215	ALA	3.9
1	B	198	ILE	3.9
1	C	133	GLY	3.9
1	C	193	GLU	3.9
1	C	128	CYS	3.9
1	C	120	PRO	3.9
1	C	165	GLU	3.9
1	C	144	ASN	3.9
1	B	175	ARG	3.9
1	C	86	ASN	3.8
1	B	103	MET	3.8
1	C	138	PRO	3.8
1	C	158	GLY	3.8
1	C	129	SER	3.8
1	A	132	ARG	3.8
1	B	87	THR	3.8
1	B	98	LEU	3.7
1	A	100	ALA	3.7
1	C	124	VAL	3.7
1	A	134	THR	3.7
1	A	168	PHE	3.7
1	A	166	GLY	3.7
1	A	202	GLY	3.6
1	C	102[A]	SER	3.6
1	C	106	LYS	3.6
1	A	144	ASN	3.6
1	A	193	GLU	3.6
1	A	127	LEU	3.6
1	A	131	LEU	3.5
1	B	162[A]	GLU	3.5
1	A	179	SER	3.5
1	A	162[A]	GLU	3.5
1	B	160	THR	3.5
1	A	181	TRP	3.4
1	B	112	PHE	3.4
1	A	160	THR	3.4
1	C	76	VAL	3.4
1	A	136	ALA	3.4
1	B	163	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	81	MET	3.4
1	C	114	THR	3.3
1	A	124	VAL	3.3
1	C	135	VAL	3.3
1	B	166	GLY	3.3
1	B	91	LYS	3.3
1	A	86	ASN	3.3
1	B	147	ILE	3.2
1	B	159	ILE	3.2
1	B	86	ASN	3.2
1	C	116	HIS	3.2
1	A	89	LYS	3.2
1	A	125	LYS	3.2
1	B	124	VAL	3.2
1	C	160	THR	3.2
1	A	116	HIS	3.2
1	C	214	THR	3.1
1	B	217	CYS	3.1
1	B	88	LEU	3.1
1	B	156	PHE	3.1
1	B	116	HIS	3.1
1	B	188	ASP	3.1
1	C	212	SER	3.1
1	B	96	ASN	3.1
1	A	215	ALA	3.1
1	A	88	LEU	3.0
1	C	96	ASN	3.0
1	A	90	SER	3.0
1	B	115	ASN	3.0
1	B	196	VAL	3.0
1	A	91	LYS	3.0
1	A	106	LYS	3.0
1	B	133	GLY	2.9
1	A	157	LEU	2.9
1	A	163	VAL	2.9
1	C	126	ALA	2.9
1	B	105	LYS	2.9
1	C	97	LYS	2.9
1	B	121	PHE	2.8
1	C	85	ILE	2.8
1	A	195	CYS	2.8
1	B	143	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASN	2.8
1	B	89	LYS	2.8
1	C	111	PHE	2.8
1	C	98	LEU	2.8
1	A	187	ASN	2.8
1	B	167	GLN	2.8
1	A	170	TYR	2.7
1	A	182	LYS	2.7
1	B	144	ASN	2.7
1	A	143	GLU	2.7
1	A	188	ASP	2.7
1	A	154	SER	2.7
1	B	100	ALA	2.7
1	C	218	GLU	2.7
1	B	97	LYS	2.7
1	B	139	ARG	2.7
1	C	90	SER	2.6
1	B	119	MET	2.6
1	A	205	ASN	2.6
1	A	206	ASP	2.6
1	A	87	THR	2.6
1	B	107	SER	2.6
1	B	104	GLY	2.6
1	A	155	ALA	2.6
1	A	156	PHE	2.5
1	A	191	SER	2.5
1	B	117	GLU	2.5
1	C	130	GLU	2.5
1	B	106	LYS	2.5
1	C	188	ASP	2.5
1	C	125	LYS	2.4
1	A	180	ASN	2.4
1	A	197	THR	2.4
1	B	195	CYS	2.4
1	C	122	SER	2.4
1	B	136	ALA	2.3
1	B	76	VAL	2.3
1	B	93	GLU	2.3
1	B	158	GLY	2.3
1	C	104	GLY	2.3
1	C	117	GLU	2.3
1	A	217	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	156	PHE	2.2
1	A	146	ALA	2.2
1	C	110	LYS	2.2
1	B	192	GLY	2.2
1	A	183	LYS	2.1
1	A	161	ASP	2.1
1	B	80	ASN	2.1
1	B	81	MET	2.1
1	B	122	SER	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	C	702[A]	11/12	0.36	0.79	2.48	87,87,88,88	11
2	MAN	C	702[B]	11/12	0.36	0.79	2.48	82,82,83,83	11
2	MAN	B	602	11/12	0.36	0.54	1.26	41,45,47,51	0
2	MAN	A	502[A]	11/12	0.69	0.35	-0.23	23,24,27,29	11
2	MAN	A	502[B]	11/12	0.69	0.35	-0.25	24,27,30,32	11
2	MAN	A	501[B]	12/12	0.35	1.08	-	30,32,33,34	12
2	MAN	B	601	12/12	0.50	0.56	-	50,55,57,59	0
2	MAN	C	701	12/12	0.59	0.91	-	89,91,91,91	0
2	MAN	A	501[A]	12/12	0.35	1.08	-	27,31,33,34	12

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
3	CA	C	705	1/1	0.71	0.51	1.28	42,42,42,42	0
4	CL	A	506	1/1	0.63	0.54	1.16	26,26,26,26	0
4	CL	C	706	1/1	0.87	0.86	0.56	43,43,43,43	0
3	CA	A	505	1/1	0.86	0.33	0.43	23,23,23,23	0
4	CL	B	606	1/1	0.53	0.36	-0.02	50,50,50,50	0
3	CA	C	704	1/1	0.79	0.39	-0.31	44,44,44,44	0
3	CA	B	603	1/1	0.92	0.14	-1.41	24,24,24,24	0
3	CA	C	703	1/1	0.88	0.25	-1.51	40,40,40,40	0
3	CA	B	604	1/1	0.83	0.11	-1.72	29,29,29,29	0
3	CA	A	504	1/1	0.78	0.12	-1.83	24,24,24,24	0
3	CA	A	503	1/1	0.95	0.12	-3.45	22,22,22,22	0
3	CA	B	605	1/1	0.49	0.34	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.