Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:11 PM GMT

PDB ID	:	4KRM
Title	:	Nanobody/VHH domain 7D12 in complex with domain III of the extracellular region of EGFR, pH 3.5
Authors	:	Ferguson, K.M.; Schmitz, K.R.
Deposited on	:	2013-05-16
Resolution	:	2.65 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 ①) were used in the production of this report:

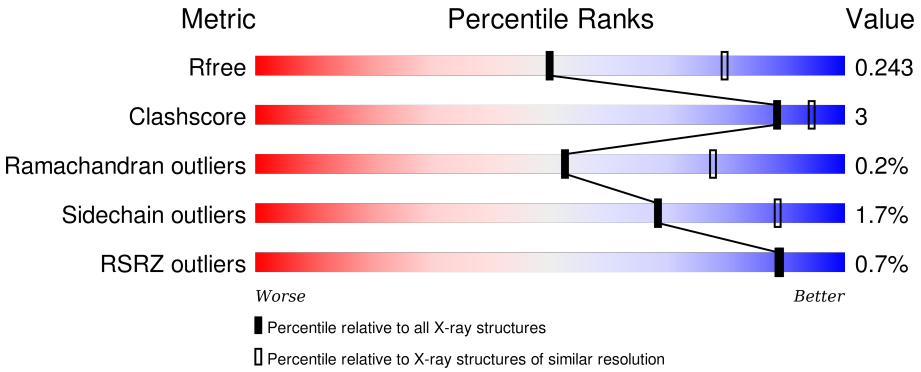
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	214	89% · 8%
1	C	214	87% 5% 8%
1	E	214	88% · 8%
1	G	214	88% · 7%
1	I	214	% 86% 5% 9%

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Mol	Chain	Length	Quality of chain
1	K	214	86% 6% 8%
2	B	133	87% 5% 7%
2	D	133	83% 9% 7%
2	F	133	79% 11% 8%
2	H	133	84% 7% 7%
2	J	133	86% 7% 7%
2	L	133	86% 6% 7%

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
4	NAG	E	606	-	-	-	X
4	NAG	G	606	-	-	-	X
4	NAG	K	606	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28686 atoms, of which 13827 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	197	Total	C	H	N	O	S	0	0	0
			2885	924	1412	254	286	9			
1	C	197	Total	C	H	N	O	S	0	0	0
			2906	927	1426	257	287	9			
1	E	197	Total	C	H	N	O	S	0	0	0
			2885	923	1414	257	282	9			
1	G	198	Total	C	H	N	O	S	0	0	0
			2912	930	1425	260	287	10			
1	I	195	Total	C	H	N	O	S	0	0	0
			2851	912	1399	254	278	8			
1	K	196	Total	C	H	N	O	S	0	0	0
			2847	913	1395	253	277	9			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	EXPRESSION TAG	UNP P00533
A	308	GLU	-	EXPRESSION TAG	UNP P00533
A	309	GLU	-	EXPRESSION TAG	UNP P00533
A	310	LYS	-	EXPRESSION TAG	UNP P00533
A	515	HIS	-	EXPRESSION TAG	UNP P00533
A	516	HIS	-	EXPRESSION TAG	UNP P00533
A	517	HIS	-	EXPRESSION TAG	UNP P00533
A	518	HIS	-	EXPRESSION TAG	UNP P00533
A	519	HIS	-	EXPRESSION TAG	UNP P00533
A	520	HIS	-	EXPRESSION TAG	UNP P00533
C	307	LEU	-	EXPRESSION TAG	UNP P00533
C	308	GLU	-	EXPRESSION TAG	UNP P00533
C	309	GLU	-	EXPRESSION TAG	UNP P00533
C	310	LYS	-	EXPRESSION TAG	UNP P00533
C	515	HIS	-	EXPRESSION TAG	UNP P00533
C	516	HIS	-	EXPRESSION TAG	UNP P00533
C	517	HIS	-	EXPRESSION TAG	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
C	518	HIS	-	EXPRESSION TAG	UNP P00533
C	519	HIS	-	EXPRESSION TAG	UNP P00533
C	520	HIS	-	EXPRESSION TAG	UNP P00533
E	307	LEU	-	EXPRESSION TAG	UNP P00533
E	308	GLU	-	EXPRESSION TAG	UNP P00533
E	309	GLU	-	EXPRESSION TAG	UNP P00533
E	310	LYS	-	EXPRESSION TAG	UNP P00533
E	515	HIS	-	EXPRESSION TAG	UNP P00533
E	516	HIS	-	EXPRESSION TAG	UNP P00533
E	517	HIS	-	EXPRESSION TAG	UNP P00533
E	518	HIS	-	EXPRESSION TAG	UNP P00533
E	519	HIS	-	EXPRESSION TAG	UNP P00533
E	520	HIS	-	EXPRESSION TAG	UNP P00533
G	307	LEU	-	EXPRESSION TAG	UNP P00533
G	308	GLU	-	EXPRESSION TAG	UNP P00533
G	309	GLU	-	EXPRESSION TAG	UNP P00533
G	310	LYS	-	EXPRESSION TAG	UNP P00533
G	515	HIS	-	EXPRESSION TAG	UNP P00533
G	516	HIS	-	EXPRESSION TAG	UNP P00533
G	517	HIS	-	EXPRESSION TAG	UNP P00533
G	518	HIS	-	EXPRESSION TAG	UNP P00533
G	519	HIS	-	EXPRESSION TAG	UNP P00533
G	520	HIS	-	EXPRESSION TAG	UNP P00533
I	307	LEU	-	EXPRESSION TAG	UNP P00533
I	308	GLU	-	EXPRESSION TAG	UNP P00533
I	309	GLU	-	EXPRESSION TAG	UNP P00533
I	310	LYS	-	EXPRESSION TAG	UNP P00533
I	515	HIS	-	EXPRESSION TAG	UNP P00533
I	516	HIS	-	EXPRESSION TAG	UNP P00533
I	517	HIS	-	EXPRESSION TAG	UNP P00533
I	518	HIS	-	EXPRESSION TAG	UNP P00533
I	519	HIS	-	EXPRESSION TAG	UNP P00533
I	520	HIS	-	EXPRESSION TAG	UNP P00533
K	307	LEU	-	EXPRESSION TAG	UNP P00533
K	308	GLU	-	EXPRESSION TAG	UNP P00533
K	309	GLU	-	EXPRESSION TAG	UNP P00533
K	310	LYS	-	EXPRESSION TAG	UNP P00533
K	515	HIS	-	EXPRESSION TAG	UNP P00533
K	516	HIS	-	EXPRESSION TAG	UNP P00533
K	517	HIS	-	EXPRESSION TAG	UNP P00533
K	518	HIS	-	EXPRESSION TAG	UNP P00533
K	519	HIS	-	EXPRESSION TAG	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
K	520	HIS	-	EXPRESSION TAG	UNP P00533

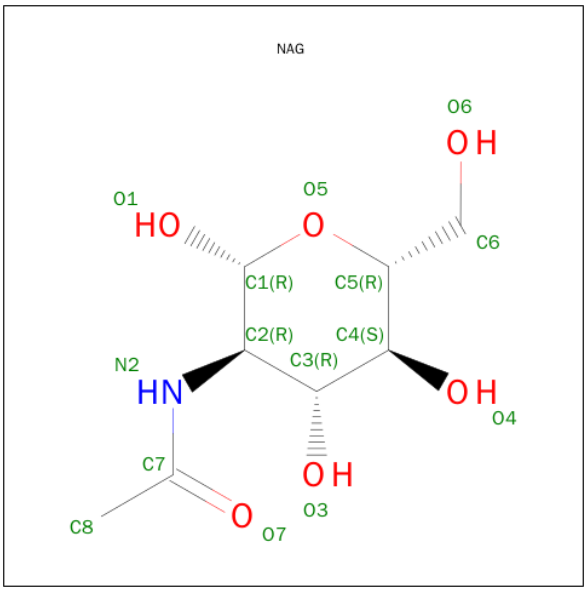
- Molecule 2 is a protein called Nanobody/VHH domain 7D12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	124	Total	C	H	N	O	S	0	0	0
			1753	568	835	159	187	4			
2	D	124	Total	C	H	N	O	S	0	0	0
			1717	562	810	155	186	4			
2	F	122	Total	C	H	N	O	S	0	0	0
			1666	549	782	151	180	4			
2	H	124	Total	C	H	N	O	S	0	0	0
			1770	571	846	162	187	4			
2	J	124	Total	C	H	N	O	S	0	0	0
			1771	572	845	160	190	4			
2	L	124	Total	C	H	N	O	S	0	0	0
			1732	565	821	156	186	4			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	4	Total	C	H	N	O	0	0
			94	28	44	2	20		
3	C	4	Total	C	H	N	O	0	0
			94	28	44	2	20		
3	E	4	Total	C	H	N	O	0	0
			94	28	44	2	20		
3	G	4	Total	C	H	N	O	0	0
			94	28	44	2	20		
3	I	4	Total	C	H	N	O	0	0
			94	28	44	2	20		
3	K	4	Total	C	H	N	O	0	0
			94	28	44	2	20		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	I	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	I	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	K	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	K	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

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

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

- Molecule 6 is water.

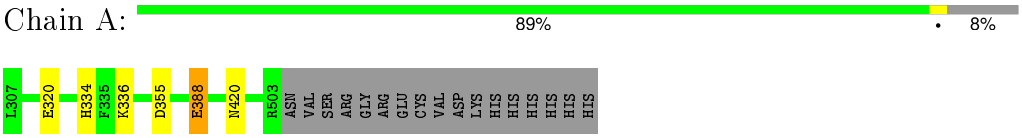
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	8	Total O 8 8	0	0
6	C	12	Total O 12 12	0	0
6	D	3	Total O 3 3	0	0
6	E	14	Total O 14 14	0	0
6	F	3	Total O 3 3	0	0
6	G	10	Total O 10 10	0	0
6	H	5	Total O 5 5	0	0
6	I	7	Total O 7 7	0	0
6	J	10	Total O 10 10	0	0
6	K	5	Total O 5 5	0	0
6	L	6	Total O 6 6	0	0

3 Residue-property plots (i)

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.

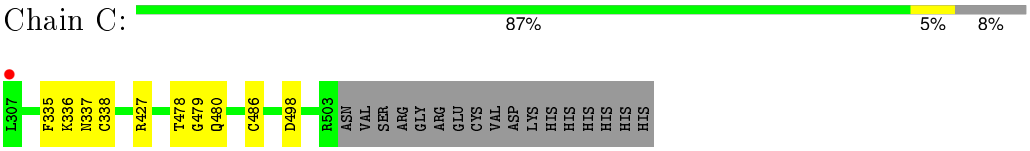
- Molecule 1: Epidermal growth factor receptor

Chain A:



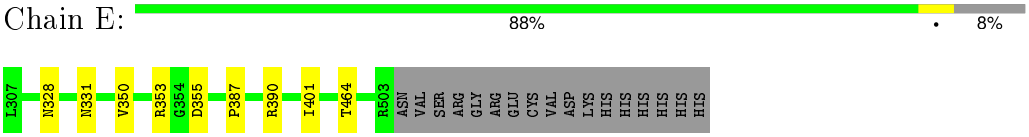
- Molecule 1: Epidermal growth factor receptor

Chain C:



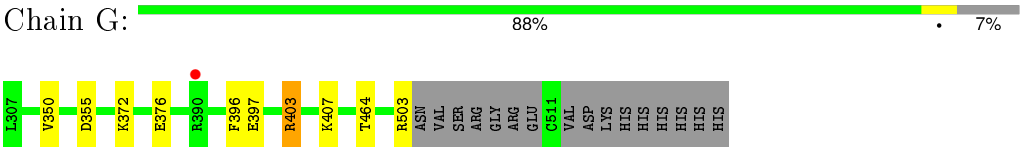
- Molecule 1: Epidermal growth factor receptor

Chain E:



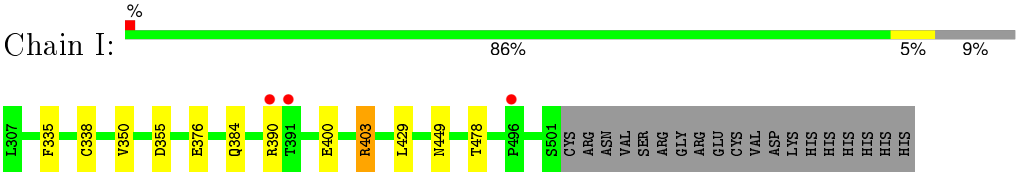
- Molecule 1: Epidermal growth factor receptor

Chain G:



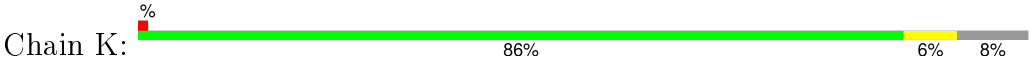
- Molecule 1: Epidermal growth factor receptor

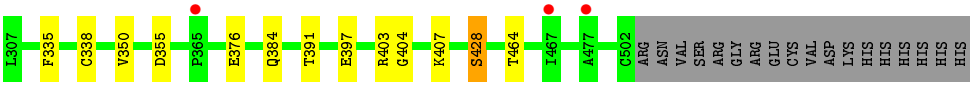
Chain I:



- Molecule 1: Epidermal growth factor receptor

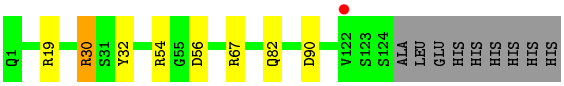
Chain K:





• Molecule 2: Nanobody/VHH domain 7D12

Chain B:



• Molecule 2: Nanobody/VHH domain 7D12

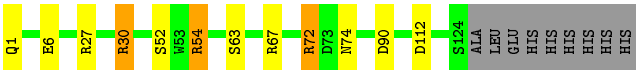
Chain D:

• Molecule 2: Nanobody/VHH domain 7D12

Chain F:

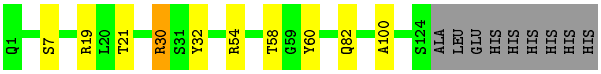
• Molecule 2: Nanobody/VHH domain 7D12

Chain H:



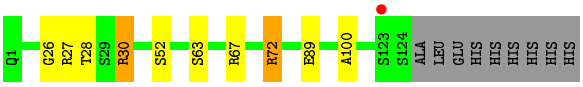
• Molecule 2: Nanobody/VHH domain 7D12

Chain J:



• Molecule 2: Nanobody/VHH domain 7D12

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.70Å 147.25Å 254.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.65 49.51 – 2.66	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.51-2.65) 96.1 (49.51-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.208 , 0.244 0.207 , 0.243	Depositor DCC
R_{free} test set	4233 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 83025 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28686	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, 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	0.29	0/1501	0.49	0/2040
1	C	0.28	0/1508	0.49	0/2048
1	E	0.30	0/1499	0.48	0/2037
1	G	0.29	0/1514	0.48	0/2055
1	I	0.29	0/1479	0.47	0/2009
1	K	0.28	0/1480	0.45	0/2013
2	B	0.32	0/938	0.47	0/1273
2	D	0.30	0/927	0.44	0/1261
2	F	0.30	0/904	0.47	0/1232
2	H	0.31	0/944	0.46	0/1280
2	J	0.30	0/946	0.46	0/1283
2	L	0.30	0/931	0.45	0/1265
All	All	0.29	0/14571	0.47	0/19796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1473	1412	1408	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1480	1426	1422	6	0
1	E	1471	1414	1410	7	0
1	G	1487	1425	1421	6	0
1	I	1452	1399	1397	8	0
1	K	1452	1395	1390	6	0
2	B	918	835	835	5	0
2	D	907	810	810	8	0
2	F	884	782	782	10	0
2	H	924	846	846	9	0
2	J	926	845	845	7	0
2	L	911	821	821	6	0
3	A	50	44	43	0	0
3	C	50	44	43	0	0
3	E	50	44	43	0	0
3	G	50	44	43	0	0
3	I	50	44	43	0	0
3	K	50	44	43	0	0
4	A	28	28	26	2	0
4	C	14	13	13	0	0
4	E	28	28	26	0	0
4	G	28	28	26	0	0
4	I	28	28	26	0	0
4	K	28	28	26	0	0
5	C	28	0	25	1	0
6	A	9	0	0	0	0
6	B	8	0	0	0	0
6	C	12	0	0	1	0
6	D	3	0	0	0	0
6	E	14	0	0	0	0
6	F	3	0	0	0	0
6	G	10	0	0	2	0
6	H	5	0	0	0	0
6	I	7	0	0	2	0
6	J	10	0	0	0	0
6	K	5	0	0	0	0
6	L	6	0	0	0	0
All	All	14859	13827	13813	72	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 3.

All (72) 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:I:384:GLN:NE2	6:I:705:HOH:O	2.14	0.80
1:E:328:ASN:OD1	1:E:331:ASN:ND2	2.19	0.76
1:A:336:LYS:HG2	4:A:605:NAG:O7	1.87	0.75
2:F:67:ARG:NH2	2:F:90:ASP:OD1	2.19	0.74
1:K:376:GLU:OE2	1:K:403:ARG:NH1	2.25	0.70
1:E:328:ASN:OD1	1:E:331:ASN:CG	2.32	0.69
2:F:52:SER:O	2:F:72:ARG:NH1	2.27	0.67
2:D:52:SER:O	2:D:72:ARG:NH1	2.28	0.66
1:A:388:GLU:HG2	1:A:420:ASN:HD22	1.60	0.66
2:H:67:ARG:NH2	2:H:90:ASP:OD1	2.30	0.65
2:B:67:ARG:NH1	2:B:90:ASP:OD1	2.29	0.64
2:D:67:ARG:NH2	2:D:90:ASP:OD1	2.36	0.59
2:L:89:GLU:OE1	2:L:89:GLU:N	2.36	0.58
5:C:607:NAG:H82	2:D:107:THR:HG22	1.85	0.58
1:A:320:GLU:OE2	1:A:334:HIS:ND1	2.37	0.57
1:G:503:ARG:O	6:G:710:HOH:O	2.18	0.57
1:E:387:PRO:HG2	1:E:390:ARG:HG3	1.87	0.57
1:E:350:VAL:HG11	2:F:100:ALA:HB3	1.87	0.56
1:C:486:CYS:SG	6:C:709:HOH:O	2.58	0.56
1:I:355:ASP:OD2	2:J:30:ARG:NH1	2.38	0.56
1:G:396:PHE:O	6:G:701:HOH:O	2.18	0.55
1:E:355:ASP:OD2	2:F:30:ARG:NH1	2.40	0.55
1:I:449:ASN:HB2	6:I:706:HOH:O	2.06	0.55
2:H:52:SER:O	2:H:72:ARG:NH1	2.39	0.55
2:D:72:ARG:NE	2:D:74:ASN:OD1	2.39	0.55
2:F:26:GLY:O	2:F:28:THR:N	2.41	0.54
1:K:350:VAL:HG11	2:L:100:ALA:HB3	1.89	0.54
2:L:26:GLY:O	2:L:28:THR:N	2.44	0.51
1:C:336:LYS:O	1:C:337:ASN:HB2	2.10	0.51
1:A:355:ASP:OD2	2:B:30:ARG:NH1	2.42	0.51
1:K:404:GLY:O	1:K:407:LYS:NZ	2.46	0.49
1:I:376:GLU:OE1	1:I:403:ARG:NH1	2.44	0.48
2:L:52:SER:O	2:L:72:ARG:NH1	2.46	0.48
2:D:63:SER:O	2:D:67:ARG:NH1	2.46	0.48
2:B:54:ARG:HG3	2:B:56:ASP:H	1.79	0.48
2:F:30:ARG:HD2	2:F:32:TYR:CE2	2.49	0.47
2:D:22:CYS:HB3	2:D:79:VAL:HG13	1.95	0.47
2:H:72:ARG:NE	2:H:74:ASN:OD1	2.46	0.47
1:G:376:GLU:OE1	1:G:403:ARG:NH1	2.47	0.47
2:L:63:SER:O	2:L:67:ARG:NH1	2.44	0.47
1:G:355:ASP:OD2	2:H:30:ARG:NH1	2.45	0.47
2:J:30:ARG:HD2	2:J:32:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:VAL:HG23	2:H:112:ASP:OD1	2.15	0.47
1:C:427:ARG:NH2	1:C:498:ASP:OD1	2.43	0.46
2:B:19:ARG:NH1	2:B:82:GLN:HG2	2.31	0.46
2:F:72:ARG:NE	2:F:74:ASN:OD1	2.47	0.46
1:C:478:THR:HB	1:C:480:GLN:HG2	1.98	0.46
2:H:1:GLN:O	2:H:27:ARG:N	2.48	0.46
2:J:19:ARG:NH1	2:J:82:GLN:HG2	2.32	0.45
1:A:336:LYS:HG2	4:A:605:NAG:C7	2.47	0.45
1:C:478:THR:HG22	1:C:479:GLY:H	1.81	0.45
1:C:335:PHE:HA	1:C:338:CYS:SG	2.57	0.45
2:J:7:SER:OG	2:J:21:THR:OG1	2.33	0.45
1:E:328:ASN:CG	1:E:331:ASN:ND2	2.69	0.45
1:I:350:VAL:HG11	2:J:100:ALA:HB3	1.97	0.45
2:F:22:CYS:HB3	2:F:79:VAL:HG13	1.99	0.44
2:H:63:SER:O	2:H:67:ARG:NH1	2.52	0.43
1:G:372:LYS:NZ	1:G:397:GLU:OE2	2.52	0.43
1:E:353:ARG:NH1	2:F:110:GLU:O	2.46	0.43
1:K:335:PHE:HA	1:K:338:CYS:SG	2.59	0.43
2:H:6:GLU:OE1	2:H:6:GLU:N	2.53	0.42
1:K:355:ASP:OD2	2:L:30:ARG:NH1	2.44	0.42
2:H:54:ARG:HD3	2:H:54:ARG:H	1.84	0.42
2:D:58:THR:CG2	2:D:60:TYR:CE1	3.03	0.42
1:I:335:PHE:HA	1:I:338:CYS:SG	2.59	0.41
1:K:397:GLU:O	1:K:428:SER:OG	2.34	0.41
2:B:30:ARG:HD2	2:B:32:TYR:CE2	2.56	0.41
1:I:350:VAL:CG1	2:J:100:ALA:HB3	2.51	0.41
2:D:12:VAL:HG21	2:D:18:LEU:HG	2.03	0.41
1:I:400:GLU:HA	1:I:429:LEU:HA	2.04	0.40
2:F:68:PHE:CD1	2:F:83:MET:HA	2.56	0.40
2:J:58:THR:CG2	2:J:60:TYR:CE1	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	195/214 (91%)	186 (95%)	9 (5%)	0	100	100
1	C	195/214 (91%)	190 (97%)	5 (3%)	0	100	100
1	E	195/214 (91%)	183 (94%)	12 (6%)	0	100	100
1	G	195/214 (91%)	187 (96%)	8 (4%)	0	100	100
1	I	193/214 (90%)	186 (96%)	7 (4%)	0	100	100
1	K	194/214 (91%)	183 (94%)	11 (6%)	0	100	100
2	B	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
2	D	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
2	F	120/133 (90%)	116 (97%)	2 (2%)	2 (2%)	11	25
2	H	122/133 (92%)	121 (99%)	1 (1%)	0	100	100
2	J	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
2	L	122/133 (92%)	120 (98%)	1 (1%)	1 (1%)	24	47
All	All	1897/2082 (91%)	1828 (96%)	66 (4%)	3 (0%)	52	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	14	THR
2	F	27	ARG
2	L	27	ARG

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	161/188 (86%)	160 (99%)	1 (1%)	90	97
1	C	163/188 (87%)	163 (100%)	0	100	100
1	E	160/188 (85%)	158 (99%)	2 (1%)	76	91
1	G	163/188 (87%)	160 (98%)	3 (2%)	66	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	157/188 (84%)	154 (98%)	3 (2%)	65 87
1	K	157/188 (84%)	153 (98%)	4 (2%)	55 82
2	B	90/104 (86%)	89 (99%)	1 (1%)	80 93
2	D	87/104 (84%)	84 (97%)	3 (3%)	44 72
2	F	83/104 (80%)	81 (98%)	2 (2%)	57 82
2	H	91/104 (88%)	88 (97%)	3 (3%)	45 73
2	J	92/104 (88%)	90 (98%)	2 (2%)	60 84
2	L	88/104 (85%)	86 (98%)	2 (2%)	58 83
All	All	1492/1752 (85%)	1466 (98%)	26 (2%)	68 88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	GLU
2	B	30	ARG
2	D	30	ARG
2	D	58	THR
2	D	72	ARG
1	E	401	ILE
1	E	464	THR
2	F	30	ARG
2	F	72	ARG
1	G	403	ARG
1	G	407	LYS
1	G	464	THR
2	H	30	ARG
2	H	54	ARG
2	H	72	ARG
1	I	390	ARG
1	I	403	ARG
1	I	478	THR
2	J	30	ARG
2	J	54	ARG
1	K	384	GLN
1	K	391	THR
1	K	428	SER
1	K	464	THR
2	L	30	ARG
2	L	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	483	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

26 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	$\#\|Z\| > 2$
3	NAG	A	601	1,3	14,14,15	0.36	0	15,19,21	0.27	0
3	NAG	A	602	3	14,14,15	0.46	0	15,19,21	0.37	0
3	BMA	A	603	3	11,11,12	0.43	0	14,15,17	1.13	2 (14%)
3	MAN	A	604	3	11,11,12	1.01	1 (9%)	14,15,17	2.15	4 (28%)
3	NAG	C	601	1,3	14,14,15	0.27	0	15,19,21	0.29	0
3	NAG	C	602	3	14,14,15	0.51	0	15,19,21	0.23	0
3	BMA	C	603	3	11,11,12	0.32	0	14,15,17	1.06	0
3	MAN	C	604	3	11,11,12	1.05	1 (9%)	14,15,17	1.94	4 (28%)
5	NAG	C	606	1,5	14,14,15	0.33	0	15,19,21	0.30	0
5	NAG	C	607	5	14,14,15	0.25	0	15,19,21	0.42	0
3	NAG	E	601	1,3	14,14,15	0.26	0	15,19,21	0.34	0
3	NAG	E	602	3	14,14,15	0.46	0	15,19,21	0.31	0
3	BMA	E	603	3	11,11,12	0.46	0	14,15,17	1.02	2 (14%)
3	MAN	E	604	3	11,11,12	0.99	1 (9%)	14,15,17	2.05	4 (28%)
3	NAG	G	601	1,3	14,14,15	0.40	0	15,19,21	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	G	602	3	14,14,15	0.44	0	15,19,21	0.32	0
3	BMA	G	603	3	11,11,12	0.35	0	14,15,17	1.24	2 (14%)
3	MAN	G	604	3	11,11,12	0.87	1 (9%)	14,15,17	1.76	4 (28%)
3	NAG	I	601	1,3	14,14,15	0.27	0	15,19,21	0.32	0
3	NAG	I	602	3	14,14,15	0.38	0	15,19,21	0.23	0
3	BMA	I	603	3	11,11,12	0.31	0	14,15,17	0.80	0
3	MAN	I	604	3	11,11,12	1.03	1 (9%)	14,15,17	1.85	5 (35%)
3	NAG	K	601	1,3	14,14,15	0.30	0	15,19,21	0.41	0
3	NAG	K	602	3	14,14,15	0.59	1 (7%)	15,19,21	0.25	0
3	BMA	K	603	3	11,11,12	0.41	0	14,15,17	1.11	2 (14%)
3	MAN	K	604	3	11,11,12	0.80	1 (9%)	14,15,17	1.82	4 (28%)

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	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
3	BMA	A	603	3	-	0/2/19/22	0/1/1/1
3	MAN	A	604	3	-	0/2/19/22	0/1/1/1
3	NAG	C	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	602	3	-	0/6/23/26	0/1/1/1
3	BMA	C	603	3	-	0/2/19/22	0/1/1/1
3	MAN	C	604	3	-	0/2/19/22	0/1/1/1
5	NAG	C	606	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	607	5	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	602	3	-	0/6/23/26	0/1/1/1
3	BMA	E	603	3	-	0/2/19/22	0/1/1/1
3	MAN	E	604	3	-	0/2/19/22	0/1/1/1
3	NAG	G	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	602	3	-	0/6/23/26	0/1/1/1
3	BMA	G	603	3	-	0/2/19/22	0/1/1/1
3	MAN	G	604	3	-	0/2/19/22	0/1/1/1
3	NAG	I	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	602	3	-	0/6/23/26	0/1/1/1
3	BMA	I	603	3	-	0/2/19/22	0/1/1/1
3	MAN	I	604	3	-	0/2/19/22	0/1/1/1
3	NAG	K	601	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	602	3	-	0/6/23/26	0/1/1/1
3	BMA	K	603	3	-	0/2/19/22	0/1/1/1
3	MAN	K	604	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	602	NAG	O5-C1	-2.12	1.40	1.43
3	K	604	MAN	C1-C2	2.11	1.57	1.52
3	G	604	MAN	C1-C2	2.22	1.57	1.52
3	A	604	MAN	C1-C2	2.26	1.57	1.52
3	I	604	MAN	C1-C2	2.32	1.57	1.52
3	C	604	MAN	C1-C2	2.70	1.58	1.52
3	E	604	MAN	C1-C2	2.74	1.58	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	604	MAN	O2-C2-C3	-2.73	104.64	110.12
3	K	604	MAN	O2-C2-C3	-2.70	104.69	110.12
3	G	604	MAN	O2-C2-C3	-2.66	104.76	110.12
3	C	604	MAN	O2-C2-C3	-2.66	104.77	110.12
3	I	604	MAN	O2-C2-C3	-2.53	105.03	110.12
3	A	604	MAN	O2-C2-C3	-2.22	105.65	110.12
3	I	604	MAN	C3-C4-C5	-2.14	106.47	110.20
3	A	603	BMA	C3-C4-C5	2.04	113.75	110.20
3	E	603	BMA	C3-C4-C5	2.05	113.77	110.20
3	K	603	BMA	C3-C4-C5	2.12	113.89	110.20
3	G	603	BMA	C3-C4-C5	2.12	113.89	110.20
3	K	603	BMA	C1-C2-C3	2.19	112.13	109.54
3	G	603	BMA	C1-C2-C3	2.20	112.15	109.54
3	E	603	BMA	C1-C2-C3	2.21	112.15	109.54
3	A	603	BMA	C1-C2-C3	2.25	112.21	109.54
3	K	604	MAN	C1-C2-C3	2.53	112.53	109.54
3	I	604	MAN	C1-C2-C3	2.62	112.64	109.54
3	G	604	MAN	C1-C2-C3	2.65	112.68	109.54
3	C	604	MAN	C1-C2-C3	2.98	113.07	109.54
3	K	604	MAN	O5-C1-C2	3.11	115.90	110.86
3	G	604	MAN	O5-C1-C2	3.11	115.90	110.86
3	A	604	MAN	C1-C2-C3	3.16	113.27	109.54
3	I	604	MAN	O5-C1-C2	3.37	116.33	110.86
3	C	604	MAN	O5-C1-C2	3.39	116.36	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	604	MAN	C1-C2-C3	3.40	113.56	109.54
3	I	604	MAN	C1-O5-C5	3.61	116.83	112.25
3	E	604	MAN	O5-C1-C2	3.61	116.72	110.86
3	G	604	MAN	C1-O5-C5	3.71	116.95	112.25
3	A	604	MAN	O5-C1-C2	3.91	117.20	110.86
3	C	604	MAN	C1-O5-C5	4.23	117.62	112.25
3	K	604	MAN	C1-O5-C5	4.29	117.69	112.25
3	E	604	MAN	C1-O5-C5	4.65	118.15	112.25
3	A	604	MAN	C1-O5-C5	5.44	119.15	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	607	NAG	1	0

5.6 Ligand geometry

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	605	1	14,14,15	0.54	0	15,19,21	1.14	0
4	NAG	A	606	1	14,14,15	0.34	0	15,19,21	0.24	0
4	NAG	C	605	1	14,14,15	0.52	0	15,19,21	1.10	1 (6%)
4	NAG	E	605	1	14,14,15	0.43	0	15,19,21	0.69	1 (6%)
4	NAG	E	606	1	14,14,15	0.55	0	15,19,21	0.32	0
4	NAG	G	605	1	14,14,15	0.33	0	15,19,21	0.43	0
4	NAG	G	606	1	14,14,15	0.26	0	15,19,21	0.46	0
4	NAG	I	605	1	14,14,15	0.23	0	15,19,21	0.46	0
4	NAG	I	606	1	14,14,15	0.28	0	15,19,21	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	K	605	1	14,14,15	0.63	0	15,19,21	0.50	0
4	NAG	K	606	1	14,14,15	0.18	0	15,19,21	0.37	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
4	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	NAG	C	605	1	-	0/6/23/26	0/1/1/1
4	NAG	E	605	1	-	0/6/23/26	0/1/1/1
4	NAG	E	606	1	-	0/6/23/26	0/1/1/1
4	NAG	G	605	1	-	0/6/23/26	0/1/1/1
4	NAG	G	606	1	-	0/6/23/26	0/1/1/1
4	NAG	I	605	1	-	0/6/23/26	0/1/1/1
4	NAG	I	606	1	-	0/6/23/26	0/1/1/1
4	NAG	K	605	1	-	0/6/23/26	0/1/1/1
4	NAG	K	606	1	-	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(^{o})	Ideal(^{o})
4	C	605	NAG	C4-C3-C2	-2.23	107.76	111.23
4	E	605	NAG	C1-O5-C5	2.54	115.47	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	NAG	2	0

5.7 Other polymers (i)

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, 95^{th} 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	197/214 (92%)	0.09	0 100 100	40, 52, 69, 78	0
1	C	197/214 (92%)	0.11	1 (0%) 91 92	39, 51, 68, 80	0
1	E	197/214 (92%)	0.13	0 100 100	41, 53, 65, 78	0
1	G	198/214 (92%)	0.11	1 (0%) 91 92	42, 54, 72, 84	0
1	I	195/214 (91%)	0.20	3 (1%) 76 75	42, 59, 82, 92	0
1	K	196/214 (91%)	0.30	3 (1%) 76 75	48, 67, 86, 94	0
2	B	124/133 (93%)	0.24	1 (0%) 87 87	39, 52, 65, 76	0
2	D	124/133 (93%)	0.14	0 100 100	42, 57, 71, 84	0
2	F	122/133 (91%)	0.28	3 (2%) 61 59	42, 65, 83, 87	0
2	H	124/133 (93%)	0.17	0 100 100	43, 54, 70, 75	0
2	J	124/133 (93%)	0.18	0 100 100	41, 52, 66, 82	0
2	L	124/133 (93%)	0.20	1 (0%) 87 87	47, 57, 69, 83	0
All	All	1922/2082 (92%)	0.17	13 (0%) 89 89	39, 55, 77, 94	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	122	VAL	3.4
2	L	123	SER	2.9
2	F	88	PRO	2.7
1	I	391	THR	2.7
1	K	365	PRO	2.4
1	I	390	ARG	2.4
1	G	390	ARG	2.3
1	C	307	LEU	2.3
1	K	467	ILE	2.3
1	K	477	ALA	2.2
2	F	91	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	122	VAL	2.0
1	I	496	PRO	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)

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, 95^{th} 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
5	NAG	C	606	14/15	0.93	0.19	0.92	64,77,78,82	0
3	NAG	G	602	14/15	0.92	0.19	0.65	59,72,81,93	0
3	NAG	I	601	14/15	0.96	0.20	0.33	51,59,71,84	0
3	NAG	A	602	14/15	0.94	0.18	0.32	55,67,84,90	0
3	NAG	K	601	14/15	0.96	0.20	0.21	51,62,74,87	0
3	NAG	C	601	14/15	0.97	0.19	0.08	46,55,65,76	0
3	NAG	K	602	14/15	0.93	0.19	-0.18	63,77,91,92	0
3	NAG	E	601	14/15	0.92	0.18	-0.41	50,61,73,81	0
3	NAG	C	602	14/15	0.92	0.16	-0.47	49,68,81,89	0
3	NAG	A	601	14/15	0.96	0.16	-0.78	41,53,67,77	0
3	NAG	G	601	14/15	0.95	0.15	-0.81	48,58,69,76	0
3	NAG	I	602	14/15	0.95	0.13	-1.35	56,67,80,81	0
3	NAG	E	602	14/15	0.90	0.13	-1.95	62,77,90,98	0
3	MAN	K	604	11/12	0.76	0.22	-	102,113,135,136	0
3	MAN	I	604	11/12	0.72	0.29	-	90,109,128,132	0
5	NAG	C	607	14/15	0.84	0.41	-	68,85,93,97	0
3	BMA	K	603	11/12	0.69	0.23	-	91,106,127,140	0
3	MAN	C	604	11/12	0.72	0.26	-	96,105,127,128	0
3	BMA	G	603	11/12	0.74	0.28	-	88,100,120,125	0
3	BMA	A	603	11/12	0.72	0.28	-	80,99,121,122	0
3	MAN	G	604	11/12	0.78	0.20	-	97,106,121,128	0
3	BMA	C	603	11/12	0.81	0.17	-	86,100,120,121	0
3	MAN	A	604	11/12	0.76	0.20	-	86,103,118,124	0
3	MAN	E	604	11/12	0.70	0.32	-	94,111,130,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	BMA	I	603	11/12	0.83	0.22	-	76,95,118,121	0
3	BMA	E	603	11/12	0.69	0.23	-	89,107,128,131	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
4	NAG	K	606	14/15	0.80	0.43	5.23	80,96,112,116	0
4	NAG	G	606	14/15	0.82	0.41	5.17	75,89,99,102	0
4	NAG	E	606	14/15	0.81	0.33	4.53	81,94,107,111	0
4	NAG	I	606	14/15	0.87	0.21	1.43	54,75,88,94	0
4	NAG	A	606	14/15	0.84	0.22	1.23	69,88,98,106	0
4	NAG	A	605	14/15	0.68	0.37	-	77,93,112,113	0
4	NAG	C	605	14/15	0.77	0.25	-	79,95,107,116	0
4	NAG	E	605	14/15	0.79	0.26	-	80,96,113,119	0
4	NAG	G	605	14/15	0.91	0.13	-	69,87,106,119	0
4	NAG	I	605	14/15	0.79	0.28	-	85,101,118,121	0
4	NAG	K	605	14/15	0.77	0.22	-	89,103,119,122	0

6.5 Other polymers (i)

There are no such residues in this entry.