Full wwPDB X-ray Structure Validation Report ⓘ

Dec 30, 2023 – 08:34 am GMT

PDB ID	:	7NZE
Title	:	Crystal structure of HLA-DR4 in complex with a human collagen type II peptide
Authors	:	Ge, C.; Dobritzsch, D.; Holmdahl, R.
Deposited on	:	2021-03-24
Resolution	:	2.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

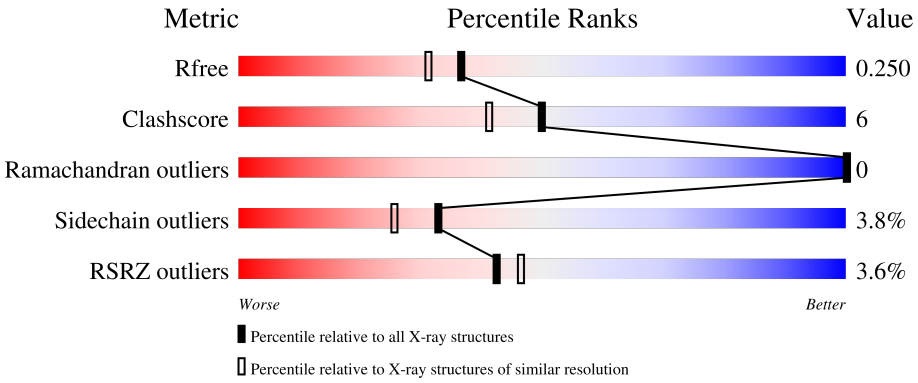
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AAA	182	2% 84% 14%
1	CCC	182	4% 87% 12%
2	BBB	191	5% 85% 12%
2	DDD	191	3% 84% 15%
3	EEE	15	80% 7% 13%

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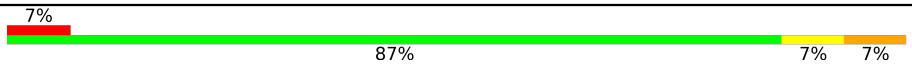
Mol	Chain	Length	Quality of chain
3	FFF	15	

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	BBB	201	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12951 atoms, of which 6169 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	179	Total	C	H	N	O	S	35	3	0
			2936	967	1442	246	276	5			
1	CCC	182	Total	C	H	N	O	S	38	2	0
			2970	980	1460	248	277	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	46	ARG	GLU	conflict	UNP P01903
AAA	183	SER	PRO	conflict	UNP P01903
CCC	46	ARG	GLU	conflict	UNP P01903
CCC	183	SER	PRO	conflict	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	190	Total	C	H	N	O	S	50	0	0
			3078	998	1498	282	295	5			
2	DDD	191	Total	C	H	N	O	S	49	1	0
			3096	1003	1507	283	298	5			

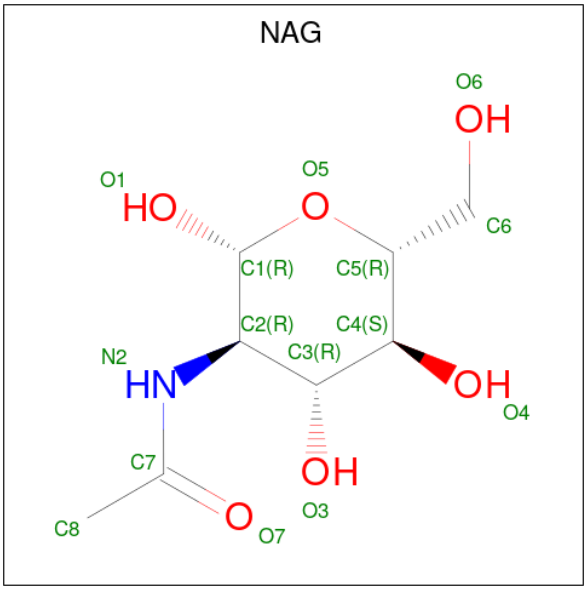
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	71	LYS	ARG	conflict	UNP A2BFX2
BBB	74	ALA	GLU	conflict	UNP A2BFX2
BBB	86	GLY	VAL	conflict	UNP A2BFX2
DDD	71	LYS	ARG	conflict	UNP A2BFX2
DDD	74	ALA	GLU	conflict	UNP A2BFX2
DDD	86	GLY	VAL	conflict	UNP A2BFX2

- Molecule 3 is a protein called Collagen alpha-1(II) chain.

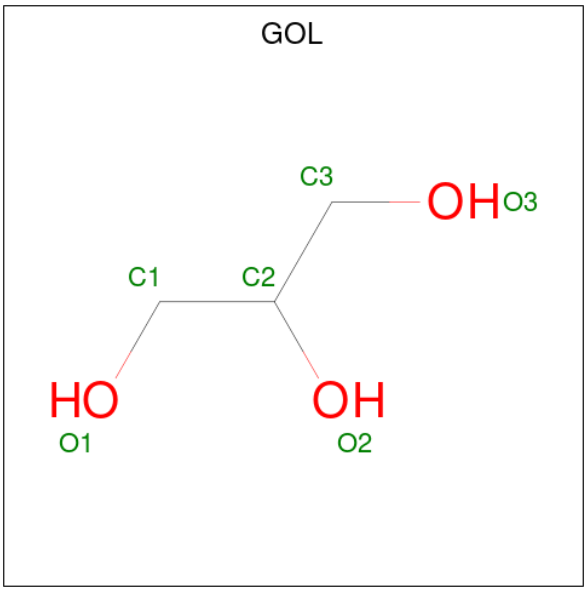
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EEE	13	Total	C	H	N	O	0	0	0
			178	57	86	16	19			
3	FFF	15	Total	C	H	N	O	0	0	0
			206	65	102	18	21			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	CCC	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C H O 14 3 8 3	2	0
5	BBB	1	Total C H O 14 3 8 3	2	0
5	DDD	1	Total C H O 14 3 8 3	2	0
5	DDD	1	Total C H O 14 3 8 3	2	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	111	Total O 112 112	0	1
6	BBB	70	Total O 70 70	0	0
6	CCC	84	Total O 84 84	0	0
6	DDD	73	Total O 73 73	0	0
6	EEE	1	Total O 1 1	0	0
6	FFF	7	Total O 7 7	0	0

3 Residue-property plots (i)

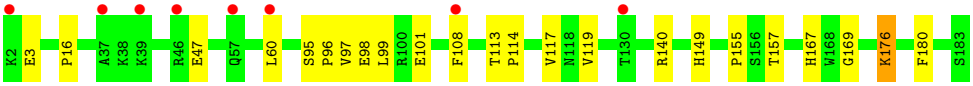
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain AAA:

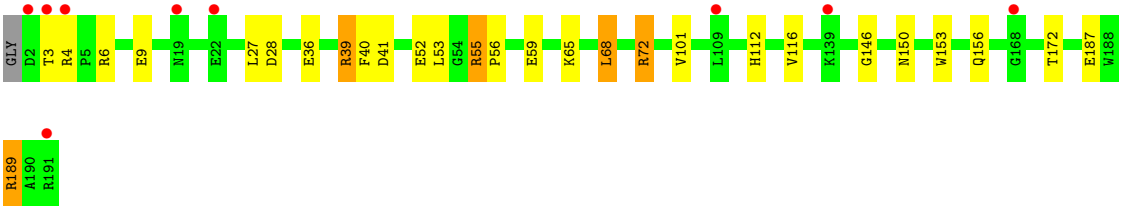
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain CCC:



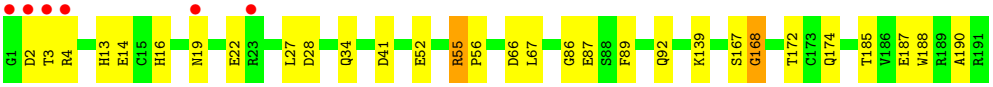
• Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain BBB:



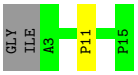
• Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain DDD:



• Molecule 3: Collagen alpha-1(II) chain

Chain EEE:



• Molecule 3: Collagen alpha-1(II) chain

Chain FFF:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.42Å 71.84Å 125.72Å 90.00° 111.33° 90.00°	Depositor
Resolution (Å)	47.01 – 2.05 46.96 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.01-2.05) 97.9 (46.96-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.245 0.199 , 0.250	Depositor DCC
R_{free} test set	3061 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.001 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.002 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12951	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	AAA	0.84	1/1548 (0.1%)	0.95	0/2109
1	CCC	0.82	0/1563	1.02	3/2129 (0.1%)
2	BBB	0.84	1/1624 (0.1%)	1.03	1/2207 (0.0%)
2	DDD	0.84	0/1636	0.97	0/2223
3	EEE	0.81	0/94	0.89	0/122
3	FFF	0.86	0/106	0.94	0/138
All	All	0.83	2/6571 (0.0%)	0.99	4/8928 (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	DDD	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	146	GLY	C-O	5.21	1.31	1.23
1	AAA	158	GLU	CD-OE2	-5.14	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	140	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	BBB	189	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	CCC	108[A]	PHE	CB-CA-C	5.02	120.44	110.40
1	CCC	108[B]	PHE	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DDD	168	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1494	1442	1438	19	0
1	CCC	1510	1460	1452	13	0
2	BBB	1580	1498	1490	22	2
2	DDD	1589	1507	1501	25	0
3	EEE	92	86	85	1	0
3	FFF	104	102	102	1	0
4	AAA	14	14	13	0	0
4	BBB	14	14	13	0	0
4	CCC	14	14	13	0	0
5	AAA	6	8	8	0	0
5	BBB	6	8	8	0	0
5	DDD	12	16	16	0	0
6	AAA	112	0	0	2	0
6	BBB	70	0	0	0	0
6	CCC	84	0	0	0	0
6	DDD	73	0	0	2	0
6	EEE	1	0	0	0	0
6	FFF	7	0	0	0	0
All	All	6782	6169	6139	73	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (73) 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:BBB:55:ARG:O	2:BBB:59:GLU:OE1	1.90	0.89
1:AAA:101:GLU:OE1	6:AAA:301:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:98:GLU:HB2	1:CCC:101:GLU:HG3	1.65	0.79
2:BBB:150:ASN:HD21	2:BBB:156:GLN:HE21	1.36	0.74
2:DDD:52:GLU:CD	2:DDD:55:ARG:HH12	1.91	0.73
2:BBB:55:ARG:C	2:BBB:59:GLU:OE1	2.31	0.69
1:AAA:89:VAL:O	1:AAA:176:LYS:HE2	1.95	0.66
1:CCC:95:SER:HB2	1:CCC:96:PRO:HD2	1.77	0.66
2:DDD:172:THR:HG22	2:DDD:187:GLU:HG2	1.79	0.63
2:DDD:13:HIS:HD2	2:DDD:28:ASP:OD1	1.83	0.61
1:CCC:3:GLU:OE1	2:DDD:16:HIS:HD2	1.85	0.59
2:DDD:52:GLU:CD	2:DDD:55:ARG:NH1	2.55	0.59
2:DDD:168:GLY:N	6:DDD:302:HOH:O	2.27	0.59
2:BBB:172:THR:HG22	2:BBB:187:GLU:HG2	1.83	0.59
2:DDD:13:HIS:CD2	2:DDD:28:ASP:OD1	2.56	0.59
2:BBB:56:PRO:HA	2:BBB:59:GLU:OE1	2.04	0.58
1:AAA:98:GLU:HB2	1:AAA:101:GLU:CG	2.35	0.57
1:AAA:175:LEU:HD12	1:AAA:175:LEU:N	2.20	0.57
2:BBB:36:GLU:OE2	2:BBB:39:ARG:HD2	2.07	0.55
2:BBB:56:PRO:CA	2:BBB:59:GLU:OE1	2.56	0.54
2:DDD:52:GLU:OE1	2:DDD:55:ARG:NH1	2.40	0.54
2:DDD:55:ARG:NH1	2:DDD:55:ARG:HG3	2.25	0.52
1:AAA:95:SER:HB2	1:AAA:96:PRO:HD2	1.92	0.51
2:DDD:87:GLU:OE2	2:DDD:92:GLN:NE2	2.42	0.51
2:DDD:19:ASN:HD22	2:DDD:22:GLU:CD	2.13	0.51
1:AAA:164[A]:ARG:NH2	1:AAA:173:PRO:HG2	2.25	0.50
1:AAA:72:ILE:CG2	1:AAA:76:ARG:HH21	2.24	0.50
2:BBB:172:THR:CG2	2:BBB:187:GLU:HG2	2.42	0.50
1:AAA:98:GLU:HB2	1:AAA:101:GLU:HG3	1.93	0.50
2:BBB:68:LEU:HG	2:BBB:72:ARG:HH12	1.77	0.49
3:FFF:14:GLU:OE1	3:FFF:15:PRO:HD2	2.12	0.49
1:AAA:21:GLU:OE2	1:AAA:137:PHE:O	2.30	0.49
1:AAA:17:ASP:OD1	2:BBB:6:ARG:NE	2.45	0.49
1:AAA:72:ILE:HG21	1:AAA:76:ARG:HH21	1.79	0.48
2:BBB:150:ASN:ND2	2:BBB:156:GLN:HE21	2.09	0.48
1:CCC:95:SER:HB2	1:CCC:96:PRO:CD	2.43	0.47
1:AAA:158:GLU:HA	1:AAA:158:GLU:OE1	2.14	0.47
2:DDD:67:LEU:HD21	3:EEE:11:PRO:HG3	1.96	0.46
2:BBB:55:ARG:N	2:BBB:56:PRO:CD	2.78	0.46
2:DDD:55:ARG:HG3	2:DDD:55:ARG:HH11	1.80	0.46
2:DDD:188:TRP:CH2	2:DDD:190:ALA:HA	2.50	0.46
2:DDD:55:ARG:HB2	2:DDD:56:PRO:HD3	1.97	0.45
2:DDD:188:TRP:CZ3	2:DDD:190:ALA:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:3:GLU:OE1	2:DDD:16:HIS:CD2	2.68	0.44
2:BBB:52:GLU:HA	2:BBB:55:ARG:HE	1.82	0.44
2:DDD:27:LEU:HD23	2:DDD:41:ASP:HA	1.99	0.44
1:CCC:113:THR:OG1	1:CCC:114:PRO:HA	2.18	0.44
2:BBB:56:PRO:HA	2:BBB:59:GLU:CD	2.38	0.44
1:AAA:11:GLU:HA	1:AAA:21:GLU:O	2.18	0.44
2:BBB:101:VAL:HA	2:BBB:116:VAL:O	2.19	0.43
1:CCC:176:LYS:HD2	1:CCC:176:LYS:HA	1.86	0.43
1:AAA:107:CYS:HB2	1:AAA:121:TRP:CH2	2.53	0.43
1:AAA:50:ARG:NH1	6:AAA:311:HOH:O	2.49	0.43
1:AAA:94:ASN:HB2	1:AAA:104:VAL:HB	2.01	0.43
1:AAA:29:ASP:HB3	2:BBB:153:TRP:CE2	2.53	0.42
1:AAA:175:LEU:N	1:AAA:175:LEU:CD1	2.82	0.42
2:BBB:52:GLU:O	2:BBB:55:ARG:HG3	2.19	0.42
2:BBB:112:HIS:NE2	1:CCC:157:THR:O	2.46	0.42
1:AAA:70:LEU:HB2	2:BBB:9:GLU:HB2	2.01	0.42
2:BBB:27:LEU:HD23	2:BBB:41:ASP:HA	2.01	0.42
1:CCC:119:VAL:HB	1:CCC:149:HIS:CE1	2.54	0.42
1:CCC:16:PRO:HG2	2:DDD:4:ARG:NH1	2.35	0.42
1:CCC:97:VAL:HG11	1:CCC:180:PHE:CG	2.55	0.42
2:DDD:174:GLN:HG3	2:DDD:185:THR:HG22	2.01	0.42
2:BBB:4:ARG:O	2:BBB:6:ARG:NH1	2.52	0.42
2:DDD:168:GLY:CA	6:DDD:302:HOH:O	2.68	0.42
2:DDD:14:GLU:OE1	2:DDD:16:HIS:HE1	2.02	0.41
2:BBB:27:LEU:HA	2:BBB:40:PHE:O	2.20	0.41
1:CCC:167[A]:HIS:CD2	1:CCC:169:GLY:H	2.39	0.40
2:DDD:86:GLY:HA2	2:DDD:89:PHE:CE1	2.57	0.40
1:CCC:114:PRO:O	1:CCC:167[A]:HIS:HE1	2.05	0.40
2:DDD:55:ARG:HH11	2:DDD:55:ARG:CG	2.33	0.40

All (2) 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)
2:BBB:59:GLU:OE2	2:BBB:59:GLU:OE2[2_556]	1.19	1.01
2:BBB:59:GLU:CD	2:BBB:59:GLU:OE2[2_556]	1.97	0.23

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	AAA	180/182 (99%)	176 (98%)	4 (2%)	0	100	100
1	CCC	182/182 (100%)	179 (98%)	3 (2%)	0	100	100
2	BBB	188/191 (98%)	179 (95%)	9 (5%)	0	100	100
2	DDD	190/191 (100%)	183 (96%)	7 (4%)	0	100	100
3	EEE	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	FFF	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	764/776 (98%)	739 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	167/166 (101%)	162 (97%)	5 (3%)	41	34
1	CCC	168/166 (101%)	162 (96%)	6 (4%)	35	28
2	BBB	172/172 (100%)	163 (95%)	9 (5%)	23	14
2	DDD	173/172 (101%)	167 (96%)	6 (4%)	36	29
3	EEE	8/9 (89%)	8 (100%)	0	100	100
3	FFF	9/9 (100%)	8 (89%)	1 (11%)	6	1
All	All	697/694 (100%)	670 (96%)	27 (4%)	33	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	19	SER
1	AAA	46	ARG
1	AAA	62[A]	ASN
1	AAA	62[B]	ASN
2	BBB	3	THR
2	BBB	28	ASP
2	BBB	39	ARG
2	BBB	53	LEU
2	BBB	55	ARG
2	BBB	65	LYS
2	BBB	68	LEU
2	BBB	72	ARG
2	BBB	189	ARG
1	CCC	47	GLU
1	CCC	60	LEU
1	CCC	99	LEU
1	CCC	117	VAL
1	CCC	155	PRO
1	CCC	176	LYS
2	DDD	3	THR
2	DDD	34	GLN
2	DDD	55	ARG
2	DDD	66	ASP
2	DDD	139	LYS
2	DDD	167	SER
3	FFF	14	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	BBB	201	2	14,14,15	1.64	2 (14%)	17,19,21	2.33	5 (29%)
4	NAG	CCC	201	1	14,14,15	0.72	0	17,19,21	2.01	5 (29%)
4	NAG	AAA	201	1	14,14,15	0.85	0	17,19,21	1.78	4 (23%)
5	GOL	AAA	202	-	5,5,5	0.11	0	5,5,5	0.32	0
5	GOL	BBB	202	-	5,5,5	0.08	0	5,5,5	0.30	0
5	GOL	DDD	202	-	5,5,5	0.08	0	5,5,5	0.24	0
5	GOL	DDD	201	-	5,5,5	0.09	0	5,5,5	0.33	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	BBB	201	2	1/1/7/7	3/6/23/26	0/1/1/1
4	NAG	CCC	201	1	-	2/6/23/26	0/1/1/1
4	NAG	AAA	201	1	-	2/6/23/26	0/1/1/1
5	GOL	AAA	202	-	-	2/4/4/4	-
5	GOL	BBB	202	-	-	0/4/4/4	-
5	GOL	DDD	202	-	-	1/4/4/4	-
5	GOL	DDD	201	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	201	NAG	C1-C2	3.93	1.58	1.52
4	BBB	201	NAG	C2-N2	3.48	1.52	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	201	NAG	C2-N2-C7	7.10	133.02	122.90
4	CCC	201	NAG	C3-C4-C5	-4.65	101.95	110.24
4	AAA	201	NAG	C1-O5-C5	3.71	117.22	112.19
4	CCC	201	NAG	O5-C5-C6	3.58	112.82	107.20
4	AAA	201	NAG	C2-N2-C7	3.58	128.00	122.90
4	BBB	201	NAG	O5-C1-C2	3.47	116.77	111.29
4	CCC	201	NAG	C1-O5-C5	3.34	116.72	112.19
4	CCC	201	NAG	O5-C1-C2	-2.87	106.76	111.29
4	BBB	201	NAG	C1-C2-N2	2.80	115.27	110.49
4	AAA	201	NAG	C6-C5-C4	-2.78	106.49	113.00
4	BBB	201	NAG	O7-C7-N2	2.67	126.87	121.95
4	CCC	201	NAG	O4-C4-C5	2.42	115.30	109.30
4	AAA	201	NAG	O5-C5-C4	2.01	115.72	110.83
4	BBB	201	NAG	C1-O5-C5	2.01	114.92	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	BBB	201	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	201	NAG	C3-C2-N2-C7
5	AAA	202	GOL	O2-C2-C3-O3
4	CCC	201	NAG	O5-C5-C6-O6
4	AAA	201	NAG	C8-C7-N2-C2
4	AAA	201	NAG	O7-C7-N2-C2
4	CCC	201	NAG	C4-C5-C6-O6
5	AAA	202	GOL	C1-C2-C3-O3
4	BBB	201	NAG	O5-C5-C6-O6
4	BBB	201	NAG	C1-C2-N2-C7
5	DDD	202	GOL	C1-C2-C3-O3

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, 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	AAA	179/182 (98%)	0.08	4 (2%)	62	66	28, 40, 72, 100	0
1	CCC	182/182 (100%)	0.09	8 (4%)	34	37	29, 44, 73, 86	0
2	BBB	190/191 (99%)	0.12	9 (4%)	31	33	26, 47, 77, 122	0
2	DDD	191/191 (100%)	0.05	6 (3%)	49	53	29, 49, 74, 109	0
3	EEE	13/15 (86%)	0.01	0	100	100	53, 59, 76, 86	0
3	FFF	15/15 (100%)	0.30	1 (6%)	17	19	33, 39, 64, 74	0
All	All	770/776 (99%)	0.09	28 (3%)	42	46	26, 46, 75, 122	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DDD	3	THR	7.6
1	AAA	79	TYR	4.4
1	CCC	2	LYS	4.3
2	BBB	4	ARG	4.2
2	BBB	2	ASP	3.5
1	CCC	46	ARG	3.2
2	BBB	3	THR	3.0
2	BBB	19	ASN	2.9
2	DDD	23	ARG	2.8
3	FFF	15	PRO	2.7
1	AAA	78	ASN	2.7
1	AAA	75	LYS	2.6
2	DDD	1	GLY	2.6
1	CCC	60	LEU	2.6
2	DDD	2[A]	ASP	2.4
2	BBB	22	GLU	2.4
2	DDD	4	ARG	2.3
2	BBB	109	LEU	2.3
1	CCC	130	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	DDD	19	ASN	2.3
1	CCC	57	GLN	2.2
1	CCC	37	ALA	2.2
2	BBB	168	GLY	2.2
1	CCC	39	LYS	2.2
1	CCC	108[A]	PHE	2.1
2	BBB	139	LYS	2.1
2	BBB	191	ARG	2.1
1	AAA	77	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
4	NAG	BBB	201	14/15	0.52	0.39	30,98,108,110	3
4	NAG	CCC	201	14/15	0.86	0.23	30,67,76,80	3
4	NAG	AAA	201	14/15	0.89	0.15	30,74,85,89	3
5	GOL	DDD	202	6/6	0.90	0.12	45,63,65,66	2
5	GOL	DDD	201	6/6	0.94	0.12	38,43,45,47	2
5	GOL	AAA	202	6/6	0.96	0.10	35,44,45,45	2
5	GOL	BBB	202	6/6	0.96	0.10	38,45,47,47	2

6.5 Other polymers (i)

There are no such residues in this entry.