

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 - 05:07 PM JST

PDB ID	:	8W86
Title	:	HLA-DQ2.5-B/C hordein peptide in complex with DQN0385AE02
Authors	:	Irie, M.; Tsushima, T.; Teranishi-Ikawa, Y.; Takahashi, N.; Ishii, S.; Okura,
		Y.; Fukami, T.A.; Torizawa, T.
Deposited on	:	2023-08-31
Resolution	:	2.24 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.24 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	А	223	6% 79%	15%	5%
1	Е	223	^{2%} 46% 6% 48%		
2	В	213	92%		7%•
2	F	213	46% · 50%		
3	С	189	% 82%	13%	• •
3	G	189	% 81%	14%	•••



Mol	Chain	Length	Quality of chain		
4	D	230	% 70%	16%	14%
4	Н	230	2% 70%	13%	17%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11188 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	911	Total	С	Ν	0	\mathbf{S}	0	0	0
1 A	211	1538	976	250	306	6	0	0	0	
1	1 5	116	Total	С	Ν	0	S	0	0	0
	110	872	557	146	165	4	0	0	0	

• Molecule 1 is a protein called DQN0385AE02 Fab heavy chain.

• Molecule 2 is a protein called DQN0385AE02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D 911	911	Total	С	Ν	0	\mathbf{S}	0	0	0
	211	1595	1002	261	327	5	0	0	0	
9	E	106	Total	С	Ν	0	S	0	0	0
2	Г		807	513	128	163	3	0	0	U

• Molecule 3 is a protein called HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	181	Total	С	Ν	0	S	0	0	0
3 0	101	1440	927	235	276	2	0	0	0	
2	C 191	101	Total	С	Ν	0	S	0	0	0
9 G	G	101	1422	916	234	270	2	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	47	SER	CYS	engineered mutation	UNP P01909
С	184	LEU	-	expression tag	UNP P01909
С	185	GLU	-	expression tag	UNP P01909
С	186	VAL	-	expression tag	UNP P01909
С	187	LEU	-	expression tag	UNP P01909
С	188	PHE	-	expression tag	UNP P01909
С	189	GLN	-	expression tag	UNP P01909
G	47	SER	CYS	engineered mutation	UNP P01909



Chain	Residue	Modelled	Actual	Comment	Reference
G	184	LEU	-	expression tag	UNP P01909
G	185	GLU	-	expression tag	UNP P01909
G	186	VAL	-	expression tag	UNP P01909
G	187	LEU	-	expression tag	UNP P01909
G	188	PHE	-	expression tag	UNP P01909
G	189	GLN	-	expression tag	UNP P01909

• Molecule 4 is a protein called MHC class II HLA-DQ-beta-1 - B/C hordein peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4		107	Total	С	Ν	0	\mathbf{S}	0	0	0
4 D	191	1605	1015	283	300	7	0	0	0	
4	п	102	Total	С	Ν	0	S	0	0	0
4 П	192	1529	975	265	282	$\overline{7}$	0	0	0	

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	984	GLY	-	linker	PDB ?
D	985	SER	-	linker	PDB ?
D	986	GLY	-	linker	PDB ?
D	987	GLY	-	linker	PDB ?
D	988	GLY	-	linker	PDB ?
D	989	GLY	-	linker	PDB ?
D	990	SER	-	linker	PDB ?
D	991	ILE	-	linker	PDB ?
D	992	GLU	-	linker	PDB ?
D	993	GLY	-	linker	PDB ?
D	994	ARG	-	linker	PDB ?
D	995	GLY	-	linker	PDB ?
D	996	SER	-	linker	PDB ?
D	997	GLY	-	linker	PDB ?
D	998	GLY	-	linker	PDB ?
D	999	GLY	-	linker	PDB ?
D	1000	SER	-	linker	PDB ?
D	1191	LEU	-	expression tag	UNP 019712
D	1192	GLU	-	expression tag	UNP 019712
D	1193	VAL	-	expression tag	UNP 019712
D	1194	LEU	-	expression tag	UNP 019712
D	1195	PHE	-	expression tag	UNP 019712
D	1196	GLN	-	expression tag	UNP 019712



Chain	Residue	Modelled	Actual	Comment	Reference
Н	984	GLY	-	linker	PDB ?
Н	985	SER	-	linker	PDB ?
Н	986	GLY	-	linker	PDB ?
Н	987	GLY	-	linker	PDB ?
Н	988	GLY	-	linker	PDB ?
Н	989	GLY	-	linker	PDB ?
Н	990	SER	-	linker	PDB ?
Н	991	ILE	-	linker	PDB ?
Н	992	GLU	-	linker	PDB ?
Н	993	GLY	-	linker	PDB ?
Н	994	ARG	-	linker	PDB ?
Н	995	GLY	-	linker	PDB ?
Н	996	SER	-	linker	PDB ?
Н	997	GLY	-	linker	PDB ?
Н	998	GLY	-	linker	PDB ?
Н	999	GLY	-	linker	PDB ?
Н	1000	SER	-	linker	PDB ?
Н	1191	LEU	-	expression tag	UNP 019712
Н	1192	GLU	-	expression tag	UNP 019712
Н	1193	VAL	-	expression tag	UNP 019712
Н	1194	LEU	-	expression tag	UNP 019712
Н	1195	PHE	-	expression tag	UNP 019712
Н	1196	GLN	-	expression tag	UNP 019712

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	С	1	Total 14	C 8	N 1	O 5	0	0
5	G	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
6	В	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
6	С	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
6	D	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
6	Е	15	Total O 15 15	0	0
6	F	25	$\begin{array}{cc} \text{Total} & \text{O} \\ 25 & 25 \end{array}$	0	0
6	G	60	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 60 & 60 \end{array}$	0	0
6	Н	58	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 58 & 58 \end{array}$	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.



 \bullet Molecule 1: DQN0385AE02 Fab heavy chain



A ASIN A ASIN COLLECTION A ASIN A ASI ARG GLY GLU CYS • Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain Chain C: 82% 13% CEL CEL • Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain Chain G: 81% 14% GLN • Molecule 4: MHC class II HLA-DQ-beta-1 - B/C hordein peptide chimeric protein Chain D: 70% 14% 16% GLN PPRO GLY SER GLY GLY GLY CLY GLY CLY GLY CLY GLY SER ARG GLY ARG THR GLU ALA LEU ASN HIS LEU GLU VAL LEU PHE GLN • Molecule 4: MHC class II HLA-DQ-beta-1 - B/C hordein peptide chimeric protein Chain H: 70% 13% 17% ALA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	73.70Å 127.19Å 130.37Å	Deperitor
a, b, c, α , β , γ	90.00° 104.45° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	126.22 - 2.24	Depositor
Resolution (A)	126.24 - 2.24	EDS
% Data completeness	69.1 (126.22 - 2.24)	Depositor
(in resolution range)	$69.1 \ (126.24 - 2.24)$	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.50 (at 2.22 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
D D.	0.241 , 0.280	Depositor
Π, Π_{free}	0.234 , 0.279	DCC
R_{free} test set	4001 reflections $(5.16%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	51.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.31, 37.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11188	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: 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).

Mal	Chain	Bo	ond lengths	Bond angles	
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.38	0/1578	0.63	0/2165
1	Е	0.39	0/894	0.58	0/1218
2	В	0.43	1/1631~(0.1%)	0.61	0/2224
2	F	0.44	0/826	0.62	0/1122
3	С	0.45	0/1482	0.67	0/2026
3	G	0.44	0/1464	0.65	0/2004
4	D	0.42	0/1645	0.65	0/2242
4	Н	0.44	0/1567	0.64	0/2139
All	All	0.42	1/11087~(0.0%)	0.63	0/15140

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	4	MET	SD-CE	-5.62	1.46	1.77

There are no bond angle outliers.

There are no chirality outliers.

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	А	1538	0	1414	20	0
1	Е	872	0	808	9	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	1595	0	1506	4	0
2	F	807	0	781	2	0
3	С	1440	0	1382	18	0
3	G	1422	0	1352	15	0
4	D	1605	0	1544	24	0
4	Н	1529	0	1461	18	0
5	С	14	0	13	1	0
5	G	14	0	13	0	0
6	А	34	0	0	0	0
6	В	52	0	0	0	0
6	С	54	0	0	0	0
6	D	54	0	0	0	0
6	Ε	15	0	0	0	0
6	F	25	0	0	0	0
6	G	60	0	0	1	0
6	Н	58	0	0	0	0
All	All	11188	0	10274	90	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 4.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:200:ILE:HA	1:A:215:ARG:HA	1.62	0.79
3:C:75:LEU:HD23	4:D:1032:TYR:HB2	1.65	0.79
4:D:1085:LEU:O	4:D:1089:THR:HG22	1.85	0.76
4:D:1116:VAL:HG22	4:D:1160:MET:HG2	1.74	0.70
1:A:113:LEU:HD23	1:A:154:PRO:HD3	1.75	0.69
3:C:75:LEU:HD21	4:D:1037:ILE:HD13	1.77	0.65
1:A:129:LEU:HD11	1:A:146:LEU:HD13	1.77	0.65
2:B:119:PRO:HD3	2:B:131:VAL:HG22	1.79	0.64
1:A:159:TRP:HA	1:A:201:CYS:HA	1.80	0.61
1:A:155:VAL:HG12	1:A:205:HIS:CD2	2.35	0.60
1:E:5:VAL:HG13	1:E:23:ALA:HB3	1.84	0.60
3:C:99:VAL:HG11	3:C:182:PRO:HB3	1.83	0.59
4:D:1170:VAL:HG22	4:D:1189:ARG:HG2	1.84	0.59
3:G:107:LEU:HD22	3:G:155:LEU:HD21	1.85	0.58
3:C:120:ASN:HD21	5:C:1000:NAG:C1	2.16	0.58
3:G:120:ASN:HB2	3:G:168:GLU:HB2	1.86	0.58
1:A:92:THR:HG23	1:A:115:THR:HA	1.87	0.56



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:35:MET:HB3	1:A:80:LEU:HD22	1.89	0.55
3:G:124:LEU:HB2	3:G:164:ASP:HB2	1.89	0.55
3:G:99:VAL:HG11	3:G:182:PRO:HB3	1.88	0.54
1:A:155:VAL:HG12	1:A:205:HIS:HD2	1.72	0.54
1:E:101:ILE:HG22	2:F:89:HIS:CE1	2.43	0.53
1:E:33:TYR:CE2	1:E:99:ARG:NH1	2.76	0.53
4:H:1174:HIS:HE1	4:H:1176:GLU:OE2	1.93	0.52
4:D:1049:ALA:HB3	4:H:1143:VAL:HG22	1.92	0.51
3:C:17:GLN:OE1	4:D:1006:ASP:OD2	2.28	0.51
3:C:124:LEU:HB2	3:C:164:ASP:HB2	1.92	0.51
4:H:-1:GLU:HG3	4:H:0:GLN:H	1.76	0.51
3:G:107:LEU:HD13	3:G:155:LEU:HD21	1.93	0.50
3:C:97:SER:HB2	3:C:98:PRO:HD2	1.94	0.49
1:E:33:TYR:HE2	1:E:99:ARG:NH1	2.09	0.49
4:H:1142:VAL:HG12	4:H:1161:LEU:HD12	1.93	0.49
1:A:48:TRP:CG	2:B:95:VAL:HB	2.47	0.49
1:A:32:TRP:O	3:C:69:LYS:HE2	2.13	0.49
3:C:78:ARG:HD3	4:D:1053:LEU:HD23	1.95	0.49
3:C:48:LEU:HD13	4:D:1153:TRP:CG	2.50	0.47
1:E:71:ILE:HD11	1:E:80:LEU:HD11	1.96	0.47
4:H:1129:VAL:HG22	4:H:1175:VAL:HG22	1.97	0.47
1:A:157:VAL:HG22	1:A:203:VAL:HG22	1.95	0.47
2:B:162:VAL:HG22	2:B:174:LEU:HD12	1.95	0.47
1:E:12:VAL:HG11	1:E:18:LEU:HD13	1.96	0.47
4:H:1037:ILE:HG13	4:H:1038:VAL:HG12	1.97	0.47
3:C:46:TRP:CE3	3:C:51:LEU:HB3	2.50	0.47
4:D:1176:GLU:HG2	4:D:1183:PRO:HG3	1.96	0.46
4:H:1114:LEU:HD21	4:H:1160:MET:HG2	1.95	0.46
3:G:12:GLY:HA3	6:G:1123:HOH:O	2.15	0.46
4:D:1089:THR:HG23	4:D:1090:THR:H	1.80	0.46
1:A:62:ALA:CB	1:A:64:TRP:NE1	2.79	0.46
2:F:21:ILE:HD12	2:F:73:LEU:HD23	1.98	0.46
4:D:9:TYR:OH	4:D:1053:LEU:O	2.33	0.45
1:E:33:TYR:HE2	1:E:99:ARG:HH11	1.61	0.45
3:G:17:GLN:OE1	4:H:1006:ASP:OD2	2.35	0.45
3:C:170:TRP:CE2	4:D:1004:PRO:HD2	2.51	0.45
1:E:92:THR:HG23	1:E:115:THR:HA	1.98	0.45
3:G:79:SER:HB3	4:H:1053:LEU:HD21	1.99	0.45
1:A:155:VAL:CG1	1:A:205:HIS:CD2	2.99	0.45
1:A:155:VAL:CG1	1:A:205:HIS:HD2	2.28	0.44
3:C:75:LEU:HD22	4:D:1009:TYR:CE2	2.53	0.44



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance $(Å)$	overlap (Å)
3:G:130:VAL:HG12	3:G:131:THR:H	1.82	0.44
4:H:1010:GLN:HB2	4:H:1031:ILE:HB	1.99	0.43
1:A:71:ILE:HD11	1:A:80:LEU:HD11	2.00	0.43
4:D:1055:LEU:HD21	4:H:1143:VAL:HG23	2.00	0.43
4:H:1064:GLN:HB2	4:H:1067:ILE:HD12	2.00	0.43
3:C:14:ASN:HD22	3:C:14:ASN:N	2.17	0.43
1:A:37:TRP:NE1	1:A:80:LEU:HG	2.33	0.43
4:H:-1:GLU:HG3	4:H:0:GLN:N	2.33	0.43
1:E:33:TYR:CD2	1:E:99:ARG:HD2	2.53	0.43
4:D:1076:ASP:HA	4:D:1080:ARG:HB2	2.00	0.43
1:A:19:ARG:NH2	1:A:81:TYR:CE1	2.87	0.43
1:A:32:TRP:CD1	1:A:53:ASP:OD1	2.72	0.42
4:D:1082:ASN:O	4:D:1086:GLU:HG2	2.19	0.42
4:H:9:TYR:CE2	4:H:1057:ALA:HB2	2.54	0.42
1:A:128:PRO:HB3	1:A:216:VAL:HG12	2.02	0.42
1:A:210:THR:HG22	1:A:212:VAL:HG23	2.00	0.42
2:B:148:LYS:HB2	2:B:192:ALA:HB3	2.01	0.42
3:G:10:SER:HB3	3:G:13:VAL:HG23	2.02	0.42
4:D:1181:GLN:CD	4:D:1181:GLN:H	2.23	0.42
3:C:107:LEU:HD13	3:C:155:LEU:HD13	2.02	0.41
3:G:115:PHE:CG	4:H:1034:ARG:HD2	2.55	0.41
3:C:12:GLY:O	4:D:1012:LYS:HA	2.21	0.41
3:C:169:HIS:CD2	3:C:171:GLY:H	2.38	0.41
4:D:1037:ILE:HA	4:D:1051:THR:HB	2.01	0.41
3:G:33:GLU:HB2	3:G:140:LEU:HD11	2.02	0.41
3:G:96:LYS:HD3	3:G:106:ILE:HD12	2.02	0.41
3:G:78:ARG:HE	4:H:1056:PRO:HG2	1.86	0.40
3:G:48:LEU:HD13	4:H:1153:TRP:CG	2.56	0.40
4:D:-3:GLU:N	4:D:-2:PRO:CD	2.85	0.40
3:C:75:LEU:HD11	4:D:9:TYR:CE1	2.57	0.40
4:D:1130:ARG:HB2	4:D:1174:HIS:HB3	2.04	0.40
4:D:1162:GLU:HB2	4:H:1055:LEU:HD13	2.02	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	207/223~(93%)	196 (95%)	9 (4%)	2(1%)	15	11
1	Е	114/223~(51%)	108 (95%)	5(4%)	1 (1%)	17	13
2	В	209/213~(98%)	198 (95%)	10~(5%)	1 (0%)	29	28
2	F	104/213~(49%)	101 (97%)	3~(3%)	0	100	100
3	С	179/189~(95%)	176 (98%)	3(2%)	0	100	100
3	G	179/189~(95%)	170 (95%)	9~(5%)	0	100	100
4	D	191/230~(83%)	180 (94%)	10 (5%)	1 (0%)	29	28
4	Н	184/230 (80%)	177 (96%)	7 (4%)	0	100	100
All	All	1367/1710~(80%)	1306 (96%)	56 (4%)	5(0%)	34	35

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

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	149	ASP
1	А	194	LEU
4	D	1126	GLN
2	В	210	ARG
1	Е	32	TRP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	161/187~(86%)	157~(98%)	4 (2%)	47 54
1	Е	86/187~(46%)	83~(96%)	3~(4%)	36 40
2	В	177/188~(94%)	172 (97%)	5(3%)	43 49
2	F	90/188~(48%)	86 (96%)	4 (4%)	28 30
3	С	164/173~(95%)	157 (96%)	7 (4%)	29 31



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
3	G	159/173~(92%)	151~(95%)	8 (5%)	24 24		
4	D	178/204~(87%)	172~(97%)	6 (3%)	37 42		
4	Н	166/204~(81%)	159~(96%)	7 (4%)	30 32		
All	All	1181/1504 (78%)	1137 (96%)	44 (4%)	34 38		

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All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	73	ARG
1	А	140	THR
1	А	145	CYS
1	А	146	LEU
2	В	1	ASP
2	В	47	LEU
2	В	56	GLU
2	В	121	ASP
2	В	146	GLN
3	С	14	ASN
3	С	77	LYS
3	С	85	THR
3	С	95	SER
3	С	100	THR
3	С	132	GLU
3	С	155	LEU
4	D	-1	GLU
4	D	1019	ASN
4	D	1021	THR
4	D	1051	THR
4	D	1135	ASP
4	D	1163	MET
1	Е	58	SER
1	Е	73	ARG
1	Е	115	THR
2	F	22	THR
2	F	45	LYS
2	F	47	LEU
2	F	90	TYR
3	G	47	SER
3	G	55	ARG
3	G	75	LEU
3	G	90	GLU



Mol	Chain	Res	Type
3	G	140	LEU
3	G	155	LEU
3	G	156	LEU
3	G	162	SER
4	Н	4	GLU
4	Н	1066	ASP
4	Н	1087	LEU
4	Н	1120	THR
4	Н	1126	GLN
4	H	1127	ILE
4	Н	1142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	С	120	ASN
3	С	169	HIS
4	D	1174	HIS
3	G	179	HIS
4	Н	1174	HIS

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)

2 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 Tur	Turne	Type Chain		Chain	Chain	Chain	Dec	Tinle	Bo	ond leng	ths	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2				
5	NAG	С	1000	-	14,14,15	0.35	0	17,19,21	1.18	1 (5%)				
5	NAG	G	1000	-	14,14,15	0.33	0	17,19,21	1.39	1 (5%)				

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	С	1000	-	-	0/6/23/26	0/1/1/1
5	NAG	G	1000	-	-	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	$Observed(^{o})$	$Ideal(^{o})$
5	G	1000	NAG	O5-C1-C2	-5.41	102.74	111.29
5	С	1000	NAG	O5-C1-C2	-4.59	104.04	111.29

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	С	1000	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ	>2	$OWAB(Å^2)$	Q<0.9
1	А	211/223~(94%)	0.65	14 (6%) 18	18	33, 69, 103, 115	0
1	Е	116/223~(52%)	0.41	4 (3%) 45	45	43, 63, 75, 84	0
2	В	211/213~(99%)	0.26	1 (0%) 91	91	30, 55, 80, 88	0
2	F	106/213~(49%)	0.22	1 (0%) 84	84	39, 54, 69, 82	0
3	С	181/189~(95%)	0.29	1 (0%) 89	89	30, 45, 69, 80	0
3	G	181/189~(95%)	0.23	1 (0%) 89	89	30, 44, 70, 82	0
4	D	197/230~(85%)	0.24	2 (1%) 82	83	34, 51, 70, 83	0
4	Н	192/230~(83%)	0.41	5 (2%) 56	57	33, 51, 68, 84	0
All	All	1395/1710~(81%)	0.35	29 (2%) 63	65	30, 54, 82, 115	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	161 SER		3.6
1	А	2	VAL	3.4
1	А	212	VAL	3.4
1	Е	2	VAL	3.3
1	А	219	LYS	3.2
1	А	216	VAL	3.1
1	А	196	THR	3.1
1	А	162	GLY	2.9
4	D	1104	SER	2.7
4	Н	1105	ARG	2.5
1	Е	32	TRP	2.4
1	А	81	TYR	2.4
4	D	1114	LEU	2.4
1	А	107	PHE	2.4
2	F	19	VAL	2.4
1	А	209	ASN	2.3



Mol	Chain	Res Type		RSRZ	
4	Н	-3	GLU	2.3	
1	А	218	PRO	2.3	
1	А	163	ALA	2.2	
1	А	195	GLY	2.2	
1	А	113	LEU	2.2	
4	Н	1175	VAL	2.2	
1	Е	11	VAL	2.1	
2	В	110	ALA	2.1	
3	G	159	ALA	2.1	
4	Н	1158	LEU	2.1	
1	Е	107	PHE	2.0	
4	Н	1120	THR	2.0	
3	С	159	ALA	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	NAG	С	1000	14/15	0.66	0.22	81,83,84,84	0
5	NAG	G	1000	14/15	0.76	0.22	87,89,90,90	0

6.5 Other polymers (i)

There are no such residues in this entry.

