

Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 03:33 PM JST

PDB ID	:	8W85
Title	:	HLA-DQ2.5-gamma2 gliadin peptide in complex with DQN0385AE01
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	:	2.77 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 2.77 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	.% •	67%		26%	• 5%			
1	Е	223	4%	10%	6 • 4	3%	_			
2	В	213	2%	80%		18%				
2	F	213	9% 40%	8% •	51%)				
3	С	189	.%	80%		15%	• 5%			
3	G	189	<u>2%</u>	71%		23%	• 5%			



Mol	Chain	Length	Quality of chain							
4	D	222	^{2%} 69%	14%	16%					
4	Н	222	67%	14%	20%					



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10295 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		At	oms			ZeroOcc	AltConf	Trace
1	1 1	911	Total	С	Ν	0	\mathbf{S}	0	0	0
1 A	A	211	1559	988	261	303	7		0	
1	F	E 126	Total	С	Ν	0	S	0	0	0
	Ľ		875	555	141	174	5	0	0	0

• Molecule 1 is a protein called DQN0385AE01 Fab heavy chain.

• Molecule 2 is a protein called DQN0385AE01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D D	911	Total	С	Ν	0	S	0	0	0
	D	211	1548	973	249	321	5			
0	Б	105	Total	С	Ν	0	S	0	0	0
	Г	105	736	465	120	148	3			0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	180	Total 1383	C 896	N 225	O 260	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0
3	G	179	Total 1379	C 889	N 224	O 264	S 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 - gamma2 gliadin peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	186	Total 1427	C 909	N 247	0 264	${ m S} 7$	0	0	0
4	Н	178	Total 1360	C 869	N 231	O 253	S 7	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
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
Н	986	GLY	-	linker	PDB ?
Н	987	GLY	-	linker	PDB ?

There are 42 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
5	G	1	Total 14	C 8	N 1	O 5	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: DQN0385AE01 Fab heavy chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants	150.53Å 243.91Å 136.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	50.47 - 2.77	Depositor
Resolution (A)	50.47 - 2.77	EDS
% Data completeness	65.3(50.47-2.77)	Depositor
(in resolution range)	65.3(50.47-2.77)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 2.77 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
P. P.	0.253 , 0.300	Depositor
n, n_{free}	0.251 , 0.303	DCC
R_{free} test set	2093 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	85.6	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 51.9	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10295	wwPDB-VP
Average B, all atoms $(Å^2)$	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% 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).

Mol Chain		Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/1601	0.67	0/2197	
1	Е	0.36	0/898	0.57	0/1237	
2	В	0.45	0/1584	0.71	1/2172~(0.0%)	
2	F	0.40	0/755	0.60	0/1036	
3	С	0.44	0/1425	0.65	0/1956	
3	G	0.37	0/1421	0.60	0/1951	
4	D	0.48	0/1459	0.65	0/1996	
4	Н	0.40	0/1389	0.59	0/1900	
All	All	0.43	0/10532	0.64	1/14445~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	50	TYR	C-N-CA	5.79	136.19	121.70

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	1559	0	1462	30	0
1	Е	875	0	750	19	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	1548	0	1419	24	0
2	F	736	0	639	12	0
3	С	1383	0	1299	23	0
3	G	1379	0	1280	26	0
4	D	1427	0	1344	26	0
4	Н	1360	0	1270	18	0
5	С	14	0	13	1	0
5	G	14	0	13	0	0
All	All	10295	0	9489	148	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 7.

All (148) 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:E:17:SER:HB3	1:E:85:ASN:HA	1.52	0.89
1:A:92:THR:HG23	1:A:115:THR:HA	1.62	0.80
3:G:113:ASN:H	3:G:142:LYS:NZ	1.80	0.78
1:A:6:GLU:HB3	1:A:112:THR:HB	1.67	0.77
2:B:53:THR:HG23	2:B:53:THR:O	1.87	0.75
3:C:75:LEU:HD21	4:D:1037:ILE:HD13	1.70	0.73
3:G:113:ASN:H	3:G:142:LYS:HZ3	1.33	0.72
1:A:159:TRP:CD1	1:A:168:VAL:HG11	2.26	0.71
1:A:156:THR:HB	1:A:204:ASN:HB3	1.72	0.70
1:A:200:ILE:HG13	1:A:215:LYS:HA	1.73	0.70
2:B:7:SER:OG	2:B:8:PRO:HD3	1.92	0.69
2:B:89:HIS:NE2	2:B:95:VAL:HG13	2.08	0.69
3:C:10:SER:HB3	3:C:13:VAL:HG23	1.75	0.69
4:H:1172:THR:HG21	4:H:1174:HIS:NE2	2.07	0.69
1:E:17:SER:CB	1:E:85:ASN:HA	2.21	0.68
1:A:68:ARG:NH2	1:A:91:ASP:OD2	2.25	0.67
1:A:101:ILE:HG22	2:B:89:HIS:CE1	2.30	0.66
2:B:105:ILE:H	2:B:165:GLN:HE22	1.44	0.65
3:C:145:HIS:CD2	4:D:1031:ILE:HD12	2.32	0.64
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.80	0.62
1:E:104:ASP:HB2	2:F:49:TYR:CE2	2.35	0.62
3:C:68:LEU:HG	4:D:1009:TYR:HD1	1.66	0.61
3:C:120:ASN:HD21	5:C:1000:NAG:C1	2.14	0.61
2:F:55:ALA:HB3	2:F:58:ILE:HB	1.82	0.60
3:G:145:HIS:CE1	4:H:1031:ILE:HD12	2.36	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:53:THR:O	2:B:53:THR:CG2	2.48	0.60
3:C:120:ASN:HB2	3:C:168:GLU:HB2	1.84	0.60
3:G:120:ASN:HB2	3:G:168:GLU:HB2	1.85	0.59
1:A:159:TRP:HD1	1:A:168:VAL:HG11	1.65	0.59
3:C:145:HIS:NE2	4:D:1031:ILE:HD12	2.18	0.59
4:D:1037:ILE:HG13	4:D:1038:VAL:HG23	1.84	0.59
4:D:1119:VAL:HG21	4:D:1129:VAL:HG21	1.85	0.58
1:E:35:ILE:HG12	1:E:99:ARG:HB2	1.86	0.58
3:G:48:LEU:HD11	3:G:51:LEU:HD12	1.85	0.57
1:A:84:MET:HE1	1:A:114:VAL:HG11	1.86	0.57
1:A:37:TRP:HD1	1:A:71:ILE:HD12	1.70	0.57
3:C:48:LEU:HD13	4:D:1153:TRP:CD1	2.40	0.57
3:C:75:LEU:HD23	4:D:1032:TYR:HB2	1.87	0.57
4:D:2:GLN:HG3	4:D:1081:HIS:CD2	2.39	0.57
4:D:1101:ILE:HD11	4:D:1173:CYS:HB2	1.87	0.56
4:H:1021:THR:HB	4:H:1080:ARG:HE	1.71	0.56
1:A:142:ALA:HB2	1:A:188:THR:HG23	1.87	0.56
4:H:7:ALA:HB3	4:H:1061:TRP:CE2	2.40	0.56
1:E:6:GLU:OE2	1:E:109:GLY:HA3	2.06	0.54
2:B:200:LEU:HD13	2:B:204:VAL:HG23	1.89	0.54
3:G:54:PHE:HE2	4:H:1089:THR:HG21	1.73	0.53
2:B:55:ALA:HB2	2:B:58:ILE:HG23	1.91	0.53
2:B:55:ALA:CB	2:B:58:ILE:HG23	2.37	0.53
1:A:175:LEU:HD12	1:A:181:TYR:CE1	2.44	0.53
2:B:48:ILE:HG12	2:B:53:THR:HA	1.89	0.53
3:G:106:ILE:HD12	3:G:154:THR:HG22	1.92	0.52
3:G:50:VAL:HG12	4:H:1089:THR:HG22	1.92	0.52
4:D:1174:HIS:HD2	4:D:1185:THR:HG22	1.74	0.52
1:A:40:GLN:HB2	1:A:46:LEU:HD23	1.92	0.52
1:E:31:SER:HB2	1:E:33:TYR:CE2	2.45	0.51
3:G:33:GLU:HB2	3:G:140:LEU:HD21	1.91	0.51
4:D:1038:VAL:HG12	4:D:1039:ARG:H	1.74	0.51
1:E:104:ASP:HB3	4:H:8:GLN:HE21	1.75	0.51
4:D:1148:ILE:HB	4:D:1156:GLN:HG2	1.92	0.51
3:G:164:ASP:HB3	3:G:177:LEU:HD12	1.92	0.51
3:G:162:SER:HB2	3:G:179:HIS:CE1	2.46	0.51
4:D:1037:ILE:HG13	4:D:1038:VAL:N	2.25	0.51
1:E:58:SER:HB3	3:G:42:LYS:HZ1	1.76	0.50
3:G:162:SER:HB2	3:G:179:HIS:HE1	1.76	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.50
2:F:93:SER:HB3	3:G:59:GLN:HE22	1.77	0.50



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:170:THR:HG23	1:A:185:SER:HB2	1.93	0.49
1:A:159:TRP:CD1	1:A:168:VAL:CG1	2.96	0.48
1:A:131:PRO:HB3	1:A:143:LEU:HB3	1.95	0.48
2:B:162:VAL:HG22	2:B:174:LEU:HD12	1.95	0.48
3:C:10:SER:CB	3:C:13:VAL:HG23	2.40	0.48
1:E:58:SER:HB3	3:G:42:LYS:NZ	2.28	0.48
3:C:68:LEU:HG	4:D:1009:TYR:CD1	2.48	0.48
1:A:5:VAL:HG13	1:A:23:ALA:HB3	1.94	0.48
4:H:1172:THR:CG2	4:H:1174:HIS:NE2	2.77	0.48
4:D:1101:ILE:HD12	4:D:1186:VAL:HG12	1.96	0.47
4:H:1172:THR:HG22	4:H:1174:HIS:CD2	2.50	0.47
1:A:143:LEU:HB2	1:A:216:VAL:HG11	1.96	0.47
2:B:7:SER:HB3	2:B:22:THR:OG1	2.15	0.47
3:C:15:LEU:HD23	3:C:24:GLN:HB3	1.96	0.47
1:E:40:GLN:HG3	1:E:46:LEU:HD23	1.97	0.47
2:B:89:HIS:CD2	2:B:95:VAL:HG13	2.49	0.47
3:C:145:HIS:CD2	4:D:1031:ILE:CD1	2.97	0.47
4:D:1119:VAL:HG21	4:D:1129:VAL:CG2	2.45	0.47
3:C:124:LEU:HB2	3:C:164:ASP:HB2	1.95	0.47
4:D:1117:CYS:HB2	4:D:1131:TRP:CZ2	2.50	0.46
1:A:152:PRO:HD2	1:A:207:PRO:CB	2.45	0.46
3:G:14:ASN:HB2	4:H:1011:PHE:HB3	1.97	0.46
1:E:48:TRP:HE1	1:E:51:CYS:HB2	1.80	0.46
1:E:101:ILE:HG22	2:F:89:HIS:NE2	2.29	0.46
3:C:164:ASP:OD1	3:C:179:HIS:HD2	1.99	0.46
4:H:1186:VAL:HG12	4:H:1187:GLU:H	1.81	0.46
4:D:1131:TRP:HE1	4:D:1159:VAL:HG12	1.82	0.45
4:D:1135:ASP:OD1	4:D:1135:ASP:O	2.34	0.45
2:B:53:THR:OG1	2:B:58:ILE:HD11	2.16	0.45
2:B:188:HIS:O	2:B:210:ARG:NH1	2.44	0.45
1:A:52:ILE:CG2	1:A:80:LEU:HD11	2.47	0.45
3:C:99:VAL:HG21	3:C:180:TRP:HZ2	1.81	0.45
4:H:1076:ASP:HA	4:H:1080:ARG:HB2	1.98	0.45
3:G:97:SER:HA	4:H:1120:THR:HG21	1.99	0.45
3:C:79:SER:O	3:C:82:THR:OG1	2.34	0.44
2:F:33:LEU:HD11	2:F:88:CYS:HB2	1.98	0.44
3:G:26:THR:HG22	3:G:36:TYR:HB3	1.99	0.44
3:C:124:LEU:HD23	3:C:129:SER:HA	1.99	0.44
4:D:1076:ASP:HA	4:D:1080:ARG:HB2	1.99	0.44
3:C:134:VAL:HA	3:C:152:TYR:O	2.18	0.44
3:C:145:HIS:NE2	4:D:1031:ILE:CD1	2.80	0.44



<u> </u>		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:37:TRP:CD1	1:E:82:LEU:HD13	2.52	0.44
1:A:73:ARG:HD3	1:A:75:ASN:OD1	2.18	0.43
3:C:50:VAL:HG22	4:D:1089:THR:HG22	2.00	0.43
3:G:42:LYS:O	3:G:58:PRO:HG2	2.17	0.43
1:A:99:ARG:NH1	1:A:106:ASN:OD1	2.52	0.43
1:E:12:VAL:HG12	1:E:116:VAL:HG22	2.00	0.43
3:G:145:HIS:CE1	4:H:1031:ILE:CD1	3.01	0.43
2:B:114:VAL:HG22	2:B:206:LYS:HG3	2.01	0.43
2:F:33:LEU:CD2	2:F:35:TRP:NE1	2.82	0.43
1:A:124:PRO:HA	1:A:150:TYR:HB3	2.00	0.42
1:A:22:CYS:HB3	1:A:80:LEU:HB3	2.01	0.42
1:A:52:ILE:HG21	1:A:80:LEU:HD11	2.00	0.42
1:E:104:ASP:OD2	2:F:55:ALA:HA	2.19	0.42
3:C:107:LEU:HD23	3:C:107:LEU:HA	1.91	0.42
2:B:119:PRO:HD3	2:B:131:VAL:HG22	2.01	0.42
3:G:130:VAL:HG11	3:G:153:LEU:HD11	2.01	0.42
4:H:1097:PRO:HG2	4:H:1184:ILE:HD12	2.02	0.42
1:A:186:VAL:HG21	2:B:134:LEU:HD13	2.01	0.42
3:C:155:LEU:HD13	3:C:157:PRO:HD3	2.00	0.42
3:G:75:LEU:HD21	4:H:1037:ILE:HD11	2.01	0.42
2:B:33:LEU:HD11	2:B:88:CYS:HB2	2.02	0.42
2:B:112:PRO:HB3	2:B:138:PHE:CD2	2.55	0.42
2:F:8:PRO:HG2	2:F:21:ILE:HG12	2.02	0.42
3:G:91:VAL:HG22	3:G:111:VAL:HG22	2.02	0.41
1:E:101:ILE:HG22	2:F:89:HIS:CD2	2.55	0.41
2:F:8:PRO:HD2	2:F:21:ILE:HG23	2.02	0.41
2:B:55:ALA:C	2:B:57:GLY:H	2.22	0.41
4:D:1084:GLN:HA	4:D:1087:LEU:HD12	2.02	0.41
1:E:101:ILE:HG22	2:F:89:HIS:CE1	2.55	0.41
3:G:96:LYS:HG3	3:G:108:ILE:HD11	2.01	0.41
1:A:101:ILE:HG22	2:B:89:HIS:NE2	2.36	0.41
2:B:89:HIS:CD2	2:B:95:VAL:CG1	3.03	0.41
4:D:9:LEU:HD21	4:D:1057:ALA:HB2	2.02	0.41
1:A:121:THR:HG22	1:A:208:SER:HB3	2.03	0.41
3:G:26:THR:HG22	3:G:36:TYR:CB	2.51	0.41
1:A:164:LEU:HD21	1:A:187:VAL:HG21	2.03	0.41
1:E:32:TRP:HZ3	3:G:65:ILE:HG21	1.86	0.41
4:H:1186:VAL:HG12	4:H:1187:GLU:N	2.36	0.41
1:E:53:ASP:HB3	1:E:58:SER:H	1.86	0.41
1:A:12:VAL:HG13	1:A:116:VAL:HG22	2.03	0.40
4:H:1172:THR:CG2	4:H:1174:HIS:CD2	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	Perce	entiles
1	А	207/223~(93%)	187 (90%)	17 (8%)	3~(1%)	11	19
1	Е	122/223~(55%)	106 (87%)	16 (13%)	0	100	100
2	В	209/213~(98%)	185 (88%)	20 (10%)	4 (2%)	8	14
2	F	103/213~(48%)	83 (81%)	17 (16%)	3(3%)	4	6
3	С	178/189~(94%)	166 (93%)	12 (7%)	0	100	100
3	G	177/189~(94%)	164 (93%)	9~(5%)	4 (2%)	6	10
4	D	178/222~(80%)	169~(95%)	9~(5%)	0	100	100
4	Н	168/222~(76%)	153 (91%)	14 (8%)	1 (1%)	25	42
All	All	1342/1694~(79%)	1213 (90%)	114 (8%)	15 (1%)	14	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	32	TRP
2	В	51	ALA
2	В	100	GLY
2	В	137	ASN
1	А	149	ASP
2	В	109	VAL
2	F	100	GLY
3	G	103	GLN
4	Н	1121	ASP
2	F	50	TYR
3	G	102	GLY
2	F	15	VAL
3	G	104	PRO
3	G	157	PRO



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Mol	Chain	Res	Type
1	А	154	PRO

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	168/188~(89%)	152 (90%)	16 (10%)	8 15
1	Ε	82/188~(44%)	75~(92%)	7 (8%)	10 19
2	В	168/187~(90%)	158 (94%)	10 (6%)	19 33
2	F	71/187~(38%)	64 (90%)	7 (10%)	8 13
3	С	151/173~(87%)	145 (96%)	6 (4%)	31 51
3	G	151/173~(87%)	140 (93%)	11 (7%)	14 25
4	D	150/196~(76%)	145 (97%)	5(3%)	38 58
4	Н	142/196~(72%)	130 (92%)	12 (8%)	10 19
All	All	1083/1488~(73%)	1009 (93%)	74 (7%)	16 28

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	GLN
1	А	7	SER
1	А	30	SER
1	А	31	SER
1	А	39	ARG
1	А	70	THR
1	А	73	ARG
1	А	84	MET
1	А	118	SER
1	А	120	SER
1	А	148	LYS
1	А	175	LEU
1	А	183	LEU
1	А	188	THR



Mol	Chain	Res	Type
1	A	196	THR
1	A	200	ILE
2	В	27	GLN
2	В	53	THR
2	В	65	SER
2	В	79	GLU
2	В	94	VAL
2	В	113	SER
2	В	114	VAL
2	В	153	LEU
2	В	165	GLN
2	В	180	LEU
3	С	28	GLU
3	С	151	SER
3	С	155	LEU
3	С	156	LEU
3	С	176	LEU
3	С	178	LYS
4	D	1021	THR
4	D	1066	ASP
4	D	1081	HIS
4	D	1098	THR
4	D	1163	MET
1	Е	2	VAL
1	Е	12	VAL
1	Е	32	TRP
1	Е	59	ILE
1	Е	86	SER
1	Е	99	ARG
1	Е	127	PHE
2	F	4	MET
2	F	12	SER
2	F	14	SER
2	F	31	SER
2	F	33	LEU
2	F	49	TYR
2	F	77	SER
3	G	15	LEU
3	G	24	GLN
3	G	48	LEU
3	G	92	THR
3	G	105	ASN

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Mol	Chain	Res	Type
3	G	122	THR
3	G	124	LEU
3	G	129	SER
3	G	155	LEU
3	G	176	LEU
3	G	177	LEU
4	Н	1018	THR
4	Н	1026	LEU
4	Н	1043	ASP
4	Н	1050	VAL
4	Н	1075	VAL
4	Н	1086	GLU
4	Н	1088	ARG
4	Н	1116	VAL
4	Н	1127	ILE
4	Н	1139	THR
4	Н	1160	MET
4	Н	1185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	24	GLN
3	С	120	ASN
3	С	179	HIS
4	D	1019	ASN
4	D	1174	HIS
3	G	7	HIS
3	G	145	HIS
3	G	179	HIS
4	Н	8	GLN

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).

Mal	Turne	Chain	Dec	Bog Link Bond lengths			B	ond ang	les	
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	С	1000	-	14,14,15	0.33	0	17,19,21	1.26	1 (5%)
5	NAG	G	1000	-	14,14,15	0.26	0	17,19,21	0.35	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
5	NAG	С	1000	-	-	2/6/23/26	0/1/1/1
5	NAG	G	1000	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	1000	NAG	O5-C1-C2	-4.80	103.70	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	С	1000	NAG	C4-C5-C6-O6
5	С	1000	NAG	O5-C5-C6-O6
5	G	1000	NAG	C4-C5-C6-O6



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, 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	А	211/223~(94%)	0.00	2 (0%) 84 89	44, 69, 91, 104	0
1	Е	126/223~(56%)	0.35	10 (7%) 12 15	94, 115, 133, 144	0
2	В	211/213~(99%)	0.11	4 (1%) 66 75	52, 79, 102, 107	0
2	F	105/213~(49%)	1.01	19 (18%) 1 1	100, 121, 137, 141	0
3	С	180/189~(95%)	0.02	1 (0%) 89 92	46, 66, 88, 99	0
3	G	179/189~(94%)	0.22	4 (2%) 62 70	72, 93, 122, 139	0
4	D	186/222~(83%)	0.03	5 (2%) 54 63	50, 71, 94, 111	0
4	Н	178/222~(80%)	0.55	15 (8%) 11 13	74, 95, 108, 116	0
All	All	1376/1694~(81%)	0.23	60 (4%) 34 41	44, 84, 124, 144	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	75	ILE	6.9
2	F	62	PHE	6.8
2	F	19	VAL	5.4
4	Н	1163	MET	5.3
2	F	82	ASP	5.0
2	F	20	THR	4.9
2	F	80	PRO	4.7
1	Е	17	SER	4.7
4	Н	1076	ASP	4.4
4	Н	1061	TRP	4.4
2	F	13	ALA	4.2
1	Е	127	PHE	4.2
2	F	21	ILE	4.1
4	D	1167	ARG	4.1
4	Н	9	LEU	4.1
2	F	83	PHE	4.1



8W8	35
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Mol	Chain	Res	Type	RSRZ
4	Н	1060	TYR	3.6
4	Н	1115	LEU	3.6
3	G	181	GLU	3.6
4	Н	8	GLN	3.6
1	Е	128	PRO	3.5
1	А	1	GLN	3.4
1	Е	126	VAL	3.4
2	F	81	GLU	3.4
1	Ε	125	SER	3.3
4	D	1168	GLY	3.3
2	F	53	THR	3.3
4	Н	1032	TYR	3.2
4	Н	1047	PHE	3.1
4	Н	1067	ILE	3.0
2	В	56	TYR	2.9
1	Ε	8	GLY	2.9
2	F	77	SER	2.8
4	Н	1188	TRP	2.7
4	Н	1038	VAL	2.6
3	G	182	PRO	2.6
4	Н	1003	SER	2.6
2	F	49	TYR	2.6
2	\mathbf{F}	85	VAL	2.6
2	В	180	LEU	2.6
2	F	54	LEU	2.4
1	Ε	85	ASN	2.4
3	G	180	TRP	2.3
1	Ε	120	SER	2.3
4	Н	1101	ILE	2.3
1	E	4	LEU	2.3
1	A	164	LEU	2.2
2	В	178	LEU	2.2
2	F	59	PRO	2.2
4	D	1174	HIS	2.2
4	D	0	ILE	2.1
1	Е	86	SER	2.1
2	В	53	THR	2.1
4	D	1171	TYR	2.1
3	С	173	ASP	2.1
4	Н	1007	PHE	2.1
2	F	12	SER	2.0
2	F	84	ALA	2.0



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Mol	Chain	Res	Type	RSRZ
3	G	163	TYR	2.0
2	F	74	THR	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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q < 0.9
5	NAG	G	1000	14/15	0.76	0.17	170,170,171,171	0
5	NAG	С	1000	14/15	0.81	0.23	108,109,109,110	0

6.5 Other polymers (i)

There are no such residues in this entry.

