

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 10:11 AM JST

PDB ID	:	8W83
Title	:	HLA-DQ2.5-alpha1 gliadin peptide in complex with DQN0344AE02
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Deposited on	:	2023-08-31
Resolution	:	2.82 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 2.82 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	3617 (2.84 - 2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	228	86%	10% •
1	Е	228	81%	14% • 5%
1	Ι	228	82%	12% • 5%
1	М	228	78%	12% 10%
2	В	215	87%	10% •
2	F	215	% 81%	14% ••



Mol	Chain	Length	Quality of chain						
2	J	215	89%	8% •					
2	Ν	215	% 	13% •					
3	С	189	81%	12% • 5%					
3	G	189	80%	14% • 5%					
3	K	189	83%	11% • 5%					
3	О	189	81%	12% • 6%					
4	D	226	66% 13%	• 20%					
4	Н	226	68% 11%	21%					
4	L	226	69% 10%	21%					
4	Р	226	68% 13%	• 18%					



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23643 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	Δ	210	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	219	1620	1025	269	317	9	0	0	0
1	F	217	Total	С	Ν	0	S	0	0	0
		217	1605	1017	262	317	9			
1	т	217	Total	С	Ν	0	S	0	0	0
	1	217	1589	1007	261	312	9		0	0
1	1 M	M 906	Total	С	Ν	0	S	0	0	0
1 1/1	200	1506	945	254	298	9	0	0	0	

• Molecule 1 is a protein called DQN0344AE02 Fab heavy chain.

• Molecule 2 is a protein called DQN0344AE02 Fab light chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	Р	914	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	214	1620	1016	266	333	5	0	0	0
0	Б	919	Total	С	Ν	0	S	0	0	0
	Г	212	1522	954	253	310	5	0		0
0	т	J 209	Total	С	Ν	0	S	0	0	0
	1		1548	971	252	321	4	0	0	U
0	2 N	N 212	Total	С	Ν	0	S	0	0	0
			1529	961	245	318	5			U

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	170	Total	С	Ν	0	S	0	0	0
<u></u> Э	U	179	1407	907	227	271	2	0	0	0
2	C	170	Total	С	Ν	0	S O O	0	0	
<u></u> Э	G	179	1357	871	215	269	2	0	0	0
2	K	K 179	Total	С	Ν	0	S	0	0	0
<u></u> Э	Λ		1354	874	219	259	2			0
2	2 0	170	Total	С	Ν	0	S	0	0	0
3 0	178	1370	881	227	260	2	0		0	



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
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
K	47	SER	CYS	engineered mutation	UNP P01909
K	184	LEU	-	expression tag	UNP P01909
K	185	GLU	-	expression tag	UNP P01909
K	186	VAL	-	expression tag	UNP P01909
K	187	LEU	-	expression tag	UNP P01909
K	188	PHE	-	expression tag	UNP P01909
K	189	GLN	-	expression tag	UNP P01909
0	47	SER	CYS	engineered mutation	UNP P01909
0	184	LEU	-	expression tag	UNP P01909
0	185	GLU	-	expression tag	UNP P01909
0	186	VAL	-	expression tag	UNP P01909
0	187	LEU	-	expression tag	UNP P01909
0	188	PHE	-	expression tag	UNP P01909
0	189	GLN	-	expression tag	UNP P01909

There are 28 discrepancies between the modelled and reference sequences:

• Molecule 4 is a protein called MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Л	181	Total	С	Ν	0	S	0	0	0
4	D	101	1428	917	239	266	6	0	0	0
4	Ц	178	Total	С	Ν	0	S	0	0	0
4	11	170	1347	861	228	252	6			
4	т	170	Total	С	Ν	0	S	0	0	0
4			1344	851	239	247	$\overline{7}$	0	0	0
4	4 P	P 186	Total	С	Ν	0	S	0	0	0
4			1441	916	252	266	7			U



Chain	Residue	Modelled	Actual	Comment	Reference
D	984	GLY	Ticuar	linker	PDR ?
D	985	SEB	_	linker	PDB ?
D	986	GLY		linker	PDB ?
D	987	GLY	_	linker	PDB ?
D	988	GLY	_	linker	PDB ?
D	989	GLY	_	linker	PDB ?
D	990	SEB	_	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	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

There are 92 discrepancies between the modelled and reference sequences:



Н

Comment

expression tag

Reference

UNP 019712

Actual

-

Continued from previous page... Chain Residue Modelled

VAL

1193

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



Chain	Residue	Modelled	Actual	Comment	Reference	
Р	999	GLY	-	linker	PDB ?	
Р	1000	SER	-	linker	PDB ?	
Р	1191	LEU	-	expression tag	UNP 019712	
Р	1192	GLU	-	expression tag	UNP 019712	
Р	1193	VAL	-	expression tag	UNP 019712	
Р	1194	LEU	-	expression tag	UNP 019712	
Р	1195	PHE	-	expression tag	UNP 019712	
Р	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 C N O 14 8 1 5	0	0
5	G	1	Total C N O 14 8 1 5	0	0
5	K	1	Total C N O 14 8 1 5	0	0
5	Ο	1	Total C N O 14 8 1 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.

- Chain A: 86% 10% • Molecule 1: DQN0344AE02 Fab heavy chain Chain E: 81% 14% • 5% LYS SER THR SER SER GLY GLY • Molecule 1: DQN0344AE02 Fab heavy chain Chain I: 82% 12% • 5% • Molecule 1: DQN0344AE02 Fab heavy chain Chain M: 78% 12% 10% SER SER SER SER SER LYS VAL GLU GLU PRO PRO PRO CYS SER CYS CYS
- Molecule 1: DQN0344AE02 Fab heavy chain



• Molecule 2: DQN0344AE02 Fab light chain





PHE

• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain



• Molecule 4: MHC class II HLA-DQ-beta-1 - alpha1 gliadin peptide chimeric protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	87.49Å 174.24Å 129.66Å	Depositor
a, b, c, α , β , γ	90.00° 93.17° 90.00°	Depositor
Bosolution(A)	54.86 - 2.82	Depositor
Resolution (A)	54.86 - 2.82	EDS
% Data completeness	47.7 (54.86-2.82)	Depositor
(in resolution range)	47.7(54.86-2.82)	EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.76 (at 2.81 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
P. P.	0.278 , 0.321	Depositor
n, n_{free}	0.271 , 0.315	DCC
R_{free} test set	2141 reflections $(4.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , -0.5	EDS
L-test for $twinning^2$	$ < L >=0.43, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	23643	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.15% 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	Bond lengths		angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.17	0/1664	0.35	0/2279
1	Е	0.18	0/1649	0.35	0/2260
1	Ι	0.19	0/1633	0.38	0/2239
1	М	0.18	0/1543	0.35	0/2110
2	В	0.18	0/1655	0.35	0/2253
2	F	0.21	0/1554	0.40	0/2127
2	J	0.17	0/1583	0.35	0/2163
2	N	0.17	0/1563	0.34	0/2139
3	С	0.19	0/1449	0.36	0/1985
3	G	0.19	0/1397	0.36	0/1924
3	Κ	0.18	0/1395	0.39	0/1920
3	0	0.19	0/1410	0.37	0/1933
4	D	0.19	0/1462	0.38	0/1998
4	Н	0.19	0/1381	0.38	0/1893
4	L	0.18	0/1374	0.35	0/1876
4	Р	0.18	0/1474	0.36	0/2010
All	All	0.18	0/24186	0.36	0/33109

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 (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.



8W83	,
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1620	0	1502	11	0
1	Е	1605	0	1477	24	0
1	Ι	1589	0	1446	14	0
1	М	1506	0	1387	14	0
2	В	1620	0	1539	15	0
2	F	1522	0	1392	22	0
2	J	1548	0	1425	7	0
2	Ν	1529	0	1376	10	0
3	С	1407	0	1330	9	0
3	G	1357	0	1221	16	0
3	Κ	1354	0	1242	8	0
3	0	1370	0	1278	10	0
4	D	1428	0	1361	15	0
4	Н	1347	0	1226	16	0
4	L	1344	0	1234	11	0
4	Р	1441	0	1364	17	0
5	С	14	0	13	0	0
5	G	14	0	13	0	0
5	Κ	14	0	13	0	0
5	0	14	0	13	0	0
All	All	23643	0	21852	197	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 (197) 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)
2:B:150:LYS:NZ	2:B:196:GLU:HB2	1.88	0.89
3:C:164:ASP:HB3	3:C:179:HIS:HA	1.56	0.87
1:M:160:VAL:HG22	1:M:210:HIS:CD2	2.11	0.84
1:M:40:GLN:HE22	2:N:38:GLN:HE22	1.22	0.83
3:G:14:ASN:HB3	3:G:68:LEU:HD11	1.66	0.75
4:P:1064:GLN:HB2	4:P:1067:ILE:HB	1.69	0.74
2:B:29:ILE:HB	2:B:92:HIS:HB2	1.69	0.74
1:E:37:TRP:HD1	1:E:71:ILE:HD13	1.51	0.74
2:F:151:VAL:HG12	2:F:190:HIS:HD2	1.52	0.72
4:L:2:PHE:H	4:L:1082:ASN:HD21	1.38	0.71
4:P:2:PHE:H	4:P:1082:ASN:HD21	1.40	0.68
4:H:1131:TRP:HE1	4:H:1159:VAL:HG12	1.59	0.68
2:F:114:PRO:HD2	2:F:202:LEU:HG	1.76	0.67
3:K:33:GLU:HB2	3:K:140:LEU:HD11	1.77	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:160:VAL:HG22	1:M:210:HIS:HD2	1.60	0.65
2:J:149:TRP:CG	2:J:180:LEU:HD13	2.31	0.65
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.79	0.65
4:P:1101:ILE:HD11	4:P:1173:CYS:HB2	1.80	0.63
2:B:186:ASP:HA	2:B:189:LYS:HD3	1.80	0.62
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.81	0.62
3:K:48:LEU:HD11	4:L:1153:TRP:CD2	2.35	0.61
1:E:160:VAL:HG12	1:E:210:HIS:ND1	2.16	0.61
3:0:49:PRO:HA	3:O:52:ARG:HE	1.66	0.60
1:E:173:VAL:HG12	1:E:192:VAL:HG22	1.83	0.60
2:F:37:GLN:HB2	2:F:47:LEU:HD21	1.83	0.60
4:D:1097:PRO:HB3	4:D:1122:PHE:HB3	1.82	0.60
1:E:178:ALA:HA	1:E:188:LEU:HB3	1.83	0.60
2:F:65:SER:HB2	2:F:72:THR:HB	1.83	0.59
3:O:49:PRO:HA	3:O:52:ARG:NE	2.17	0.59
4:H:1131:TRP:NE1	4:H:1159:VAL:HG12	2.17	0.59
1:A:20:LEU:HD12	1:A:82:LEU:HD23	1.83	0.59
4:L:1094:ARG:HD3	4:L:1179:SER:HA	1.85	0.59
3:C:145:HIS:CE1	4:D:1031:ILE:HD12	2.38	0.59
2:J:149:TRP:CD1	2:J:180:LEU:HD13	2.38	0.59
4:P:1064:GLN:CB	4:P:1067:ILE:HB	2.33	0.58
3:K:91:VAL:HG22	3:K:111:VAL:HG13	1.85	0.58
4:P:1037:ILE:HG12	4:P:1038:VAL:HG23	1.86	0.57
3:O:124:LEU:HD11	3:O:166:LYS:HD2	1.87	0.57
4:P:1116:VAL:HG22	4:P:1160:MET:HG2	1.87	0.57
2:F:151:VAL:HG12	2:F:190:HIS:CD2	2.36	0.57
2:F:119:PHE:CB	2:F:134:VAL:HB	2.35	0.56
2:B:29:ILE:HB	2:B:92:HIS:CB	2.35	0.56
2:J:121:PRO:HD3	2:J:133:VAL:HG22	1.87	0.56
1:I:131:VAL:HG22	1:I:152:VAL:HG22	1.88	0.56
1:E:22:CYS:HB3	1:E:80:LEU:HB3	1.88	0.55
3:G:107:LEU:HD12	3:G:153:LEU:HD23	1.89	0.55
1:I:84:MET:HB3	1:I:87:LEU:HD21	1.88	0.55
3:G:60:PHE:HB3	4:H:3:PRO:HG3	1.89	0.55
4:P:1010:GLN:HB2	4:P:1031:ILE:HB	1.89	0.55
1:I:22:CYS:HB3	1:I:80:LEU:HB3	1.89	0.55
2:B:150:LYS:HZ2	2:B:196:GLU:HB2	1.65	0.55
2:N:48:ILE:HG13	2:N:54:LEU:HA	1.89	0.54
1:E:37:TRP:CD1	1:E:71:ILE:HD13	2.37	0.53
3:G:123:TRP:CD1	3:G:134:VAL:HG23	2.43	0.53
2:N:137:LEU:HD21	2:N:197:VAL:HG21	1.90	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:158:GLU:HG2	1:E:159:PRO:HA	1.90	0.53
2:N:191:LYS:HA	2:N:212:ARG:HE	1.73	0.53
4:P:1131:TRP:CD1	4:P:1159:VAL:HG12	2.44	0.53
2:B:146:LYS:HB3	2:B:198:THR:HB	1.89	0.53
4:P:1130:ARG:HB2	4:P:1174:HIS:HB3	1.91	0.53
4:L:1131:TRP:CD1	4:L:1159:VAL:HG12	2.44	0.53
2:F:133:VAL:HB	2:F:180:LEU:HB3	1.90	0.53
3:G:48:LEU:HD12	4:H:1153:TRP:CG	2.44	0.53
4:L:1016:TYR:HB2	4:L:1025:ARG:HB3	1.91	0.52
1:M:162:VAL:HG22	1:M:208:VAL:HG12	1.91	0.52
2:F:11:LEU:HD11	2:F:19:VAL:HG13	1.92	0.52
1:A:169:LEU:HD23	1:A:192:VAL:HG21	1.91	0.52
3:O:107:LEU:HD21	3:O:180:TRP:CD2	2.44	0.52
1:M:84:MET:HB2	1:M:87:LEU:HD21	1.91	0.52
4:P:1076:ASP:HA	4:P:1080:ARG:HB2	1.92	0.52
1:A:33:TYR:HE2	4:D:1067:ILE:HD11	1.75	0.51
1:A:136:PRO:HG3	1:A:148:LEU:HB3	1.92	0.51
3:O:14:ASN:HB2	4:P:1011:PHE:HB3	1.91	0.51
2:B:150:LYS:HZ1	2:B:196:GLU:HB2	1.74	0.51
1:M:33:TYR:CD2	1:M:99:ARG:NH2	2.79	0.51
4:L:1010:GLN:HG3	4:L:1031:ILE:HB	1.93	0.51
3:K:99:VAL:HG11	3:K:182:PRO:HB3	1.92	0.51
1:E:178:ALA:HB2	1:E:188:LEU:HD23	1.91	0.51
2:B:147:VAL:HG21	2:B:176:LEU:HD22	1.93	0.51
4:D:1129:VAL:HG22	4:D:1175:VAL:HG22	1.91	0.51
3:O:48:LEU:HD12	4:P:1153:TRP:CE2	2.46	0.51
1:A:178:ALA:HB2	1:A:188:LEU:HD23	1.92	0.51
3:G:48:LEU:HD12	4:H:1153:TRP:CD2	2.46	0.51
3:C:33:GLU:HB2	3:C:140:LEU:HD11	1.92	0.50
2:J:21:ILE:HD12	2:J:73:LEU:HD23	1.92	0.50
4:P:1018:THR:HB	4:P:1023:ARG:HB2	1.92	0.50
2:J:163:SER:OG	2:J:177:SER:OG	2.30	0.50
1:M:49:MET:SD	1:M:95:TYR:HE2	2.35	0.50
3:C:14:ASN:HB2	4:D:1011:PHE:HB3	1.93	0.50
4:D:1131:TRP:CD1	4:D:1159:VAL:HG12	2.46	0.50
1:A:12:VAL:HG11	1:A:87:LEU:HD12	1.94	0.50
2:N:126:LEU:HD13	2:N:131:ALA:HB2	1.94	0.49
1:I:92:THR:HG23	1:I:120:THR:HA	1.95	0.49
2:B:48:ILE:HA	2:B:54:LEU:HA	1.94	0.49
2:F:121:PRO:HG3	2:F:133:VAL:HG22	1.94	0.49
1:I:28:THR:O	1:I:33:TYR:OH	2.29	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:G:48:LEU:HD12	4:H:1153:TRP:CD1	2.48	0.49
2:J:161:GLN:HB2	2:J:179:THR:HB	1.94	0.48
4:D:1101:ILE:HD11	4:D:1173:CYS:HB2	1.95	0.48
2:N:21:ILE:HD12	2:N:73:LEU:HD23	1.94	0.48
4:D:1076:ASP:HA	4:D:1080:ARG:HB2	1.96	0.48
1:E:174:HIS:CD2	2:F:138:ASN:HD21	2.32	0.48
1:A:41:ALA:HB3	1:A:44:GLN:HB2	1.94	0.47
3:G:72:LEU:HD13	4:H:1009:TYR:HB2	1.95	0.47
4:H:4:GLN:OE1	4:H:1028:SER:OG	2.31	0.47
1:A:178:ALA:HA	1:A:188:LEU:HB3	1.97	0.47
4:H:4:GLN:HG2	4:H:1078:VAL:HG11	1.95	0.47
1:E:34:TRP:HB3	1:E:51:CYS:SG	2.54	0.47
1:E:158:GLU:HG2	1:E:159:PRO:CA	2.45	0.47
1:I:34:TRP:HB3	1:I:51:CYS:SG	2.55	0.47
4:L:1116:VAL:HG12	4:L:1160:MET:HG3	1.97	0.47
2:B:21:ILE:HD12	2:B:73:LEU:HD23	1.97	0.47
3:K:68:LEU:HD13	4:L:1009:TYR:HD2	1.80	0.47
2:B:48:ILE:HG12	2:B:54:LEU:HB3	1.96	0.46
1:E:178:ALA:HB1	1:E:186:TYR:HB3	1.96	0.46
3:O:120:ASN:HB2	3:O:168:GLU:HB2	1.96	0.46
3:G:114:ILE:HD13	3:G:119:VAL:HG11	1.97	0.46
2:F:55:ALA:HB3	2:F:58:ILE:HD13	1.97	0.46
3:G:48:LEU:HD12	4:H:1153:TRP:CE2	2.50	0.46
4:H:1116:VAL:HG12	4:H:1160:MET:HB3	1.96	0.46
3:O:48:LEU:HD13	3:O:51:LEU:HD13	1.97	0.46
4:P:1129:VAL:HG22	4:P:1175:VAL:HG22	1.98	0.46
4:L:1114:LEU:HD11	4:L:1160:MET:HB3	1.97	0.46
3:C:145:HIS:CE1	4:D:1031:ILE:CD1	2.99	0.46
1:I:160:VAL:CG1	1:I:210:HIS:ND1	2.79	0.46
1:M:49:MET:SD	1:M:95:TYR:CE2	3.09	0.46
4:H:1117:CYS:SG	4:H:1131:TRP:CZ2	3.08	0.45
1:A:150:CYS:SG	1:A:164:TRP:CH2	3.09	0.45
1:E:160:VAL:CG1	1:E:210:HIS:ND1	2.80	0.45
4:H:1103:PRO:HA	4:H:1115:LEU:HA	1.98	0.45
2:B:145:ALA:HB2	2:B:199:HIS:HD2	1.81	0.45
3:G:123:TRP:CD1	3:G:134:VAL:CG2	2.99	0.45
1:E:37:TRP:CD2	1:E:82:LEU:HD12	2.52	0.45
3:O:44:THR:HG21	3:O:56:PHE:HB3	1.99	0.45
1:I:154:ASP:HA	1:I:185:LEU:CB	2.47	0.45
1:I:20:LEU:HB2	1:I:82:LEU:HB3	1.99	0.45
1:E:12:VAL:HG11	1:E:87:LEU:HD12	2.00	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:94:ILE:HD13	2:F:94:ILE:H	1.80	0.44
1:A:92:THR:HG23	1:A:120:THR:HA	1.98	0.44
4:D:7:LEU:HD21	4:D:1067:ILE:HG21	2.00	0.44
2:N:35:TRP:HB2	2:N:48:ILE:HG22	1.99	0.44
1:A:84:MET:HB3	1:A:87:LEU:HD21	1.99	0.44
4:D:1132:PHE:HB2	4:D:1172:THR:HG23	1.98	0.44
1:E:179:VAL:HG11	2:F:161:GLN:HB3	1.98	0.44
3:O:114:ILE:HD13	3:O:119:VAL:HG11	2.00	0.44
3:C:136:GLU:HA	3:C:151:SER:HA	1.99	0.44
1:I:35:MET:HB3	1:I:80:LEU:HD22	1.98	0.44
2:F:151:VAL:CG1	2:F:190:HIS:CD2	3.00	0.44
3:G:124:LEU:HB2	3:G:164:ASP:HB2	1.99	0.44
1:I:37:TRP:HE1	1:I:80:LEU:HG	1.82	0.44
2:F:7:SER:HG	2:F:22:THR:HG1	1.61	0.43
2:F:151:VAL:O	2:F:152:ASP:OD1	2.36	0.43
4:P:1149:ARG:NH2	4:P:1155:PHE:HZ	2.15	0.43
4:P:2:PHE:N	4:P:1082:ASN:HD21	2.12	0.43
1:E:177:PRO:HG2	2:F:163:SER:HB2	2.00	0.43
2:F:33:LEU:HB3	2:F:51:VAL:HG22	2.00	0.43
3:K:72:LEU:HD13	4:L:1009:TYR:HB2	1.98	0.43
3:G:110:LEU:HG	3:G:150:ILE:HG12	2.00	0.43
1:M:3:GLN:HG3	1:M:25:SER:HB3	2.00	0.43
1:M:149:GLY:HA3	1:M:191:VAL:HA	2.00	0.43
2:B:94:ILE:HD13	2:B:94:ILE:H	1.83	0.43
3:C:124:LEU:HD11	3:C:166:LYS:HD2	2.01	0.43
4:D:1037:ILE:HD12	4:D:1038:VAL:HG23	1.99	0.43
2:F:137:LEU:HD13	2:F:176:LEU:HB3	2.01	0.43
1:I:178:ALA:HB1	1:I:186:TYR:HB3	1.99	0.43
1:E:34:TRP:HB2	1:E:100:ASP:O	2.19	0.42
4:D:7:LEU:HD23	4:D:1061:TRP:CD1	2.54	0.42
3:G:48:LEU:HD23	3:G:49:PRO:HD2	2.01	0.42
4:H:1131:TRP:HE1	4:H:1159:VAL:CG1	2.30	0.42
4:H:1084:GLN:HA	4:H:1087:LEU:HD12	2.00	0.42
1:I:154:ASP:HA	1:I:185:LEU:HB3	2.01	0.42
4:D:1120:THR:HG22	4:D:1156:GLN:HG3	2.02	0.42
1:E:92:THR:HG23	1:E:120:THR:HA	2.00	0.42
1:M:12:VAL:HG23	1:M:121:VAL:HG22	2.01	0.42
4:P:1148:ILE:HB	4:P:1156:GLN:HG3	2.00	0.42
1:E:158:GLU:CG	1:E:159:PRO:HA	2.49	0.42
4:H:1098:THR:OG1	4:H:1120:THR:OG1	2.33	0.42
1:I:151:LEU:O	1:I:188:LEU:O	2.37	0.42



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:134:VAL:HG12	2:J:179:THR:HA	2.01	0.42
2:N:65:SER:HG	2:N:72:THR:HG1	1.68	0.41
1:E:84:MET:HB3	1:E:87:LEU:HD21	2.02	0.41
3:G:124:LEU:HD12	3:G:177:LEU:HD11	2.02	0.41
1:M:6:GLU:OE2	1:M:97:CYS:SG	2.78	0.41
1:E:6:GLU:OE2	1:E:97:CYS:SG	2.78	0.41
2:F:30:TYR:HD2	2:F:92:HIS:NE2	2.18	0.41
2:N:118:ILE:HB	2:N:208:LYS:HB3	2.01	0.41
2:B:129:GLY:HA2	2:B:184:LYS:HB2	2.01	0.41
3:G:104:PRO:HB3	3:G:156:LEU:HG	2.01	0.41
3:C:91:VAL:HB	3:C:178:LYS:HD3	2.02	0.41
1:E:174:HIS:CD2	2:F:138:ASN:ND2	2.89	0.41
3:K:24:GLN:HE21	3:K:24:GLN:HB3	1.71	0.41
1:E:191:VAL:HG21	2:F:136:LEU:HD11	2.03	0.41
3:K:88:VAL:HA	3:K:89:PRO:HD3	1.97	0.41
1:M:34:TRP:HB2	1:M:100:ASP:O	2.21	0.41
4:L:1050:VAL:HG22	4:L:1051:THR:HG23	2.03	0.40
1:M:92:THR:HG23	1:M:120:THR:HA	2.03	0.40
3:C:72:LEU:HD13	4:D:1009:TYR:HB2	2.03	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	215/228~(94%)	204 (95%)	11 (5%)	0	100	100
1	E	213/228~(93%)	193 (91%)	19 (9%)	1 (0%)	29	59
1	Ι	213/228~(93%)	192 (90%)	18 (8%)	3(1%)	11	32
1	М	200/228~(88%)	190 (95%)	10 (5%)	0	100	100
2	В	212/215~(99%)	200 (94%)	9 (4%)	3 (1%)	11	32



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	F	210/215~(98%)	186 (89%)	19 (9%)	5(2%)	6	19
2	J	207/215~(96%)	188 (91%)	16 (8%)	3~(1%)	11	32
2	Ν	210/215~(98%)	191 (91%)	18 (9%)	1 (0%)	29	59
3	С	177/189~(94%)	170 (96%)	7 (4%)	0	100	100
3	G	177/189~(94%)	166 (94%)	10 (6%)	1 (1%)	25	54
3	Κ	177/189~(94%)	171 (97%)	4 (2%)	2(1%)	14	39
3	Ο	176/189~(93%)	168 (96%)	8 (4%)	0	100	100
4	D	173/226~(76%)	163 (94%)	9(5%)	1 (1%)	25	54
4	Н	170/226~(75%)	156 (92%)	12 (7%)	2(1%)	13	37
4	L	171/226~(76%)	157 (92%)	11 (6%)	3~(2%)	8	26
4	Р	178/226~(79%)	169 (95%)	9 (5%)	0	100	100
All	All	3079/3432~(90%)	2864 (93%)	190 (6%)	25 (1%)	19	47

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All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	141	TYR
2	В	139	ASN
2	F	158	GLY
4	Н	1121	ASP
2	J	139	ASN
4	L	1121	ASP
4	D	1121	ASP
2	F	30	TYR
4	Н	1133	ARG
1	Ι	86	SER
1	Ι	152	VAL
3	K	12	GLY
3	Κ	139	PHE
2	В	30	TYR
2	В	144	GLU
1	Ι	221	VAL
2	J	144	GLU
2	Ν	139	ASN
2	F	183	SER
2	J	30	TYR
4	L	1033	ASN
2	F	152	ASP



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Mol	Chain	Res	Type
3	G	12	GLY
1	Е	136	PRO
4	L	1124	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	173/193~(90%)	167~(96%)	6 (4%)	36	68
1	Е	172/193~(89%)	166 (96%)	6 (4%)	36	68
1	Ι	166/193~(86%)	161 (97%)	5(3%)	41	73
1	М	160/193~(83%)	154 (96%)	6 (4%)	33	65
2	В	181/188~(96%)	172~(95%)	9~(5%)	24	55
2	F	159/188~(85%)	149 (94%)	10 (6%)	18	44
2	J	168/188~(89%)	164 (98%)	4 (2%)	49	80
2	Ν	159/188~(85%)	149 (94%)	10 (6%)	18	44
3	С	158/173~(91%)	144 (91%)	14 (9%)	9	27
3	G	146/173~(84%)	138~(94%)	8 (6%)	21	50
3	Κ	145/173~(84%)	135~(93%)	10 (7%)	15	40
3	Ο	149/173~(86%)	139~(93%)	10 (7%)	16	41
4	D	155/200~(78%)	144 (93%)	11 (7%)	14	38
4	Н	139/200~(70%)	133~(96%)	6 (4%)	29	60
4	L	$13\overline{6/200}~(68\%)$	$1\overline{32}\ (97\%)$	4 (3%)	42	74
4	Р	153/200~(76%)	145 (95%)	8 (5%)	23	53
All	All	2519/3016 (84%)	2392 (95%)	127 (5%)	24	55

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	16	ARG



Mol	Chain	Res	Type
1	А	65	THR
1	А	75	ASN
1	А	148	LEU
1	А	174	HIS
1	А	206	CYS
2	В	11	LEU
2	В	29	ILE
2	В	54	LEU
2	В	94	ILE
2	В	96	GLU
2	В	106	GLU
2	В	176	LEU
2	В	184	LYS
2	В	186	ASP
3	С	59	GLN
3	С	64	ASN
3	С	68	LEU
3	С	78	ARG
3	С	86	ASN
3	С	101	LEU
3	С	110	LEU
3	С	120	ASN
3	С	136	GLU
3	С	150	ILE
3	С	155	LEU
3	С	164	ASP
3	С	176	LEU
3	С	177	LEU
4	D	1005	GLU
4	D	1014	MET
4	D	1034	ARG
4	D	1037	ILE
4	D	1038	VAL
4	D	1050	VAL
4	D	1055	LEU
4	D	1059	GLU
4	D	1069	GLU
4	D	1114	LEU
4	D	1128	LYS
1	Е	2	VAL
1	Е	6	GLU
1	Е	44	GLN



Mol	Chain	Res	Type
1	Е	82	LEU
1	Е	151	LEU
1	Е	217	VAL
2	F	11	LEU
2	F	33	LEU
2	F	47	LEU
2	F	94	ILE
2	F	109	ARG
2	F	127	LYS
2	F	140	PHE
2	F	152	ASP
2	F	176	LEU
2	F	212	ARG
3	G	21	PRO
3	G	27	HIS
3	G	48	LEU
3	G	59	GLN
3	G	64	ASN
3	G	118	VAL
3	G	138	SER
3	G	155	LEU
4	Н	1005	GLU
4	Н	1010	GLN
4	Н	1048	ARG
4	Н	1050	VAL
4	Н	1161	LEU
4	Н	1171	TYR
1	I	105	TYR
1	I	117	THR
1	Ι	151	LEU
1	Ι	180	LEU
1	Ι	202	GLN
2	J	11	LEU
2	J	99	PHE
2	J	176	LEU
2	J	196	GLU
3	K	24	GLN
3	K	26	THR
3	K	68	LEU
3	K	75	LEU
3	K	86	ASN
3	K	97	SER



Mol	Chain	R os	Typo
2		102	стм
3 	K V	103	GLN
<u>う</u>	Λ V	120	ASN
<u>3</u>	K	155	LEU
3	K	177	LEU
4	L	1026	LEU
4	L	1050	VAL
4	L	1093	ARG
4	L	1115	LEU
1	M	13	GLN
1	M	99	ARG
1	М	105	TYR
1	М	131	VAL
1	М	188	LEU
1	М	199	LEU
2	N	11	LEU
2	N	28	ASN
2	N	78	LEU
2	N	96	GLU
2	Ν	118	ILE
2	Ν	135	CYS
2	N	163	SER
2	N	167	GLN
2	N	176	LEU
2	N	196	GLU
3	0	33	GLU
3	0	48	LEU
3	0	63	THR
3	0	64	ASN
3	0	68	LEU
3	0	69	LYS
3	0	132	GLU
3	0	142	LYS
3	0	155	LEU
3	0	176	LEU
4	Р	4	GLN
4	Р	1037	ILE
4	Р	1064	GLN
4	Р	1082	ASN
4	P	1086	GLU
4	Р	1094	ARG
4	P	1161	LEU
4	P	1163	MET
I	1	1100	

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	89	GLN
2	В	138	ASN
2	В	139	ASN
3	С	145	HIS
4	D	1019	ASN
1	Е	83	GLN
1	Е	174	HIS
2	F	6	GLN
2	F	138	ASN
2	F	190	HIS
3	G	17	GLN
2	J	138	ASN
4	L	1082	ASN
4	L	1174	HIS
1	М	40	GLN
1	М	83	GLN
1	М	210	HIS
3	0	17	GLN
3	0	71	ASN
3	0	179	HIS
4	Р	1082	ASN

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)

4 ligands are modelled in this entry.



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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	Tink	Bo	ond leng	ths	B	ond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	С	1000	-	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	G	1000	-	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	0	1000	-	14,14,15	0.38	0	17,19,21	0.30	0
5	NAG	K	1000	-	14,14,15	0.24	0	17,19,21	0.38	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	-	-	0/6/23/26	0/1/1/1
5	NAG	G	1000	-	-	1/6/23/26	0/1/1/1
5	NAG	0	1000	-	-	0/6/23/26	0/1/1/1
5	NAG	Κ	1000	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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 (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	<RSRZ $>$	#	#RSR	Z>2	$OWAB(Å^2)$	Q<0.9
1	А	219/228~(96%)	-0.57	0	100	100	24, 30, 41, 50	0
1	Е	217/228~(95%)	-0.46	1 (0	9%) 9	1 88	20, 34, 56, 66	0
1	Ι	217/228~(95%)	-0.42	0	100	100	31, 38, 50, 56	0
1	М	206/228~(90%)	-0.04	7 (3	8%) 4	5 35	26, 37, 86, 93	0
2	В	214/215~(99%)	-0.50	0	100	100	23, 36, 48, 55	0
2	F	212/215~(98%)	-0.35	2 (0	0%) 8	4 80	26, 42, 60, 69	0
2	J	209/215~(97%)	-0.48	0	100	100	30, 39, 47, 51	0
2	Ν	212/215~(98%)	-0.16	3 (1	.%) 7	5 69	34, 51, 73, 82	0
3	С	179/189~(94%)	-0.59	0	100	100	15, 31, 40, 45	0
3	G	179/189~(94%)	-0.45	0	100	100	23, 36, 50, 52	0
3	Κ	179/189~(94%)	-0.51	0	100	100	26, 40, 53, 58	0
3	Ο	178/189~(94%)	-0.43	0	100	100	28, 39, 54, 64	0
4	D	181/226~(80%)	-0.45	0	100	100	27, 32, 43, 50	0
4	Н	178/226~(78%)	-0.51	0	100	100	26, 35, 46, 53	0
4	L	179/226~(79%)	-0.46	0	100	100	29, 41, 55, 58	0
4	Р	186/226~(82%)	-0.46	0	100	100	28, 38, 50, 56	0
All	All	3145/3432 (91%)	-0.42	13 (0%) 9	92 91	15, 37, 67, 93	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	М	151	LEU	4.4
1	М	133	PRO	3.2
1	М	203	THR	2.6
1	М	131	VAL	2.5
1	Е	201	THR	2.4



Mol	Chain	Res	Type	RSRZ
1	М	130	SER	2.3
2	F	207	THR	2.3
2	Ν	128	SER	2.3
2	Ν	207	THR	2.1
1	М	154	ASP	2.1
1	М	173	VAL	2.1
2	F	129	GLY	2.0
2	Ν	193	TYR	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	0	1000	14/15	0.87	0.25	64,64,64,64	0
5	NAG	G	1000	14/15	0.88	0.22	62,62,62,62	0
5	NAG	С	1000	14/15	0.89	0.20	52,52,52,52	0
5	NAG	K	1000	14/15	0.91	0.17	57,57,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.

