

Full wwPDB X-ray Structure Validation Report (i)

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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	:	2.35
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)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain				
1	А	217		68%		28%	
1	С	217	62%			33%	5%
2	В	218			23%	7% • •	
2	D	218		61%		30%	6% •
3	Q	9	22% 33% 11%			33%	
3	Х	9	44%	6	44%		11%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7204 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.

• Molecule 1 is a protein called Immunoglobulin light chain (IgG2a).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	215	Total	С	Ν	0	S	0	0	0
	A	210	1660	1037	282	336	5	0	0	0
1	C	217	Total	С	Ν	0	S	0	0	0
		217	1674	1044	284	340	6	0		0

• Molecule 2 is a protein called Immunoglobulin heavy chain (IgG2a).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
9	В	210	Total	С	Ν	0	S	0	0	0
	D	210	1598	1004	271	315	8	0	0	0
0	П	911	Total	С	Ν	0	S	0	0	0
	D	211	1609	1010	275	316	8		0	0

• Molecule 3 is a protein called Podoplanin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	Х	9	Total C N O 68 44 10 14	0	0	0
3	Q	6	Total C N O 42 28 7 7	0	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Zn 1 1	0	0
4	В	1	Total Zn 1 1	0	0
4	С	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0





• Molecule 5 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	Х	1	Total 14	C 8	N 1	O 5	0	0
5	Q	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	160	Total O 160 160	0	0
6	В	116	Total O 116 116	0	0
6	С	111	Total O 111 111	0	0
6	D	120	Total O 120 120	0	0
6	Х	7	Total O 7 7	0	0
6	Q	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. 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. 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: Immunoglobulin light chain (IgG2a)

A100 Y102 D31 <mark>A32</mark> W33 M34 E42 K43 G94 C95 <u>К96</u> V97 Ξ T108 V109 T110 Y145 F146 P147 E148 E148 P149 D173 L174 <mark>Y175</mark> T176 L177 Q105 G106 T116 V169 L170 P189 N196

• Molecule 3: Podoplanin

Chain X:	44	%	44%	11%
G1 72 74 75 16 16 19 19				
• Molecule 3:	Podoplani	n		
Chain Q:	22%	33%	11%	33%
2212 1213 1213 1214 1215 1217 1217 1217 1217 1217 1217 1217				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	277.91Å 38.24Å 95.91Å	Deneiten
a, b, c, α , β , γ	90.00° 108.99° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\mathbf{\hat{A}})$	19.86 - 2.20	Depositor
Resolution (A)	19.86 - 2.38	EDS
% Data completeness	98.0 (19.86-2.20)	Depositor
(in resolution range)	98.5(19.86-2.38)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.48 (at 2.38 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.4_4	Depositor
D D	0.227 , 0.271	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.287 , 0.293	DCC
R_{free} test set	1938 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	33.2	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 54.8	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.004 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.59% 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: A2G, ZN $\,$

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	
WIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.34	0/1698	0.55	0/2305
1	С	0.38	0/1712	0.56	0/2324
2	В	0.36	0/1636	0.65	3/2227~(0.1%)
2	D	0.35	0/1647	0.61	1/2241~(0.0%)
3	Q	0.52	0/43	0.78	0/58
3	Х	0.41	0/69	0.71	0/93
All	All	0.36	0/6805	0.60	4/9248~(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	В	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	112	SER	N-CA-C	7.08	130.12	111.00
2	D	177	LEU	CA-CB-CG	7.05	131.50	115.30
2	В	177	LEU	CA-CB-CG	5.92	128.91	115.30
2	В	77	ARG	NE-CZ-NH1	-5.61	117.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	В	111	VAL	Peptide
2	В	112	SER	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	А	1660	0	1603	51	0
1	С	1674	0	1615	69	0
2	В	1598	0	1557	76	0
2	D	1609	0	1570	59	0
3	Q	42	0	46	5	0
3	Х	68	0	72	3	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
5	Q	14	0	12	0	0
5	Х	14	0	12	0	0
6	А	160	0	0	12	0
6	В	116	0	0	11	2
6	С	111	0	0	17	3
6	D	120	0	0	12	1
6	Q	7	0	0	2	0
6	Х	7	0	0	0	0
All	All	7204	0	6487	257	3

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 20.

All (257) 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:D:200:PRO:HD2	6:D:517:HOH:O	1.52	1.09
2:B:12:VAL:O	2:B:112:SER:HB2	1.56	1.03
2:D:6:GLN:HE21	2:D:92:CYS:H	0.98	0.92
1:A:2:ILE:HD11	1:A:25:SER:HB2	1.51	0.92



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:X:6:LEU:HA	3:X:9:LEU:HD22	1.51	0.92
2:B:6:GLN:HE21	2:B:92:CYS:H	1.10	0.91
1:C:2:ILE:HD11	1:C:93:HIS:CD2	2.07	0.89
2:D:75:LYS:HB2	2:D:75:LYS:NZ	1.88	0.87
1:A:106:ILE:H	1:A:166:GLN:HE22	1.21	0.87
2:B:83:ARG:NH2	2:B:85:GLU:HG3	1.90	0.86
1:A:109:ALA:O	1:A:110:ASP:HB2	1.74	0.86
1:C:7:THR:HG22	1:C:22:SER:HB2	1.57	0.86
2:B:194:THR:HB	2:B:209:LYS:HA	1.59	0.85
1:C:83:LEU:HB3	1:C:106:ILE:CD1	2.07	0.83
2:D:149:PRO:O	6:D:517:HOH:O	1.94	0.83
2:B:18:MET:HE1	2:B:109:VAL:HG13	1.62	0.82
1:C:195:GLU:O	1:C:205:ILE:O	2.00	0.80
1:C:54:ARG:NH2	6:C:501:HOH:O	2.16	0.79
1:C:2:ILE:HD11	1:C:93:HIS:CG	2.20	0.77
1:C:138:ASN:ND2	6:D:306:HOH:O	2.14	0.77
2:D:6:GLN:NE2	2:D:92:CYS:H	1.79	0.77
2:B:153:THR:HG23	2:B:196:ASN:OD1	1.85	0.77
2:B:138:LEU:HG	2:B:210:ILE:HG21	1.67	0.76
2:B:14:PRO:HD3	2:B:112:SER:HB3	1.69	0.74
2:B:123:PRO:HG3	2:B:208:LYS:HG3	1.71	0.73
1:C:160:LEU:HD11	2:D:169:VAL:HB	1.70	0.73
1:C:213:CYS:SG	6:C:466:HOH:O	2.46	0.73
1:A:7:THR:HG23	2:D:21:PHE:CZ	2.24	0.72
2:B:147:PRO:O	2:B:199:HIS:HE1	1.73	0.72
2:B:83:ARG:HH21	2:B:85:GLU:HG3	1.55	0.70
2:B:18:MET:CE	2:B:109:VAL:HG13	2.22	0.70
1:C:4:LEU:HD23	1:C:23:CYS:SG	2.32	0.69
1:C:83:LEU:HB3	1:C:106:ILE:HD13	1.74	0.69
2:D:75:LYS:HB2	2:D:75:LYS:HZ2	1.57	0.69
1:A:4:LEU:HD11	1:A:90:GLN:HG3	1.74	0.69
2:B:114:LYS:HD3	2:B:173:ASP:HA	1.74	0.69
1:A:7:THR:HG22	6:A:382:HOH:O	1.92	0.69
2:D:100:ALA:O	6:D:323:HOH:O	2.09	0.69
2:B:153:THR:HG22	2:B:196:ASN:HB2	1.74	0.68
2:B:171:GLN:O	2:B:171:GLN:HG3	1.91	0.68
2:B:11:LEU:HD23	2:B:116:THR:HG22	1.74	0.68
2:D:6:GLN:HE21	2:D:92:CYS:N	1.83	0.68
2:D:96:LYS:HG2	6:D:271:HOH:O	1.93	0.68
2:B:114:LYS:HB2	2:B:146:PHE:CE1	2.30	0.67
1:C:145:ASN:O	1:C:196:ALA:HA	1.94	0.67



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:202:SER:OG	2:B:204:THR:HG23	1.96	0.66
2:B:43:LYS:HD3	6:B:224:HOH:O	1.95	0.65
1:A:60:ASP:OD2	6:A:304:HOH:O	2.15	0.65
1:C:2:ILE:CD1	1:C:93:HIS:CD2	2.80	0.65
3:Q:214:LYS:HB2	3:Q:214:LYS:NZ	2.12	0.65
2:B:112:SER:OG	2:B:113:SER:N	2.30	0.65
2:D:153:THR:HG23	2:D:157:GLY:N	2.10	0.65
2:B:97:VAL:O	2:B:98:ARG:HB3	1.96	0.65
2:D:135:SER:HB3	2:D:185:SER:OG	1.97	0.65
2:D:97:VAL:O	2:D:98:ARG:HB3	1.97	0.64
1:C:157:ASN:OD1	1:C:157:ASN:N	2.28	0.63
1:A:122:SER:O	1:A:126:THR:HG23	1.99	0.63
2:B:114:LYS:HD2	2:B:146:PHE:CZ	2.33	0.63
3:Q:212:GLY:N	6:Q:336:HOH:O	2.31	0.63
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.80	0.63
2:D:153:THR:HG22	2:D:196:ASN:OD1	1.99	0.62
2:D:190:SER:HB2	6:D:290:HOH:O	2.00	0.61
2:B:85:GLU:CD	2:B:85:GLU:H	2.03	0.61
1:A:36:TYR:HE1	1:A:89:SER:HB3	1.65	0.61
1:A:190:ASN:O	1:A:210:ASN:HA	2.01	0.61
1:C:83:LEU:HB3	1:C:106:ILE:HD11	1.83	0.61
2:D:138:LEU:HG	2:D:210:ILE:HG21	1.83	0.61
1:A:60:ASP:OD1	6:A:471:HOH:O	2.16	0.61
2:B:83:ARG:HD2	2:B:85:GLU:HG2	1.83	0.61
2:D:114:LYS:HE2	2:D:173:ASP:OD2	2.00	0.60
2:B:85:GLU:OE2	6:B:396:HOH:O	2.16	0.60
1:C:190:ASN:HB3	6:C:316:HOH:O	2.02	0.60
2:D:75:LYS:HB2	2:D:75:LYS:HZ3	1.65	0.60
2:D:96:LYS:HE3	6:D:271:HOH:O	2.01	0.59
2:B:1:GLN:HA	2:B:1:GLN:OE1	2.03	0.59
2:D:105:GLN:C	2:D:105:GLN:HE21	2.04	0.59
1:A:142:LYS:HD3	1:A:173:TYR:CE2	2.38	0.59
1:C:104:LEU:C	1:C:104:LEU:HD23	2.23	0.59
1:A:189:HIS:O	1:A:211:ARG:HD3	2.02	0.59
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.84	0.59
2:D:31:ASP:HB3	2:D:96:LYS:HD2	1.85	0.58
1:C:190:ASN:ND2	6:C:316:HOH:O	2.36	0.58
1:A:109:ALA:O	1:A:110:ASP:CB	2.49	0.58
1:C:106:ILE:H	1:C:166:GLN:HE22	1.50	0.58
1:A:108:ARG:HG3	1:A:171:SER:HB2	1.84	0.58
2:B:116:THR:HB	6:B:448:HOH:O	2.03	0.58



	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:147:PRO:O	2:D:199:HIS:HE1	1.85	0.58
1:C:198:HIS:CD2	1:C:200:THR:HG23	2.38	0.57
2:D:11:LEU:HB2	2:D:147:PRO:HG3	1.86	0.57
2:D:52(A):ASN:HB3	2:D:53(A):ASN:H	1.69	0.57
2:B:199:HIS:HD2	2:B:202:SER:OG	1.88	0.57
2:B:155:ASN:OD1	6:B:410:HOH:O	2.18	0.57
2:B:194:THR:HG23	6:B:410:HOH:O	2.04	0.56
3:Q:214:LYS:HG3	3:Q:214:LYS:O	2.05	0.56
2:D:153:THR:CG2	2:D:157:GLY:N	2.69	0.56
2:B:114:LYS:HE3	2:B:173:ASP:OD2	2.06	0.56
1:C:2:ILE:HA	1:C:26:SER:OG	2.05	0.56
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.88	0.56
2:D:199:HIS:HD2	2:D:202:SER:OG	1.89	0.55
1:C:185:GLU:OE2	1:C:189:HIS:NE2	2.39	0.55
2:D:105:GLN:NE2	2:D:106:GLY:O	2.40	0.55
2:D:202:SER:O	2:D:204:THR:HG23	2.06	0.55
1:A:2:ILE:CG2	1:A:90:GLN:NE2	2.70	0.55
2:B:83:ARG:HB2	2:B:85:GLU:OE2	2.08	0.54
2:D:18:MET:HE1	2:D:109:VAL:HG22	1.89	0.54
2:B:194:THR:CG2	6:B:410:HOH:O	2.55	0.54
2:B:94:GLY:HA2	6:B:215:HOH:O	2.08	0.54
2:B:153:THR:CG2	2:B:196:ASN:HB2	2.38	0.54
2:D:125:ALA:O	2:D:213:ARG:NH1	2.41	0.54
2:D:188:TRP:CG	2:D:189:PRO:HA	2.43	0.54
2:B:83:ARG:NH2	2:B:85:GLU:CG	2.68	0.54
1:A:2:ILE:HG21	1:A:90:GLN:NE2	2.22	0.53
2:D:52:ARG:O	2:D:55:HIS:HA	2.08	0.53
2:D:9:GLY:HA2	2:D:18:MET:HE3	1.88	0.53
1:C:190:ASN:HB2	1:C:211:ARG:HB2	1.91	0.53
2:B:209:LYS:HE3	2:B:211:GLU:OE1	2.09	0.53
2:D:18:MET:CE	2:D:109:VAL:HG22	2.39	0.53
2:D:5:GLN:NE2	6:D:430:HOH:O	2.42	0.52
1:A:137:ASN:HB3	1:A:138:ASN:OD1	2.09	0.52
1:C:163:TRP:NE1	6:C:429:HOH:O	2.32	0.52
1:C:37:LEU:HD13	1:C:86:TYR:CZ	2.45	0.52
1:C:157:ASN:O	6:C:414:HOH:O	2.19	0.52
1:C:79:GLU:OE1	6:C:492:HOH:O	2.19	0.52
2:B:162:GLY:N	6:B:343:HOH:O	2.15	0.52
1:A:137:ASN:HD22	1:A:174:SER:HB3	1.75	0.52
1:C:24:ARG:NH1	6:C:399:HOH:O	2.23	0.51
2:B:83:ARG:HD2	2:B:85:GLU:CG	2.40	0.51



	A t ama 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1:GLN:OE1	2:B:1:GLN:CA	2.58	0.51
2:B:187:THR:O	2:B:191:GLN:HB2	2.10	0.51
1:A:151:ASP:HA	1:A:191:SER:HB3	1.93	0.51
1:A:113:PRO:HG3	1:A:144:ILE:HD11	1.92	0.51
2:B:189:PRO:HB3	2:B:212:PRO:HG3	1.93	0.50
2:B:35:ASP:OD2	2:B:98:ARG:HD2	2.11	0.50
2:D:194:THR:HB	2:D:209:LYS:HA	1.94	0.50
1:C:45:LYS:HG3	6:C:260:HOH:O	2.12	0.50
3:X:6:LEU:HD12	3:X:7:GLU:N	2.27	0.50
3:Q:212:GLY:N	6:Q:409:HOH:O	2.44	0.50
1:A:165:ASP:OD1	6:A:287:HOH:O	2.19	0.49
2:B:170:LEU:HB2	2:B:175:TYR:CE2	2.47	0.49
2:B:116:THR:CB	6:B:448:HOH:O	2.61	0.49
2:B:118:ALA:HB1	2:B:204:THR:HG21	1.95	0.49
1:C:155:ARG:NH1	6:C:469:HOH:O	2.41	0.49
1:A:45:LYS:HD3	6:A:482:HOH:O	2.11	0.49
2:B:105:GLN:NE2	6:B:305:HOH:O	2.31	0.49
2:D:2:VAL:HG11	2:D:102:TYR:CG	2.48	0.49
1:C:54:ARG:NH2	6:C:454:HOH:O	2.46	0.48
2:D:153:THR:HG23	2:D:157:GLY:H	1.78	0.48
1:A:136:LEU:HD12	1:A:136:LEU:N	2.29	0.48
1:C:195:GLU:O	1:C:196:ALA:HB3	2.13	0.48
1:A:135:PHE:C	1:A:136:LEU:HD12	2.33	0.48
2:D:105:GLN:HE21	2:D:106:GLY:N	2.12	0.47
2:D:121:VAL:HG21	2:D:206:VAL:HG22	1.95	0.47
1:A:2:ILE:HG21	1:A:90:GLN:CD	2.35	0.47
2:B:64:LYS:HB2	2:B:64:LYS:NZ	2.28	0.47
1:C:74:LYS:NZ	6:C:371:HOH:O	2.32	0.47
1:A:142:LYS:O	1:A:142:LYS:HG3	2.15	0.47
1:C:27:GLN:NE2	6:C:331:HOH:O	2.47	0.47
2:D:33:TRP:CZ3	3:Q:216:PRO:HG3	2.49	0.47
1:A:9:LEU:HD22	2:D:77:ARG:HD2	1.97	0.47
2:B:83:ARG:HH21	2:B:85:GLU:CG	2.24	0.47
1:C:185:GLU:OE1	1:C:188:ARG:NE	2.39	0.47
2:B:31:ASP:C	2:B:52(A):ASN:OD1	2.53	0.47
1:C:141:PRO:O	1:C:198:HIS:HE1	1.98	0.47
2:B:13:GLN:HA	2:B:112:SER:CB	2.45	0.47
2:B:114:LYS:HD2	2:B:146:PHE:CE2	2.49	0.47
2:D:114:LYS:HB2	2:D:146:PHE:CE1	2.49	0.47
1:C:3:GLN:CD	1:C:26:SER:HB3	2.35	0.47
1:C:185:GLU:HB2	1:C:188:ARG:HH11	1.80	0.47



	A t ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:96:LYS:NZ	6:D:393:HOH:O	2.48	0.47
2:B:85:GLU:CD	2:B:85:GLU:N	2.69	0.46
1:C:151:ASP:OD1	1:C:189:HIS:ND1	2.37	0.46
1:A:198:HIS:HD2	1:A:200:THR:OG1	1.97	0.46
1:C:137:ASN:ND2	1:C:174:SER:HB3	2.31	0.46
1:C:155:ARG:NE	6:C:469:HOH:O	2.20	0.46
1:C:190:ASN:O	1:C:210:ASN:HA	2.14	0.46
1:C:198:HIS:HD2	1:C:200:THR:OG1	1.99	0.46
1:A:116:SER:O	1:A:134:CYS:HA	2.16	0.46
1:A:2:ILE:O	1:A:2:ILE:HG23	2.16	0.45
1:A:140:TYR:CG	1:A:141:PRO:HA	2.51	0.45
2:B:38:ARG:HA	2:B:89:ILE:O	2.16	0.45
2:B:43:LYS:HE2	2:B:46:GLU:CD	2.37	0.45
2:B:153:THR:OG1	2:B:157:GLY:N	2.49	0.45
2:B:42:GLU:CD	2:B:42:GLU:H	2.19	0.45
1:C:195:GLU:OE1	6:C:505:HOH:O	2.21	0.45
1:C:76:SER:O	1:C:77:SER:C	2.55	0.45
2:D:64:LYS:HB2	2:D:64:LYS:HE3	1.74	0.45
2:D:199:HIS:CD2	2:D:202:SER:OG	2.69	0.45
2:B:123:PRO:HG3	2:B:208:LYS:CG	2.41	0.44
2:B:205:LYS:O	2:B:206:VAL:HG13	2.17	0.44
2:B:6:GLN:HE21	2:B:92:CYS:N	1.94	0.44
1:A:76:SER:HB2	6:A:284:HOH:O	2.17	0.44
2:D:34:MET:SD	2:D:94:GLY:HA3	2.58	0.44
2:D:4:LEU:HG	2:D:92:CYS:SG	2.58	0.44
1:A:62:PHE:CD1	1:A:75:ILE:HG12	2.53	0.44
2:B:52:ARG:O	2:B:55:HIS:HA	2.18	0.44
2:D:82(B):SER:OG	6:D:347:HOH:O	2.21	0.44
2:B:93:SER:OG	2:B:99:ASN:HA	2.17	0.44
1:C:33:LEU:HD13	1:C:33:LEU:C	2.38	0.44
1:C:54:ARG:NH1	1:C:58:VAL:O	2.51	0.44
1:C:170:ASP:O	1:C:171:SER:HB2	2.17	0.44
2:D:70:THR:O	2:D:78:MET:HB2	2.17	0.44
1:C:106:ILE:N	1:C:106:ILE:HD12	2.33	0.44
1:C:108:ARG:HG2	1:C:109:ALA:N	2.32	0.44
1:C:25:SER:OG	1:C:69:THR:HA	2.17	0.43
1:C:34:HIS:O	1:C:88:CYS:HA	2.18	0.43
1:A:79:GLU:O	1:A:82:ASP:HB2	2.18	0.43
1:A:113:PRO:HG3	1:A:144:ILE:CD1	2.48	0.43
1:C:137:ASN:HD22	1:C:174:SER:HB3	1.82	0.43
2:B:11:LEU:CD2	2:B:116:THR:HG22	2.46	0.43



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:94:VAL:HA	1:C:95:PRO:HD3	1.85	0.43
2:D:188:TRP:CD1	2:D:189:PRO:HA	2.53	0.43
2:B:172:SER:O	2:B:173:ASP:HB2	2.19	0.43
3:X:3:LYS:HA	3:X:4:PRO:HD3	1.80	0.43
2:B:114:LYS:HG2	2:B:173:ASP:CG	2.39	0.43
1:C:27(B):LEU:HD22	1:C:71:PHE:CE1	2.53	0.43
1:A:2:ILE:CG2	1:A:2:ILE:O	2.65	0.43
1:C:119:PRO:HD2	6:D:274:HOH:O	2.19	0.43
1:C:207:LYS:HE2	6:C:455:HOH:O	2.19	0.43
1:A:80:ALA:HA	1:A:106:ILE:HG13	2.00	0.43
2:B:11:LEU:HD11	2:B:112:SER:HA	2.01	0.43
2:B:177:LEU:HD12	2:B:177:LEU:C	2.39	0.43
2:B:188:TRP:CG	2:B:189:PRO:HA	2.53	0.43
2:D:126:PRO:HD3	2:D:138:LEU:HD12	2.01	0.42
1:A:125:LEU:O	1:A:183:LYS:HD3	2.19	0.42
1:A:162:SER:OG	2:B:167:PRO:HD2	2.19	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.80	0.42
1:A:160:LEU:HD11	2:B:171:GLN:HG2	2.01	0.42
2:B:188:TRP:CD1	2:B:189:PRO:HA	2.55	0.42
2:D:200:PRO:CD	6:D:517:HOH:O	2.33	0.42
1:A:2:ILE:N	6:A:272:HOH:O	2.52	0.42
2:B:77:ARG:NH1	6:B:494:HOH:O	2.15	0.42
2:B:191:GLN:HE21	2:B:191:GLN:HB3	1.67	0.42
1:C:50:LYS:HB2	1:C:53:ASN:HD22	1.83	0.42
1:C:125:LEU:C	1:C:127:SER:H	2.22	0.42
2:D:152:LEU:C	2:D:152:LEU:HD23	2.40	0.42
1:C:104:LEU:C	1:C:104:LEU:CD2	2.88	0.42
1:A:79:GLU:CD	6:A:413:HOH:O	2.58	0.42
1:A:137:ASN:HD22	1:A:174:SER:CB	2.32	0.42
2:B:83:ARG:HD2	2:B:85:GLU:OE2	2.20	0.42
1:C:136:LEU:HD12	1:C:136:LEU:N	2.34	0.42
2:D:170:LEU:HD12	2:D:174:LEU:O	2.19	0.42
1:C:43:SER:HB2	1:C:44:PRO:HD2	2.02	0.41
2:D:59:TYR:OH	2:D:69:ILE:HG22	2.19	0.41
1:C:116:SER:O	1:C:134:CYS:HA	2.19	0.41
1:A:136:LEU:HD21	1:A:146:VAL:HG22	2.03	0.41
1:C:198:HIS:CD2	1:C:200:THR:H	2.39	0.41
1:A:79:GLU:OE2	6:A:413:HOH:O	2.21	0.41
1:C:18:GLN:HE21	1:C:18:GLN:HB2	1.67	0.41
1:A:110:ASP:HB2	6:A:254:HOH:O	2.20	0.41
2:D:87:THR:HA	2:D:109:VAL:O	2.21	0.41



31	Eï I

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:HG3	6:A:305:HOH:O	2.21	0.41
1:A:86:TYR:O	1:A:101:GLY:HA2	2.21	0.41
1:C:27:GLN:C	1:C:69:THR:HG22	2.41	0.41
2:B:111:VAL:O	2:B:111:VAL:HG22	2.20	0.40
1:C:27(A):SER:HA	1:C:68:GLY:O	2.21	0.40
1:C:54:ARG:NE	6:C:337:HOH:O	2.51	0.40
6:A:275:HOH:O	2:B:176:THR:HG21	2.22	0.40

All (3) 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)
6:C:431:HOH:O	6:D:420:HOH:O[1_545]	2.17	0.03
6:B:320:HOH:O	6:C:244:HOH:O[1_556]	2.18	0.02
6:B:446:HOH:O	6:C:230:HOH:O[1_556]	2.18	0.02

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	А	213/217~(98%)	204 (96%)	8 (4%)	1 (0%)	29 31
1	С	215/217~(99%)	200~(93%)	10 (5%)	5(2%)	6 3
2	В	206/218~(94%)	198 (96%)	5 (2%)	3~(2%)	10 8
2	D	207/218~(95%)	202~(98%)	2(1%)	3~(1%)	11 8
3	Q	4/9~(44%)	4 (100%)	0	0	100 100
3	Х	7/9~(78%)	7~(100%)	0	0	100 100
All	All	852/888~(96%)	815 (96%)	25 (3%)	12 (1%)	11 8

All (12) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	110	ASP
2	В	52(A)	ASN
2	В	113	SER
1	С	110	ASP
2	D	52(A)	ASN
2	В	112	SER
2	D	43	LYS
1	С	109	ALA
1	С	68	GLY
1	С	196	ALA
1	С	2	ILE
2	D	98	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	193/195~(99%)	178~(92%)	15 (8%)	12	13
1	С	195/195~(100%)	182 (93%)	13 (7%)	16	18
2	В	180/186~(97%)	159~(88%)	21 (12%)	5	4
2	D	181/186~(97%)	159 (88%)	22 (12%)	5	4
3	Q	5/8~(62%)	3~(60%)	2(40%)	0	0
3	Х	8/8~(100%)	7~(88%)	1 (12%)	4	4
All	All	762/778~(98%)	688~(90%)	74 (10%)	8	7

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

Mol	Chain	Res	Type
1	А	2	ILE
1	А	7	THR
1	А	9	LEU
1	А	11	LEU
1	А	22	SER
1	А	24	ARG
1	А	27(B)	LEU



Mol	Chain	Res	Type
1	А	79	GLU
1	А	103	LYS
1	А	108	ARG
1	А	110	ASP
1	А	155	ARG
1	А	157	ASN
1	А	181	LEU
1	А	199	LYS
2	В	1	GLN
2	В	12	VAL
2	В	42	GLU
2	В	46	GLU
2	В	61	GLU
2	В	70	THR
2	В	98	ARG
2	В	110	THR
2	В	111	VAL
2	В	113	SER
2	В	116	THR
2	В	138	LEU
2	В	171	GLN
2	В	174	LEU
2	В	176	THR
2	В	177	LEU
2	В	194	THR
2	В	196	ASN
2	В	204	THR
2	В	206	VAL
2	В	209	LYS
1	С	1	ASP
1	С	3	GLN
1	С	7	THR
1	С	9	LEU
1	С	12	PRO
1	С	27(B)	LEU
1	С	60	ASP
1	C	63	SER
1	С	67	SER
1	С	157	ASN
1	С	160	LEU
1	С	163	TRP
1	С	212	GLU



Mol	Chain	Res	Type
2	D	3	GLN
2	D	4	LEU
2	D	12	VAL
2	D	42	GLU
2	D	70	THR
2	D	75	LYS
2	D	85	GLU
2	D	98	ARG
2	D	105	GLN
2	D	108	THR
2	D	110	THR
2	D	116	THR
2	D	127	VAL
2	D	136	VAL
2	D	138	LEU
2	D	153	THR
2	D	174	LEU
2	D	176	THR
2	D	177	LEU
2	D	190	SER
2	D	194	THR
2	D	213	ARG
3	Х	9	LEU
3	Q	214	LYS
3	Q	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	137	ASN
1	А	161	ASN
1	А	166	GLN
1	А	198	HIS
2	В	3	GLN
2	В	99	ASN
2	В	171	GLN
2	В	191	GLN
2	В	199	HIS
1	С	18	GLN
1	С	42	GLN
1	С	53	ASN
1	С	93	HIS



Mol	Chain	Res	Type
1	С	137	ASN
1	С	161	ASN
1	С	166	GLN
1	С	198	HIS
2	D	3	GLN
2	D	6	GLN
2	D	13	GLN
2	D	99	ASN
2	D	105	GLN
2	D	199	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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	T in le	Bo	ond leng	\mathbf{ths}	В	ond ang	les
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A2G	Х	800	3	14,14,15	0.62	0	17,19,21	1.29	1 (5%)
5	A2G	Q	800	3	14,14,15	0.60	0	17,19,21	1.08	2 (11%)



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	A2G	Х	800	3	-	1/6/23/26	0/1/1/1
5	A2G	Q	800	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Х	800	A2G	C2-N2-C7	-3.78	117.52	122.90
5	Q	800	A2G	C6-C5-C4	-2.44	107.28	113.00
5	Q	800	A2G	C4-C3-C2	-2.30	107.64	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	800	A2G	O5-C5-C6-O6
5	Х	800	A2G	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

