

Full wwPDB X-ray Structure Validation Report (i)

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onent C8
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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 2.51 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	$5346 \ (2.50-2.50)$
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	y of chain	
1	А	554	5%	26%	8% 14%
2	В	537	4%	36%	11% • 6%
3	С	182	2% 54%	30%	7% • 9%



30JY

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9234 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 Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	478	Total 3799	C 2359	N 666	O 736	S 38	0	0	0

• Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	В	504	Total 4050	C 2521	N 722	0 771	Р 1	S 35	0	0	0

• Molecule 3 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	165	Total 1295	C 828	N 224	O 239	${S \atop 4}$	0	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0

• Molecule 5 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	А	1	Total C O	0	0	
5	А	1	$\begin{array}{ccc} 10tar & C & O \\ 11 & 6 & 5 \end{array}$	0	0	
	Δ	1	Total C O	0	0	
6	А	1	11 6 5	0	0	
5	Λ	1	Total C O	0	0	
0	Л	1	11 6 5	0		
5	В	1	Total C O	0	0	
0	D	1	11 6 5	0	0	
5	В	1	Total C O	0	0	
0	D	1	11 6 5	0	0	
Б	р	1	Total C O	0	0	
0	D		11 6 5	0	0	
5	р	1	Total C O	0	0	
0	D		11 6 5	0	U	



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: Complement component C8 alpha chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	139.57Å 139.57Å 127.16Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{Posolution} \left(\mathbf{\hat{A}} \right)$	45.69 - 2.51	Depositor
Resolution (A)	45.69 - 2.51	EDS
% Data completeness	93.1 (45.69-2.51)	Depositor
(in resolution range)	$93.1 \ (45.69 - 2.51)$	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.27 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
P. P.	0.249 , 0.337	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.248 , 0.335	DCC
R_{free} test set	2267 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 37.2	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9234	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.67% 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: BMA, CA, TPO

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	nd lengths	Bo	ond angles
MIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.80	4/3873~(0.1%)	0.82	0/5207
2	В	0.86	5/4131~(0.1%)	0.89	3/5574~(0.1%)
3	С	0.70	0/1323	0.82	1/1794~(0.1%)
All	All	0.81	9/9327~(0.1%)	0.85	4/12575~(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
3	С	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
2	В	16	TRP	CG-CD1	9.82	1.50	1.36
1	А	515	TRP	CG-CD1	9.75	1.50	1.36
1	А	518	TRP	CG-CD1	9.59	1.50	1.36
1	А	512	TRP	CG-CD1	9.27	1.49	1.36
2	В	497	TRP	CG-CD1	9.19	1.49	1.36
2	В	19	TRP	CG-CD1	9.09	1.49	1.36
1	А	14	TRP	CG-CD1	9.08	1.49	1.36
2	В	467	CYS	CB-SG	-7.94	1.68	1.82
2	В	500	TRP	CG-CD1	7.77	1.47	1.36

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	480	CYS	CA-CB-SG	-6.48	102.34	114.00
3	С	89	LEU	CA-CB-CG	5.43	127.78	115.30
2	В	520	GLN	N-CA-C	5.40	125.58	111.00
2	В	152	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	107	LYS	Peptide
2	В	96	SER	Peptide
3	С	110	THR	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	3799	0	3596	118	1
2	В	4050	0	3853	224	1
3	С	1295	0	1259	45	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	44	0	40	1	0
5	В	44	0	40	3	0
All	All	9234	0	8788	373	1

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 21.

All (373) 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:B:93:GLY:O	2:B:261:TYR:CD2	2.04	1.09
2:B:520:GLN:NE2	2:B:520:GLN:HA	1.52	1.08
1:A:322:GLU:HB3	1:A:392:ARG:HB2	1.34	1.08
2:B:516:ASN:O	2:B:518:PRO:HD3	1.56	1.04



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:146:CYS:O	2:B:148:PRO:HD3	1.58	1.03
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.19	1.02
1:A:156:ARG:HD2	2:B:404:TYR:CE2	1.98	0.99
1:A:25:ASP:HB3	1:A:54:CYS:O	1.64	0.97
2:B:26:GLN:O	2:B:27:LYS:HG2	1.63	0.97
3:C:155:THR:H	3:C:158:GLN:HE21	1.12	0.96
1:A:368:HIS:HE1	1:A:370:LYS:HG3	1.30	0.94
2:B:82:ARG:HH11	2:B:82:ARG:H	1.11	0.94
2:B:490:ILE:HB	2:B:518:PRO:HD2	1.49	0.94
2:B:489:PRO:HB3	2:B:520:GLN:HG2	1.50	0.92
2:B:520:GLN:NE2	2:B:520:GLN:CA	2.34	0.91
2:B:94:ASP:O	2:B:95:GLN:HG3	1.72	0.90
2:B:187:GLU:HG3	2:B:190:VAL:HG22	1.52	0.89
2:B:266:ARG:NH1	2:B:285:ASP:OD2	2.09	0.86
2:B:41:PHE:CE2	2:B:479:ALA:HB2	2.12	0.85
2:B:349:CYS:O	2:B:351:GLY:N	2.13	0.81
2:B:457:ASN:HD21	2:B:491:ASP:H	1.25	0.81
1:A:257:PHE:HE1	1:A:387:GLU:HG3	1.46	0.81
1:A:7:VAL:O	1:A:41:GLY:HA3	1.82	0.79
2:B:457:ASN:ND2	2:B:491:ASP:H	1.79	0.79
3:C:78:GLN:HB2	3:C:171:ALA:CB	2.13	0.79
1:A:74:GLU:OE2	1:A:74:GLU:HA	1.80	0.78
2:B:353:LEU:HD23	2:B:353:LEU:O	1.83	0.78
1:A:550:GLN:OE1	1:A:550:GLN:HA	1.83	0.77
1:A:191:ALA:HB3	2:B:220:ARG:HG2	1.67	0.76
2:B:349:CYS:SG	2:B:350:ARG:HG3	2.25	0.76
1:A:495:GLY:HA3	1:A:499:GLU:OE1	1.85	0.76
2:B:217:GLN:O	2:B:218:SER:O	2.03	0.75
3:C:155:THR:H	3:C:158:GLN:NE2	1.84	0.75
2:B:82:ARG:H	2:B:82:ARG:NH1	1.82	0.75
3:C:101:GLY:HA3	3:C:122:ARG:HE	1.52	0.74
1:A:257:PHE:CE1	1:A:387:GLU:HG3	2.23	0.73
2:B:503:CYS:C	2:B:505:GLY:H	1.91	0.73
2:B:520:GLN:HA	2:B:520:GLN:HE21	1.52	0.72
2:B:187:GLU:HG3	2:B:190:VAL:CG2	2.18	0.71
2:B:519:PRO:O	2:B:520:GLN:NE2	2.21	0.71
2:B:352:ILE:C	2:B:354:ASN:H	1.94	0.71
2:B:82:ARG:HH11	2:B:82:ARG:N	1.88	0.70
2:B:260:HIS:HD2	2:B:262:GLU:H	1.39	0.70
2:B:485:ARG:HG2	2:B:485:ARG:NH1	1.96	0.70
1:A:512:TRP:CE3	1:A:530:ARG:HG3	2.27	0.70



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:93:GLY:HA2	2:B:94:ASP:HB3	1.73	0.70
2:B:381:ILE:HG23	2:B:386:TYR:HD1	1.57	0.70
1:A:368:HIS:CE1	1:A:370:LYS:HG3	2.21	0.70
2:B:380:HIS:CE1	2:B:397:GLU:HG3	2.28	0.69
2:B:500:TRP:CE3	2:B:508:LYS:HG3	2.28	0.69
2:B:270:LEU:HD11	2:B:282:LEU:HD22	1.74	0.68
2:B:489:PRO:HB3	2:B:520:GLN:CG	2.22	0.67
1:A:59:THR:O	1:A:60:CYS:HB2	1.94	0.67
3:C:78:GLN:HB2	3:C:171:ALA:HB2	1.74	0.66
2:B:19:TRP:CZ2	2:B:31:ARG:HD2	2.31	0.66
1:A:445:PRO:O	1:A:446:LEU:HG	1.95	0.66
2:B:94:ASP:C	2:B:95:GLN:HG3	2.14	0.66
2:B:349:CYS:C	2:B:351:GLY:H	1.98	0.66
2:B:414:GLU:HG3	2:B:418:GLU:HG3	1.77	0.65
2:B:379:GLU:OE2	2:B:379:GLU:HA	1.97	0.65
2:B:70:GLY:HA2	2:B:82:ARG:CZ	2.27	0.65
2:B:143:ALA:HB2	2:B:160:TYR:CD1	2.31	0.65
2:B:444:LYS:HG2	5:B:541:BMA:O6	1.98	0.64
2:B:352:ILE:C	2:B:354:ASN:N	2.51	0.64
2:B:394:LEU:HG	2:B:394:LEU:O	1.97	0.64
3:C:41:ARG:O	3:C:44:GLN:HG2	1.98	0.64
3:C:110:THR:OG1	3:C:111:ASP:O	2.15	0.64
2:B:355:GLU:O	2:B:359:ARG:HD3	1.98	0.64
2:B:364:TPO:O2P	2:B:364:TPO:HA	1.98	0.64
3:C:46:GLN:HB3	3:C:49:ARG:HD3	1.80	0.64
3:C:41:ARG:HA	3:C:44:GLN:HE21	1.63	0.63
2:B:69:GLU:HA	2:B:69:GLU:OE1	1.98	0.63
1:A:512:TRP:CH2	1:A:548:LYS:HB3	2.34	0.62
2:B:213:GLY:O	2:B:214:ILE:C	2.38	0.62
3:C:57:VAL:HG13	3:C:64:MET:HE3	1.80	0.62
2:B:293:GLU:HB2	2:B:412:LYS:HB2	1.80	0.62
2:B:390:PRO:HG2	2:B:391:THR:H	1.65	0.62
1:A:490:ARG:N	1:A:490:ARG:HE	1.98	0.62
2:B:96:SER:C	2:B:98:GLU:H	2.03	0.61
2:B:214:ILE:O	2:B:218:SER:OG	2.13	0.61
1:A:322:GLU:HB3	1:A:392:ARG:CB	2.22	0.61
2:B:317:THR:O	2:B:320:ASN:HB2	2.01	0.61
3:C:146:GLU:O	3:C:149:VAL:HG12	2.00	0.61
2:B:269:ARG:HH11	2:B:269:ARG:CB	2.15	0.60
1:A:249:LEU:C	1:A:251:LYS:H	2.06	0.60
2:B:9:ILE:O	2:B:43:GLY:HA3	2.02	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:190:VAL:C	2:B:192:GLU:H	2.04	0.59
2:B:490:ILE:CB	2:B:518:PRO:HD2	2.28	0.59
2:B:503:CYS:C	2:B:505:GLY:N	2.54	0.59
2:B:352:ILE:O	2:B:354:ASN:N	2.36	0.59
2:B:298:GLY:HA2	2:B:374:ARG:O	2.03	0.59
1:A:204:ASN:HD22	1:A:490:ARG:HD2	1.68	0.59
2:B:90:ASN:ND2	2:B:94:ASP:HB2	2.18	0.59
2:B:93:GLY:O	2:B:261:TYR:CE2	2.55	0.59
1:A:138:TYR:HB3	1:A:181:ASN:HD22	1.69	0.58
2:B:246:GLU:OE1	2:B:249:HIS:NE2	2.25	0.58
3:C:47:GLY:O	3:C:49:ARG:N	2.37	0.58
2:B:349:CYS:SG	2:B:350:ARG:N	2.76	0.58
2:B:290:TYR:CZ	2:B:419:LEU:HD13	2.39	0.57
2:B:40:GLN:OE1	2:B:452:ALA:HB3	2.03	0.57
2:B:66:VAL:HG23	2:B:66:VAL:O	2.04	0.57
2:B:427:TYR:O	2:B:428:SER:C	2.41	0.57
2:B:512:ARG:HH22	2:B:527:SER:HA	1.69	0.57
2:B:92:CYS:O	2:B:93:GLY:C	2.42	0.57
2:B:115:TYR:OH	2:B:149:HIS:HD2	1.87	0.57
2:B:453:PRO:HB3	2:B:515:ASN:HB2	1.87	0.57
2:B:123:SER:HA	2:B:135:PRO:HA	1.86	0.57
2:B:506:ARG:CZ	5:B:542:BMA:O2	2.53	0.57
1:A:261:ARG:NH2	1:A:322:GLU:OE2	2.24	0.56
2:B:466:ARG:HG3	2:B:467:CYS:N	2.19	0.56
2:B:179:GLU:HG3	2:B:322:HIS:HD2	1.68	0.56
1:A:154:GLU:O	1:A:156:ARG:N	2.39	0.56
1:A:275:LYS:NZ	2:B:285:ASP:OD2	2.28	0.56
3:C:45:GLU:C	3:C:47:GLY:H	2.09	0.56
2:B:349:CYS:HB2	2:B:353:LEU:HD13	1.87	0.56
3:C:47:GLY:C	3:C:49:ARG:H	2.10	0.55
1:A:284:MET:HG3	1:A:307:TYR:CD1	2.42	0.55
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.06	0.55
1:A:258:ILE:CD1	1:A:339:SER:HB3	2.36	0.55
2:B:216:SER:OG	2:B:217:GLN:N	2.40	0.55
2:B:478:LEU:C	2:B:480:CYS:H	2.10	0.54
1:A:511:SER:N	1:A:544:CYS:SG	2.80	0.54
3:C:78:GLN:HB2	3:C:171:ALA:HB3	1.87	0.54
1:A:547:ARG:NH2	2:B:12:GLU:OE2	2.41	0.54
1:A:296:ASN:O	1:A:300:TYR:HD1	1.91	0.54
2:B:179:GLU:HG3	2:B:322:HIS:CD2	2.43	0.54
1:A:195:ILE:N	1:A:195:ILE:HD12	2.22	0.54



	A h C	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:382:LYS:O	1:A:385:ALA:N	2.38	0.54
2:B:24:PRO:HB2	2:B:62:CYS:HB2	1.89	0.54
1:A:160:TYR:OH	1:A:165:GLU:OE1	2.26	0.54
2:B:20:THR:O	2:B:29:ARG:HB2	2.08	0.54
3:C:78:GLN:CB	3:C:171:ALA:CB	2.84	0.54
1:A:473:PHE:O	1:A:474:ASN:HB2	2.08	0.53
2:B:97:ASP:N	2:B:97:ASP:OD2	2.41	0.53
2:B:93:GLY:N	2:B:94:ASP:HA	2.23	0.53
2:B:365:MET:O	2:B:365:MET:HG2	2.09	0.53
2:B:400:ASP:CG	2:B:401:ALA:N	2.61	0.53
2:B:269:ARG:HH11	2:B:269:ARG:HB2	1.71	0.53
2:B:179:GLU:CD	2:B:179:GLU:H	2.10	0.53
2:B:352:ILE:HG22	2:B:356:ILE:N	2.24	0.53
1:A:254:GLU:HG2	1:A:256:LYS:HG2	1.90	0.52
1:A:296:ASN:OD1	1:A:299:MET:HG2	2.09	0.52
1:A:191:ALA:HB3	2:B:220:ARG:CG	2.39	0.52
2:B:96:SER:CA	2:B:98:GLU:H	2.23	0.52
1:A:33:LEU:HB3	1:A:468:ARG:HH12	1.75	0.52
2:B:181:GLU:HA	2:B:237:VAL:HG22	1.92	0.52
2:B:150:TYR:CZ	2:B:155:ARG:HG3	2.44	0.52
1:A:486:ARG:O	1:A:487:CYS:SG	2.68	0.52
2:B:128:PHE:CE2	2:B:443:GLN:HG3	2.44	0.52
2:B:93:GLY:HA2	2:B:94:ASP:CB	2.38	0.52
2:B:221:GLY:O	2:B:225:ILE:HG12	2.10	0.51
1:A:82:HIS:NE2	2:B:95:GLN:CB	2.73	0.51
3:C:38:SER:HB2	3:C:127:SER:HB3	1.93	0.51
2:B:352:ILE:HB	2:B:356:ILE:HB	1.92	0.51
1:A:59:THR:O	1:A:60:CYS:CB	2.59	0.51
1:A:300:TYR:CE2	1:A:452:ASN:HB3	2.45	0.51
2:B:348:LYS:HG3	2:B:348:LYS:O	2.09	0.51
1:A:73:LYS:HB2	1:A:93:ASP:OD2	2.11	0.51
2:B:59:ASN:O	2:B:60:ARG:C	2.48	0.51
3:C:172:ASP:O	3:C:174:PHE:N	2.44	0.51
1:A:190:LEU:HD23	1:A:190:LEU:O	2.11	0.51
1:A:191:ALA:O	1:A:193:THR:HG23	2.11	0.51
1:A:434:ILE:O	1:A:437:VAL:HG12	2.11	0.51
1:A:521:CYS:SG	1:A:526:GLN:NE2	2.82	0.51
3:C:81:GLN:NE2	3:C:94:LEU:HD21	2.26	0.51
3:C:16:ILE:O	3:C:91:ARG:NH2	2.43	0.51
2:B:381:ILE:HG23	2:B:386:TYR:CD1	2.42	0.51
2:B:352:ILE:O	2:B:356:ILE:N	2.43	0.50



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:478:LEU:O	2:B:479:ALA:HB3	2.11	0.50
3:C:128:VAL:HG23	3:C:145:PHE:HE1	1.77	0.50
2:B:121:LEU:HD11	2:B:296:LEU:HD11	1.93	0.50
2:B:93:GLY:O	2:B:261:TYR:CG	2.61	0.50
2:B:380:HIS:HE1	2:B:397:GLU:HG3	1.73	0.50
2:B:381:ILE:HG22	2:B:382:THR:N	2.27	0.50
3:C:128:VAL:HG23	3:C:145:PHE:CE1	2.47	0.50
1:A:269:ALA:HB3	1:A:317:MET:HB2	1.92	0.50
2:B:500:TRP:CD2	2:B:508:LYS:HG3	2.46	0.50
3:C:41:ARG:HG2	3:C:42:PHE:H	1.76	0.50
2:B:518:PRO:HB2	2:B:519:PRO:HD3	1.94	0.50
1:A:166:ARG:HG2	1:A:168:TYR:CD2	2.45	0.50
3:C:21:ASN:O	3:C:22:PHE:C	2.48	0.50
3:C:155:THR:HG23	3:C:158:GLN:NE2	2.27	0.50
1:A:293:ASP:OD2	1:A:293:ASP:N	2.45	0.50
2:B:260:HIS:CD2	2:B:262:GLU:H	2.24	0.49
2:B:8:PRO:HB3	2:B:43:GLY:HA2	1.94	0.49
2:B:59:ASN:O	2:B:60:ARG:O	2.30	0.49
1:A:25:ASP:OD1	1:A:55:SER:HA	2.11	0.49
2:B:481:GLU:N	2:B:481:GLU:OE1	2.42	0.49
3:C:169:GLU:CG	3:C:170:ALA:H	2.25	0.49
1:A:155:TRP:HB3	1:A:174:LYS:HA	1.94	0.49
1:A:518:TRP:CH2	1:A:552:GLN:HB2	2.47	0.49
1:A:195:ILE:HD12	1:A:195:ILE:H	1.78	0.49
3:C:57:VAL:CG1	3:C:64:MET:HE3	2.43	0.49
2:B:269:ARG:NH1	2:B:269:ARG:HB3	2.28	0.49
1:A:515:TRP:CZ3	1:A:530:ARG:HD2	2.47	0.48
2:B:75:GLN:H	2:B:95:GLN:NE2	2.11	0.48
1:A:368:HIS:HE1	1:A:370:LYS:CG	2.14	0.48
2:B:91:ASP:C	2:B:93:GLY:N	2.66	0.48
1:A:247:ASN:C	1:A:249:LEU:H	2.17	0.48
1:A:267:GLN:HG2	1:A:427:ILE:HD11	1.95	0.48
2:B:19:TRP:CH2	2:B:31:ARG:HD2	2.48	0.48
2:B:247:VAL:CG1	2:B:403:GLN:NE2	2.76	0.48
2:B:352:ILE:O	2:B:355:GLU:N	2.47	0.48
2:B:141:TYR:CD2	2:B:258:MET:HG2	2.48	0.48
2:B:485:ARG:NH1	2:B:485:ARG:CG	2.72	0.48
2:B:512:ARG:NH2	2:B:527:SER:HA	2.28	0.48
3:C:135:LEU:HA	3:C:136:PRO:C	2.33	0.48
2:B:489:PRO:HB3	2:B:520:GLN:CB	2.44	0.48
1:A:184:LYS:HG2	1:A:272:LYS:HB3	1.94	0.48



	is as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:431:MET:HE2	2:B:47:ASN:HD22	1.79	0.48
2:B:320:ASN:O	2:B:324:CYS:HB2	2.13	0.48
2:B:500:TRP:HB3	2:B:506:ARG:HG2	1.96	0.48
1:A:371:LYS:HG3	1:A:380:ALA:HA	1.95	0.48
2:B:270:LEU:HD13	2:B:279:TYR:CE2	2.49	0.48
2:B:187:GLU:CG	2:B:190:VAL:HG22	2.36	0.48
1:A:313:THR:O	1:A:314:SER:HB3	2.14	0.48
2:B:377:ALA:HB1	2:B:381:ILE:HD11	1.96	0.48
2:B:429:SER:O	2:B:433:GLN:HG2	2.14	0.48
2:B:208:GLY:H	2:B:412:LYS:NZ	2.12	0.47
1:A:518:TRP:CZ3	1:A:528:ARG:HB2	2.49	0.47
2:B:226:ARG:NH1	2:B:471:CYS:HB2	2.29	0.47
2:B:348:LYS:NZ	2:B:351:GLY:HA2	2.30	0.47
2:B:355:GLU:HA	2:B:358:ASP:HB2	1.96	0.47
2:B:269:ARG:CB	2:B:269:ARG:NH1	2.78	0.47
2:B:484:TYR:O	2:B:485:ARG:HB2	2.15	0.47
2:B:489:PRO:HB3	2:B:520:GLN:HB2	1.96	0.47
3:C:109:GLU:O	3:C:110:THR:HB	2.14	0.47
1:A:71:GLN:HE21	1:A:71:GLN:HB3	1.60	0.47
1:A:191:ALA:O	1:A:193:THR:N	2.48	0.47
2:B:189:ASN:OD1	2:B:240:HIS:CE1	2.68	0.47
1:A:82:HIS:NE2	2:B:95:GLN:HB2	2.29	0.46
1:A:107:ASP:C	1:A:109:ASP:H	2.19	0.46
1:A:68:GLN:O	1:A:81:ARG:NE	2.38	0.46
3:C:41:ARG:O	3:C:44:GLN:CG	2.62	0.46
3:C:79:VAL:HG13	3:C:177:LEU:HB3	1.98	0.46
1:A:138:TYR:HB3	1:A:181:ASN:ND2	2.30	0.46
1:A:6:ALA:HB1	1:A:40:GLY:H	1.80	0.46
2:B:512:ARG:NH2	2:B:527:SER:OG	2.48	0.46
1:A:262:ILE:O	1:A:322:GLU:HA	2.15	0.46
1:A:82:HIS:NE2	2:B:95:GLN:HB3	2.31	0.46
2:B:210:PHE:HE2	2:B:413:VAL:HG22	1.81	0.46
2:B:348:LYS:HZ1	2:B:351:GLY:HA2	1.79	0.46
1:A:14:TRP:CH2	1:A:50:ASP:HB2	2.51	0.46
1:A:154:GLU:C	1:A:156:ARG:H	2.19	0.46
2:B:29:ARG:HD3	2:B:56:CYS:SG	2.56	0.46
2:B:96:SER:HB2	2:B:99:ALA:N	2.30	0.46
2:B:226:ARG:HG2	2:B:471:CYS:O	2.16	0.46
2:B:70:GLY:HA2	2:B:82:ARG:NH1	2.30	0.45
2:B:151:ILE:HG22	2:B:152:LEU:HG	1.98	0.45
2:B:502:SER:HA	2:B:506:ARG:CG	2.46	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:56:CYS:O	2:B:57:VAL:HG13	2.16	0.45
2:B:327:ASN:CG	2:B:328:ASP:N	2.70	0.45
3:C:16:ILE:HD13	3:C:16:ILE:N	2.31	0.45
2:B:299:ILE:O	2:B:398:TRP:CH2	2.69	0.45
1:A:89:GLN:HG3	1:A:91:CYS:O	2.17	0.45
1:A:107:ASP:OD1	1:A:107:ASP:N	2.49	0.45
2:B:23:ASP:HA	2:B:24:PRO:HD3	1.85	0.45
2:B:173:TYR:O	2:B:174:GLU:C	2.53	0.45
2:B:183:TYR:O	2:B:186:PHE:HB3	2.16	0.45
1:A:443:LEU:H	1:A:443:LEU:HG	1.63	0.45
1:A:447:GLU:HG3	1:A:450:ARG:HH21	1.82	0.45
1:A:16:GLU:OE1	1:A:16:GLU:HA	2.16	0.44
1:A:350:LEU:HA	1:A:412:THR:HG22	1.98	0.44
2:B:235:LYS:O	2:B:308:LYS:HB2	2.16	0.44
2:B:129:THR:HB	2:B:217:GLN:HG2	1.98	0.44
2:B:162:VAL:HG22	2:B:250:TYR:HE1	1.83	0.44
1:A:165:GLU:O	3:C:70:ARG:NH2	2.50	0.44
2:B:383:THR:HA	2:B:388:GLU:OE2	2.18	0.44
2:B:516:ASN:OD1	2:B:516:ASN:N	2.25	0.44
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.80	0.44
2:B:96:SER:C	2:B:98:GLU:N	2.64	0.44
1:A:66:CYS:O	1:A:67:GLY:C	2.55	0.44
2:B:23:ASP:OD2	2:B:272:LEU:HG	2.18	0.44
1:A:452:ASN:OD1	1:A:455:ARG:NH2	2.51	0.44
2:B:371:VAL:HG21	2:B:385:ALA:O	2.17	0.44
2:B:408:ILE:HG22	2:B:411:VAL:HG23	2.00	0.44
2:B:316:TYR:CD2	2:B:353:LEU:HD12	2.53	0.44
1:A:353:GLN:NE2	2:B:387:GLN:OE1	2.44	0.43
2:B:50:ASP:OD1	2:B:50:ASP:N	2.36	0.43
2:B:11:CYS:HB2	2:B:39:SER:HB3	2.00	0.43
2:B:349:CYS:C	2:B:351:GLY:N	2.67	0.43
2:B:355:GLU:C	2:B:357:LYS:N	2.71	0.43
1:A:253:ASN:OD1	1:A:253:ASN:N	2.37	0.43
2:B:204:PHE:HE2	2:B:443:GLN:NE2	2.16	0.43
1:A:152:ASN:O	1:A:155:TRP:HD1	2.01	0.43
1:A:168:TYR:CD2	1:A:168:TYR:N	2.86	0.43
1:A:319:GLY:C	1:A:320:ILE:HG12	2.38	0.43
3:C:71:LYS:HA	3:C:75:ILE:O	2.19	0.43
2:B:325:ALA:C	2:B:327:ASN:H	2.22	0.43
2:B:520:GLN:CA	2:B:520:GLN:HE21	2.17	0.43
1:A:192:ASP:OD2	2:B:227:ARG:NH2	2.38	0.43



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)) overlap (Å)		
1:A:117:PRO:HD3	1:A:176:PHE:CD2	2.54	0.43		
2:B:34:TYR:HB2	2:B:445:GLU:OE2	2.19	0.43		
2:B:141:TYR:CG	2:B:258:MET:HG2	2.54	0.43		
2:B:190:VAL:C	2:B:192:GLU:N	2.72	0.43		
2:B:478:LEU:O	2:B:481:GLU:OE1	2.36	0.43		
1:A:245:PHE:HD1	1:A:390:ILE:HG21	1.84	0.43		
3:C:37:GLY:HA3	3:C:128:VAL:HG22	2.00	0.43		
2:B:183:TYR:HB3	2:B:234:THR:HB	2.00	0.43		
2:B:127:LEU:HD12	2:B:127:LEU:HA	1.80	0.42		
2:B:151:ILE:HD13	2:B:167:PRO:HG3	2.01	0.42		
1:A:170:GLY:C	1:A:172:ASP:H	2.23	0.42		
1:A:337:ILE:HG23	1:A:341:ASP:HB2	2.01	0.42		
1:A:528:ARG:NH2	5:A:558:BMA:O5	2.52	0.42		
2:B:283:PHE:CZ	2:B:439:LEU:HD13	2.54	0.42		
3:C:104:HIS:O	3:C:120:LEU:HA	2.19	0.42		
2:B:205:LYS:CE	2:B:418:GLU:OE1	2.68	0.42		
2:B:209:ILE:H	2:B:209:ILE:HG13	1.44	0.42		
2:B:457:ASN:HD21	2:B:491:ASP:N	2.03	0.42		
2:B:506:ARG:CZ	5:B:542:BMA:HO2	2.31	0.42		
2:B:514:CYS:O	2:B:515:ASN:CB	2.68	0.42		
2:B:212:LEU:C	2:B:214:ILE:H	2.23	0.42		
3:C:34:VAL:HG21	3:C:137:VAL:HG21	2.00	0.42		
2:B:30:TYR:CE1	2:B:271:PRO:HG3	2.55	0.42		
1:A:81:ARG:O	1:A:84:VAL:HB	2.20	0.42		
2:B:130:ASN:HD22	2:B:216:SER:HB2	1.84	0.42		
2:B:118:ILE:HG23	2:B:119:GLY:N	2.35	0.42		
2:B:201:SER:O	2:B:202:PHE:O	2.37	0.42		
1:A:211:LYS:HE2	1:A:477:VAL:HG22	2.01	0.41		
1:A:368:HIS:CG	1:A:369:CYS:N	2.88	0.41		
2:B:42:HIS:H	2:B:466:ARG:HH22	1.67	0.41		
2:B:179:GLU:O	2:B:180:TYR:CG	2.73	0.41		
3:C:78:GLN:HB3	3:C:176:VAL:HB	2.02	0.41		
1:A:155:TRP:CB	1:A:174:LYS:HA	2.50	0.41		
1:A:512:TRP:HH2	1:A:548:LYS:HB3	1.84	0.41		
2:B:187:GLU:CG	2:B:190:VAL:CG2	2.94	0.41		
1:A:518:TRP:CZ2	1:A:528:ARG:HD2	2.55	0.41		
2:B:408:ILE:CG2	2:B:411:VAL:HG23	2.50	0.41		
2:B:441:GLU:HA	2:B:444:LYS:NZ	2.35	0.41		
3:C:169:GLU:HG3	3:C:170:ALA:H	1.85	0.41		
2:B:128:PHE:CD2	2:B:443:GLN:HG3	2.55	0.41		
2:B:243:SER:O	2:B:299:ILE:O	2.39	0.41		



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:427:TYR:O	2:B:429:SER:N	2.53	0.41
3:C:44:GLN:HG3	3:C:45:GLU:OE1	2.20	0.41
3:C:47:GLY:C	3:C:49:ARG:N	2.73	0.41
1:A:246:LEU:HD21	1:A:488:GLN:OE1	2.21	0.41
1:A:33:LEU:N	1:A:463:GLU:OE1	2.28	0.41
1:A:284:MET:HE3	1:A:434:ILE:HD11	2.03	0.41
1:A:379:ARG:H	1:A:379:ARG:HG3	1.67	0.41
2:B:416:LEU:HD12	2:B:416:LEU:HA	1.85	0.41
3:C:41:ARG:HG2	3:C:42:PHE:N	2.35	0.41
2:B:356:ILE:HG13	2:B:364:TPO:O	2.20	0.41
2:B:381:ILE:HG13	2:B:386:TYR:CE1	2.56	0.41
1:A:249:LEU:C	1:A:251:LYS:N	2.72	0.41
2:B:208:GLY:HA2	2:B:412:LYS:HE2	2.02	0.41
3:C:119:TYR:CD1	3:C:128:VAL:HG12	2.56	0.41
1:A:72:CYS:SG	1:A:77:ARG:HB3	2.61	0.41
1:A:330:ALA:O	1:A:334:SER:OG	2.35	0.41
1:A:332:MET:SD	1:A:338:THR:HA	2.61	0.41
1:A:490:ARG:N	1:A:490:ARG:NE	2.67	0.41
2:B:108:CYS:C	2:B:110:HIS:H	2.23	0.41
2:B:247:VAL:HG13	2:B:403:GLN:HE22	1.86	0.41
2:B:327:ASN:CG	2:B:328:ASP:H	2.24	0.41
1:A:550:GLN:HG3	1:A:551:THR:H	1.86	0.41
2:B:79:CYS:SG	2:B:79:CYS:O	2.79	0.41
1:A:438:LEU:HD11	1:A:453:LEU:HD12	2.03	0.40
2:B:230:ARG:HE	2:B:230:ARG:HB2	1.59	0.40
3:C:55:LEU:HD22	3:C:131:TYR:CZ	2.56	0.40
3:C:105:VAL:HG13	3:C:120:LEU:HG	2.03	0.40
1:A:170:GLY:O	1:A:172:ASP:N	2.54	0.40
2:B:130:ASN:HD22	2:B:216:SER:CB	2.34	0.40
2:B:383:THR:HB	2:B:384:LEU:HD12	2.02	0.40
1:A:160:TYR:OH	1:A:165:GLU:CD	2.59	0.40
1:A:346:PHE:O	1:A:349:SER:OG	2.39	0.40
2:B:75:GLN:N	2:B:95:GLN:NE2	2.69	0.40
1:A:207:LEU:HD23	1:A:490:ARG:HG2	2.03	0.40
1:A:433:PRO:HD3	2:B:48:PHE:HA	2.02	0.40
2:B:111:GLU:HG3	2:B:155:ARG:HH12	1.86	0.40
2:B:138:ASP:HB2	2:B:260:HIS:HA	2.03	0.40
1:A:431:MET:CE	2:B:47:ASN:HD22	2.34	0.40
1:A:515:TRP:CH2	1:A:530:ARG:HD2	2.57	0.40
2:B:150:TYR:CE2	2:B:155:ARG:HG3	2.56	0.40
2:B:179:GLU:CG	2:B:322:HIS:HD2	2.34	0.40



All (1) 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)	
1:A:10:GLN:NE2	2:B:520:GLN:O[2_545]	2.07	0.13	

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	464/554~(84%)	386~(83%)	55~(12%)	23~(5%)	2	2
2	В	495/537~(92%)	412 (83%)	55 (11%)	28 (6%)	1	1
3	С	161/182~(88%)	146 (91%)	11 (7%)	4 (2%)	5	8
All	All	1120/1273 (88%)	944 (84%)	121 (11%)	55 (5%)	2	2

All (55) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	194	GLY
1	А	369	CYS
2	В	202	PHE
2	В	218	SER
2	В	350	ARG
2	В	363	ASP
2	В	519	PRO
3	С	48	HIS
3	С	173	GLN
1	А	24	GLN
1	А	67	GLY
1	А	73	LYS
1	А	155	TRP
1	А	192	ASP
2	В	57	VAL
2	В	66	VAL



Mol	Chain	Res	Type
2	В	93	GLY
2	В	214	ILE
2	B	215	SER
2	В	326	LYS
2	В	327	ASN
2	В	353	LEU
2	В	388	GLU
2	В	485	ARG
3	С	46	GLN
3	С	169	GLU
1	А	157	GLU
1	А	171	ASP
1	А	210	VAL
1	А	250	ASN
1	А	371	LYS
1	А	471	PRO
1	А	492	GLY
2	В	174	GLU
2	В	351	GLY
2	В	381	ILE
2	В	383	THR
2	В	390	PRO
1	А	248	GLU
2	В	60	ARG
2	В	95	GLN
2	В	173	TYR
2	В	503	CYS
1	А	64	ALA
1	А	110	CYS
1	А	203	ALA
1	А	383	ALA
1	А	446	LEU
1	А	491	LEU
2	В	147	SER
2	В	378	SER
2	В	428	SER
1	А	314	SER
2	В	191	THR
1	А	373	GLY



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	Pe	erce	entil	\mathbf{es}
1	А	412/466~(88%)	351~(85%)	61 (15%)		3	5	
2	В	446/472~(94%)	356~(80%)	90 (20%)		1	2	
3	С	134/149~(90%)	110 (82%)	24 (18%)		2	3	
All	All	992/1087~(91%)	817 (82%)	175 (18%)		2	3	

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	12	SER
1	А	19	ASP
1	А	33	LEU
1	А	34	LEU
1	А	45	SER
1	А	60	CYS
1	А	68	GLN
1	А	71	GLN
1	А	72	CYS
1	А	74	GLU
1	А	89	GLN
1	А	92	LEU
1	А	99	ASP
1	А	104	ARG
1	А	106	ILE
1	А	107	ASP
1	А	109	ASP
1	А	112	GLN
1	А	132	GLU
1	А	156	ARG
1	A	168	TYR
1	А	173	GLU
1	A	183	LEU
1	A	184	LYS
1	А	188	GLU
1	А	190	LEU



1 A 201 ASP 1 A 205 ASP 1 A 206 LEU 1 A 210 VAL 1 A 245 PHE 1 A 246 LEU 1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 205 ASP 1 A 206 LEU 1 A 210 VAL 1 A 245 PHE 1 A 246 LEU 1 A 246 LEU 1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 206 LEU 1 A 210 VAL 1 A 245 PHE 1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 210 VAL 1 A 245 PHE 1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 245 PHE 1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 246 LEU 1 A 247 ASN 1 A 248 GLU	
1 A 247 ASN 1 A 248 GLU	
1 A 248 GLU	
1 A 253 ASN	
1 A 272 LYS	
1 A 286 GLN	
1 A 293 ASP	
1 A 320 ILE	
1 A 332 MET	
1 A 334 SER	
1 A 340 ARG	
1 A 352 ILE	
1 A 376 LYS	
1 A 381 ARG	
1 A 382 LYS	
1 A 388 ASP	
1 A 394 ARG	
1 A 408 ARG	
1 A 439 ARG	
1 A 442 SER	
1 A 443 LEU	
1 A 453 LEU	
1 A 489 CYS	
1 A 490 ARG	
1 A 511 SER	
1 A 517 SER	
1 A 519 SER	
1 A 530 ARG	
1 A 549 VAL	
1 A 550 GLN	
2 B 7 MET	
2 B 23 ASP	
2 B 27 LYS	
2 B 34 TYR	
2 B 35 LEU	
2 B 50 ASP	\neg
2 B 56 CYS	



2 B 57 VAL 2 B 63 ARG 2 B 65 GLN 2 B 68 CYS 2 B 82 ARG 2 B 83 ARG 2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 102 ARG 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 188 ARG 2 B
2 B 63 ARG 2 B 65 GLN 2 B 68 CYS 2 B 82 ARG 2 B 83 ARG 2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 102 ARG 2 B 102 ARG 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 188 ARG 2 B 188 ARG 2 B </td
2 B 65 GLN 2 B 68 CYS 2 B 82 ARG 2 B 83 ARG 2 B 95 GLN 2 B 97 ASP 2 B 97 ASP 2 B 102 ARG 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 68 CYS 2 B 82 ARG 2 B 95 GLN 2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 102 ARG 2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 82 ARG 2 B 93 ARG 2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 102 ARG 2 B 102 ARG 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 83 ARG 2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 102 ARG 2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 95 GLN 2 B 97 ASP 2 B 102 ARG 2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 97 ASP 2 B 102 ARG 2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 163 GLU 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 188 ARG 2 B 188 ARG 2 B 182 GLU
2 B 102 ARG 2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 188 ARG 2 B 188 ARG
2 B 111 GLU 2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 125 ILE 2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 188 ARG 2 B 192 GLU
2 B 127 LEU 2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 179 GLU 2 B 188 ARG 2 B 192 GLU
2 B 131 SER 2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 147 SER 2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 152 LEU 2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 163 GLU 2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 164 SER 2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 169 THR 2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 170 GLN 2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 173 TYR 2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 179 GLU 2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 187 GLU 2 B 188 ARG 2 B 192 GLU
2 B 188 ARG 2 B 192 GLU
2 B 192 GLU
2 B 201 SER
2 B 209 ILE
2 B 215 SER
2 B 217 GLN
2 B 218 SER
2 B 220 ARG
2 B 222 LYS
2 B 227 ARG
2 B 229 LYS
2 B 230 ARG
2 B 234 THR
2 B 236 SER
2 B 237 VAL
2 B 250 TYR
2 B 255 ARG
2 B 266 ARG
2 B 269 ARG
2 B 273 GLU

Continued from previous page...



Mol	Chain	Res	Type
2	В	281	ASP
2	В	303	THR
2	В	315	ASP
2	В	345	SER
2	В	350	ARG
2	В	352	ILE
2	В	356	ILE
2	В	358	ASP
2	В	359	ARG
2	В	361	LYS
2	В	362	ARG
2	В	365	MET
2	В	368	ASP
2	В	379	GLU
2	В	383	THR
2	В	386	TYR
2	В	388	GLU
2	В	394	LEU
2	В	396	GLN
2	В	400	ASP
2	В	405	ASN
2	В	408	ILE
2	В	410	LYS
2	В	411	VAL
2	В	419	LEU
2	В	423	THR
2	В	429	SER
2	В	440	GLU
2	В	457	ASN
2	В	462	LEU
2	В	463	LYS
2	В	466	ARG
2	В	468	ASP
2	В	484	TYR
2	В	485	ARG
2	В	486	LYS
2	В	503	CYS
2	В	507	ARG
2	В	513	GLN
2	В	515	ASN
2	В	520	GLN
3	С	16	ILE



	5	1	1 0
\mathbf{Mol}	Chain	\mathbf{Res}	Type
3	С	19	LYS
3	С	32	LEU
3	С	41	ARG
3	С	45	GLU
3	С	54	THR
3	С	62	THR
3	С	67	SER
3	С	70	ARG
3	С	82	LEU
3	С	85	ASP
3	С	86	THR
3	С	95	GLN
3	С	105	VAL
3	С	121	GLU
3	С	127	SER
3	С	134	SER
3	С	135	LEU
3	С	138	SER
3	С	146	GLU
3	С	150	GLN
3	С	169	GLU
3	С	172	ASP
3	С	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	10	GLN
1	А	71	GLN
1	А	89	GLN
1	А	146	GLN
1	А	270	HIS
1	А	368	HIS
1	А	474	ASN
2	В	47	ASN
2	В	95	GLN
2	В	130	ASN
2	В	149	HIS
2	В	170	GLN
2	В	223	HIS
2	В	260	HIS
2	В	320	ASN



Mol	Chain	\mathbf{Res}	Type
2	В	322	HIS
2	В	327	ASN
2	В	403	GLN
2	В	405	ASN
2	В	457	ASN
2	В	499	ASN
2	В	515	ASN
3	С	44	GLN
3	С	81	GLN
3	С	95	GLN
3	С	125	GLN
3	С	158	GLN
3	С	175	HIS

Continued from previous page...

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Turne	Chain	Dec	Link	Bond lengths			Bond angles		
	Type		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPO	В	364	2	8,10,11	1.13	1 (12%)	10,14,16	1.14	1 (10%)

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
2	TPO	В	364	2	-	5/9/11/13	-



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	364	TPO	P-OG1	2.38	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	364	TPO	O3P-P-O2P	2.05	115.47	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	364	TPO	N-CA-CB-CG2
2	В	364	TPO	N-CA-CB-OG1
2	В	364	TPO	C-CA-CB-CG2
2	В	364	TPO	CA-CB-OG1-P
2	В	364	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	364	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	BMA	А	556	1	11,11,12	0.70	0	$15,\!15,\!17$	1.53	3 (20%)
5	BMA	В	539	2	11,11,12	0.52	0	$15,\!15,\!17$	1.11	1 (6%)
5	BMA	В	541	2	11,11,12	0.71	0	$15,\!15,\!17$	1.28	2 (13%)
5	BMA	А	558	1	11,11,12	0.70	0	15,15,17	1.77	3 (20%)
5	BMA	А	557	1	11,11,12	0.73	0	15,15,17	1.96	3 (20%)
5	BMA	В	542	2	11,11,12	0.83	0	15,15,17	1.09	1 (6%)
5	BMA	В	540	2	11,11,12	0.70	0	15,15,17	1.77	4 (26%)
5	BMA	А	559	1	11,11,12	1.02	1 (9%)	15,15,17	3.01	5 (33%)

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	BMA	А	556	1	-	2/2/19/22	0/1/1/1
5	BMA	В	539	2	-	0/2/19/22	0/1/1/1
5	BMA	В	541	2	-	2/2/19/22	0/1/1/1
5	BMA	А	558	1	-	2/2/19/22	0/1/1/1
5	BMA	А	557	1	-	2/2/19/22	0/1/1/1
5	BMA	В	542	2	-	2/2/19/22	0/1/1/1
5	BMA	В	540	2	-	0/2/19/22	0/1/1/1
5	BMA	А	559	1	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	559	BMA	C2-C3	2.06	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	559	BMA	C1-O5-C5	-8.10	101.22	112.19
5	А	557	BMA	C1-O5-C5	-5.09	105.29	112.19
5	А	559	BMA	O5-C5-C6	4.77	114.68	107.20
5	А	558	BMA	O5-C5-C6	4.36	114.04	107.20
5	А	559	BMA	C3-C4-C5	4.11	117.57	110.24
5	А	558	BMA	C1-O5-C5	-3.71	107.17	112.19
5	А	557	BMA	O5-C5-C6	3.67	112.95	107.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	540	BMA	C1-C2-C3	-3.62	105.21	109.67
5	А	559	BMA	C2-C3-C4	3.53	117.00	110.89
5	А	559	BMA	O2-C2-C1	3.26	115.81	109.15
5	В	542	BMA	O5-C5-C6	3.11	112.08	107.20
5	В	540	BMA	O5-C5-C6	2.82	111.62	107.20
5	А	556	BMA	O2-C2-C1	2.75	114.79	109.15
5	А	558	BMA	C3-C4-C5	2.53	114.75	110.24
5	В	539	BMA	O2-C2-C1	2.28	113.81	109.15
5	А	557	BMA	C3-C4-C5	2.27	114.29	110.24
5	В	541	BMA	O5-C5-C6	2.15	110.58	107.20
5	В	541	BMA	O3-C3-C4	-2.14	105.41	110.35
5	А	556	BMA	O5-C5-C6	2.10	110.50	107.20
5	В	540	BMA	O5-C5-C4	-2.08	105.78	110.83
5	А	556	BMA	O4-C4-C3	-2.02	105.67	110.35
5	В	540	BMA	C3-C4-C5	-2.01	106.65	110.24

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
5	А	557	BMA	O5-C5-C6-O6
5	В	541	BMA	O5-C5-C6-O6
5	А	557	BMA	C4-C5-C6-O6
5	А	559	BMA	O5-C5-C6-O6
5	В	541	BMA	C4-C5-C6-O6
5	А	558	BMA	C4-C5-C6-O6
5	А	556	BMA	C4-C5-C6-O6
5	А	558	BMA	O5-C5-C6-O6
5	А	559	BMA	C4-C5-C6-O6
5	А	556	BMA	O5-C5-C6-O6
5	В	542	BMA	O5-C5-C6-O6
5	В	542	BMA	C4-C5-C6-O6

All (12) torsion outliers are listed below:

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	541	BMA	1	0
5	А	558	BMA	1	0
5	В	542	BMA	2	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	<RSRZ $>$	> #RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	478/554~(86%)	0.44	27 (5%)	24 25	23, 54, 78, 94	1 (0%)
2	В	503/537~(93%)	0.32	20 (3%)	38 41	26, 48, 74, 86	0
3	С	165/182~(90%)	0.21	4 (2%) 5	59 62	28, 53, 77, 83	0
All	All	1146/1273~(90%)	0.35	51 (4%)	33 36	23, 50, 77, 94	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	108	CYS	7.8
1	А	281	ASP	6.6
1	А	491	LEU	6.0
1	А	492	GLY	4.8
2	В	93	GLY	4.6
2	В	216	SER	4.4
1	А	371	LYS	4.1
2	В	502	SER	4.0
1	А	527	GLU	4.0
2	В	346	VAL	3.9
1	А	409	SER	3.8
1	А	3	THR	3.7
1	А	521	CYS	3.6
1	А	507	LYS	3.5
2	В	345	SER	3.4
2	В	109	GLN	3.4
3	С	173	GLN	3.4
1	А	509	ASP	3.3
1	А	494	LEU	3.2
1	А	386	VAL	3.0
1	А	490	ARG	3.0
2	В	192	GLU	3.0
1	А	99	ASP	2.9



Mol	Chain	\mathbf{Res}	Type	RSRZ
3	С	174	PHE	2.9
1	А	164	CYS	2.8
2	В	234	THR	2.7
2	В	66	VAL	2.7
1	А	98	ASP	2.7
3	С	16	ILE	2.6
2	В	389	LEU	2.6
1	А	23	CYS	2.6
2	В	503	CYS	2.6
2	В	505	GLY	2.6
2	В	94	ASP	2.6
2	В	315	ASP	2.6
2	В	173	TYR	2.5
1	А	506	ALA	2.5
3	С	42	PHE	2.5
1	А	377	THR	2.4
2	В	57	VAL	2.4
1	А	372	PHE	2.2
1	А	252	TYR	2.2
1	А	522	ARG	2.2
1	А	517	SER	2.1
1	А	410	THR	2.1
1	A	389	ILE	2.1
1	A	508	ALA	2.0
2	В	347	GLY	2.0
1	А	103	VAL	2.0
2	В	170	GLN	2.0
2	В	518	PRO	2.0

Continued from previous page...

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	TPO	В	364	11/12	0.68	0.24	69,71,79,79	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	В	542	11/12	0.60	0.30	56,60,62,62	0
5	BMA	А	559	11/12	0.67	0.33	79,81,81,82	0
5	BMA	В	540	11/12	0.83	0.32	63,67,67,70	0
5	BMA	А	556	11/12	0.91	0.14	47,51,56,59	0
5	BMA	А	558	11/12	0.93	0.12	$63,\!65,\!67,\!67$	0
5	BMA	А	557	11/12	0.94	0.18	$58,\!61,\!61,\!62$	0
5	BMA	В	539	11/12	0.94	0.13	56,59,62,64	0
5	BMA	В	541	11/12	0.96	0.12	39,42,44,46	0
4	CA	В	538	1/1	0.96	0.15	38,38,38,38	0
4	CA	А	555	1/1	0.98	0.09	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.

