

Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 12:20 PM EDT

PDB ID	:	1QU7
Title	:	FOUR HELICAL-BUNDLE STRUCTURE OF THE CYTOPLASMIC DO-
		MAIN OF A SERINE CHEMOTAXIS RECEPTOR
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Deposited on	:	1999-07-07
Resolution	:	2.60 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

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 2.60 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	Whole archive $(\#Entries)$	Similar resolution (#Entries, resolution range(Å))		
Rfree	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	227	26%	64%	10%		
1	В	227	28%	59%	9% •		



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3430 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 METHYL-ACCEPTING CHEMOTAXIS PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	227	Total	С	Ν	0	S	0	0	0
1	I A	221	1643	989	302	347	5	0		
1	р	221	Total	С	Ν	0	S	0	0	0
I D	221	1600	966	292	337	5	0	0	0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	304	GLN	GLU	engineered mutation	UNP P02942
А	493	GLN	GLU	engineered mutation	UNP P02942
В	304	GLN	GLU	engineered mutation	UNP P02942
В	493	GLN	GLU	engineered mutation	UNP P02942

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	87	Total O 87 87	0	0
2	В	100	Total O 100 100	0	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: METHYL-ACCEPTING CHEMOTAXIS PROTEIN I



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	132.44Å 132.44 Å 134.59 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	100.00 - 2.60	Depositor
Resolution (A)	43.65 - 2.59	EDS
% Data completeness	(Not available) (100.00-2.60)	Depositor
(in resolution range)	59.2(43.65-2.59)	EDS
R_{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 2.58 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.243 , 0.276	Depositor
n, n_{free}	0.265 , 0.312	DCC
R_{free} test set	1452 reflections (4.92%)	wwPDB-VP
Wilson B-factor $(Å^2)$	35.6	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 83.6	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3430	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.13% 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)

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	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.62	1/1646~(0.1%)	0.80	0/2226	
1	В	0.59	0/1603	0.78	0/2168	
All	All	0.61	1/3249~(0.0%)	0.79	0/4394	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	335	GLU	CD-OE2	6.89	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1643	0	1632	278	0
1	В	1600	0	1600	251	0
2	А	87	0	0	27	0
2	В	100	0	0	29	0
All	All	3430	0	3232	462	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 71.

All (462) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:406:LEU:HD23	1:B:375:THR:HG22	1.20	1.18
1:A:438:ALA:HB2	1:B:343:VAL:HG11	1.26	1.16
1:B:312:LEU:HB3	1:B:470:ILE:HD11	1.25	1.08
1:B:432:SER:O	1:B:436:GLU:HG2	1.61	1.00
1:A:312:LEU:HB3	1:A:470:ILE:HD11	1.44	0.99
1:B:467:SER:O	1:B:470:ILE:HG22	1.68	0.93
1:A:294:ARG:HH11	1:A:294:ARG:HB3	1.36	0.89
1:A:516:ARG:O	1:A:518:GLN:N	2.05	0.89
1:A:338:GLN:HE21	1:A:338:GLN:HA	1.39	0.87
1:B:345:ASP:O	1:B:348:VAL:HG12	1.73	0.87
1:A:517:ILE:C	1:A:519:GLN:H	1.78	0.86
1:B:412:GLN:HB2	2:B:652:HOH:O	1.75	0.85
1:A:425:VAL:O	1:A:428:VAL:HG12	1.77	0.85
1:B:420:LEU:HD23	1:B:420:LEU:C	1.97	0.84
1:B:354:ILE:HD11	1:B:428:VAL:HG22	1.59	0.84
1:B:483:VAL:O	1:B:486:GLN:HB2	1.77	0.84
1:A:347:VAL:HG22	1:B:434:LEU:HB3	1.60	0.82
1:A:459:ILE:HG12	1:B:319:ASN:ND2	1.95	0.82
1:A:336:THR:HG22	1:B:445:ILE:HG12	1.60	0.81
1:A:300:ALA:HA	1:A:303:GLU:HG2	1.62	0.81
1:B:312:LEU:HB3	1:B:470:ILE:CD1	2.10	0.80
1:B:450:THR:HA	2:B:640:HOH:O	1.81	0.79
1:A:438:ALA:CB	1:B:343:VAL:HG11	2.10	0.79
1:A:361:ILE:HD11	1:B:420:LEU:HD21	1.63	0.78
1:B:463:SER:HA	1:B:466:GLN:HB2	1.63	0.78
1:A:332:SER:HB3	1:B:448:ALA:HB2	1.65	0.78
1:A:472:GLN:HB2	2:B:756:HOH:O	1.82	0.78
1:A:481:ASP:HA	1:A:484:THR:HG22	1.66	0.77
1:A:329:LEU:HD21	1:B:451:ARG:HD3	1.66	0.77
1:A:422:GLU:O	1:A:425:VAL:HG22	1.86	0.76
1:A:497:ALA:O	1:A:501:LEU:HD13	1.86	0.76
1:A:325:GLN:HE21	1:B:455:ILE:HD11	1.51	0.75
1:A:325:GLN:HE21	1:B:455:ILE:CD1	1.99	0.74
1:B:454:ASP:O	1:B:458:GLU:HG2	1.87	0.74
1:A:516:ARG:C	1:A:518:GLN:H	1.91	0.74
1:B:316:VAL:CG2	1:B:466:GLN:HG2	2.18	0.74
1:B:302:LEU:HB2	1:B:480:MET:HE2	1.69	0.74
1:A:503:GLU:HG3	2:A:628:HOH:O	1.88	0.73
1:B:441:THR:O	1:B:445:ILE:HG12	1.89	0.73
1:B:316:VAL:HG21	1:B:466:GLN:HG2	1.68	0.73
1:A:446:VAL:O	1:A:450:THR:HB	1.89	0.73
1:B:302:LEU:CD2	1:B:481:ASP:HB2	2.18	0.73



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlan (Å)		
1·B·302·LEU·HB2	1.B.480.MET.CE	2.18	0.72		
1:A:329:LEU:O	1.B.448.ALA.HB1	1.89	0.72		
1.A.330.ALA.HB1	$1 \cdot A \cdot 452 \cdot VAL \cdot CG1$	2.19	0.72		
1.B.318.GLN.HG3	1.B.319.ASN.H	1 54	0.72		
1:A:300:ALA:HA	1:A:303:GLU:CG	2.19	0.72		
1.B.415.ABG.O	1.B.418.LVS.HB3	1.89	0.72		
1.B.336.THB.HA	1.B.339.ABG.HD3	1.80	0.72		
1:A:327:SEB:O	1.A.331.LEU.HD23	1.10	0.72		
1:B:311:GLN:OE1	1:B:312:LEU:HD12	1.89	0.71		
1·B·432·SEB·HB2	2·B·613·HOH·O	1.89	0.71		
1.B.354.ILE.HG13	1·B·355·SEB·N	2.05	0.71		
1.B.312.LEU.CB	1.B.470.ILE.HD11	2.00	0.71		
1·B·378·LEU·HD23	1.B.378.LEU.C	2.10	0.71		
1:A:459:ILE:HG12	1·B·319·ASN·HD21	1 53	0.70		
1:A:378:LEU:HA	1.A.381.ASN.HD22	1.56	0.70		
1.R.381.ASN.O	1.R.384.VAL:HG22	1.00	0.70		
1.A.459.ILE.HA	1.B.319 ASN HD21	1.52	0.70		
1.B.371.ILE.O	1.B.375.THB.HG23	1.01	0.70		
1.A.406.LEU.HD23	1.B.375.THB.CG2	2.12	0.70		
1:A:338:GLN:HA	1:A:338:GLN:NE2	2.12	0.10		
1.A.304.GLN.HG3	1.A.305.THB.N	2.00	0.69		
1.B.452.VAL:O	1.B.456.MET.HG2	1.92	0.69		
1:B:301:SEB:O	1.B.305.THB.HG23	1.02	0.69		
1:A:395:GLY:O	1.A.398.VAL:HG13	1.02	0.69		
1·A·329·LEU·HD11	1.B.451.ARG.HB2	1.01	0.69		
1.B.450.THB.HG23	2·B·651·HOH·O	1.10	0.68		
1.B.361.ILE.HG22	1·B·362·ALA·N	2.09	0.68		
1:A:361:ILE:HG23	1·B·417·ILE·HD12	1.76	0.68		
1:A:361:ILE:CG1	1.B.420.LEU.HD21	2.24	0.67		
1.A.333.ALA.HB2	1.B.448.ALA.HB3	1.77	0.67		
1:A:361:ILE:CD1	1:B:420:LEU:HD21	2.25	0.67		
1:A·481:ASP·HA	1:A:484:THB:CG2	2.24	0.67		
1:A:420:LEU:HD11	1.B.360.LYS.HD2	1.77	0.67		
1:A:343:VAL:HG12	1.B.438.ALA.HB2	1.76	0.66		
1:A:365:ILE:HG13	1:A:417:ILE:HD11	1.77	0.66		
1:A:451:ARG:HB2	1:B:329:LEU:HD21	1.78	0.66		
1:B:355:SER:HB2	1:B:428:VAL:HG11	1.78	0.66		
1:A:452:VAL:O	1:A:456:MET:HB2	1.96	0.66		
1:B:373:PHE:HA	2:B:645:HOH:O	1.95	0.66		
1:B:443:ALA:O	1:B:446:VAL:HG12	1.95	0.65		
1:B:420:LEU:HD23	1:B:421:ILE:N	2.10	0.65		



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:375:THR:OG1	1:B:406:LEU:HD23	1.95	0.65	
1:A:418:LYS:O	1:A:421:ILE:HG22	1.97	0.65	
1:B:311:GLN:O	1:B:314:ALA:HB3	1.96	0.65	
1:A:493:GLN:O	1:A:496:ALA:HB3	1.97	0.65	
1:B:436:GLU:HA	2:B:616:HOH:O	1.95	0.65	
1:A:315:THR:CB	1:B:466:GLN:HE22	2.09	0.65	
1:B:416:GLU:HB3	2:B:620:HOH:O	1.96	0.64	
1:A:312:LEU:HB3	1:A:470:ILE:CD1	2.25	0.64	
1:B:443:ALA:HB3	2:B:610:HOH:O	1.98	0.64	
1:A:361:ILE:HD11	1:B:420:LEU:CD2	2.27	0.64	
1:B:514:VAL:O	1:B:518:GLN:HB3	1.97	0.64	
1:A:313:THR:O	1:A:316:VAL:HG12	1.97	0.64	
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.63	0.64	
1:B:454:ASP:C	1:B:458:GLU:HG2	2.18	0.64	
1:A:406:LEU:CD2	1:B:375:THR:HG22	2.13	0.64	
1:A:417:ILE:C	1:A:417:ILE:HD13	2.18	0.64	
1:A:339:ARG:HA	1:A:342:LYS:HE2	1.79	0.64	
1:A:350:THR:O	1:A:354:ILE:HD13	1.97	0.64	
1:B:443:ALA:HB1	2:B:625:HOH:O	1.96	0.64	
1:A:361:ILE:O	1:A:364:ILE:N	2.27	0.63	
1:B:450:THR:HG21	2:B:636:HOH:O	1.97	0.63	
1:A:479:GLU:O	1:A:483:VAL:HG22	1.98	0.63	
1:B:511:ALA:O	1:B:514:VAL:HG22	1.99	0.63	
1:A:420:LEU:HD22	1:B:361:ILE:HD11	1.79	0.63	
1:A:447:SER:O	1:A:450:THR:HG22	1.99	0.63	
1:B:468:ARG:O	1:B:472:GLN:HG3	1.98	0.62	
1:A:332:SER:HB3	1:B:448:ALA:CB	2.29	0.62	
1:A:417:ILE:HG22	1:B:364:ILE:HG21	1.80	0.62	
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.14	0.62	
1:B:378:LEU:C	1:B:378:LEU:CD2	2.68	0.62	
1:B:520:GLN:HA	2:B:637:HOH:O	1.99	0.62	
1:A:396:PHE:HA	1:B:396:PHE:CZ	2.34	0.62	
1:A:304:GLN:HG3	1:A:305:THR:CG2	2.30	0.62	
1:B:316:VAL:HG21	1:B:466:GLN:CG	2.29	0.62	
1:A:336:THR:HG21	1:B:444:GLU:C	2.20	0.62	
1:A:517:ILE:C	1:A:519:GLN:N	2.49	0.61	
1:A:503:GLU:O	1:A:506:SER:N	2.32	0.61	
1:B:347:VAL:O	1:B:351:MET:HG2	2.00	0.61	
1:A:300:ALA:CA	1:A:303:GLU:HG2	2.28	0.61	
1:A:330:ALA:HB1	1:A:452:VAL:HG11	1.81	0.61	
1:A:364:ILE:CG2	1:B:417:ILE:HD11	2.31	0.60	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:295:THR:HG23	2:A:765:HOH:O	2.01	0.60	
1:B:305:THR:HG22	2:B:756:HOH:O	2.01	0.60	
1:B:302:LEU:HD22	1:B:481:ASP:HB2	1.83	0.60	
1:B:302:LEU:HD23	1:B:481:ASP:HB2	1.82	0.60	
1:A:326:ALA:O	1:A:330:ALA:HB2	2.02	0.60	
1:A:378:LEU:HD21	1:B:402:GLU:CG	2.32	0.60	
1:B:318:GLN:C	1:B:320:ALA:H	2.05	0.60	
1:B:517:ILE:C	1:B:519:GLN:H	2.04	0.60	
1:B:320:ALA:HB1	2:B:760:HOH:O	2.02	0.60	
1:B:465:GLU:OE1	1:B:465:GLU:HA	2.02	0.59	
1:A:317:LYS:HG3	1:A:318:GLN:N	2.16	0.59	
1:A:483:VAL:C	1:A:485:GLN:N	2.52	0.59	
1:B:309:MET:O	1:B:312:LEU:HB2	2.03	0.59	
1:A:325:GLN:HG3	1:A:326:ALA:N	2.17	0.59	
1:A:428:VAL:O	1:A:432:SER:HB2	2.03	0.59	
1:A:393:GLY:O	1:A:396:PHE:N	2.36	0.58	
1:B:451:ARG:O	1:B:454:ASP:N	2.35	0.58	
1:A:329:LEU:HD11	1:B:448:ALA:O	2.03	0.58	
1:A:354:ILE:HG22	1:A:355:SER:N	2.18	0.58	
1:A:454:ASP:O	1:A:458:GLU:HG2	2.03	0.58	
1:A:315:THR:HB	1:B:466:GLN:HE22	1.69	0.58	
2:A:695:HOH:O	1:B:339:ARG:HB3	2.02	0.58	
1:A:316:VAL:O	1:A:320:ALA:HB2	2.04	0.58	
1:A:336:THR:C	1:B:445:ILE:HD11	2.23	0.57	
1:A:380:LEU:C	1:A:380:LEU:HD23	2.24	0.57	
1:B:510:GLU:O	1:B:513:ALA:HB3	2.03	0.57	
1:B:427:LYS:C	1:B:429:ASP:N	2.58	0.57	
1:A:467:SER:OG	1:A:468:ARG:N	2.37	0.57	
1:A:392:GLN:N	1:A:392:GLN:OE1	2.36	0.57	
1:A:449:VAL:HG12	1:A:449:VAL:O	2.03	0.57	
1:B:318:GLN:CG	1:B:319:ASN:H	2.17	0.57	
1:B:354:ILE:CG1	1:B:355:SER:N	2.67	0.57	
1:A:394:ARG:O	1:A:397:ALA:HB3	2.05	0.57	
1:A:420:LEU:HD22	1:B:361:ILE:CD1	2.35	0.57	
1:B:378:LEU:HD23	1:B:378:LEU:O	2.04	0.57	
1:A:481:ASP:CA	1:A:484:THR:HG22	2.34	0.56	
1:A:455:ILE:HG22	1:A:456:MET:HE2	1.87	0.56	
1:A:314:ALA:HB3	2:A:654:HOH:O	2.05	0.56	
1:A:402:GLU:O	1:A:406:LEU:HD13	2.05	0.56	
1:A:304:GLN:CG	1:A:305:THR:N	2.69	0.56	
1:B:350:THR:O	1:B:353:ASP:HB2	2.04	0.56	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:306:ALA:O	1:A:310:GLU:HG3	2.06	0.56
1:A:415:ARG:O	1:A:418:LYS:N	2.34	0.56
1:B:451:ARG:O	1:B:454:ASP:HB2	2.06	0.56
1:B:483:VAL:HA	1:B:486:GLN:HG3	1.88	0.56
1:A:364:ILE:O	1:A:367:VAL:HB	2.06	0.55
1:B:412:GLN:O	1:B:416:GLU:HG3	2.05	0.55
1:A:433:THR:O	1:A:436:GLU:HB3	2.07	0.55
1:B:334:SER:O	1:B:338:GLN:HG3	2.07	0.55
1:A:483:VAL:C	1:A:485:GLN:H	2.10	0.55
1:A:492:GLU:HB3	2:A:678:HOH:O	2.06	0.55
1:B:311:GLN:OE1	1:B:311:GLN:C	2.45	0.55
1:B:468:ARG:O	1:B:471:ASP:HB3	2.05	0.55
1:A:503:GLU:O	1:A:504:GLN:C	2.43	0.55
2:A:695:HOH:O	1:B:339:ARG:CB	2.53	0.55
1:B:357:SER:HB3	2:B:778:HOH:O	2.06	0.55
1:A:315:THR:OG1	1:B:466:GLN:NE2	2.39	0.55
1:A:393:GLY:O	1:A:394:ARG:C	2.45	0.55
1:A:361:ILE:HG21	1:A:421:ILE:CD1	2.36	0.55
1:A:515:PHE:O	2:A:741:HOH:O	2.18	0.55
1:A:304:GLN:HB2	2:A:702:HOH:O	2.07	0.54
1:A:378:LEU:HD12	2:A:680:HOH:O	2.06	0.54
1:B:402:GLU:OE1	1:B:402:GLU:HA	2.06	0.54
1:B:511:ALA:HA	2:B:712:HOH:O	2.07	0.54
1:A:300:ALA:C	1:A:303:GLU:HG2	2.28	0.54
1:A:325:GLN:O	1:A:329:LEU:N	2.35	0.54
1:A:393:GLY:O	1:A:395:GLY:N	2.40	0.54
1:B:318:GLN:O	1:B:320:ALA:N	2.41	0.54
1:B:427:LYS:C	1:B:429:ASP:H	2.10	0.54
1:A:336:THR:HB	1:B:445:ILE:HD13	1.88	0.54
1:B:318:GLN:C	1:B:320:ALA:N	2.61	0.54
1:A:352:ARG:C	1:A:354:ILE:H	2.11	0.53
1:B:334:SER:HB2	1:B:449:VAL:HG12	1.90	0.53
1:A:422:GLU:HG3	1:A:423:ASP:N	2.23	0.53
1:A:359:GLN:C	1:A:361:ILE:N	2.61	0.53
1:A:332:SER:CB	1:B:448:ALA:HB2	2.36	0.53
1:A:399:VAL:O	1:A:403:VAL:HG23	2.08	0.53
1:B:365:ILE:HG13	1:B:417:ILE:HG21	1.91	0.53
1:B:455:ILE:O	1:B:459:ILE:HG23	2.09	0.53
1:A:376:ASN:ND2	1:A:404:ARG:HE	2.07	0.53
1:A:434:LEU:HD12	2:B:749:HOH:O	2.08	0.53
1:A:466:GLN:O	1:A:470:ILE:HB	2.09	0.53



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:516:ARG:O	1:A:519:GLN:N	2.42	0.53	
1:A:304:GLN:HG3	1:A:305:THR:HG22	1.91	0.52	
1:A:420:LEU:HD13	1:B:361:ILE:HG13	1.91	0.52	
1:A:434:LEU:HD21	2:A:627:HOH:O	2.09	0.52	
1:A:474:GLY:O	1:A:477:VAL:HG23	2.09	0.52	
2:A:663:HOH:O	1:B:329:LEU:HD23	2.09	0.52	
1:B:454:ASP:HA	2:B:604:HOH:O	2.09	0.52	
1:A:315:THR:HG23	2:A:654:HOH:O	2.08	0.52	
1:A:345:ASP:HA	2:A:728:HOH:O	2.09	0.52	
1:A:367:VAL:O	1:A:371:ILE:HD13	2.10	0.52	
1:B:455:ILE:HG22	1:B:456:MET:HE2	1.89	0.52	
1:A:361:ILE:O	1:A:364:ILE:HB	2.09	0.52	
1:B:330:ALA:HB2	1:B:452:VAL:HG12	1.92	0.52	
1:B:340:GLY:O	1:B:344:VAL:HB	2.10	0.52	
1:B:440:GLU:HA	2:B:610:HOH:O	2.10	0.52	
1:A:378:LEU:O	1:A:379:ALA:C	2.48	0.52	
1:A:422:GLU:HG3	1:A:423:ASP:H	1.74	0.52	
1:A:330:ALA:CB	1:A:452:VAL:CG1	2.88	0.52	
1:B:343:VAL:O	1:B:347:VAL:HG23	2.10	0.52	
1:A:402:GLU:HB3	1:B:378:LEU:HD11	1.92	0.51	
1:B:321:GLU:OE1	1:B:321:GLU:HA	2.09	0.51	
1:A:418:LYS:O	1:A:422:GLU:HG2	2.10	0.51	
1:B:395:GLY:O	1:B:398:VAL:HG22	2.10	0.51	
1:A:379:ALA:O	1:A:382:ALA:HB3	2.11	0.51	
1:A:496:ALA:O	1:A:499:ALA:N	2.43	0.51	
1:A:518:GLN:CB	2:A:658:HOH:O	2.58	0.51	
1:B:506:SER:O	1:B:510:GLU:HG2	2.10	0.51	
1:A:485:GLN:OE1	1:A:485:GLN:HA	2.10	0.51	
1:B:479:GLU:O	1:B:480:MET:C	2.49	0.51	
1:A:480:MET:O	1:A:484:THR:HG22	2.11	0.51	
1:B:318:GLN:CG	1:B:319:ASN:N	2.73	0.51	
1:B:328:HIS:C	1:B:330:ALA:N	2.63	0.51	
1:B:323:ALA:CB	1:B:459:ILE:HD11	2.41	0.51	
1:A:376:ASN:HD21	1:A:404:ARG:HE	1.59	0.51	
1:B:514:VAL:HG23	1:B:515:PHE:N	2.26	0.51	
1:A:331:LEU:HA	1:A:334:SER:HB3	1.94	0.50	
1:A:517:ILE:HA	2:A:665:HOH:O	2.11	0.50	
1:B:321:GLU:OE1	1:B:324:ARG:HB2	2.11	0.50	
1:B:391:GLU:OE1	1:B:391:GLU:HA	2.11	0.50	
1:A:395:GLY:O	1:A:396:PHE:C	2.50	0.50	
1:A:404:ARG:O	1:A:408:GLN:HG3	2.12	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:510:GLU:O	1:A:511:ALA:C	2.50	0.50	
1:A:512:VAL:O	1:A:513:ALA:C	2.50	0.50	
1:A:420:LEU:CD1	1:B:361:ILE:HG13	2.40	0.50	
1:A:498:ALA:O	1:A:502:GLU:HG3	2.11	0.50	
1:B:327:SER:HB2	1:B:456:MET:HB2	1.94	0.50	
1:A:374:GLN:HG3	2:A:743:HOH:O	2.12	0.50	
1:A:402:GLU:HG3	2:A:641:HOH:O	2.10	0.50	
1:A:434:LEU:N	1:A:434:LEU:HD23	2.27	0.50	
1:A:469:GLY:O	1:A:472:GLN:HG2	2.12	0.50	
1:A:456:MET:SD	1:B:456:MET:SD	3.09	0.49	
1:A:309:MET:CE	1:A:473:VAL:HG12	2.41	0.49	
1:A:440:GLU:C	1:A:442:MET:H	2.14	0.49	
1:A:451:ARG:C	1:A:453:THR:N	2.66	0.49	
1:A:316:VAL:HG23	1:A:466:GLN:HB2	1.94	0.49	
1:A:475:LEU:O	1:A:478:ALA:HB3	2.12	0.49	
1:A:294:ARG:HH11	1:A:294:ARG:CB	2.15	0.49	
1:A:501:LEU:HD21	1:B:501:LEU:HD21	1.93	0.49	
2:A:754:HOH:O	1:B:333:ALA:HA	2.11	0.49	
1:B:306:ALA:O	1:B:309:MET:HB2	2.12	0.49	
1:B:328:HIS:HA	2:B:607:HOH:O	2.12	0.49	
1:B:332:SER:C	1:B:334:SER:H	2.15	0.49	
1:B:360:LYS:C	1:B:360:LYS:HD3	2.32	0.49	
1:A:361:ILE:CG2	1:A:421:ILE:CD1	2.90	0.49	
1:B:340:GLY:HA3	1:B:442:MET:HG2	1.94	0.49	
1:A:384:VAL:O	1:A:388:ARG:HG3	2.12	0.49	
1:B:375:THR:OG1	1:B:407:ALA:HB2	2.13	0.49	
1:A:438:ALA:HB2	1:B:343:VAL:CG1	2.18	0.48	
1:A:463:SER:HA	1:A:466:GLN:HG3	1.94	0.48	
1:A:474:GLY:HA2	1:A:477:VAL:CG2	2.43	0.48	
1:B:316:VAL:HG23	1:B:466:GLN:HG2	1.94	0.48	
1:B:353:ASP:HB3	2:B:758:HOH:O	2.12	0.48	
1:A:376:ASN:HD21	1:A:404:ARG:NE	2.12	0.48	
1:A:359:GLN:C	1:A:361:ILE:H	2.16	0.48	
1:A:415:ARG:O	1:A:416:GLU:C	2.52	0.48	
1:A:303:GLU:O	1:A:307:ALA:HB3	2.14	0.48	
1:A:347:VAL:CG2	1:B:434:LEU:HB3	2.38	0.48	
1:A:481:ASP:O	1:A:485:GLN:HB2	2.14	0.48	
1:A:503:GLU:HA	2:A:768:HOH:O	2.12	0.48	
1:B:426:GLY:O	1:B:429:ASP:HB3	2.13	0.48	
1:B:513:ALA:HA	2:B:706:HOH:O	2.14	0.48	
1:A:304:GLN:OE1	1:B:472:GLN:HB3	2.13	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:352:ARG:C	1:A:354:ILE:N	2.66	0.48	
1:A:496:ALA:O	1:A:498:ALA:N	2.47	0.48	
1:B:318:GLN:OE1	1:B:319:ASN:N	2.46	0.48	
1:B:350:THR:OG1	1:B:351:MET:N	2.47	0.48	
1:B:454:ASP:O	1:B:457:GLY:N	2.46	0.48	
1:B:479:GLU:O	1:B:482:ARG:N	2.46	0.48	
1:A:353:ASP:HA	1:A:356:THR:HG23	1.94	0.47	
1:A:361:ILE:CG1	1:B:420:LEU:CD2	2.92	0.47	
1:A:417:ILE:HD13	1:A:417:ILE:O	2.14	0.47	
1:A:430:VAL:O	1:A:434:LEU:HG	2.14	0.47	
1:A:481:ASP:O	1:A:484:THR:HG22	2.14	0.47	
1:B:331:LEU:O	1:B:335:GLU:OE1	2.32	0.47	
1:A:299:ALA:O	1:A:303:GLU:OE2	2.32	0.47	
1:A:403:VAL:O	1:A:404:ARG:C	2.51	0.47	
1:A:424:SER:O	1:A:426:GLY:N	2.47	0.47	
1:B:302:LEU:HB2	1:B:480:MET:HE1	1.93	0.47	
1:B:488:ALA:O	1:B:492:GLU:HG2	2.13	0.47	
1:A:374:GLN:HG2	1:B:406:LEU:HD21	1.96	0.47	
1:A:458:GLU:OE1	1:A:458:GLU:HA	2.15	0.47	
1:A:487:ASN:HB2	1:B:487:ASN:OD1	2.14	0.47	
1:A:425:VAL:C	1:A:428:VAL:HG12	2.35	0.47	
1:A:459:ILE:O	1:A:463:SER:HB3	2.14	0.47	
1:B:328:HIS:C	1:B:330:ALA:H	2.16	0.47	
1:B:334:SER:HB2	1:B:449:VAL:CG1	2.44	0.47	
1:B:446:VAL:HG13	2:B:609:HOH:O	2.14	0.47	
1:A:431:GLY:O	1:A:435:VAL:HG12	2.14	0.47	
1:B:324:ARG:NH1	1:B:327:SER:HB3	2.29	0.47	
1:B:504:GLN:O	1:B:507:ARG:HB3	2.15	0.47	
1:B:300:ALA:HB3	2:B:770:HOH:O	2.14	0.47	
1:B:311:GLN:OE1	1:B:312:LEU:N	2.48	0.47	
1:A:313:THR:C	1:A:316:VAL:HG12	2.34	0.47	
1:A:352:ARG:O	1:A:354:ILE:N	2.47	0.47	
1:B:360:LYS:HD3	1:B:360:LYS:O	2.15	0.47	
1:B:399:VAL:O	1:B:403:VAL:HG23	2.15	0.47	
1:A:309:MET:HE2	1:A:473:VAL:HG12	1.96	0.46	
1:A:342:LYS:HG3	2:A:642:HOH:O	2.15	0.46	
1:A:302:LEU:HB2	2:A:623:HOH:O	2.14	0.46	
1:A:415:ARG:O	1:A:418:LYS:HB3	2.16	0.46	
1:B:356:THR:OG1	1:B:357:SER:N	2.49	0.46	
1:B:432:SER:C	1:B:435:VAL:HG12	2.36	0.46	
1:A:469:GLY:O	1:A:471:ASP:N	2.48	0.46	



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:342:LYS:HA	1:B:345:ASP:HB3	1.97	0.46	
1:B:348:VAL:O	1:B:352:ARG:HG2	2.15	0.46	
1:B:385:GLU:OE2	1:B:385:GLU:HA	2.15	0.46	
1:A:420:LEU:HB2	2:A:783:HOH:O	2.15	0.46	
1:B:415:ARG:HD2	2:B:742:HOH:O	2.16	0.46	
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.81	0.46	
1:A:356:THR:OG1	1:A:357:SER:N	2.48	0.46	
1:A:364:ILE:HG22	1:B:417:ILE:HD11	1.98	0.46	
1:A:465:GLU:HA	1:A:468:ARG:HD3	1.98	0.46	
1:A:482:ARG:O	1:A:485:GLN:HB3	2.16	0.46	
1:A:343:VAL:HG12	1:B:438:ALA:CB	2.44	0.45	
1:A:459:ILE:HD11	1:B:323:ALA:HB2	1.97	0.45	
1:A:466:GLN:NE2	1:B:315:THR:OG1	2.49	0.45	
1:A:430:VAL:HG12	1:A:431:GLY:N	2.31	0.45	
1:A:420:LEU:HD13	1:B:361:ILE:CG1	2.46	0.45	
1:B:495:ALA:HA	2:B:699:HOH:O	2.15	0.45	
1:A:357:SER:C	1:A:359:GLN:H	2.20	0.45	
1:A:304:GLN:HG3	1:A:305:THR:H	1.81	0.45	
1:A:338:GLN:HE21	1:A:338:GLN:CA	2.11	0.45	
1:B:370:GLY:O	1:B:373:PHE:HB3	2.16	0.45	
1:B:432:SER:HA	2:B:608:HOH:O	2.16	0.45	
1:A:316:VAL:CG2	1:A:466:GLN:HB2	2.47	0.45	
1:A:496:ALA:O	1:A:497:ALA:C	2.55	0.45	
1:B:517:ILE:O	1:B:519:GLN:N	2.50	0.45	
1:A:367:VAL:HG12	1:A:371:ILE:HD13	1.97	0.45	
1:A:446:VAL:O	1:A:446:VAL:HG12	2.15	0.45	
1:B:309:MET:HE1	1:B:470:ILE:O	2.17	0.45	
1:A:304:GLN:HG3	1:A:305:THR:HG23	1.97	0.45	
1:B:332:SER:C	1:B:334:SER:N	2.69	0.45	
1:A:326:ALA:HB2	1:B:455:ILE:HG21	1.98	0.45	
1:A:485:GLN:O	1:A:487:ASN:N	2.50	0.45	
1:A:394:ARG:O	1:A:398:VAL:HG12	2.17	0.45	
1:B:327:SER:HB2	1:B:456:MET:CB	2.47	0.45	
1:B:508:LEU:O	1:B:511:ALA:N	2.49	0.45	
1:B:412:GLN:HG3	1:B:413:ALA:N	2.32	0.44	
1:B:514:VAL:CG2	1:B:515:PHE:N	2.80	0.44	
1:A:396:PHE:HD1	1:A:396:PHE:H	1.63	0.44	
1:A:297:GLN:HA	1:A:300:ALA:HB3	1.99	0.44	
1:A:442:MET:O	1:A:445:ILE:N	2.51	0.44	
1:A:378:LEU:HD21	1:B:402:GLU:HG2	1.99	0.44	
1:A:510:GLU:HA	1:A:510:GLU:OE2	2.18	0.44	



	lo do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:B:341:GLY:O	1:B:342:LYS:HD2	2.17	0.44	
1:B:354:ILE:CG1	1:B:355:SER:H	2.30	0.44	
1:B:404:ARG:HD3	1:B:408:GLN:NE2	2.33	0.44	
1:B:510:GLU:HG3	1:B:511:ALA:N	2.32	0.44	
1:B:304:GLN:CD	1:B:304:GLN:C	2.77	0.44	
1:A:485:GLN:C	1:A:487:ASN:N	2.71	0.43	
1:A:517:ILE:C	1:A:520:GLN:H	2.19	0.43	
1:B:315:THR:O	1:B:318:GLN:HG3	2.17	0.43	
1:B:489:ALA:O	1:B:492:GLU:HB2	2.17	0.43	
1:A:512:VAL:O	1:A:516:ARG:HB3	2.18	0.43	
1:B:483:VAL:HA	1:B:486:GLN:CG	2.48	0.43	
1:A:389:ALA:O	1:A:390:GLY:C	2.57	0.43	
1:A:329:LEU:O	1:A:332:SER:HB3	2.18	0.43	
1:A:330:ALA:CB	1:A:452:VAL:HG11	2.46	0.43	
1:A:456:MET:HE2	1:A:456:MET:N	2.32	0.43	
1:A:459:ILE:O	1:A:463:SER:CB	2.67	0.43	
1:A:449:VAL:O	1:A:449:VAL:CG1	2.65	0.43	
1:B:353:ASP:O	3:ASP:O 1:B:354:ILE:C		0.43	
1:B:388:ARG:C	1:B:390:GLY:H	2.22	0.43	
1:A:361:ILE:HG21	1:A:421:ILE:HD12	2.01	0.43	
1:A:363:ASP:N	1:A:363:ASP:OD2	2.50	0.43	
1:A:404:ARG:O	1:A:407:ALA:HB3	2.19	0.43	
1:A:463:SER:O	1:A:466:GLN:HB2	2.19	0.43	
1:B:427:LYS:HA	2:B:611:HOH:O	2.19	0.43	
1:A:353:ASP:C	1:A:353:ASP:OD2	2.56	0.42	
1:A:363:ASP:HB3	2:A:672:HOH:O	2.18	0.42	
1:A:406:LEU:CD1	1:A:406:LEU:N	2.82	0.42	
1:A:417:ILE:O	1:A:417:ILE:HG12	2.18	0.42	
1:B:314:ALA:O	1:B:315:THR:C	2.58	0.42	
1:A:451:ARG:C	1:A:453:THR:H	2.21	0.42	
1:B:316:VAL:O	1:B:320:ALA:HB2	2.19	0.42	
1:B:426:GLY:O	1:B:429:ASP:CB	2.67	0.42	
1:B:508:LEU:O	1:B:509:THR:C	2.58	0.42	
1:A:339:ARG:HB3	2:A:757:HOH:O	2.18	0.42	
1:A:417:ILE:O	1:A:417:ILE:CG1	2.66	0.42	
1:B:316:VAL:HG21	1:B:466:GLN:HB3	2.02	0.42	
1:B:357:SER:C	1:B:359:GLN:H	2.23	0.42	
1:B:394:ARG:O	1:B:398:VAL:HG13	2.19	0.42	
1:B:406:LEU:HD12	1:B:406:LEU:HA	1.55	0.42	
1:B:428:VAL:HG12	1:B:428:VAL:O	2.19	0.42	
1:A:303:GLU:O	1:A:307:ALA:CB	2.68	0.42	



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:377:ILE:HD13	1:B:377:ILE:HA	1.94	0.42
1:A:452:VAL:O	1:A:456:MET:HE3	2.20	0.42
1:A:356:THR:O	1:A:359:GLN:HB3	2.20	0.42
1:A:361:ILE:HG12	1:B:420:LEU:CD2	2.49	0.42
1:A:364:ILE:HG21	1:B:417:ILE:CD1	2.49	0.42
1:A:493:GLN:HG3	2:A:698:HOH:O	2.20	0.42
1:B:315:THR:OG1	1:B:316:VAL:N	2.53	0.41
1:B:315:THR:O	1:B:317:LYS:N	2.53	0.41
1:B:449:VAL:HG12	1:B:449:VAL:O	2.20	0.41
1:A:303:GLU:O	1:A:304:GLN:C	2.58	0.41
1:A:469:GLY:C	1:A:471:ASP:N	2.73	0.41
1:B:358:SER:C	2:B:639:HOH:O	2.59	0.41
1:B:422:GLU:O	1:B:423:ASP:C	2.57	0.41
1:A:307:ALA:HB3	2:A:614:HOH:O	2.19	0.41
1:A:383:ALA:O	1:A:386:ALA:HB3	2.20	0.41
1:A:458:GLU:OE1	1:A:458:GLU:CA	2.68	0.41
1:A:348:VAL:HG13	1:A:352:ARG:NH2	2.36	0.41
1:B:321:GLU:OE1	1:B:460:ALA:HB1	2.20	0.41
1:B:354:ILE:CD1	1:B:428:VAL:HG22	2.40	0.41
1:B:432:SER:O	1:B:435:VAL:HG12	2.20	0.41
1:A:354:ILE:CD1	1:B:427:LYS:HE3	2.50	0.41
1:A:425:VAL:HA	1:A:428:VAL:HG12	2.02	0.41
1:B:318:GLN:O	1:B:322:ASN:HB3	2.21	0.41
1:A:331:LEU:HA	1:A:334:SER:CB	2.51	0.41
1:A:420:LEU:C	1:A:420:LEU:HD23	2.41	0.41
1:B:514:VAL:O	1:B:518:GLN:CB	2.66	0.41
1:A:336:THR:HG22	1:B:441:THR:O	2.21	0.41
1:A:337:ALA:N	1:B:445:ILE:HD11	2.36	0.41
1:A:352:ARG:NH2	2:A:724:HOH:O	2.53	0.41
1:A:399:VAL:HG22	1:B:396:PHE:HZ	1.85	0.41
1:A:483:VAL:HB	1:B:483:VAL:CG1	2.50	0.41
1:B:306:ALA:HA	1:B:309:MET:HB2	2.03	0.41
1:B:420:LEU:C	1:B:420:LEU:CD2	2.72	0.41
1:A:474:GLY:HA2	1:A:477:VAL:HG22	2.02	0.41
1:B:325:GLN:OE1	1:B:326:ALA:N	2.54	0.41
1:B:430:VAL:O	1:B:430:VAL:HG12	2.20	0.41
1:A:335:GLU:O	1:A:339:ARG:HG3	2.21	0.41
1:A:442:MET:C	1:A:444:GLU:N	2.73	0.41
1:B:380:LEU:HA	1:B:380:LEU:HD13	1.86	0.41
1:B:404:ARG:O	1:B:408:GLN:HG2	2.20	0.41
1:A:300:ALA:HA	1:A:303:GLU:HG3	2.02	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HB2	1:B:434:LEU:CD1	2.51	0.40
1:A:349:GLN:HG3	1:A:350:THR:N	2.36	0.40
1:B:324:ARG:HG3	1:B:324:ARG:HH11	1.86	0.40
1:A:311:GLN:H	1:A:311:GLN:HG3	1.64	0.40
1:A:440:GLU:C	1:A:442:MET:N	2.74	0.40
1:B:517:ILE:C	1:B:519:GLN:N	2.74	0.40
1:B:455:ILE:CG2	1:B:456:MET:HE2	2.49	0.40
1:A:442:MET:HE2	1:A:442:MET:HA	2.04	0.40
1:A:481:ASP:O	1:A:484:THR:CG2	2.69	0.40
1:B:324:ARG:NH1	1:B:324:ARG:HG3	2.37	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	Percentiles
1	А	225/227~(99%)	164 (73%)	46 (20%)	15 (7%)	1 1
1	В	219/227~(96%)	169 (77%)	40 (18%)	10 (5%)	2 3
All	All	444/454~(98%)	333~(75%)	86 (19%)	25~(6%)	2 2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	394	ARG
1	А	517	ILE
1	А	391	GLU
1	А	496	ALA
1	В	389	ALA
1	В	424	SER
1	В	454	ASP
1	В	455	ILE



Mol	Chain	Res	Type
1	В	518	GLN
1	А	296	GLU
1	А	304	GLN
1	А	349	GLN
1	А	497	ALA
1	В	319	ASN
1	А	318	GLN
1	А	353	ASP
1	А	425	VAL
1	А	468	ARG
1	А	486	GLN
1	В	309	MET
1	В	316	VAL
1	В	418	LYS
1	В	519	GLN
1	А	403	VAL
1	А	470	ILE

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	167/171~(98%)	156~(93%)	11 (7%)	16 33
1	В	164/171~(96%)	143~(87%)	21 (13%)	4 8
All	All	331/342~(97%)	299~(90%)	32 (10%)	8 15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	294	ARG
1	А	321	GLU
1	А	354	ILE
1	А	356	THR
1	А	398	VAL
1	А	402	GLU



Mol	Chain	Res	Type
1	А	417	ILE
1	А	430	VAL
1	А	456	MET
1	А	477	VAL
1	А	493	GLN
1	В	311	GLN
1	В	316	VAL
1	В	318	GLN
1	В	319	ASN
1	В	322	ASN
1	В	325	GLN
1	В	335	GLU
1	В	380	LEU
1	В	385	GLU
1	В	398	VAL
1	В	404	ARG
1	В	406	LEU
1	В	420	LEU
1	В	434	LEU
1	В	458	GLU
1	В	466	GLN
1	В	481	ASP
1	В	483	VAL
1	В	490	LEU
1	В	503	GLU
1	В	518	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	304	GLN
1	А	311	GLN
1	А	318	GLN
1	А	319	ASN
1	А	322	ASN
1	А	325	GLN
1	А	338	GLN
1	А	346	ASN
1	А	374	GLN
1	А	376	ASN
1	А	381	ASN
1	А	466	GLN



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Mol	Chain	Res	Type
1	А	486	GLN
1	А	493	GLN
1	В	319	ASN
1	В	466	GLN
1	В	518	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	227/227~(100%)	0.08	7 (3%) 49 42	13, 71, 116, 139	0
1	В	221/227~(97%)	0.10	10 (4%) 33 26	8, 70, 110, 128	0
All	All	448/454~(98%)	0.09	17 (3%) 40 33	8, 71, 114, 139	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	449	VAL	4.2
1	В	438	ALA	4.0
1	А	330	ALA	3.9
1	В	442	MET	3.7
1	В	330	ALA	3.5
1	А	333	ALA	3.3
1	А	448	ALA	3.1
1	В	344	VAL	3.0
1	В	445	ILE	3.0
1	А	319	ASN	2.9
1	А	297	GLN	2.7
1	А	455	ILE	2.7
1	В	343	VAL	2.5
1	В	452	VAL	2.4
1	В	447	SER	2.3
1	А	296	GLU	2.0
1	В	424	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

