

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 02:26 PM JST

PDB ID	:	8H1S
Title	:	Crystal structure of apo-LptDE complex
Authors	:	Luo, Q.; Huang, Y.
Deposited on	:	2022-10-03
Resolution	:	3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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

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 3.28 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	1177 (3.32 - 3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 chai	n	
1	А	924	3% 63%	25%	• 11%
1	С	924	63%	26%	• 11%
2	В	207	8%	15%	20%
2	D	207	13%	22%	20%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15855 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	С	824	Total 6634	C 4179	N 1155	O 1283	${ m S}$ 17	0	0	0
1	А	825	Total 6641	C 4181	N 1157	0 1286	S 17	0	0	0

• Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	а	166	Total	С	Ν	0	S	0	0	0
	D	100	1290	790	237	259	4	0		
0	р	166	Total	С	Ν	0	S	0	0	0
	D		1290	790	237	259	4	0	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: LPS-assembly protein LptD

• Molecule 1: LPS-assembly protein LptD













4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	113.03Å 160.49Å 218.07Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	43.09 - 3.28	Depositor
Resolution (A)	43.09 - 3.28	EDS
% Data completeness	96.4 (43.09-3.28)	Depositor
(in resolution range)	96.4 (43.09-3.28)	EDS
R_{merge}	0.67	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.00 (at 3.25 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.242 , 0.279	Depositor
n, n_{free}	0.242 , 0.275	DCC
R_{free} test set	2952 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	80.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 27.9	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15855	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 27.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1179e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.54	0/6808	0.73	1/9234~(0.0%)	
1	С	0.53	0/6799	0.73	2/9218~(0.0%)	
2	В	0.47	1/1302~(0.1%)	0.65	0/1758	
2	D	0.44	0/1302	0.67	0/1758	
All	All	0.53	1/16211~(0.0%)	0.72	3/21968~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	93	GLU	CG-CD	5.54	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	729	PRO	N-CA-CB	6.13	110.66	103.30
1	С	486	LEU	CA-CB-CG	-5.87	101.80	115.30
1	А	729	PRO	N-CA-CB	5.56	109.98	103.30

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	6641	0	6295	174	0
1	С	6634	0	6291	173	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 13.

All (390) 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:C:444:VAL:HG23	1:C:869:TRP:HB2	1.45	0.94
1:A:628:GLN:OE1	1:A:688:PHE:CZ	2.21	0.93
1:C:150:ALA:HB2	1:C:185:SER:HB3	1.56	0.88
1:C:727:LEU:HD13	1:C:732:LEU:HD22	1.55	0.87
1:C:191:ASP:HB2	1:C:206:GLY:HA3	1.60	0.81
1:C:270:CYS:HB3	1:C:274:SER:HB3	1.60	0.81
1:C:151:PRO:HB2	1:C:154:GLU:HB2	1.61	0.81
2:D:64:THR:HG22	2:D:66:ASN:H	1.45	0.80
1:C:412:ASN:HD21	1:C:414:THR:HG23	1.45	0.79
1:A:482:PRO:HB3	2:B:130:LEU:HD23	1.63	0.79
1:A:466:ARG:HB3	1:A:490:THR:HG23	1.65	0.78
1:C:117:ILE:HG13	1:C:139:ILE:HD11	1.63	0.78
1:C:171:GLN:H	1:C:198:LEU:HD21	1.49	0.77
1:A:563:TRP:HB2	2:B:24:LEU:HD22	1.67	0.76
1:A:191:ASP:HB2	1:A:206:GLY:HA3	1.67	0.75
1:C:711:ARG:HH11	1:C:711:ARG:HG2	1.49	0.75
1:C:419:ARG:NH2	1:C:461:ASP:OD1	2.20	0.74
1:A:117:ILE:HG13	1:A:139:ILE:HD11	1.68	0.74
2:D:40:SER:HB3	2:D:72:VAL:HG22	1.70	0.73
1:C:470:GLN:OE1	1:C:485:ARG:NH2	2.22	0.73
1:C:836:ARG:NH1	1:C:848:GLU:OE1	2.21	0.73
2:B:121:LYS:HB2	2:B:144:MET:HE2	1.70	0.72
1:A:143:ARG:H	1:A:146:MET:HE3	1.55	0.71
1:A:644:GLN:HE21	1:A:712:VAL:HG11	1.56	0.71
1:A:418:SER:O	1:A:459:ARG:NH2	2.24	0.71
1:A:359:ARG:NH1	1:A:369:GLU:OE1	2.23	0.71
1:A:647:LEU:O	1:A:673:ARG:NH2	2.21	0.70
1:C:852:GLY:HA3	1:C:865:ILE:HD13	1.72	0.70
1:C:332:SER:HA	1:C:337:GLY:O	1.91	0.70
1:A:900:ILE:HG13	1:A:901:VAL:HG23	1.72	0.69
2:D:57:GLU:HG3	2:D:63:VAL:HG23	1.75	0.68



Chain Non-H H(added) Symm-Clashes Mol H(model) Clashes В 1277 2 1290 250 0 $\mathbf{2}$ D 1290 0 1277 36 0 All All 0 0 1585515140390

Continued from previous page...

		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:142:VAL:HA	1:A:146:MET:HE1	1.74	0.68		
1:C:444:VAL:CG2	1:C:869:TRP:HB2	2.21	0.68		
2:D:84:SER:HB2	2:D:93:GLU:HG3	1.74	0.67		
1:C:444:VAL:HG21	1:C:848:GLU:HB2	1.76	0.66		
1:A:862:LEU:HD11	1:A:890:LEU:HD11	1.77	0.66		
1:C:723:LYS:NZ	1:C:724:ARG:HH22	1.94	0.66		
1:C:429:ILE:HG12	1:C:473:GLN:OE1	1.95	0.66		
1:A:794:ARG:HD2	2:B:93:GLU:OE2	1.95	0.66		
1:C:560:THR:HG22	1:C:565:TYR:HB2	1.78	0.65		
1:A:174:THR:HB	1:A:192:GLU:HG3	1.79	0.65		
2:B:20:CYS:SG	2:B:21:GLY:N	2.63	0.65		
1:A:836:ARG:NH1	1:A:848:GLU:OE1	2.30	0.65		
1:A:383:VAL:HG22	1:A:410:LEU:HD13	1.79	0.64		
1:C:647:LEU:O	1:C:673:ARG:NH2	2.31	0.64		
1:A:628:GLN:OE1	1:A:688:PHE:CE2	2.51	0.64		
1:C:682:LEU:HD12	1:C:705:TYR:CE2	2.32	0.63		
1:C:825:TRP:CD1	1:C:826:PRO:HD2	2.32	0.63		
1:A:170:LYS:HD3	1:A:198:LEU:HD21	1.79	0.63		
1:C:633:ARG:HD3	1:C:663:TRP:CZ2	2.33	0.63		
2:D:159:LEU:HD21	2:D:164:LEU:HD21	1.81	0.63		
1:C:853:PHE:HE1	1:C:864:LEU:HD23	1.64	0.62		
1:A:828:VAL:O	1:A:830:GLN:N	2.32	0.62		
2:B:38:ASP:HB3	2:B:70:HIS:HA	1.81	0.62		
1:C:794:ARG:HD2	2:D:93:GLU:OE2	1.99	0.62		
1:A:713:GLN:HB2	1:A:718:THR:HG23	1.81	0.62		
1:C:723:LYS:NZ	1:C:724:ARG:HH12	1.98	0.62		
1:C:711:ARG:HG2	1:C:711:ARG:NH1	2.15	0.62		
1:C:727:LEU:HD22	1:C:732:LEU:HD13	1.80	0.62		
1:C:359:ARG:NH1	1:C:369:GLU:OE1	2.24	0.61		
1:C:214:GLY:HA3	1:C:242:LYS:HE3	1.83	0.61		
1:A:419:ARG:NH2	1:A:461:ASP:OD1	2.34	0.61		
1:A:171:GLN:O	1:A:171:GLN:HG3	2.00	0.61		
1:C:212:ASP:OD1	1:C:213:LYS:N	2.33	0.60		
1:C:229:GLY:HA3	1:C:254:ARG:HH12	1.67	0.60		
1:C:682:LEU:HD12	1:C:705:TYR:HE2	1.66	0.60		
2:D:121:LYS:HB2	2:D:144:MET:HE2	1.84	0.60		
1:A:629:THR:HG22	1:A:687:ARG:O	2.00	0.59		
1:A:182:ARG:HG2	1:A:187:GLN:HG3	1.83	0.59		
1:C:669:THR:HG22	2:D:139:GLN:NE2	2.18	0.59		
1:C:367:MET:HG3	1:C:388:LEU:HB2	1.85	0.59		
1:C:412:ASN:ND2	1:C:414:THR:HG23	2.17	0.59		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:649:VAL:HG13	1:A:652:THR:HB	1.84	0.59	
1:C:455:THR:HG23	1:C:468:ASN:HB2	1.85	0.59	
1:A:904:LYS:C	1:A:906:GLU:H	2.07	0.59	
1:C:854:GLU:OE1	1:C:863:ARG:NH1	2.36	0.59	
1:A:853:PHE:HE1	1:A:864:LEU:HD23	1.67	0.59	
1:C:323:SER:OG	1:C:324:GLY:N	2.22	0.58	
1:C:418:SER:O	1:C:459:ARG:NH2	2.35	0.58	
1:A:379:SER:HB2	1:A:414:THR:HG22	1.86	0.58	
1:C:723:LYS:HZ2	1:C:724:ARG:HH12	1.51	0.57	
1:C:282:ASN:HB3	1:C:297:ASN:HB3	1.85	0.57	
1:A:628:GLN:OE1	1:A:688:PHE:CE1	2.57	0.57	
1:A:682:LEU:HD12	1:A:705:TYR:CE2	2.40	0.57	
2:D:64:THR:HG21	2:D:66:ASN:OD1	2.05	0.56	
1:A:171:GLN:HE21	1:A:173:ALA:HA	1.69	0.56	
1:C:681:SER:OG	1:C:704:ILE:HG12	2.05	0.56	
1:C:828:VAL:O	1:C:830:GLN:N	2.39	0.56	
1:C:521:ILE:HD13	1:C:532:LYS:HD3	1.87	0.56	
2:D:34:LEU:HD23	2:D:34:LEU:H	1.70	0.56	
2:D:138:ALA:HA	2:D:141:ARG:NH1	2.20	0.56	
1:A:194:ASN:HB2	1:A:203:GLU:HB3	1.86	0.56	
1:A:470:GLN:OE1	1:A:485:ARG:NH2	2.38	0.56	
1:C:152:SER:O	1:C:183:GLN:NE2	2.39	0.56	
1:A:644:GLN:NE2	1:A:712:VAL:HG11	2.19	0.56	
1:A:172:ILE:CG2	1:A:195:LEU:HB3	2.36	0.56	
1:A:282:ASN:HB3	1:A:297:ASN:HB2	1.88	0.56	
1:C:321:ARG:CZ	1:C:322:GLN:HE22	2.18	0.55	
1:A:227:ASP:OD1	1:A:227:ASP:N	2.39	0.55	
1:A:341:VAL:HG13	1:A:359:ARG:HG2	1.89	0.55	
1:A:917:ARG:C	1:A:919:ARG:H	2.09	0.55	
1:A:254:ARG:HG2	1:A:260:ILE:HG12	1.87	0.55	
1:A:628:GLN:NE2	1:A:688:PHE:CE2	2.75	0.55	
1:C:410:LEU:HD11	1:C:412:ASN:HB2	1.87	0.55	
1:C:617:ARG:HB3	2:D:22:PHE:CD2	2.41	0.55	
2:B:96:LEU:HD11	2:B:137:ALA:HB1	1.88	0.55	
1:A:662:LEU:HA	1:A:704:ILE:HD11	1.87	0.55	
2:B:100:ILE:HG13	2:B:148:LEU:HD13	1.87	0.55	
1:C:343:PRO:HB3	1:C:357:TYR:CD1	2.42	0.55	
1:C:95:LEU:O	1:C:97:THR:N	2.39	0.54	
2:D:49:VAL:HG22	2:D:53:LYS:HE3	1.89	0.54	
1:A:150:ALA:O	1:A:152:SER:N	2.40	0.54	
1:C:459:ARG:NH1	2:D:43:ASN:OD1	2.40	0.54	



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:D:35:LYS:O	2:D:62:LYS:N	2.40	0.54	
1:C:662:LEU:HA	1:C:704:ILE:HD11	1.88	0.54	
1:C:777:TYR:CZ	1:C:779:PRO:HG3	2.42	0.54	
1:A:171:GLN:NE2	1:A:173:ALA:HA	2.23	0.54	
1:A:628:GLN:CD	1:A:688:PHE:CE2	2.81	0.54	
1:C:230:GLU:HA	1:C:254:ARG:O	2.08	0.54	
1:C:237:GLU:HA	1:C:248:SER:HA	1.90	0.54	
1:A:854:GLU:OE1	1:A:863:ARG:NH1	2.39	0.53	
1:C:400:ASP:OD2	1:C:533:ARG:NH2	2.40	0.53	
1:C:553:PRO:HD2	1:C:572:TYR:O	2.07	0.53	
1:C:335:ASP:N	1:C:335:ASP:OD1	2.41	0.53	
1:C:690:GLU:OE2	1:C:696:ARG:HD2	2.08	0.53	
1:A:332:SER:HA	1:A:337:GLY:O	2.08	0.53	
1:A:466:ARG:HB3	1:A:490:THR:CG2	2.36	0.53	
1:A:716:GLY:O	1:A:717:LEU:HD23	2.09	0.53	
1:A:874:ASP:OD1	2:B:90:ARG:NH2	2.41	0.53	
2:D:100:ILE:HG12	2:D:148:LEU:HD13	1.90	0.53	
1:A:828:VAL:HG13	1:A:829:PRO:HD2	1.89	0.53	
1:C:104:LEU:HD12	1:C:107:ARG:NH1	2.23	0.53	
1:C:332:SER:O	1:C:887:GLY:HA2	2.08	0.53	
1:C:572:TYR:OH	1:C:603:SER:HB3	2.08	0.53	
1:A:727:LEU:HD23	1:A:728:ASP:O	2.09	0.53	
1:C:423:GLU:HG3	1:C:455:THR:HB	1.90	0.53	
2:B:96:LEU:HB2	2:B:144:MET:HE1	1.91	0.53	
1:C:158:TYR:CD1	1:C:182:ARG:HG3	2.44	0.53	
1:C:206:GLY:O	1:C:208:VAL:HG23	2.09	0.53	
2:D:86:THR:HG22	2:D:92:ALA:HB2	1.91	0.53	
1:A:777:TYR:CZ	1:A:779:PRO:HG3	2.44	0.53	
1:C:847:LEU:HA	1:C:870:LEU:HD12	1.91	0.52	
1:C:316:PRO:HG2	1:C:323:SER:HB3	1.90	0.52	
1:A:180:VAL:O	1:A:181:LEU:HD12	2.10	0.52	
1:C:323:SER:HG	1:C:344:TYR:HH	1.55	0.52	
1:C:383:VAL:HG22	1:C:410:LEU:HD13	1.90	0.52	
1:A:834:LEU:HD11	1:A:865:ILE:HD12	1.91	0.52	
2:D:123:TYR:CZ	2:D:137:ALA:HB2	2.45	0.52	
1:C:110:ASP:OD1	1:C:112:SER:OG	2.28	0.52	
1:A:406:TRP:CE2	1:A:430:SER:HB3	2.44	0.52	
1:C:453:ARG:HB2	1:C:470:GLN:HG3	1.93	0.51	
1:C:620:THR:HA	1:C:624:THR:O	2.10	0.51	
1:A:508:THR:HA	1:A:550:HIS:O	2.10	0.51	
1:C:374:TYR:OH	1:C:412:ASN:OD1	2.27	0.51	



	lo ao pagom	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
2:B:96:LEU:HB2	2:B:144:MET:CE	2.40	0.51		
1:A:104:LEU:HB3	1:A:107:ARG:HG3	1.93	0.51		
1:C:557:LEU:O	1:C:568:PRO:HD2	2.10	0.51		
1:A:354:ALA:HB2	1:A:372:PHE:HD1	1.76	0.51		
1:C:488:GLN:HA	1:C:510:PHE:O	2.11	0.51		
1:A:819:HIS:HD2	1:A:841:TYR:OH	1.94	0.51		
2:B:84:SER:HB2	2:B:93:GLU:HG3	1.93	0.51		
1:C:721:ASP:C	1:C:723:LYS:H	2.13	0.50		
1:A:412:ASN:HD21	1:A:414:THR:HG23	1.76	0.50		
1:A:613:LEU:O	1:A:632:PRO:HD2	2.11	0.50		
1:A:633:ARG:HD3	1:A:663:TRP:CZ2	2.46	0.50		
1:C:114:LEU:HD22	1:C:239:VAL:HG23	1.92	0.50		
1:A:621:PHE:O	1:A:624:THR:OG1	2.22	0.50		
1:A:911:LYS:O	2:B:81:ARG:NH1	2.45	0.50		
1:A:746:GLN:OE1	1:A:748:ARG:HD3	2.12	0.50		
1:A:819:HIS:CE1	1:A:821:PHE:CE2	2.99	0.50		
1:C:95:LEU:C	1:C:97:THR:H	2.14	0.50		
1:C:727:LEU:CD2	1:C:732:LEU:HD13	2.40	0.50		
1:A:169:GLU:OE1	1:A:169:GLU:N	2.45	0.50		
1:C:581:LEU:O	1:C:586:LYS:HE3	2.11	0.50		
1:C:282:ASN:CB	1:C:297:ASN:HB3	2.40	0.50		
1:C:819:HIS:NE2	1:C:839:TYR:HB3	2.27	0.50		
1:C:428:ARG:HG3	1:C:473:GLN:HE22	1.76	0.50		
1:A:852:GLY:HA3	1:A:865:ILE:HD13	1.94	0.50		
1:A:819:HIS:HD2	1:A:841:TYR:CZ	2.30	0.50		
1:A:399:PRO:HG3	1:A:878:LEU:HD21	1.93	0.49		
1:A:572:TYR:OH	1:A:603:SER:HB2	2.12	0.49		
1:C:133:TYR:HE2	1:C:856:ASP:HB3	1.76	0.49		
2:B:49:VAL:HG22	2:B:53:LYS:HE3	1.94	0.49		
1:A:915:GLY:O	1:A:917:ARG:N	2.45	0.49		
1:C:482:PRO:HB3	2:D:130:LEU:HD23	1.93	0.49		
1:A:514:ASP:OD1	1:A:515:ARG:N	2.46	0.49		
1:A:608:LYS:HE3	1:A:635:MET:SD	2.53	0.49		
1:A:710:ARG:NH2	1:A:734:ASN:O	2.46	0.49		
1:A:812:GLU:HA	1:A:815:ILE:HG13	1.95	0.49		
1:C:521:ILE:CD1	1:C:532:LYS:HD3	2.43	0.49		
1:C:487:PRO:CD	1:C:512:ARG:HB3	2.42	0.48		
1:C:753:TRP:HB3	1:C:777:TYR:HD1	1.78	0.48		
1:C:102:ARG:CG	1:C:275:ASN:HB3	2.43	0.48		
2:B:32:PHE:C	2:B:34:LEU:H	2.16	0.48		
1:A:515:ARG:NH2	1:A:542:ALA:O	2.46	0.48		



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:274:SER:O	1:C:276:ALA:N	2.46	0.48	
1:C:874:ASP:OD1	2:D:90:ARG:NH2	2.47	0.48	
1:A:487:PRO:CD	1:A:512:ARG:HB3	2.43	0.48	
1:C:662:LEU:HB3	1:C:663:TRP:CD1	2.49	0.48	
1:C:298:ALA:HB3	1:C:310:THR:HG23	1.94	0.48	
1:C:133:TYR:CE2	1:C:856:ASP:HB3	2.49	0.47	
1:C:277:TRP:CD2	1:C:894:LEU:HD22	2.49	0.47	
1:A:444:VAL:HG22	2:B:85:TYR:CE2	2.49	0.47	
1:A:487:PRO:HD3	1:A:512:ARG:HB3	1.96	0.47	
1:C:676:ASP:OD1	1:C:712:VAL:HG22	2.14	0.47	
1:A:485:ARG:HG3	2:B:131:ILE:HD12	1.95	0.47	
1:C:919:ARG:HH11	1:C:919:ARG:HA	1.78	0.47	
2:D:50:ARG:HG2	2:D:54:GLU:OE2	2.15	0.47	
1:C:819:HIS:CD2	1:C:839:TYR:HB3	2.49	0.47	
1:A:561:ARG:HB3	1:A:563:TRP:CZ3	2.49	0.47	
1:A:896:GLY:O	1:A:897:LEU:HD12	2.15	0.47	
1:C:777:TYR:OH	1:C:779:PRO:HG3	2.14	0.47	
1:C:102:ARG:HG3	1:C:275:ASN:HB3	1.96	0.47	
1:C:406:TRP:CE2	1:C:430:SER:HB3	2.50	0.47	
1:C:822:SER:HB2	1:C:913:ILE:HG12	1.96	0.47	
1:A:174:THR:CB	1:A:192:GLU:HG3	2.44	0.47	
1:A:175:LEU:O	1:A:192:GLU:HA	2.15	0.47	
1:A:721:ASP:C	1:A:723:LYS:H	2.18	0.47	
1:A:731:GLY:O	1:A:733:ASP:N	2.44	0.47	
1:A:834:LEU:C	1:A:834:LEU:HD12	2.35	0.47	
1:C:341:VAL:HG13	1:C:359:ARG:HG2	1.97	0.47	
1:C:673:ARG:HA	1:C:673:ARG:HD3	1.70	0.47	
1:C:785:LYS:HB3	1:C:825:TRP:CZ3	2.50	0.47	
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.71	0.47	
1:A:367:MET:HG3	1:A:388:LEU:HB2	1.96	0.47	
1:A:504:PHE:CE2	1:A:555:MET:HG2	2.50	0.47	
1:A:162:LYS:HB2	1:A:177:GLY:HA3	1.96	0.47	
1:C:478:THR:HG21	1:C:880:GLN:HG2	1.96	0.46	
1:A:695:GLU:HB2	2:B:154:MET:HE1	1.96	0.46	
1:A:428:ARG:HG3	1:A:473:GLN:HE22	1.80	0.46	
1:C:476:THR:OG1	1:C:478:THR:HG22	2.16	0.46	
1:A:834:LEU:HD11	1:A:865:ILE:CD1	2.46	0.46	
1:C:836:ARG:HG2	1:C:837:TRP:N	2.30	0.46	
1:A:262:LEU:HB2	1:A:284:VAL:HB	1.97	0.46	
1:A:789:VAL:HG13	1:A:821:PHE:CD1	2.51	0.46	
1:A:504:PHE:CD2	1:A:555:MET:HG2	2.50	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:775:PHE:CZ	1:A:777:TYR:HB2	2.51	0.46	
1:C:356:LEU:HD21	1:C:368:LEU:CD1	2.46	0.46	
1:C:652:THR:HG23	1:C:668:PHE:HB3	1.97	0.46	
1:A:206:GLY:O	1:A:208:VAL:HG23	2.15	0.46	
1:A:788:ASN:HB2	1:A:822:SER:OG	2.16	0.46	
1:C:406:TRP:CZ2	1:C:430:SER:HA	2.51	0.46	
1:C:704:ILE:HB	1:C:739:SER:HB3	1.98	0.46	
2:D:29:ASP:O	2:D:157:GLN:NE2	2.49	0.46	
1:A:615:PHE:HB2	1:A:630:LEU:HB3	1.97	0.46	
2:D:100:ILE:HB	2:D:117:VAL:HG22	1.98	0.45	
1:A:317:ILE:HG13	1:A:318:ASP:H	1.80	0.45	
1:C:95:LEU:HG	1:C:96:VAL:HG23	1.96	0.45	
1:C:519:GLU:O	1:C:532:LYS:NZ	2.49	0.45	
1:A:398:PHE:CZ	1:A:876:ALA:HB2	2.51	0.45	
1:C:615:PHE:HB2	1:C:630:LEU:HB3	1.98	0.45	
1:A:667:ARG:NH2	1:A:712:VAL:O	2.47	0.45	
1:A:848:GLU:HG3	1:A:869:TRP:HB3	1.99	0.45	
1:A:812:GLU:OE1	1:A:812:GLU:N	2.46	0.45	
1:C:790:GLY:O	1:C:819:HIS:HA	2.17	0.45	
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.48	0.45	
1:C:710:ARG:HH22	1:C:736:SER:H	1.64	0.45	
1:C:723:LYS:HZ1	1:C:724:ARG:HH22	1.65	0.45	
1:C:870:LEU:HD22	1:C:882:GLU:HB3	1.99	0.45	
1:C:907:MET:CE	1:C:911:LYS:HE3	2.46	0.45	
1:A:361:MET:HB2	1:A:364:ARG:HB2	1.98	0.45	
1:A:785:LYS:HB3	1:A:825:TRP:CZ3	2.52	0.45	
1:A:903:ASN:HB3	1:A:906:GLU:OE2	2.17	0.45	
1:C:299:THR:HA	1:C:308:PHE:O	2.17	0.45	
1:A:727:LEU:HD11	1:A:732:LEU:HD13	1.99	0.45	
1:C:107:ARG:HB2	1:C:113:HIS:CE1	2.52	0.45	
1:C:399:PRO:HG2	1:C:878:LEU:HD21	1.99	0.45	
1:A:189:GLU:HB2	1:A:209:LYS:HB2	1.98	0.45	
1:C:746:GLN:NE2	1:C:748:ARG:HH21	2.15	0.45	
2:D:70:HIS:HD2	2:D:105:VAL:HG23	1.82	0.45	
1:A:98:GLU:OE1	1:A:98:GLU:HA	2.16	0.44	
1:A:533:ARG:HE	1:A:533:ARG:HB3	1.56	0.44	
1:A:738:ARG:O	1:A:764:ASN:ND2	2.40	0.44	
1:C:361:MET:HB2	1:C:364:ARG:HB2	1.99	0.44	
1:A:224:VAL:HG22	1:A:231:ALA:HB2	2.00	0.44	
1:A:887:GLY:C	1:A:888:ILE:HD12	2.38	0.44	
1:C:198:LEU:HD22	1:C:198:LEU:H	1.82	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:268:THR:HB	1:C:278:THR:HG22	2.00	0.44	
1:C:300:LEU:HB3	1:C:308:PHE:HB3	1.99	0.44	
1:A:478:THR:HG21	1:A:880:GLN:HG2	2.00	0.44	
1:A:760:ASN:N	1:A:770:SER:O	2.50	0.44	
1:C:514:ASP:OD1	1:C:515:ARG:N	2.50	0.44	
1:C:828:VAL:HG13	1:C:829:PRO:HD2	1.99	0.44	
1:A:426:TYR:CD2	1:A:452:GLN:HB3	2.53	0.44	
1:C:379:SER:HB2	1:C:414:THR:HG22	1.98	0.44	
2:B:139:GLN:O	2:B:142:SER:HB2	2.18	0.44	
1:A:407:LEU:HD12	1:A:429:ILE:HG22	2.00	0.44	
1:A:870:LEU:HD22	1:A:882:GLU:HB2	1.99	0.44	
1:C:143:ARG:O	1:C:146:MET:HG3	2.18	0.44	
1:A:231:ALA:O	1:A:253:LYS:HA	2.18	0.44	
1:A:459:ARG:NH1	2:B:43:ASN:OD1	2.43	0.44	
2:B:123:TYR:CZ	2:B:137:ALA:HB2	2.53	0.44	
1:C:330:PHE:CD2	1:C:340:LEU:HD13	2.53	0.43	
1:C:351:ASN:OD1	1:C:351:ASN:N	2.50	0.43	
1:C:669:THR:CG2	2:D:139:GLN:NE2	2.81	0.43	
1:A:367:MET:HB2	1:A:388:LEU:HD13	2.00	0.43	
1:A:429:ILE:HG12	1:A:473:GLN:OE1	2.18	0.43	
1:A:864:LEU:O	1:A:865:ILE:HD13	2.17	0.43	
1:C:277:TRP:CE2	1:C:894:LEU:HD22	2.53	0.43	
1:C:120:GLU:OE1	1:C:120:GLU:N	2.38	0.43	
1:C:780:GLU:OE1	1:C:780:GLU:N	2.49	0.43	
1:C:822:SER:HB3	1:C:836:ARG:HG3	2.00	0.43	
2:D:110:LEU:HD11	2:D:168:GLN:HG3	2.00	0.43	
1:A:476:THR:HG21	1:A:479:ASP:OD2	2.18	0.43	
1:C:604:LEU:HD21	1:C:642:LYS:HB2	1.99	0.43	
1:C:909:LEU:HD23	1:C:909:LEU:HA	1.82	0.43	
1:A:300:LEU:HB3	1:A:308:PHE:HB3	1.99	0.43	
1:C:322:GLN:O	1:C:346:PHE:HA	2.19	0.43	
1:A:541:LEU:H	1:A:541:LEU:HD12	1.83	0.43	
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.83	0.43	
1:A:708:ARG:HH21	1:A:711:ARG:HG3	1.83	0.43	
1:A:819:HIS:CD2	1:A:841:TYR:OH	2.71	0.43	
1:A:494:PHE:CD1	1:A:494:PHE:C	2.92	0.43	
1:A:833:VAL:HG13	1:A:833:VAL:O	2.18	0.43	
1:C:466:ARG:NH2	1:C:490:THR:HG21	2.34	0.43	
1:C:919:ARG:HA	1:C:919:ARG:HD3	1.65	0.43	
1:A:111:TYR:O	1:A:116:TRP:HB3	2.18	0.43	
1:A:374:TYR:OH	1:A:412:ASN:OD1	2.31	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:C:387:TYR:CG	1:C:388:LEU:N	2.87	0.43	
1:A:553:PRO:HD2	1:A:572:TYR:O	2.19	0.43	
2:B:34:LEU:HD12	2:B:35:LYS:H	1.83	0.43	
2:B:168:GLN:O	2:B:172:GLU:HG3	2.19	0.43	
1:C:171:GLN:N	1:C:198:LEU:HD21	2.26	0.43	
1:C:662:LEU:HD21	1:C:702:GLY:HA3	2.01	0.43	
1:C:701:ALA:HA	1:C:742:ALA:O	2.19	0.43	
1:C:853:PHE:CE1	1:C:864:LEU:HD23	2.50	0.43	
1:A:682:LEU:HD12	1:A:705:TYR:CD2	2.53	0.43	
1:A:180:VAL:C	1:A:181:LEU:HD12	2.39	0.42	
1:A:232:GLN:HA	1:A:252:ALA:O	2.19	0.42	
1:A:790:GLY:O	1:A:819:HIS:HA	2.19	0.42	
1:C:406:TRP:CD2	1:C:430:SER:HB3	2.54	0.42	
1:A:143:ARG:H	1:A:146:MET:CE	2.28	0.42	
1:A:606:LEU:HD12	1:A:639:VAL:CG2	2.50	0.42	
2:B:140:LEU:HD12	2:B:140:LEU:HA	1.86	0.42	
1:C:617:ARG:HB3	2:D:22:PHE:CE2	2.54	0.42	
1:A:426:TYR:HA	1:A:452:GLN:HA	2.02	0.42	
1:A:162:LYS:CB	1:A:177:GLY:HA3	2.49	0.42	
2:D:20:CYS:SG	2:D:21:GLY:N	2.87	0.42	
1:A:628:GLN:CD	1:A:688:PHE:CZ	2.90	0.42	
1:A:641:TYR:CE1	1:A:711:ARG:HB2	2.54	0.42	
1:C:759:PHE:O	1:C:760:ASN:ND2	2.53	0.42	
1:A:557:LEU:O	1:A:568:PRO:HD2	2.20	0.42	
1:C:793:TYR:HA	1:C:816:ILE:O	2.20	0.42	
1:C:804:ARG:O	1:C:806:THR:HG22	2.20	0.42	
1:C:918:GLN:O	1:C:919:ARG:NH1	2.52	0.42	
2:D:100:ILE:HB	2:D:117:VAL:CG2	2.50	0.42	
1:A:387:TYR:CG	1:A:388:LEU:N	2.88	0.42	
1:A:719:GLU:OE1	1:A:719:GLU:N	2.50	0.42	
1:C:326:LEU:HB2	1:C:343:PRO:O	2.20	0.41	
1:C:777:TYR:CE2	1:C:779:PRO:HD3	2.55	0.41	
1:C:202:GLY:O	1:C:223:GLN:HA	2.20	0.41	
2:D:84:SER:HB2	2:D:93:GLU:CG	2.45	0.41	
1:A:168:GLN:N	1:A:168:GLN:OE1	2.53	0.41	
1:C:170:LYS:O	1:C:172:ILE:N	2.53	0.41	
1:C:644:GLN:NE2	1:C:712:VAL:HG11	2.35	0.41	
1:C:617:ARG:HD3	2:D:22:PHE:CE1	2.55	0.41	
1:C:812:GLU:HA	1:C:815:ILE:HG13	2.02	0.41	
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.84	0.41	
1:A:261:MET:HB2	1:A:285:LYS:HD3	2.02	0.41	



A 4 1	A + 0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:341:VAL:HG22	1:A:359:ARG:HG2	2.02	0.41	
1:A:414:THR:O	1:A:421:LEU:HD12	2.20	0.41	
2:B:152:LEU:HD23	2:B:152:LEU:HA	1.86	0.41	
1:A:488:GLN:HB2	1:A:511:VAL:HG23	2.02	0.41	
2:D:64:THR:HG22	2:D:66:ASN:N	2.23	0.41	
1:A:340:LEU:HD12	1:A:341:VAL:N	2.35	0.41	
1:A:631:GLU:OE2	1:A:687:ARG:NH1	2.54	0.41	
1:A:634:ALA:HB1	1:A:680:LEU:HD11	2.02	0.41	
1:A:847:LEU:HA	1:A:870:LEU:HD12	2.02	0.41	
1:C:608:LYS:HD3	1:C:665:GLU:HG2	2.03	0.41	
1:A:904:LYS:C	1:A:906:GLU:N	2.72	0.41	
1:A:911:LYS:HA	1:A:911:LYS:HD3	1.76	0.41	
1:C:209:LYS:HG2	1:C:218:VAL:HG22	2.02	0.41	
1:C:252:ALA:HA	1:C:261:MET:O	2.20	0.41	
1:C:371:GLU:HA	1:C:383:VAL:O	2.21	0.41	
1:C:417:ASP:OD1	1:C:417:ASP:N	2.48	0.41	
2:D:100:ILE:CG1	2:D:148:LEU:HD13	2.50	0.41	
1:A:266:THR:HA	1:A:279:LEU:O	2.21	0.41	
1:A:503:GLN:OE1	1:A:558:PRO:HG2	2.21	0.41	
1:A:629:THR:HG23	1:A:687:ARG:H	1.85	0.41	
1:A:867:ARG:HG3	1:A:869:TRP:HZ3	1.86	0.41	
2:D:175:ALA:O	2:D:179:ALA:HB3	2.21	0.40	
1:A:853:PHE:CE1	1:A:864:LEU:HD23	2.52	0.40	
1:C:114:LEU:O	1:C:115:ASP:HB2	2.21	0.40	
1:C:550:HIS:ND1	1:C:575:THR:OG1	2.54	0.40	
2:D:70:HIS:CD2	2:D:105:VAL:HG23	2.56	0.40	
2:D:96:LEU:HB2	2:D:144:MET:HE1	2.03	0.40	
1:C:678:ASN:HB3	1:C:708:ARG:HG2	2.03	0.40	
1:A:237:GLU:HA	1:A:248:SER:HA	2.03	0.40	
1:C:322:GLN:HB2	1:C:348:LEU:HA	2.03	0.40	
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.76	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	s
1	А	823/924~(89%)	756~(92%)	53~(6%)	14~(2%)	9 37	
1	С	818/924~(88%)	751~(92%)	58 (7%)	9~(1%)	14 46	
2	В	164/207~(79%)	156~(95%)	8~(5%)	0	100 100	
2	D	164/207~(79%)	157~(96%)	7 (4%)	0	100 100	
All	All	1969/2262~(87%)	1820 (92%)	126 (6%)	23 (1%)	13 44	

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

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	96	VAL
1	С	275	ASN
1	С	829	PRO
1	А	487	PRO
1	А	829	PRO
1	С	487	PRO
1	С	488	GLN
1	А	488	GLN
1	А	902	GLY
1	А	916	TYR
1	С	207	ASN
1	С	729	PRO
1	А	729	PRO
1	А	732	LEU
1	А	918	GLN
1	А	173	ALA
1	А	434	TYR
1	А	728	ASP
1	А	904	LYS
1	С	728	ASP
1	А	229	GLY
1	С	648	PRO
1	А	317	ILE

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.



Mol	Chain	Analysed Rotameric C		Outliers	F	Perce	ntiles	3
1	А	703/784~(90%)	693~(99%)	10 (1%)		67	82	
1	С	702/784~(90%)	694 (99%)	8 (1%)		73	85	
2	В	136/169~(80%)	136 (100%)	0		100	100	
2	D	136/169~(80%)	135~(99%)	1 (1%)		84	90	
All	All	1677/1906~(88%)	1658 (99%)	19 (1%)		73	85	

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

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	119	ARG
1	С	264	ASP
1	С	325	PHE
1	С	532	LYS
1	С	867	ARG
1	С	900	ILE
1	С	901	VAL
1	С	917	ARG
2	D	146	ARG
1	А	174	THR
1	А	227	ASP
1	А	264	ASP
1	А	323	SER
1	А	325	PHE
1	А	535	ASP
1	А	628	GLN
1	А	747	TYR
1	А	916	TYR
1	А	918	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	183	GLN
1	С	452	GLN
1	С	703	GLN
1	С	746	GLN
2	D	120	GLN
2	D	157	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	А	503	GLN
1	А	628	GLN
1	А	819	HIS
1	А	891	GLN
1	А	918	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	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	825/924~(89%)	0.27	31 (3%) 40 38	52, 73, 107, 151	0
1	С	824/924~(89%)	0.31	41 (4%) 28 27	58, 79, 114, 140	0
2	В	166/207~(80%)	0.78	16 (9%) 8 8	57, 83, 124, 135	0
2	D	166/207~(80%)	0.95	27~(16%) 1 2	61, 89, 129, 143	0
All	All	1981/2262~(87%)	0.39	115 (5%) 23 23	52, 77, 116, 151	0

All (115) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	D	179	ALA	6.4
2	В	185	ALA	6.2
2	D	182	LEU	5.5
1	А	174	THR	5.4
1	А	148	ASP	5.3
1	С	729	PRO	5.2
1	С	168	GLN	4.9
1	С	290	THR	4.9
2	D	181	ALA	4.9
1	С	728	ASP	4.9
2	D	184	ALA	4.8
1	А	729	PRO	4.8
1	А	152	SER	4.8
1	А	149	GLY	4.7
2	D	37	ILE	4.6
1	А	319	ASP	4.6
2	В	29	ASP	4.3
2	В	184	ALA	4.2
2	D	180	GLU	4.0
1	А	173	ALA	4.0
1	С	152	SER	4.0



Mol	Chain	Res	Type	RSRZ
1	С	147	ASP	3.8
1	С	169	GLU	3.7
1	А	322	GLN	3.7
2	D	185	ALA	3.6
2	D	183	ARG	3.5
2	В	161	PRO	3.5
1	С	289	ALA	3.5
1	А	150	ALA	3.5
1	С	532	LYS	3.4
2	В	37	ILE	3.4
1	А	531	GLY	3.3
2	В	69	TYR	3.3
1	С	167	GLU	3.2
1	С	722	LEU	3.1
1	С	498	ASN	3.0
1	А	721	ASP	3.0
1	А	620	THR	3.0
1	С	899	GLY	3.0
2	В	31	GLN	3.0
1	А	619	THR	3.0
1	А	318	ASP	3.0
1	С	95	LEU	2.9
2	D	36	GLU	2.9
1	С	258	ALA	2.8
1	А	593	ASP	2.8
2	D	177	ALA	2.7
1	А	351	ASN	2.7
2	D	34	LEU	2.7
1	А	153	ASP	2.7
2	В	166	GLU	2.7
1	С	726	ASN	2.7
1	С	735	ASP	2.6
2	В	164	LEU	2.6
1	С	619	THR	2.6
2	D	164	LEU	2.6
1	С	291	GLY	2.6
1	С	148	ASP	2.6
2	В	34	LEU	2.6
2	D	69	TYR	2.5
1	С	721	ASP	2.5
1	А	151	PRO	2.5
1	С	322	GLN	2.5



Continued from previous page...MolChainResTypeRSRZ

2	В	178	GLU	2.5
1	С	122	LEU	2.5
1	А	725	LEU	2.4
1	С	620	THR	2.4
1	А	665	GLU	2.4
1	А	768	THR	2.4
1	С	257	ASN	2.4
2	В	173	ALA	2.4
2	D	33	ALA	2.4
1	С	521	ILE	2.3
1	С	394	HIS	2.3
2	D	166	GLU	2.3
2	В	183	ARG	2.3
2	В	182	LEU	2.3
2	D	173	ALA	2.3
2	D	175	ALA	2.3
1	А	154	GLU	2.3
1	А	724	ARG	2.3
1	С	98	GLU	2.3
1	С	730	SER	2.3
1	А	352	TYR	2.3
1	А	596	PHE	2.3
2	D	108	ASN	2.2
2	D	178	GLU	2.2
1	А	257	ASN	2.2
1	С	732	LEU	2.2
1	С	624	THR	2.2
1	С	154	GLU	2.2
1	А	918	GLN	2.2
2	D	176	LYS	2.2
1	С	626	PHE	2.2
1	С	277	TRP	2.1
1	C	596	PHE	2.1
1	A	147	ASP	2.1
1	С	531	GLY	2.1
2	D	113	MET	2.1
2	В	30	ALA	2.1
2	В	180	GLU	2.1
2	D	161	PRO	2.1
1	С	155	SER	2.1
1	А	726	ASN	2.1
1	С	506	TYR	2.1



	<i>v</i>	1	10	
Mol	Chain	Res	Type	RSRZ
1	С	590	ASN	2.1
2	D	167	ALA	2.1
1	С	523	PHE	2.0
2	D	109	ASP	2.0
2	D	22	PHE	2.0
2	D	105	VAL	2.0
1	С	486	LEU	2.0
2	D	110	LEU	2.0
1	А	899	GLY	2.0
1	А	623	GLY	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.

