



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:41 PM UTC

PDB ID : 1QVC / pdb_00001qvc
Title : CRYSTAL STRUCTURE ANALYSIS OF SINGLE STRANDED DNA BINDING PROTEIN (SSB) FROM E.COLI
Authors : Matsumoto, T.; Morimoto, Y.; Shibata, N.; Shimamoto, N.; Tsukihara, T.; Yasuoka, N.
Deposited on : 1999-07-07
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

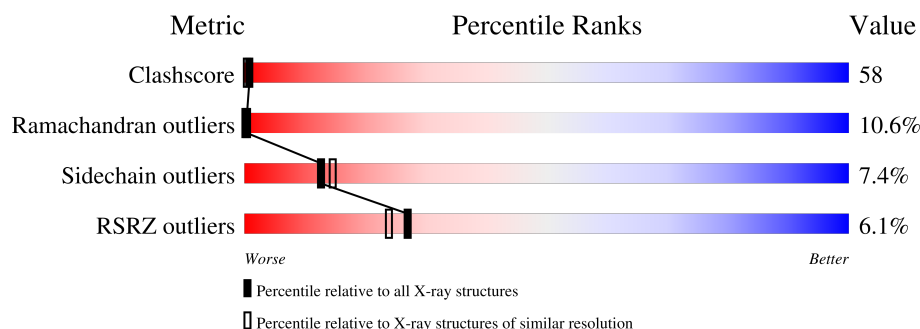
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	145	7% 37% 50% 12% .
1	B	145	6% 33% 56% 10% .
1	C	145	5% 35% 52% 12% ..
1	D	145	6% 31% 59% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4748 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 SINGLE STRANDED DNA BINDING PROTEIN MONOMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1083	665	204	210	4			
1	B	144	Total	C	N	O	S	0	0	0
			1078	662	203	209	4			
1	C	144	Total	C	N	O	S	0	0	0
			1078	662	203	209	4			
1	D	140	Total	C	N	O	S	0	0	0
			1054	648	198	204	4			

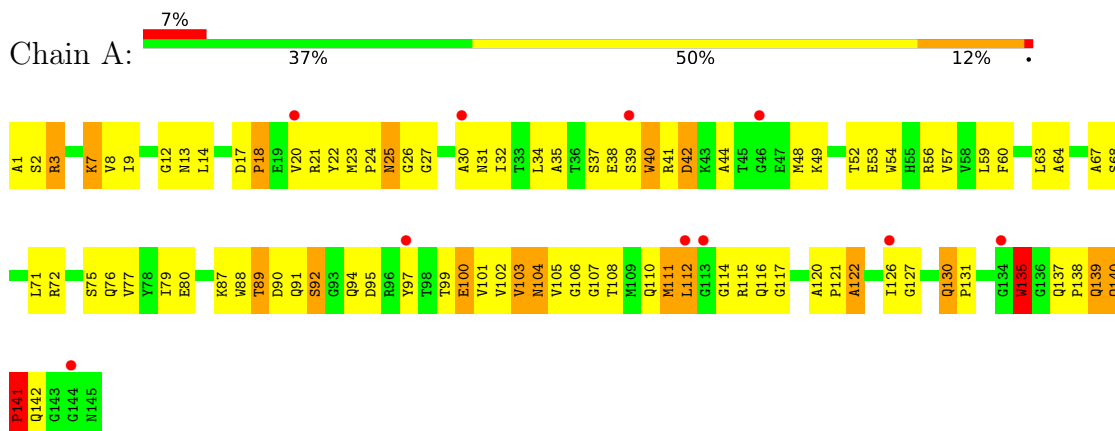
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	119	Total	O	0	0
			119	119		
2	B	118	Total	O	0	0
			118	118		
2	C	111	Total	O	0	0
			111	111		
2	D	107	Total	O	0	0
			107	107		

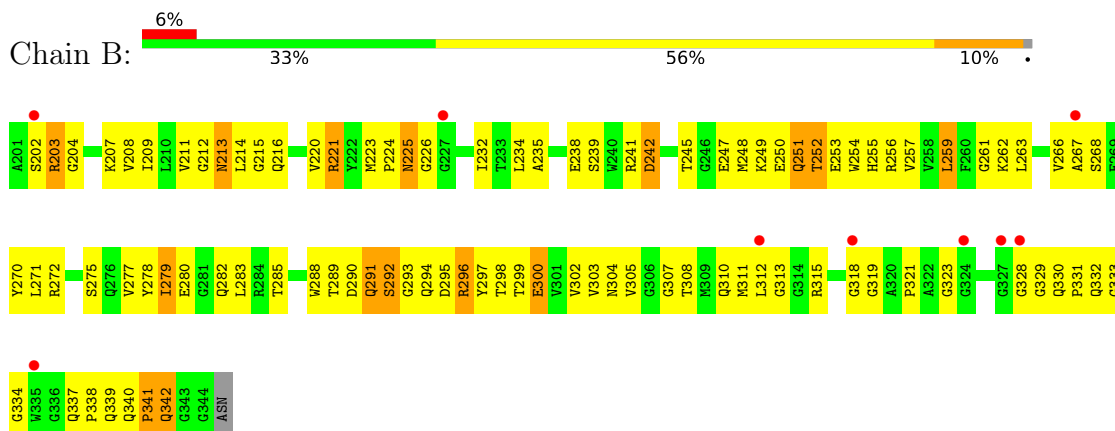
3 Residue-property plots

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.

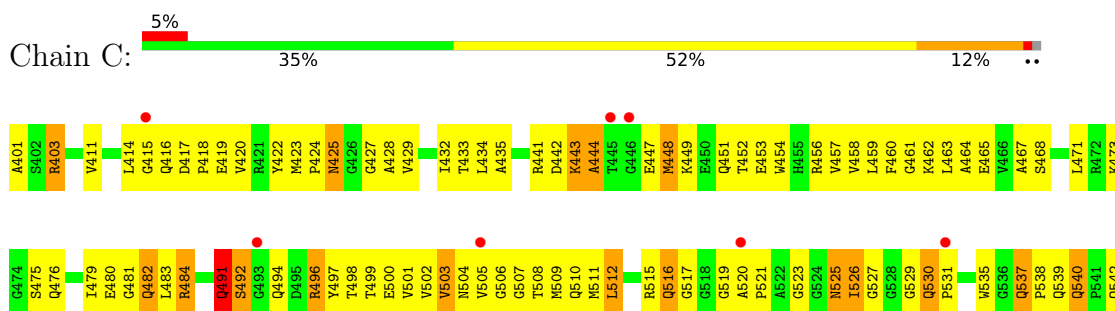
• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER



• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER



• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.37Å 62.92Å 97.79Å 90.00° 112.57° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.2 (15.00-2.20) 82.5 (15.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.317 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 98.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.020 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4748	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1102	0.81	0/1487
1	B	0.44	0/1097	0.82	1/1480 (0.1%)
1	C	0.46	0/1097	0.88	2/1480 (0.1%)
1	D	0.42	0/1072	0.86	0/1446
All	All	0.43	0/4368	0.84	3/5893 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	VAL	N-CA-C	-5.91	98.97	107.78
1	C	492	SER	N-CA-C	-5.59	107.71	114.75
1	B	279	ILE	N-CA-C	5.21	115.63	108.12

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	A	1083	0	1055	129	0
1	B	1078	0	1050	143	0
1	C	1078	0	1050	136	0
1	D	1054	0	1029	103	0
2	A	119	0	0	37	0
2	B	118	0	0	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	111	0	0	43	1
2	D	107	0	0	39	0
All	All	4748	0	4184	488	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 58.

All (488) 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)
1:A:20:VAL:HG21	1:A:68:SER:HB2	1.37	1.05
1:B:339:GLN:HG2	1:B:341:PRO:HD3	1.39	1.01
1:C:462:LYS:HD3	1:C:523:GLY:HA2	1.41	1.01
1:C:501:VAL:HA	2:C:1222:HOH:O	1.61	1.00
1:C:458:VAL:HB	2:C:1222:HOH:O	1.61	0.99
1:C:441:ARG:HA	1:C:448:MET:HA	1.43	0.97
1:B:311:MET:HG3	2:B:821:HOH:O	1.63	0.96
1:B:299:THR:HG21	2:B:1182:HOH:O	1.68	0.94
1:D:699:THR:HG21	2:D:1188:HOH:O	1.66	0.93
1:D:649:LYS:HD3	1:D:650:GLU:H	1.34	0.91
1:B:220:VAL:HG21	1:B:268:SER:HB3	1.53	0.91
1:B:271:LEU:HD23	1:B:310:GLN:HE21	1.36	0.90
1:C:491:GLN:OE1	1:C:492:SER:HB2	1.73	0.89
1:D:707:GLY:HA3	2:D:813:HOH:O	1.71	0.89
1:A:103:VAL:HG22	1:A:104:ASN:H	1.38	0.88
1:C:476:GLN:HB3	1:C:512:LEU:HG	1.56	0.88
1:B:303:VAL:HG22	1:B:304:ASN:H	1.40	0.87
1:C:499:THR:HG21	2:C:1180:HOH:O	1.73	0.86
1:C:503:VAL:HG12	2:C:857:HOH:O	1.75	0.85
1:C:498:THR:HG23	2:C:944:HOH:O	1.77	0.84
1:A:142:GLN:HA	1:A:142:GLN:HE21	1.43	0.84
1:B:252:THR:HG23	1:B:329:GLY:HA3	1.59	0.84
1:C:515:ARG:HG2	1:C:516:GLN:H	1.39	0.84
1:A:38:GLU:HA	1:B:203:ARG:HH21	1.43	0.84
1:C:500:GLU:HB2	2:C:930:HOH:O	1.77	0.84
1:C:503:VAL:HG22	1:C:504:ASN:H	1.42	0.83
1:C:457:VAL:HG11	1:C:479:ILE:HD13	1.61	0.83
1:D:670:TYR:HB3	1:D:710:GLN:HE22	1.44	0.83
1:D:738:PRO:HA	2:D:1209:HOH:O	1.79	0.82
1:A:107:GLY:HA3	2:A:803:HOH:O	1.78	0.82
1:D:620:VAL:HG21	1:D:668:SER:HB2	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:HG21	2:B:1224:HOH:O	1.79	0.81
1:C:476:GLN:HE21	1:C:512:LEU:H	1.29	0.79
1:B:220:VAL:HG12	1:B:221:ARG:H	1.46	0.79
1:D:729:GLY:HA3	1:D:735:TRP:HB3	1.63	0.78
1:D:730:GLN:HG2	2:D:1052:HOH:O	1.82	0.77
1:A:72:ARG:HA	2:A:1219:HOH:O	1.85	0.77
1:B:270:TYR:HB3	1:B:310:GLN:HE22	1.48	0.77
1:C:434:LEU:HD11	1:C:479:ILE:HD12	1.66	0.77
1:D:687:LYS:HB2	2:D:1190:HOH:O	1.83	0.77
1:C:496:ARG:HH11	1:C:496:ARG:HB2	1.49	0.77
1:D:649:LYS:HD3	1:D:650:GLU:N	1.98	0.77
1:A:76:GLN:H	1:A:112:LEU:HD11	1.50	0.77
1:A:3:ARG:HH12	1:B:238:GLU:HA	1.48	0.76
1:D:703:VAL:HG22	1:D:704:ASN:H	1.49	0.76
1:B:307:GLY:HA3	2:B:812:HOH:O	1.85	0.76
1:B:250:GLU:HB2	1:B:328:GLY:HA3	1.68	0.76
1:C:507:GLY:HA3	2:C:807:HOH:O	1.85	0.76
1:B:291:GLN:HB3	2:B:1202:HOH:O	1.86	0.75
1:A:41:ARG:H	1:A:41:ARG:HD3	1.50	0.75
1:D:703:VAL:HG13	2:D:832:HOH:O	1.85	0.75
1:D:705:VAL:N	2:D:832:HOH:O	2.18	0.75
1:B:297:TYR:HA	2:B:1006:HOH:O	1.87	0.75
1:B:313:GLY:HA2	1:D:601:ALA:N	2.00	0.74
1:B:257:VAL:HG11	1:B:279:ILE:HD13	1.69	0.74
1:D:691:GLN:HA	2:D:1100:HOH:O	1.86	0.74
1:D:663:LEU:HD23	2:D:1132:HOH:O	1.88	0.74
1:D:696:ARG:HG2	2:D:1190:HOH:O	1.88	0.73
1:C:481:GLY:HA3	1:C:500:GLU:OE1	1.88	0.73
1:B:296:ARG:HB3	2:B:1101:HOH:O	1.88	0.73
1:A:3:ARG:HE	1:C:509:MET:HE2	1.53	0.73
1:D:682:GLN:HB3	2:D:1172:HOH:O	1.89	0.72
1:B:342:GLN:HG2	2:B:1181:HOH:O	1.89	0.71
1:C:476:GLN:HG2	1:C:511:MET:HB2	1.71	0.70
1:C:484:ARG:HG2	2:D:1231:HOH:O	1.90	0.70
1:D:703:VAL:HG22	1:D:704:ASN:N	2.02	0.70
1:A:2:SER:HB2	1:C:515:ARG:HD3	1.72	0.70
1:A:87:LYS:HD2	1:B:332:GLN:CD	2.16	0.70
1:C:475:SER:HA	1:C:512:LEU:HD21	1.73	0.70
1:C:503:VAL:HG13	1:C:505:VAL:H	1.55	0.70
1:B:271:LEU:CD2	1:B:310:GLN:HE21	2.03	0.70
1:C:504:ASN:HB3	2:C:1044:HOH:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HB3	2:B:1228:HOH:O	1.91	0.69
1:A:104:ASN:H	1:A:104:ASN:HD22	1.41	0.69
1:B:290:ASP:O	1:B:291:GLN:HB2	1.92	0.69
1:B:211:VAL:HG13	2:B:821:HOH:O	1.92	0.69
1:B:291:GLN:O	1:B:292:SER:OG	2.06	0.69
1:A:12:GLY:HA3	1:A:34:LEU:HD21	1.75	0.68
1:B:310:GLN:C	1:B:311:MET:HE2	2.19	0.68
1:A:141:PRO:HB2	2:A:1037:HOH:O	1.94	0.68
1:C:483:LEU:HD13	2:D:1223:HOH:O	1.94	0.68
1:C:526:ILE:HD13	1:C:527:GLY:N	2.09	0.68
1:A:3:ARG:HD3	1:C:521:PRO:HD2	1.76	0.67
1:A:38:GLU:CA	1:B:203:ARG:HH21	2.08	0.67
1:A:3:ARG:NH1	1:B:238:GLU:HA	2.10	0.67
1:B:340:GLN:HA	2:B:1181:HOH:O	1.94	0.66
1:A:117:GLY:HA3	2:A:1114:HOH:O	1.95	0.66
1:C:503:VAL:HG13	1:C:504:ASN:N	2.09	0.66
1:B:270:TYR:CB	1:B:310:GLN:HE22	2.08	0.66
1:C:442:ASP:CG	1:C:443:LYS:H	2.04	0.66
1:C:494:GLN:HB2	2:C:1206:HOH:O	1.95	0.66
1:D:688:TRP:HZ3	1:D:690:ASP:HB2	1.60	0.65
1:A:17:ASP:HA	2:A:1219:HOH:O	1.96	0.65
1:C:542:GLN:HB3	2:C:950:HOH:O	1.96	0.65
1:A:56:ARG:HB2	1:A:99:THR:HG22	1.79	0.64
1:A:63:LEU:HD12	1:A:108:THR:CG2	2.27	0.64
1:B:303:VAL:HG22	1:B:304:ASN:N	2.10	0.64
1:A:41:ARG:HA	2:A:1227:HOH:O	1.97	0.64
1:D:634:LEU:HD13	2:D:1066:HOH:O	1.97	0.64
1:B:263:LEU:HD12	1:B:308:THR:CG2	2.27	0.64
1:B:279:ILE:HG12	2:B:955:HOH:O	1.97	0.64
1:B:300:GLU:HA	2:B:951:HOH:O	1.96	0.64
1:A:44:ALA:HB2	2:A:888:HOH:O	1.98	0.64
1:A:140:GLN:HG2	2:A:1037:HOH:O	1.97	0.64
1:D:684:ARG:HD2	2:D:941:HOH:O	1.97	0.64
1:B:339:GLN:HE21	1:B:341:PRO:HG3	1.62	0.64
1:D:688:TRP:CZ3	1:D:690:ASP:HB2	2.33	0.63
1:D:659:LEU:HD23	1:D:702:VAL:HB	1.80	0.63
1:C:415:GLY:HA3	1:C:454:TRP:HZ3	1.63	0.63
1:C:496:ARG:HH11	1:C:496:ARG:CB	2.11	0.63
1:C:463:LEU:HD22	1:C:508:THR:CG2	2.28	0.63
1:D:643:LYS:HB2	2:D:915:HOH:O	1.97	0.63
1:A:126:ILE:HG22	2:A:1055:HOH:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:ILE:HG22	2:D:879:HOH:O	1.99	0.63
1:D:715:ARG:HD2	1:D:715:ARG:N	2.14	0.62
1:A:14:LEU:HD13	1:A:75:SER:HB2	1.81	0.62
1:D:643:LYS:HA	1:D:646:GLY:O	2.00	0.62
1:D:737:GLN:HB2	1:D:738:PRO:HD3	1.82	0.62
1:B:290:ASP:O	1:B:291:GLN:CB	2.47	0.62
1:D:616:GLN:HG2	1:D:617:ASP:H	1.63	0.62
1:A:140:GLN:HG3	1:A:141:PRO:HD2	1.81	0.62
1:C:428:ALA:HB1	2:C:1242:HOH:O	1.98	0.61
1:A:1:ALA:HA	1:C:515:ARG:CA	2.30	0.61
1:B:293:GLY:HA3	2:B:1204:HOH:O	1.99	0.61
1:C:423:MET:O	1:C:425:ASN:N	2.33	0.61
1:A:48:MET:O	1:A:49:LYS:HD3	2.00	0.61
1:B:337:GLN:HA	2:B:1253:HOH:O	2.00	0.61
1:B:323:GLY:HA2	2:B:983:HOH:O	2.00	0.61
1:A:23:MET:HE2	2:A:1192:HOH:O	2.00	0.61
1:A:67:ALA:O	1:A:71:LEU:HB2	2.01	0.61
1:C:457:VAL:HG13	1:C:500:GLU:OE2	2.00	0.61
1:D:632:ILE:HG13	2:D:861:HOH:O	2.00	0.61
1:D:670:TYR:CB	1:D:710:GLN:HE22	2.12	0.61
1:A:39:SER:H	1:B:203:ARG:NH2	2.00	0.60
1:B:315:ARG:HG2	2:B:1151:HOH:O	2.00	0.60
1:C:415:GLY:HA3	1:C:454:TRP:CZ3	2.35	0.60
1:B:271:LEU:HB3	2:B:906:HOH:O	2.01	0.60
1:A:99:THR:HG21	2:A:1184:HOH:O	2.01	0.60
1:C:420:VAL:HG21	1:C:468:SER:HB2	1.81	0.60
1:A:59:LEU:HD23	1:A:102:VAL:HB	1.84	0.60
1:B:310:GLN:O	1:B:311:MET:HE2	2.01	0.60
1:A:1:ALA:HA	1:C:515:ARG:HA	1.82	0.60
1:A:104:ASN:H	1:A:104:ASN:ND2	2.00	0.59
1:A:110:GLN:HB3	2:A:814:HOH:O	2.01	0.59
1:C:459:LEU:HG	2:C:1033:HOH:O	2.02	0.59
1:C:444:ALA:HB3	2:C:949:HOH:O	2.02	0.59
1:B:272:ARG:HB3	2:B:960:HOH:O	2.02	0.59
1:A:71:LEU:HG	1:A:110:GLN:HE22	1.67	0.59
1:A:23:MET:HG3	1:A:26:GLY:O	2.03	0.59
1:B:209:ILE:HG12	2:B:1068:HOH:O	2.03	0.59
1:A:63:LEU:N	1:A:63:LEU:HD22	2.17	0.58
1:A:41:ARG:HD3	1:A:41:ARG:N	2.18	0.58
1:A:63:LEU:HD22	1:A:63:LEU:H	1.68	0.58
1:A:142:GLN:HA	1:A:142:GLN:NE2	2.14	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:PHE:HA	2:C:1191:HOH:O	2.03	0.58
1:A:9:ILE:HD12	2:B:1068:HOH:O	2.02	0.58
1:A:104:ASN:HD22	1:A:104:ASN:N	2.00	0.58
1:C:456:ARG:HG3	1:C:497:TYR:CE2	2.39	0.58
1:C:526:ILE:HD13	1:C:526:ILE:C	2.29	0.58
1:B:288:TRP:CZ3	1:B:290:ASP:HB3	2.38	0.58
1:D:628:ALA:HB3	2:D:1213:HOH:O	2.04	0.58
1:A:103:VAL:HG22	1:A:104:ASN:ND2	2.17	0.58
1:B:220:VAL:HG21	1:B:268:SER:CB	2.29	0.58
1:C:420:VAL:HG21	1:C:468:SER:CB	2.33	0.58
1:C:443:LYS:HB3	1:C:449:LYS:HD2	1.84	0.58
1:B:256:ARG:NH2	2:B:1086:HOH:O	2.36	0.58
1:B:283:LEU:HD23	2:B:951:HOH:O	2.02	0.58
1:B:241:ARG:HA	1:B:248:MET:SD	2.44	0.57
1:D:677:VAL:HG13	1:D:679:ILE:HD12	1.87	0.57
1:C:530:GLN:HE21	1:C:530:GLN:N	2.02	0.57
1:C:484:ARG:N	2:C:944:HOH:O	2.37	0.57
1:C:511:MET:C	1:C:512:LEU:HD12	2.29	0.57
1:D:614:LEU:HG	1:D:632:ILE:CG2	2.34	0.57
1:B:259:LEU:N	1:B:259:LEU:HD12	2.19	0.57
1:A:135:TRP:HA	1:A:135:TRP:CE3	2.40	0.57
1:B:263:LEU:HD12	1:B:308:THR:HG22	1.87	0.56
1:D:621:ARG:HD3	2:D:1173:HOH:O	2.04	0.56
1:A:3:ARG:HG2	1:A:3:ARG:HH11	1.69	0.56
1:A:34:LEU:HD23	1:A:35:ALA:N	2.19	0.56
1:A:103:VAL:O	1:A:106:GLY:N	2.38	0.56
1:B:303:VAL:HG13	1:B:305:VAL:HG22	1.87	0.56
1:D:643:LYS:HD3	1:D:647:GLU:HA	1.86	0.56
1:B:339:GLN:NE2	1:B:341:PRO:HG3	2.20	0.56
1:B:341:PRO:HG2	1:B:342:GLN:H	1.71	0.56
1:C:471:LEU:HD21	1:C:510:GLN:HG2	1.87	0.56
1:A:41:ARG:H	1:A:41:ARG:CD	2.18	0.56
1:C:503:VAL:CG1	1:C:505:VAL:HG22	2.35	0.56
1:B:275:SER:HB2	2:B:906:HOH:O	2.04	0.56
1:B:245:THR:HG23	1:B:247:GLU:H	1.71	0.56
1:C:414:LEU:HA	1:C:433:THR:O	2.06	0.56
1:C:443:LYS:HG3	2:C:949:HOH:O	2.05	0.56
1:D:620:VAL:CG2	1:D:668:SER:HB2	2.33	0.56
1:A:140:GLN:CG	1:A:141:PRO:HD2	2.36	0.56
1:B:302:VAL:HG21	2:B:955:HOH:O	2.06	0.56
1:C:416:GLN:HB2	2:C:996:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:THR:HG21	2:B:802:HOH:O	2.05	0.55
1:D:616:GLN:HG2	1:D:617:ASP:N	2.22	0.55
1:A:39:SER:HB3	2:A:1244:HOH:O	2.05	0.55
1:C:443:LYS:HD3	1:C:444:ALA:N	2.21	0.55
1:A:108:THR:HG21	2:A:1195:HOH:O	2.05	0.55
1:A:131:PRO:HA	2:A:1131:HOH:O	2.06	0.55
1:B:304:ASN:HB2	2:B:975:HOH:O	2.06	0.55
1:D:664:ALA:HB3	2:D:1213:HOH:O	2.06	0.55
1:D:679:ILE:HD13	2:D:1149:HOH:O	2.05	0.55
1:D:614:LEU:HG	1:D:632:ILE:HG23	1.89	0.55
1:D:634:LEU:HD11	1:D:679:ILE:HD13	1.88	0.55
1:C:529:GLY:C	1:C:530:GLN:HE21	2.15	0.55
1:B:312:LEU:N	1:D:601:ALA:HB2	2.22	0.55
1:D:619:GLU:HA	2:D:958:HOH:O	2.06	0.55
1:D:721:PRO:C	1:D:723:GLY:H	2.14	0.55
1:A:63:LEU:HD12	1:A:108:THR:HG22	1.88	0.55
1:B:271:LEU:HD22	2:B:906:HOH:O	2.06	0.55
1:B:330:GLN:N	1:B:331:PRO:HD3	2.20	0.55
1:D:632:ILE:HG22	1:D:633:THR:N	2.22	0.55
1:D:662:LYS:O	1:D:666:VAL:HG23	2.07	0.55
1:A:42:ASP:HA	2:A:1064:HOH:O	2.07	0.55
1:B:304:ASN:HB3	2:B:1236:HOH:O	2.05	0.55
1:C:423:MET:HB2	1:C:427:GLY:O	2.08	0.54
1:A:91:GLN:O	1:A:92:SER:HB2	2.06	0.54
1:C:418:PRO:HG2	2:C:1163:HOH:O	2.05	0.54
1:B:209:ILE:HD11	2:B:1232:HOH:O	2.06	0.54
1:B:313:GLY:HA3	2:B:1238:HOH:O	2.06	0.54
1:D:700:GLU:HB2	2:D:924:HOH:O	2.07	0.54
1:D:730:GLN:HB3	1:D:731:PRO:HD2	1.90	0.54
1:C:537:GLN:O	1:C:537:GLN:HG2	2.07	0.54
1:D:708:THR:OG1	2:D:811:HOH:O	2.19	0.54
1:A:105:VAL:HG12	2:C:1158:HOH:O	2.07	0.54
1:D:657:VAL:HG22	1:D:700:GLU:HB3	1.88	0.54
1:C:441:ARG:HA	1:C:448:MET:CA	2.29	0.54
1:C:504:ASN:HB2	2:C:1246:HOH:O	2.07	0.54
1:D:657:VAL:HG21	2:D:1149:HOH:O	2.09	0.53
1:A:103:VAL:HG22	1:A:104:ASN:N	2.18	0.53
1:B:339:GLN:HE21	1:B:341:PRO:CG	2.21	0.53
1:C:510:GLN:O	1:C:511:MET:HE2	2.09	0.53
1:C:511:MET:HE2	1:C:511:MET:HA	1.91	0.53
1:B:213:ASN:HA	1:B:275:SER:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:HG13	1:B:270:TYR:HD2	1.74	0.53
1:B:300:GLU:C	1:B:300:GLU:OE2	2.52	0.53
1:C:461:GLY:O	1:C:465:GLU:HG3	2.09	0.53
1:A:8:VAL:HB	1:A:100:GLU:OE1	2.09	0.53
1:C:463:LEU:HD22	1:C:508:THR:HG22	1.89	0.53
1:A:63:LEU:H	1:A:63:LEU:CD2	2.22	0.53
1:B:300:GLU:HG2	2:B:951:HOH:O	2.09	0.53
1:C:537:GLN:N	1:C:538:PRO:CD	2.72	0.53
1:C:441:ARG:HG3	1:C:448:MET:H	1.74	0.53
1:A:103:VAL:HG13	1:A:104:ASN:N	2.23	0.53
1:C:530:GLN:N	1:C:531:PRO:HD3	2.24	0.53
1:D:693:GLY:O	1:D:694:GLN:HB2	2.08	0.53
1:B:339:GLN:HG3	2:B:916:HOH:O	2.08	0.52
1:C:503:VAL:HG22	1:C:504:ASN:N	2.20	0.52
1:C:451:GLN:HG3	2:C:824:HOH:O	2.09	0.52
1:C:443:LYS:HD3	1:C:444:ALA:H	1.75	0.52
1:C:500:GLU:CD	1:C:500:GLU:C	2.78	0.52
1:A:48:MET:HB3	2:A:859:HOH:O	2.08	0.52
1:A:138:PRO:HG3	2:C:1148:HOH:O	2.09	0.52
1:D:608:VAL:HB	1:D:700:GLU:OE1	2.09	0.52
1:D:703:VAL:HG13	1:D:704:ASN:H	1.75	0.52
1:A:56:ARG:HG2	2:A:1010:HOH:O	2.09	0.52
1:B:299:THR:CG2	2:B:802:HOH:O	2.58	0.52
1:C:516:GLN:HB2	1:C:521:PRO:HD3	1.92	0.52
1:A:142:GLN:HB3	2:A:969:HOH:O	2.10	0.52
1:B:220:VAL:HG12	1:B:221:ARG:N	2.18	0.52
1:B:271:LEU:HD21	1:B:310:GLN:HG2	1.91	0.52
1:B:214:LEU:HG	1:B:232:ILE:HG23	1.91	0.51
1:B:242:ASP:OD2	1:B:242:ASP:C	2.53	0.51
1:C:432:ILE:HG12	2:C:1033:HOH:O	2.10	0.51
1:B:251:GLN:HG2	2:B:965:HOH:O	2.10	0.51
1:B:261:GLY:HA3	2:B:972:HOH:O	2.10	0.51
1:D:715:ARG:C	1:D:717:GLY:H	2.18	0.51
1:D:715:ARG:O	1:D:716:GLN:HB3	2.10	0.51
1:A:102:VAL:HG12	2:A:1128:HOH:O	2.09	0.51
1:B:234:LEU:HD21	1:B:277:VAL:HG12	1.92	0.51
1:D:703:VAL:HG22	1:D:704:ASN:OD1	2.11	0.51
1:A:110:GLN:HB3	2:A:1214:HOH:O	2.10	0.51
1:B:340:GLN:HA	1:B:340:GLN:NE2	2.25	0.51
1:D:652:THR:HB	2:D:1059:HOH:O	2.10	0.51
1:B:235:ALA:HB1	2:B:914:HOH:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:703:VAL:HG13	1:D:704:ASN:N	2.26	0.51
1:B:267:ALA:HA	1:B:271:LEU:HG	1.92	0.51
1:C:530:GLN:N	1:C:530:GLN:NE2	2.58	0.51
1:C:457:VAL:HG11	1:C:479:ILE:CD1	2.39	0.51
1:C:463:LEU:HD13	1:C:508:THR:HG22	1.93	0.51
1:D:655:HIS:HD2	2:D:836:HOH:O	1.94	0.51
1:C:456:ARG:HG3	1:C:497:TYR:HE2	1.75	0.50
1:D:632:ILE:CG2	1:D:633:THR:N	2.75	0.50
1:A:30:ALA:HB2	1:A:64:ALA:HB1	1.93	0.50
1:B:291:GLN:O	1:B:292:SER:CB	2.59	0.50
1:B:303:VAL:CG1	1:B:305:VAL:HG22	2.41	0.50
1:B:235:ALA:HB2	1:B:254:TRP:CZ3	2.46	0.50
1:C:467:ALA:HA	1:C:471:LEU:HG	1.92	0.50
1:A:111:MET:HA	1:A:111:MET:HE2	1.94	0.50
1:B:300:GLU:HB2	2:B:831:HOH:O	2.11	0.50
1:D:637:SER:CB	1:D:652:THR:HG22	2.42	0.50
1:D:655:HIS:CD2	2:D:836:HOH:O	2.64	0.50
1:A:141:PRO:HG2	2:A:1201:HOH:O	2.12	0.50
1:B:223:MET:O	1:B:225:ASN:N	2.45	0.50
1:D:689:THR:HA	2:D:1076:HOH:O	2.12	0.50
1:C:491:GLN:OE1	1:C:492:SER:CB	2.53	0.49
1:B:259:LEU:N	1:B:259:LEU:CD1	2.75	0.49
1:C:464:ALA:HB3	2:C:1191:HOH:O	2.12	0.49
1:A:20:VAL:CG2	1:A:68:SER:HB2	2.26	0.49
1:A:87:LYS:HD2	1:B:332:GLN:NE2	2.26	0.49
1:A:130:GLN:H	1:A:131:PRO:CD	2.26	0.49
1:C:429:VAL:HG22	1:C:460:PHE:CD1	2.48	0.49
1:B:303:VAL:CG2	1:B:304:ASN:H	2.20	0.49
1:D:631:ASN:HB2	2:D:1099:HOH:O	2.11	0.49
1:A:32:ILE:HG13	1:A:57:VAL:HB	1.94	0.48
1:B:300:GLU:HG2	2:B:831:HOH:O	2.13	0.48
1:D:642:ASP:CG	1:D:643:LYS:H	2.21	0.48
1:C:442:ASP:CG	1:C:443:LYS:N	2.71	0.48
1:C:482:GLN:HG2	2:C:857:HOH:O	2.14	0.48
1:A:21:ARG:HB3	2:A:1200:HOH:O	2.14	0.48
1:A:56:ARG:CB	1:A:99:THR:HG22	2.41	0.48
1:A:35:ALA:HB2	1:A:54:TRP:CZ3	2.48	0.48
1:A:104:ASN:HA	2:A:1183:HOH:O	2.13	0.48
1:A:138:PRO:HA	2:A:1026:HOH:O	2.13	0.48
1:C:467:ALA:C	2:C:1163:HOH:O	2.56	0.48
1:D:620:VAL:HG21	1:D:668:SER:CB	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:NE	2:B:1146:HOH:O	2.46	0.48
1:D:652:THR:CB	2:D:1059:HOH:O	2.62	0.48
1:A:76:GLN:HB3	1:A:111:MET:HB2	1.94	0.48
1:C:520:ALA:HB1	1:C:521:PRO:HA	1.96	0.48
1:A:103:VAL:O	1:A:104:ASN:C	2.57	0.47
1:A:142:GLN:HE21	1:A:142:GLN:CA	2.13	0.47
1:A:112:LEU:HD13	2:A:1214:HOH:O	2.13	0.47
1:A:48:MET:HB2	2:A:1244:HOH:O	2.14	0.47
1:B:245:THR:HG21	1:B:249:LYS:HZ3	1.80	0.47
1:C:459:LEU:HG	2:C:1245:HOH:O	2.14	0.47
1:C:401:ALA:N	2:C:953:HOH:O	2.47	0.47
1:D:622:TYR:CE2	1:D:628:ALA:HB2	2.49	0.47
1:C:464:ALA:CB	2:C:1191:HOH:O	2.62	0.47
1:D:656:ARG:NE	2:D:884:HOH:O	2.47	0.47
1:A:60:PHE:HE2	1:A:101:VAL:HG13	1.80	0.47
1:B:212:GLY:C	1:B:234:LEU:HD22	2.40	0.47
1:B:308:THR:OG1	2:B:1224:HOH:O	2.21	0.47
1:C:515:ARG:HG2	1:C:516:GLN:N	2.18	0.47
1:B:263:LEU:H	1:B:263:LEU:HD22	1.80	0.47
1:C:447:GLU:HB3	2:C:1205:HOH:O	2.14	0.47
1:C:456:ARG:NH2	2:C:1030:HOH:O	2.48	0.47
1:A:18:PRO:HD3	2:A:1219:HOH:O	2.15	0.46
1:B:295:ASP:C	1:B:296:ARG:HD2	2.39	0.46
1:B:321:PRO:C	1:B:323:GLY:H	2.23	0.46
1:D:687:LYS:HB2	1:D:687:LYS:NZ	2.30	0.46
1:A:14:LEU:HD21	1:A:71:LEU:HD22	1.96	0.46
1:D:690:ASP:N	2:D:1076:HOH:O	2.48	0.46
1:B:315:ARG:HA	1:B:315:ARG:NE	2.30	0.46
1:C:435:ALA:HA	1:C:453:GLU:O	2.16	0.46
1:A:120:ALA:N	1:A:121:PRO:HD3	2.31	0.46
1:A:32:ILE:CG1	1:A:57:VAL:HB	2.46	0.46
1:B:208:VAL:HB	1:B:300:GLU:OE1	2.16	0.46
1:B:223:MET:HB2	1:B:225:ASN:HD21	1.80	0.46
1:C:429:VAL:HG22	1:C:460:PHE:HD1	1.81	0.46
1:D:614:LEU:HA	1:D:633:THR:O	2.15	0.46
1:D:625:ASN:HB3	2:D:1036:HOH:O	2.15	0.46
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.80	0.46
1:C:456:ARG:HH21	1:D:696:ARG:HH22	1.63	0.46
1:A:103:VAL:HG22	1:A:104:ASN:HD22	1.79	0.45
1:B:235:ALA:HA	1:B:253:GLU:O	2.16	0.45
1:B:300:GLU:CG	2:B:831:HOH:O	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLN:HG2	1:B:333:GLY:H	1.80	0.45
1:D:648:MET:HB3	2:D:1122:HOH:O	2.15	0.45
1:D:679:ILE:HG21	2:D:1149:HOH:O	2.15	0.45
1:B:254:TRP:HE1	1:B:330:GLN:HB2	1.82	0.45
1:A:3:ARG:NE	1:C:509:MET:HE2	2.27	0.45
1:C:462:LYS:HA	1:C:465:GLU:OE1	2.17	0.45
1:C:480:GLU:O	1:C:506:GLY:HA3	2.17	0.45
1:A:3:ARG:HD2	2:A:961:HOH:O	2.15	0.45
1:B:296:ARG:NE	2:B:1101:HOH:O	2.31	0.45
1:C:435:ALA:HB2	1:C:454:TRP:CZ3	2.51	0.45
1:D:663:LEU:HD12	1:D:708:THR:CG2	2.46	0.45
1:B:300:GLU:CB	2:B:831:HOH:O	2.65	0.45
1:B:319:GLY:HA2	2:B:1153:HOH:O	2.17	0.45
2:A:1217:HOH:O	1:C:505:VAL:HG12	2.15	0.45
1:B:340:GLN:HA	1:B:340:GLN:HE21	1.82	0.45
1:D:671:LEU:HD21	1:D:710:GLN:HG2	1.99	0.45
1:A:104:ASN:OD1	1:C:526:ILE:HD12	2.17	0.45
1:A:115:ARG:HB3	1:A:116:GLN:H	1.54	0.45
1:B:272:ARG:CZ	2:B:926:HOH:O	2.64	0.45
1:B:339:GLN:CG	1:B:341:PRO:HD3	2.28	0.45
1:A:48:MET:SD	1:A:48:MET:N	2.87	0.44
1:A:140:GLN:O	1:A:141:PRO:C	2.58	0.44
1:D:719:GLY:O	1:D:720:ALA:HB2	2.18	0.44
1:C:509:MET:HB3	1:C:511:MET:HE3	1.97	0.44
1:A:122:ALA:HB1	2:A:1047:HOH:O	2.16	0.44
1:C:403:ARG:HG3	1:D:637:SER:O	2.18	0.44
1:C:540:GLN:N	2:C:1029:HOH:O	2.51	0.44
1:A:126:ILE:HG23	1:A:126:ILE:O	2.16	0.44
1:C:505:VAL:HA	2:C:1158:HOH:O	2.16	0.44
1:B:202:SER:HA	2:B:1135:HOH:O	2.17	0.44
1:B:204:GLY:O	1:D:709:MET:HE1	2.18	0.44
1:A:31:ASN:CG	2:A:843:HOH:O	2.60	0.44
1:A:71:LEU:HD21	1:A:77:VAL:HG11	1.99	0.44
1:B:207:LYS:HD2	1:B:280:GLU:HG3	2.00	0.44
1:B:270:TYR:O	1:B:318:GLY:HA2	2.18	0.44
1:A:137:GLN:N	1:A:138:PRO:HD2	2.33	0.44
1:B:257:VAL:HG12	1:B:259:LEU:CD1	2.48	0.44
1:C:484:ARG:NH2	2:C:801:HOH:O	2.30	0.44
1:C:520:ALA:HA	1:C:521:PRO:C	2.43	0.44
1:B:239:SER:HB3	1:C:519:GLY:HA2	2.00	0.43
1:B:257:VAL:HG12	1:B:259:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HG2	2:A:1167:HOH:O	2.17	0.43
1:C:415:GLY:O	1:C:473:LYS:HE2	2.17	0.43
1:A:25:ASN:HD21	1:C:542:GLN:NE2	2.16	0.43
1:C:457:VAL:HG12	2:C:1245:HOH:O	2.17	0.43
1:B:215:GLY:O	1:B:216:GLN:HG3	2.19	0.43
1:D:637:SER:HB2	1:D:652:THR:HG22	2.00	0.43
1:D:735:TRP:O	1:D:736:GLY:C	2.61	0.43
1:A:79:ILE:CG2	1:A:80:GLU:N	2.82	0.43
1:C:420:VAL:CG1	2:C:1242:HOH:O	2.67	0.43
1:B:266:VAL:HG13	1:B:270:TYR:CD2	2.53	0.43
1:C:525:ASN:N	2:C:1002:HOH:O	2.51	0.43
1:A:40:TRP:HE1	1:A:49:LYS:HB2	1.83	0.43
1:B:278:TYR:HE2	2:B:928:HOH:O	2.02	0.43
1:D:642:ASP:CG	1:D:643:LYS:N	2.77	0.43
1:B:255:HIS:HD2	2:B:827:HOH:O	2.01	0.42
1:B:263:LEU:HD22	1:B:263:LEU:N	2.33	0.42
1:B:288:TRP:HZ2	1:B:297:TYR:CE1	2.37	0.42
1:C:502:VAL:HG23	2:C:1245:HOH:O	2.18	0.42
1:D:740:GLN:HG2	2:D:1209:HOH:O	2.18	0.42
1:A:2:SER:CB	1:C:515:ARG:HD3	2.44	0.42
1:D:729:GLY:HA3	1:D:735:TRP:CB	2.42	0.42
1:A:3:ARG:NH1	1:A:3:ARG:HG2	2.34	0.42
1:C:510:GLN:C	1:C:511:MET:HE2	2.44	0.42
1:A:95:ASP:HB3	2:A:1000:HOH:O	2.20	0.42
1:C:460:PHE:HE2	1:C:501:VAL:CG1	2.33	0.42
1:D:623:MET:O	1:D:625:ASN:N	2.52	0.42
1:A:34:LEU:HD23	1:A:34:LEU:C	2.45	0.42
1:B:208:VAL:HG21	2:B:951:HOH:O	2.19	0.42
1:A:2:SER:O	1:A:3:ARG:C	2.62	0.42
1:A:37:SER:OG	1:A:52:THR:HG22	2.20	0.42
1:C:476:GLN:OE1	1:D:601:ALA:HB1	2.19	0.42
1:D:643:LYS:HG3	2:D:1048:HOH:O	2.20	0.42
1:D:721:PRO:C	1:D:723:GLY:N	2.78	0.42
1:A:130:GLN:N	1:A:131:PRO:CD	2.81	0.42
1:D:634:LEU:HD11	1:D:679:ILE:CD1	2.48	0.42
1:D:715:ARG:HD2	1:D:715:ARG:H	1.84	0.42
1:B:285:THR:HA	1:B:298:THR:HA	2.01	0.42
1:C:434:LEU:CD1	1:C:479:ILE:HD12	2.44	0.42
1:A:41:ARG:HG2	1:A:41:ARG:NH1	2.35	0.41
1:C:419:GLU:HG2	2:C:986:HOH:O	2.18	0.41
1:C:460:PHE:HE2	1:C:501:VAL:HG13	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:VAL:HG22	1:D:660:PHE:CD1	2.55	0.41
1:D:629:VAL:HG13	1:D:659:LEU:O	2.20	0.41
1:D:608:VAL:HG12	1:D:610:LEU:HG	2.00	0.41
1:D:635:ALA:HB2	1:D:654:TRP:CZ3	2.55	0.41
1:C:417:ASP:HA	1:C:418:PRO:HD3	1.83	0.41
1:B:215:GLY:C	1:B:216:GLN:HG3	2.46	0.41
1:C:496:ARG:HH11	1:C:496:ARG:CG	2.33	0.41
1:B:313:GLY:N	2:B:942:HOH:O	2.52	0.41
1:A:13:ASN:N	2:A:1141:HOH:O	2.47	0.41
1:A:20:VAL:HG12	1:A:21:ARG:N	2.35	0.41
1:C:476:GLN:HE21	1:C:512:LEU:N	2.08	0.41
1:B:288:TRP:CE3	1:B:340:GLN:HG2	2.55	0.41
1:A:7:LYS:HB2	1:A:7:LYS:HE2	1.79	0.41
1:A:22:TYR:O	1:A:23:MET:HB3	2.21	0.41
1:A:49:LYS:HG3	2:A:989:HOH:O	2.20	0.41
1:B:213:ASN:C	1:B:234:LEU:HD23	2.46	0.41
1:C:414:LEU:HD12	1:C:414:LEU:N	2.36	0.41
1:C:435:ALA:HB3	2:C:1127:HOH:O	2.20	0.41
1:C:443:LYS:O	1:C:444:ALA:C	2.64	0.41
1:C:471:LEU:HB2	2:C:1163:HOH:O	2.20	0.41
1:C:502:VAL:CG2	2:C:1245:HOH:O	2.68	0.41
1:C:516:GLN:HB3	1:C:517:GLY:H	1.51	0.41
1:D:632:ILE:HD11	1:D:667:ALA:HB1	2.03	0.41
1:A:89:THR:O	1:A:89:THR:HG23	2.20	0.41
1:B:245:THR:HG21	1:B:249:LYS:NZ	2.36	0.41
1:B:272:ARG:HH11	1:B:272:ARG:HG3	1.86	0.41
1:B:289:THR:HG22	1:B:291:GLN:H	1.86	0.41
1:B:341:PRO:HG2	1:B:342:GLN:OE1	2.22	0.41
1:C:496:ARG:NE	2:C:1009:HOH:O	2.42	0.41
1:A:35:ALA:HA	1:A:53:GLU:O	2.22	0.40
1:B:291:GLN:CB	2:B:1202:HOH:O	2.56	0.40
1:B:315:ARG:HA	1:B:315:ARG:HE	1.86	0.40
1:C:456:ARG:HG3	1:C:497:TYR:OH	2.21	0.40
1:B:256:ARG:CZ	2:B:1086:HOH:O	2.69	0.40
1:B:332:GLN:HG2	1:B:333:GLY:N	2.35	0.40
1:B:340:GLN:HE21	1:B:340:GLN:CA	2.34	0.40
1:A:88:TRP:HZ3	1:A:90:ASP:HB3	1.87	0.40
1:A:135:TRP:HA	1:A:135:TRP:HE3	1.84	0.40
1:A:139:GLN:O	1:A:140:GLN:HB3	2.20	0.40
1:B:257:VAL:HG11	1:B:279:ILE:CD1	2.46	0.40
1:D:624:PRO:O	1:D:625:ASN:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:HA	1:A:18:PRO:HD3	1.93	0.40
1:A:17:ASP:CG	2:A:871:HOH:O	2.65	0.40
1:C:422:TYR:HA	1:C:428:ALA:HA	2.03	0.40
1:D:608:VAL:CG2	1:D:683:LEU:HG	2.51	0.40
1:D:671:LEU:HD23	1:D:710:GLN:HE21	1.86	0.40
1:B:207:LYS:HG3	2:B:1068:HOH:O	2.22	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)
2:C:826:HOH:O	2:C:826:HOH:O[2_655]	1.42	0.78

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	A	143/145 (99%)	104 (73%)	18 (13%)	21 (15%)	0	0
1	B	142/145 (98%)	113 (80%)	16 (11%)	13 (9%)	0	0
1	C	142/145 (98%)	112 (79%)	19 (13%)	11 (8%)	1	0
1	D	138/145 (95%)	103 (75%)	20 (14%)	15 (11%)	0	0
All	All	565/580 (97%)	432 (76%)	73 (13%)	60 (11%)	0	0

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	104	ASN
1	B	291	GLN
1	B	292	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	PRO
1	C	444	ALA
1	C	448	MET
1	D	624	PRO
1	D	625	ASN
1	A	27	GLY
1	A	42	ASP
1	A	92	SER
1	A	127	GLY
1	A	139	GLN
1	A	141	PRO
1	B	225	ASN
1	B	341	PRO
1	C	425	ASN
1	C	491	GLN
1	D	703	VAL
1	D	715	ARG
1	D	728	GLY
1	D	736	GLY
1	A	24	PRO
1	A	94	GLN
1	A	112	LEU
1	A	122	ALA
1	B	203	ARG
1	B	224	PRO
1	C	443	LYS
1	D	603	ARG
1	D	604	GLY
1	D	722	ALA
1	D	727	GLY
1	D	732	GLN
1	A	25	ASN
1	B	221	ARG
1	B	242	ASP
1	B	251	GLN
1	C	525	ASN
1	C	539	GLN
1	D	618	PRO
1	D	738	PRO
1	A	103	VAL
1	A	135	TRP
1	B	226	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	334	GLY
1	B	342	GLN
1	C	403	ARG
1	C	424	PRO
1	C	503	VAL
1	D	694	GLN
1	A	89	THR
1	A	111	MET
1	C	537	GLN
1	D	733	GLY
1	A	114	GLY
1	A	140	GLN
1	A	18	PRO
1	A	130	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/109 (99%)	102 (94%)	6 (6%)	19	24
1	B	108/109 (99%)	101 (94%)	7 (6%)	15	18
1	C	108/109 (99%)	97 (90%)	11 (10%)	7	7
1	D	106/109 (97%)	98 (92%)	8 (8%)	12	14
All	All	430/436 (99%)	398 (93%)	32 (7%)	13	14

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

Mol	Chain	Res	Type
1	A	7	LYS
1	A	40	TRP
1	A	97	TYR
1	A	100	GLU
1	A	135	TRP
1	A	141	PRO
1	B	213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	THR
1	B	259	LEU
1	B	282	GLN
1	B	294	GLN
1	B	296	ARG
1	B	300	GLU
1	C	452	THR
1	C	482	GLN
1	C	484	ARG
1	C	491	GLN
1	C	496	ARG
1	C	512	LEU
1	C	516	GLN
1	C	526	ILE
1	C	530	GLN
1	C	535	TRP
1	C	540	GLN
1	D	641	ARG
1	D	651	GLN
1	D	679	ILE
1	D	687	LYS
1	D	691	GLN
1	D	697	TYR
1	D	711	MET
1	D	712	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	51	GLN
1	A	55	HIS
1	A	76	GLN
1	A	82	GLN
1	A	94	GLN
1	A	104	ASN
1	A	110	GLN
1	A	130	GLN
1	A	132	GLN
1	A	142	GLN
1	B	251	GLN
1	B	255	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291	GLN
1	B	310	GLN
1	B	316	GLN
1	B	330	GLN
1	B	332	GLN
1	B	339	GLN
1	C	416	GLN
1	C	431	ASN
1	C	455	HIS
1	C	494	GLN
1	C	530	GLN
1	C	532	GLN
1	C	537	GLN
1	C	542	GLN
1	D	655	HIS
1	D	676	GLN
1	D	682	GLN
1	D	694	GLN
1	D	710	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	A	145/145 (100%)	0.85	10 (6%) 23 20	29, 67, 100, 100	0
1	B	144/145 (99%)	0.62	9 (6%) 26 23	28, 57, 100, 100	0
1	C	144/145 (99%)	0.52	7 (4%) 35 31	25, 58, 100, 100	0
1	D	140/145 (96%)	0.68	9 (6%) 25 22	30, 67, 100, 100	0
All	All	573/580 (98%)	0.67	35 (6%) 27 24	25, 61, 100, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	601	ALA	4.0
1	A	113	GLY	3.8
1	D	720	ALA	3.7
1	A	30	ALA	3.7
1	D	723	GLY	3.7
1	A	20	VAL	3.6
1	A	112	LEU	3.6
1	D	640	TRP	3.5
1	C	415	GLY	3.4
1	A	134	GLY	3.3
1	B	318	GLY	2.8
1	D	642	ASP	2.8
1	B	227	GLY	2.8
1	D	697	TYR	2.8
1	B	324	GLY	2.8
1	B	335	TRP	2.7
1	B	327	GLY	2.6
1	D	724	GLY	2.5
1	C	493	GLY	2.4
1	C	446	GLY	2.3
1	D	691	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	126	ILE	2.3
1	A	97	TYR	2.3
1	B	267	ALA	2.3
1	C	520	ALA	2.3
1	B	328	GLY	2.2
1	A	39	SER	2.2
1	B	202	SER	2.2
1	A	46	GLY	2.1
1	C	445	THR	2.1
1	C	505	VAL	2.1
1	B	312	LEU	2.1
1	C	531	PRO	2.1
1	A	144	GLY	2.1
1	D	721	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.