



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:50 PM GMT

PDB ID : 1QVC
Title : CRYSTAL STRUCTURE ANALYSIS OF SINGLE STRANDED DNA BINDING PROTEIN (SSB) FROM E.COLI
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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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

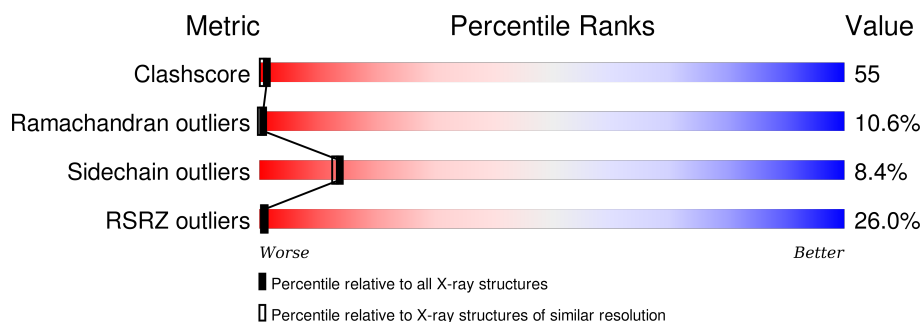
1 Overall quality at a glance

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	145	
1	C	145	
1	D	145	

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			

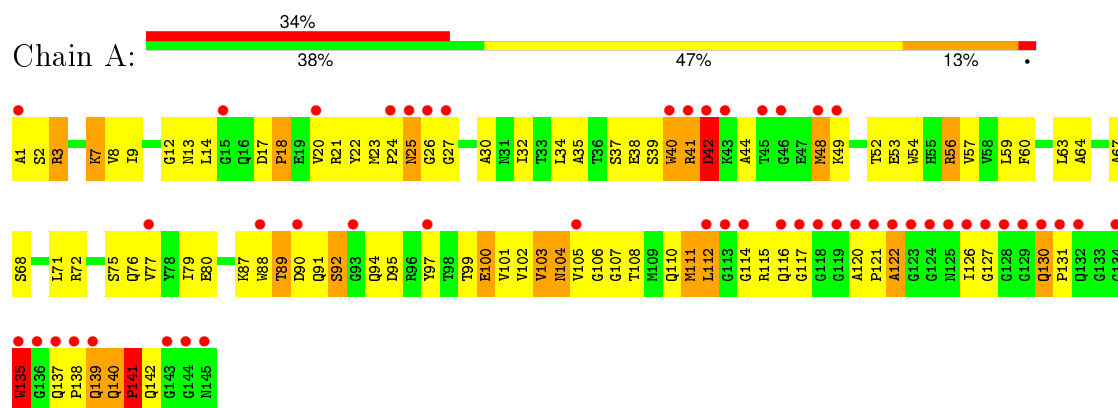
- Molecule 2 is water.

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		

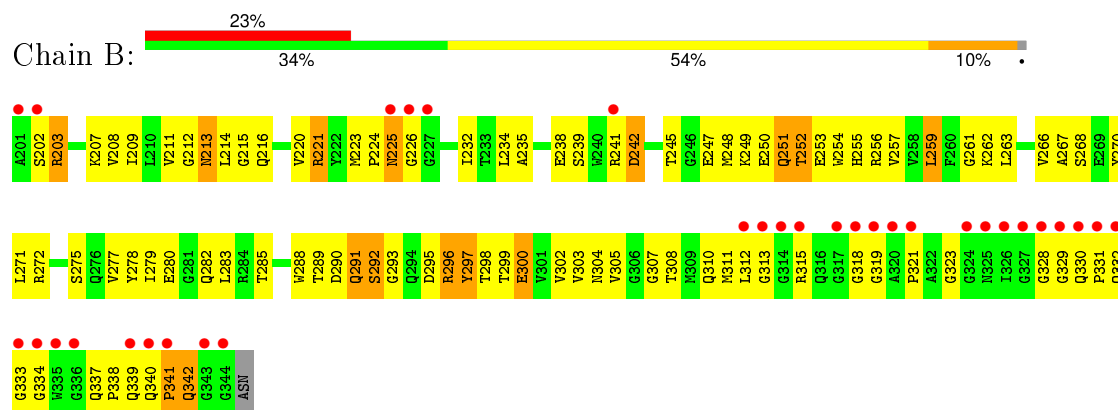
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

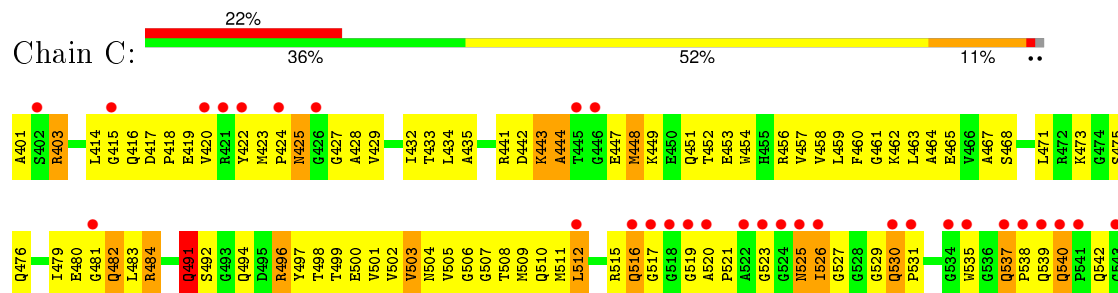
• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER



• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER

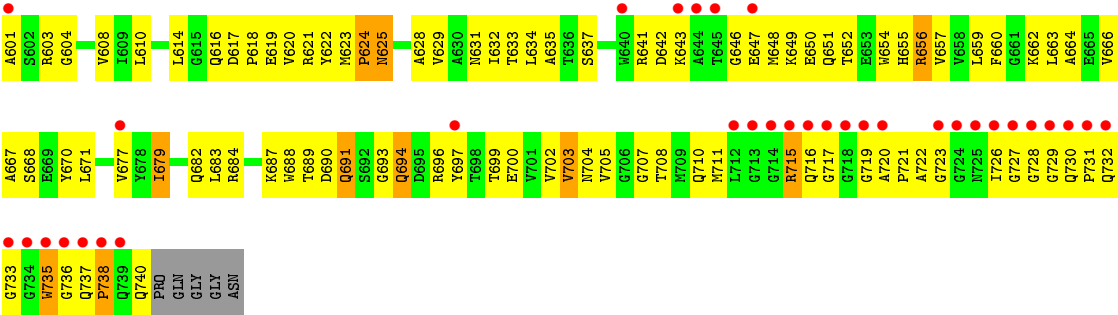


• Molecule 1: SINGLE STRANDED DNA BINDING PROTEIN MONOMER





● 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 51.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.2 (15.00-2.20) 82.7 (51.96-2.20)	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.	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.4	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 24955 reflections (0.004%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/1102	0.58	0/1487
1	B	0.35	0/1097	0.58	0/1480
1	C	0.37	0/1097	0.62	0/1480
1	D	0.34	0/1072	0.61	0/1446
All	All	0.34	0/4368	0.60	0/5893

There are no bond length outliers.

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	A	1083	0	1055	121	0
1	B	1078	0	1050	137	0
1	C	1078	0	1050	130	0
1	D	1054	0	1029	99	0
2	A	119	0	0	35	0
2	B	118	0	0	54	0
2	C	111	0	0	44	1
2	D	107	0	0	39	0
All	All	4748	0	4184	467	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 55.

All (467) 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:HE21	1:A:142:GLN:HA	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
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:B:270:TYR:HB3	1:B:310:GLN:HE22	1.48	0.77
1:A:72:ARG:HA	2:A:1219:HOH:O	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:LYS:HD3	1:D:650:GLU:N	1.98	0.77
1:C:496:ARG:HB2	1:C:496:ARG:HH11	1.49	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:C:507:GLY:HA3	2:C:807:HOH:O	1.85	0.76
1:B:250:GLU:HB2	1:B:328:GLY:HA3	1.68	0.76
1:B:291:GLN:HB3	2:B:1202:HOH:O	1.86	0.75
1:D:703:VAL:HG13	2:D:832:HOH:O	1.85	0.75
1:A:41:ARG:H	1:A:41:ARG:HD3	1.50	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:D:703:VAL:HG22	1:D:704:ASN:N	2.02	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:B:291:GLN:O	1:B:292:SER:OG	2.06	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: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:C:475:SER:HA	1:C:512:LEU:HD21	1.73	0.70
1:A:2:SER:HB2	1:C:515:ARG:HD3	1.72	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
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:A:12:GLY:HA3	1:A:34:LEU:HD21	1.75	0.68
1:A:141:PRO:HB2	2:A:1037:HOH:O	1.94	0.68
1:C:526:ILE:HD13	1:C:527:GLY:N	2.09	0.68
1:C:483:LEU:HD13	2:D:1223:HOH:O	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:503:VAL:HG13	1:C:504:ASN:N	2.09	0.66
1:A:117:GLY:HA3	2:A:1114:HOH:O	1.95	0.66
1:B:270:TYR:CB	1:B:310:GLN:HE22	2.08	0.66
1:C:494:GLN:HB2	2:C:1206:HOH:O	1.95	0.66
1:A:87:LYS:HD2	1:B:332:GLN:CD	2.16	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: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:A:44:ALA:HB2	2:A:888:HOH:O	1.98	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:496:ARG:CB	1:C:496:ARG:HH11	2.11	0.63
1:C:415:GLY:HA3	1:C:454:TRP:HZ3	1.63	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
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:D:737:GLN:HB2	1:D:738:PRO:HD3	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:O	1:A:49:LYS:HD3	2.00	0.61
1:C:442:ASP:CG	1:C:443:LYS:H	2.04	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:C:457:VAL:HG13	1:C:500:GLU:OE2	2.00	0.61
1:D:670:TYR:CB	1:D:710:GLN:HE22	2.12	0.61
1:A:67:ALA:O	1:A:71:LEU:HB2	2.01	0.61
1:D:632:ILE:HG13	2:D:861:HOH:O	2.00	0.61
1:A:39:SER:H	1:B:203:ARG:NH2	2.00	0.60
1:C:415:GLY:HA3	1:C:454:TRP:CZ3	2.35	0.60
1:B:315:ARG:HG2	2:B:1151:HOH:O	2.00	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: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:C:459:LEU:HG	2:C:1033:HOH:O	2.02	0.59
1:A:110:GLN:HB3	2:A:814:HOH:O	2.01	0.59
1:C:444:ALA:HB3	2:C:949:HOH:O	2.02	0.59
1:C:509:MET:HE2	2:C:1024:HOH:O	2.01	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:B:209:ILE:HG12	2:B:1068:HOH:O	2.03	0.59
1:A:23:MET:HG3	1:A:26:GLY: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:C:460:PHE:HA	2:C:1191:HOH:O	2.03	0.58
1:A:142:GLN:NE2	1:A:142:GLN:HA	2.14	0.58
1:A:63:LEU:HD22	1:A:63:LEU:H	1.68	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:A:9:ILE:HD12	2:B:1068:HOH:O	2.02	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:C:443:LYS:HB3	1:C:449:LYS:HD2	1.84	0.58
1:B:220:VAL:HG21	1:B:268:SER:CB	2.29	0.58
1:A:103:VAL:HG22	1:A:104:ASN:ND2	2.17	0.58
1:C:420:VAL:HG21	1:C:468:SER:CB	2.33	0.58
1:B:283:LEU:HD23	2:B:951:HOH:O	2.02	0.58
1:B:256:ARG:NH2	2:B:1086:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:530:GLN:HE21	2.02	0.57
1:C:484:ARG:N	2:C:944:HOH:O	2.37	0.57
1:D:614:LEU:HG	1:D:632:ILE:CG2	2.34	0.57
1:B:259:LEU:HD12	1:B:259:LEU:N	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: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:A:3:ARG:HH11	1:A:3:ARG:HG2	1.69	0.56
1:A:34:LEU:HD23	1:A:35:ALA:N	2.19	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:C:503:VAL:CG1	1:C:505:VAL:HG22	2.35	0.56
1:A:41:ARG:H	1:A:41:ARG:CD	2.18	0.56
1:B:275:SER:HB2	2:B:906:HOH:O	2.04	0.56
1:C:443:LYS:HG3	2:C:949:HOH:O	2.05	0.56
1:C:414:LEU:HA	1:C:433:THR:O	2.06	0.56
1:B:245:THR:HG23	1:B:247:GLU:H	1.71	0.56
1:D:620:VAL:CG2	1:D:668:SER:HB2	2.33	0.56
1:B:302:VAL:HG21	2:B:955:HOH:O	2.06	0.56
1:A:140:GLN:CG	1:A:141:PRO:HD2	2.36	0.56
1:C:416:GLN:HB2	2:C:996:HOH:O	2.06	0.56
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:C:443:LYS:HD3	1:C:444:ALA:N	2.21	0.55
1:A:39:SER:HB3	2:A:1244:HOH:O	2.05	0.55
1:B:304:ASN:HB2	2:B:975:HOH:O	2.06	0.55
1:A:108:THR:HG21	2:A:1195:HOH:O	2.05	0.55
1:D:679:ILE:HD13	2:D:1149:HOH:O	2.05	0.55
1:D:664:ALA:HB3	2:D:1213:HOH:O	2.06	0.55
1:A:131:PRO:HA	2:A:1131:HOH:O	2.06	0.55
1:D:634:LEU:HD11	1:D:679:ILE:HD13	1.88	0.55
1:D:614:LEU:HG	1:D:632:ILE:HG23	1.89	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:B:271:LEU:HD22	2:B:906:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD12	1:A:108:THR:HG22	1.88	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:B:330:GLN:N	1:B:331:PRO:HD3	2.20	0.55
1:B:304:ASN:HB3	2:B:1236:HOH:O	2.05	0.55
1:A:42:ASP:HA	2:A:1064:HOH:O	2.07	0.55
1:C:423:MET:HB2	1:C:427:GLY:O	2.08	0.54
1:C:418:PRO:HG2	2:C:1163:HOH:O	2.05	0.54
1:A:91:GLN:O	1:A:92:SER:HB2	2.06	0.54
1:B:313:GLY:HA3	2:B:1238:HOH:O	2.06	0.54
1:B:209:ILE:HD11	2:B:1232:HOH:O	2.06	0.54
1:D:730:GLN:HB3	1:D:731:PRO:HD2	1.90	0.54
1:D:700:GLU:HB2	2:D:924:HOH:O	2.07	0.54
1:D:708:THR:OG1	2:D:811:HOH:O	2.19	0.54
1:C:537:GLN:HG2	1:C:537:GLN:O	2.07	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:B:339:GLN:HE21	1:B:341:PRO:CG	2.21	0.53
1:A:103:VAL:HG22	1:A:104:ASN:N	2.18	0.53
1:C:461:GLY:O	1:C:465:GLU:HG3	2.09	0.53
1:B:266:VAL:HG13	1:B:270:TYR:HD2	1.74	0.53
1:B:213:ASN:HA	1:B:275:SER:O	2.08	0.53
1:C:526:ILE:C	1:C:526:ILE:HD13	2.29	0.53
1:C:463:LEU:HD22	1:C:508:THR:HG22	1.89	0.53
1:A:23:MET:HE2	2:A:1192:HOH:O	2.09	0.53
1:A:8:VAL:HB	1:A:100:GLU:OE1	2.09	0.53
1:A:63:LEU:CD2	1:A:63:LEU:H	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:511:MET:C	1:C:512:LEU:HD12	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:HB3	2:A:859:HOH:O	2.08	0.52
1:D:703:VAL:HG13	1:D:704:ASN:H	1.75	0.52
1:D:608:VAL:HB	1:D:700:GLU:OE1	2.09	0.52
1:A:138:PRO:HG3	2:C:1148: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:56:ARG:HG2	2:A:1010:HOH:O	2.09	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:C:432:ILE:HG12	2:C:1033:HOH:O	2.10	0.51
1:B:214:LEU:HG	1:B:232:ILE:HG23	1.91	0.51
1:D:715:ARG:O	1:D:716:GLN:HB3	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: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:102:VAL:HG12	2:A:1128:HOH:O	2.09	0.51
1:B:340:GLN:HA	1:B:340:GLN:NE2	2.25	0.51
1:A:110:GLN:HB3	2:A:1214:HOH:O	2.10	0.51
1:D:652:THR:HB	2:D:1059:HOH:O	2.10	0.51
1:D:703:VAL:HG13	1:D:704:ASN:N	2.26	0.51
1:B:235:ALA:HB1	2:B:914:HOH:O	2.11	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:B:291:GLN:O	1:B:292:SER:CB	2.59	0.50
1:C:529:GLY:C	1:C:530:GLN:HE21	2.15	0.50
1:A:30:ALA:HB2	1:A:64:ALA:HB1	1.93	0.50
1:B:303:VAL:CG1	1:B:305:VAL:HG22	2.41	0.50
1:C:467:ALA:HA	1:C:471:LEU:HG	1.92	0.50
1:B:235:ALA:HB2	1:B:254:TRP:CZ3	2.46	0.50
1:D:721:PRO:C	1:D:723:GLY:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:THR:HA	2:D:1076:HOH:O	2.12	0.50
1:B:223:MET:O	1:B:225:ASN:N	2.45	0.50
1:C:491:GLN:OE1	1:C:492:SER:CB	2.53	0.49
1:C:464:ALA:HB3	2:C:1191:HOH:O	2.12	0.49
1:B:259:LEU:N	1:B:259:LEU:CD1	2.75	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:B:300:GLU:HG2	2:B:831:HOH:O	2.13	0.48
1:A:32:ILE:HG13	1:A:57:VAL:HB	1.94	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:B:300:GLU:OE2	1:B:300:GLU:C	2.52	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:D:620:VAL:HG21	1:D:668:SER:CB	2.38	0.48
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:C:520:ALA:HB1	1:C:521:PRO:HA	1.96	0.48
1:A:76:GLN:HB3	1:A:111:MET:HB2	1.94	0.48
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:C:459:LEU:HG	2:C:1245:HOH:O	2.14	0.47
1:D:622:TYR:CE2	1:D:628:ALA:HB2	2.49	0.47
1:C:401:ALA:N	2:C:953:HOH:O	2.47	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:C:515:ARG:HG2	1:C:516:GLN:N	2.18	0.47
1:B:308:THR:OG1	2:B:1224:HOH:O	2.21	0.47
1:A:60:PHE:HE2	1:A:101:VAL:HG13	1.80	0.47
1:B:263:LEU:HD22	1:B:263:LEU:H	1.80	0.47
1:C:447:GLU:HB3	2:C:1205:HOH:O	2.14	0.47
1:B:242:ASP:C	1:B:242:ASP:OD2	2.53	0.47
1:C:456:ARG:NH2	2:C:1030:HOH:O	2.48	0.47
1:D:715:ARG:C	1:D:717:GLY:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HD3	2:A:1219:HOH:O	2.15	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:C:435:ALA:HA	1:C:453:GLU:O	2.16	0.46
1:B:315:ARG:HA	1:B:315:ARG:NE	2.30	0.46
1:A:120:ALA:N	1:A:121:PRO:HD3	2.31	0.46
1:C:429:VAL:HG22	1:C:460:PHE:HD1	1.81	0.46
1:B:208:VAL:HB	1:B:300:GLU:OE1	2.16	0.46
1:D:614:LEU:HA	1:D:633:THR:O	2.15	0.46
1:B:223:MET:HB2	1:B:225:ASN:HD21	1.80	0.46
1:A:32:ILE:CG1	1:A:57:VAL:HB	2.46	0.46
1:D:625:ASN:HB3	2:D:1036:HOH:O	2.15	0.46
1:C:456:ARG:HH21	1:D:696:ARG:HH22	1.63	0.46
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.80	0.46
1:A:103:VAL:HG22	1:A:104:ASN:HD22	1.79	0.45
1:B:332:GLN:HG2	1:B:333:GLY:H	1.80	0.45
1:D:679:ILE:HG21	2:D:1149:HOH:O	2.15	0.45
1:B:300:GLU:CG	2:B:831:HOH:O	2.64	0.45
1:B:235:ALA:HA	1:B:253:GLU:O	2.16	0.45
1:D:648:MET:HB3	2:D:1122:HOH:O	2.15	0.45
1:B:254:TRP:HE1	1:B:330:GLN:HB2	1.82	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:D:663:LEU:HD12	1:D:708:THR:CG2	2.46	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: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
1:B:340:GLN:HA	1:B:340:GLN:HE21	1.82	0.45
2:A:1217:HOH:O	1:C:505:VAL:HG12	2.15	0.45
1:D:671:LEU:HD21	1:D:710:GLN:HG2	1.99	0.45
1:B:339:GLN:CG	1:B:341:PRO:HD3	2.28	0.45
1:A:104:ASN:OD1	1:C:526:ILE:HD12	2.17	0.45
1:B:272:ARG:CZ	2:B:926:HOH:O	2.64	0.45
1:A:115:ARG:HB3	1:A:116:GLN:H	1.54	0.45
1:A:48:MET:SD	1:A:48:MET:N	2.87	0.44
1:D:719:GLY:O	1:D:720:ALA:HB2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:HB1	2:A:1047:HOH:O	2.16	0.44
1:C:505:VAL:HA	2:C:1158:HOH:O	2.16	0.44
1:A:126:ILE:O	1:A:126:ILE:HG23	2.16	0.44
1:B:202:SER:HA	2:B:1135:HOH:O	2.17	0.44
1:B:270:TYR:O	1:B:318:GLY:HA2	2.18	0.44
1:A:71:LEU:HD21	1:A:77:VAL:HG11	1.99	0.44
1:D:642:ASP:CG	1:D:643:LYS:H	2.21	0.44
1:B:207:LYS:HD2	1:B:280:GLU:HG3	2.00	0.44
1:B:257:VAL:HG12	1:B:259:LEU:CD1	2.48	0.44
1:A:137:GLN:N	1:A:138:PRO:HD2	2.33	0.44
1:C:484:ARG:NH2	2:C:801:HOH:O	2.30	0.44
1:B:257:VAL:HG12	1:B:259:LEU:HD12	2.00	0.43
1:B:239:SER:HB3	1:C:519:GLY:HA2	2.00	0.43
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:C:467:ALA:C	2:C:1163:HOH:O	2.56	0.43
1:C:457:VAL:HG12	2:C:1245:HOH:O	2.17	0.43
1:A:25:ASN:HD21	1:C:542:GLN:NE2	2.16	0.43
1:C:442:ASP:CG	1:C:443:LYS:N	2.71	0.43
1:D:637:SER:HB2	1:D:652:THR:HG22	2.00	0.43
1:B:215:GLY:O	1:B:216:GLN:HG3	2.19	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:103:VAL:O	1:A:104:ASN:C	2.57	0.43
1:A:40:TRP:HE1	1:A:49:LYS:HB2	1.83	0.43
1:C:500:GLU:CD	1:C:500:GLU:C	2.78	0.43
1:B:278:TYR:HE2	2:B:928:HOH:O	2.02	0.43
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:B:263:LEU:HD22	1:B:263:LEU:N	2.33	0.42
1:B:255:HIS:HD2	2:B:827:HOH:O	2.01	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: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:95:ASP:HB3	2:A:1000:HOH:O	2.20	0.42
1:B:212:GLY:C	1:B:234:LEU:HD22	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG21	2:B:951:HOH:O	2.19	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:A:37:SER:OG	1:A:52:THR:HG22	2.20	0.42
1:D:634:LEU:HD11	1:D:679:ILE:CD1	2.48	0.42
1:A:130:GLN:N	1:A:131:PRO:CD	2.81	0.42
1:B:295:ASP:C	1:B:296:ARG:HD2	2.39	0.42
1:D:715:ARG:HD2	1:D:715:ARG:H	1.84	0.42
1:B:321:PRO:C	1:B:323:GLY:H	2.23	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:C:460:PHE:HE2	1:C:501:VAL:HG13	1.84	0.41
1:A:41:ARG:HG2	1:A:41:ARG:NH1	2.35	0.41
1:D:629:VAL:HG22	1:D:660:PHE:CD1	2.55	0.41
1:C:419:GLU:HG2	2:C:986:HOH:O	2.18	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:C:496:ARG:CG	1:C:496:ARG:HH11	2.33	0.41
1:B:313:GLY:N	2:B:942:HOH:O	2.52	0.41
1:A:20:VAL:HG12	1:A:21:ARG:N	2.35	0.41
1:C:441:ARG:O	1:C:442:ASP:HB2	2.21	0.41
1:C:476:GLN:HE21	1:C:512:LEU:N	2.08	0.41
1:A:13:ASN:N	2:A:1141:HOH:O	2.47	0.41
1:B:288:TRP:CE3	1:B:340:GLN:HG2	2.55	0.41
1:C:516:GLN:HB3	1:C:517:GLY:H	1.51	0.41
1:A:49:LYS:HG3	2:A:989:HOH:O	2.20	0.41
1:C:502:VAL:CG2	2:C:1245:HOH:O	2.68	0.41
1:C:435:ALA:HB3	2:C:1127:HOH:O	2.20	0.41
1:D:632:ILE:HD11	1:D:667:ALA:HB1	2.03	0.41
1:A:22:TYR:O	1:A:23:MET:HB3	2.21	0.41
1:C:471:LEU:HB2	2:C:1163:HOH:O	2.20	0.41
1:C:414:LEU:N	1:C:414:LEU:HD12	2.36	0.41
1:A:7:LYS:HE2	1:A:7:LYS:HB2	1.79	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:B:272:ARG:HG3	1:B:272:ARG:HH11	1.86	0.41
1:B:245:THR:HG21	1:B:249:LYS:NZ	2.36	0.41
1:A:89:THR:HG23	1:A:89:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:GLN:CB	2:B:1202:HOH:O	2.56	0.40
1:C:456:ARG:HG3	1:C:497:TYR:OH	2.21	0.40
1:A:35:ALA:HA	1:A:53:GLU:O	2.22	0.40
1:B:315:ARG:HE	1:B:315:ARG:HA	1.86	0.40
1:B:340:GLN:CA	1:B:340:GLN:HE21	2.34	0.40
1:B:332:GLN:HG2	1:B:333:GLY:N	2.35	0.40
1:B:256:ARG:CZ	2:B:1086:HOH:O	2.69	0.40
1:B:257:VAL:HG11	1:B:279:ILE:CD1	2.46	0.40
1:A:139:GLN:O	1:A:140:GLN:HB3	2.20	0.40
1:A:135:TRP:HA	1:A:135:TRP:HE3	1.84	0.40
1:D:624:PRO:O	1:D:625:ASN:HB3	2.21	0.40
1:A:88:TRP:HZ3	1:A:90:ASP:HB3	1.87	0.40
1:D:671:LEU:HD23	1:D:710:GLN:HE21	1.86	0.40
1:A:17:ASP:HA	1:A:18:PRO:HD3	1.93	0.40
1:D:608:VAL:CG2	1:D:683:LEU:HG	2.51	0.40
1:C:422:TYR:HA	1:C:428:ALA:HA	2.03	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%)	1	0
1	C	142/145 (98%)	112 (79%)	19 (13%)	11 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Res	Type
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
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%)	98 (91%)	10 (9%)	11	10
1	B	108/109 (99%)	101 (94%)	7 (6%)	21	23
1	C	108/109 (99%)	97 (90%)	11 (10%)	9	8
1	D	106/109 (97%)	98 (92%)	8 (8%)	17	17
All	All	430/436 (99%)	394 (92%)	36 (8%)	14	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	40	TRP
1	A	41	ARG
1	A	42	ASP
1	A	48	MET
1	A	56	ARG
1	A	97	TYR
1	A	100	GLU
1	A	135	TRP
1	A	141	PRO
1	B	213	ASN
1	B	252	THR
1	B	259	LEU
1	B	282	GLN
1	B	296	ARG
1	B	297	TYR
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	656	ARG
1	D	679	ILE
1	D	691	GLN
1	D	697	TYR
1	D	711	MET
1	D	735	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN

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Mol	Chain	Res	Type
1	A	31	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
1	B	291	GLN
1	B	310	GLN
1	B	316	GLN
1	B	330	GLN
1	B	332	GLN
1	B	337	GLN
1	B	339	GLN
1	C	455	HIS
1	C	482	GLN
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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%)	1.73	50 (34%)	0 0	29, 67, 100, 100	0
1	B	144/145 (99%)	1.22	33 (22%)	1 1	28, 57, 100, 100	0
1	C	144/145 (99%)	1.25	32 (22%)	1 1	25, 58, 100, 100	0
1	D	140/145 (96%)	1.62	34 (24%)	1 1	30, 67, 100, 100	0
All	All	573/580 (98%)	1.46	149 (26%)	1 1	25, 61, 100, 100	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	TRP	10.0
1	D	601	ALA	9.6
1	D	723	GLY	9.2
1	D	720	ALA	8.6
1	B	327	GLY	8.3
1	D	724	GLY	8.3
1	B	318	GLY	7.7
1	D	725	ASN	7.3
1	A	120	ALA	7.0
1	D	729	GLY	6.8
1	A	45	THR	6.7
1	A	144	GLY	6.6
1	A	135	TRP	6.4
1	D	640	TRP	6.0
1	D	736	GLY	6.0
1	A	121	PRO	5.9
1	C	530	GLN	5.7
1	B	326	ILE	5.7
1	D	739	GLN	5.6
1	C	538	PRO	5.5
1	B	331	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	537	GLN	5.4
1	D	731	PRO	5.4
1	C	522	ALA	5.3
1	A	46	GLY	5.3
1	A	128	GLY	5.3
1	D	727	GLY	5.3
1	D	732	GLN	5.2
1	D	718	GLY	5.2
1	A	134	GLY	5.1
1	B	328	GLY	5.0
1	D	645	THR	5.0
1	D	719	GLY	4.9
1	C	520	ALA	4.7
1	A	125	ASN	4.7
1	C	541	PRO	4.7
1	C	531	PRO	4.6
1	D	737	GLN	4.6
1	C	445	THR	4.6
1	C	525	ASN	4.5
1	D	717	GLY	4.5
1	A	112	LEU	4.4
1	D	730	GLN	4.4
1	B	313	GLY	4.3
1	D	735	TRP	4.3
1	A	24	PRO	4.3
1	B	226	GLY	4.2
1	A	43	LYS	4.2
1	B	225	ASN	4.2
1	A	113	GLY	4.2
1	A	127	GLY	4.2
1	C	534	GLY	4.2
1	B	330	GLN	4.2
1	B	227	GLY	4.1
1	B	344	GLY	4.1
1	B	334	GLY	4.0
1	C	526	ILE	4.0
1	B	321	PRO	3.9
1	C	517	GLY	3.9
1	D	697	TYR	3.9
1	A	114	GLY	3.9
1	A	1	ALA	3.8
1	A	138	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	202	SER	3.7
1	A	118	GLY	3.7
1	A	105	VAL	3.7
1	C	539	GLN	3.6
1	B	343	GLY	3.6
1	A	20	VAL	3.6
1	A	131	PRO	3.5
1	A	27	GLY	3.5
1	A	40	TRP	3.5
1	D	726	ILE	3.4
1	B	324	GLY	3.4
1	A	139	GLN	3.4
1	C	540	GLN	3.4
1	B	201	ALA	3.4
1	C	422	TYR	3.3
1	A	25	ASN	3.2
1	A	145	ASN	3.2
1	D	716	GLN	3.2
1	A	122	ALA	3.2
1	B	341	PRO	3.2
1	B	317	GLY	3.2
1	A	116	GLN	3.2
1	C	512	LEU	3.2
1	A	126	ILE	3.1
1	B	332	GLN	3.1
1	C	535	TRP	3.1
1	A	129	GLY	3.0
1	D	644	ALA	3.0
1	B	312	LEU	3.0
1	C	424	PRO	2.9
1	A	143	GLY	2.9
1	A	93	GLY	2.9
1	C	402	SER	2.9
1	D	734	GLY	2.9
1	A	124	GLY	2.8
1	A	130	GLN	2.8
1	A	49	LYS	2.8
1	B	319	GLY	2.7
1	C	446	GLY	2.7
1	C	544	GLY	2.7
1	D	712	LEU	2.7
1	B	241	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	333	GLY	2.7
1	D	715	ARG	2.7
1	B	325	ASN	2.6
1	B	320	ALA	2.6
1	A	42	ASP	2.6
1	B	314	GLY	2.5
1	A	48	MET	2.5
1	A	90	ASP	2.5
1	D	728	GLY	2.5
1	D	733	GLY	2.5
1	A	136	GLY	2.5
1	C	543	GLY	2.5
1	C	481	GLY	2.5
1	A	137	GLN	2.5
1	B	315	ARG	2.5
1	B	329	GLY	2.4
1	D	738	PRO	2.4
1	D	643	LYS	2.4
1	A	123	GLY	2.3
1	A	97	TYR	2.3
1	C	523	GLY	2.3
1	C	420	VAL	2.3
1	A	41	ARG	2.3
1	A	88	TRP	2.3
1	A	15	GLY	2.2
1	D	647	GLU	2.2
1	A	132	GLN	2.2
1	C	415	GLY	2.2
1	C	519	GLY	2.2
1	A	117	GLY	2.2
1	D	714	GLY	2.2
1	C	524	GLY	2.1
1	C	518	GLY	2.1
1	A	26	GLY	2.1
1	C	426	GLY	2.1
1	A	119	GLY	2.1
1	D	713	GLY	2.0
1	C	421	ARG	2.0
1	B	339	GLN	2.0
1	B	340	GLN	2.0
1	C	516	GLN	2.0
1	A	77	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	336	GLY	2.0
1	D	677	VAL	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 carbohydrates 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.