WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jul 11, 2017 – 01:53 PM EDT

PDB ID : 3PHA

Title : The crystal structure of the W169Y mutant of alpha-glucosidase (gh31 family) from Ruminococcus obeum atcc 29174 in complex with acarbose

Authors : Tan, K.; Tesar, C.; Keigher, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)

Deposited on : unknown
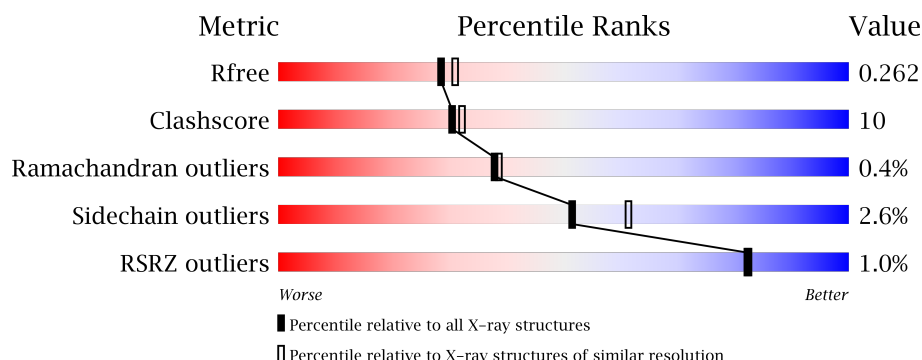
Resolution : 2.17 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		2.6%
RSRZ outliers		1.0%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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 <=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	666	.% 72% 26% •
1	B	666	2% 77% 22% •
1	C	666	.% 78% 21% •
1	D	666	.% 78% 21% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22569 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.
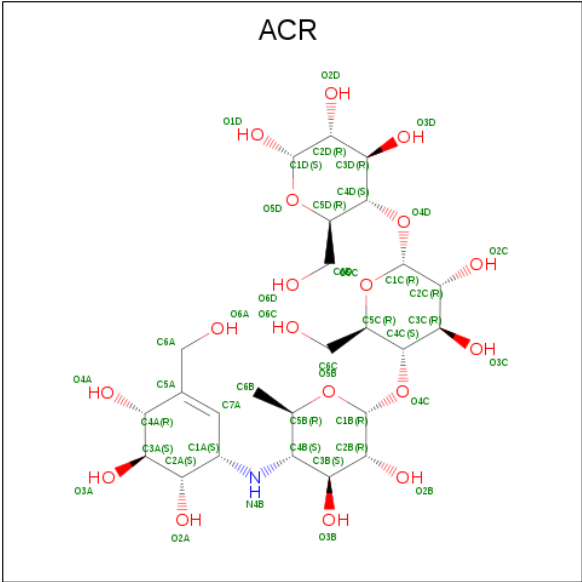
- Molecule 1 is a protein called alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total 5440	C 3491	N 890	O 1024	S 35	0	1	0
1	B	665	Total 5447	C 3494	N 892	O 1026	S 35	0	1	0
1	C	665	Total 5448	C 3495	N 892	O 1026	S 35	0	1	0
1	D	666	Total 5457	C 3498	N 896	O 1028	S 35	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A5ZY13
A	-1	ASN	-	expression tag	UNP A5ZY13
A	0	ALA	-	expression tag	UNP A5ZY13
A	169	TYR	TRP	engineered mutation	UNP A5ZY13
B	-2	SER	-	expression tag	UNP A5ZY13
B	-1	ASN	-	expression tag	UNP A5ZY13
B	0	ALA	-	expression tag	UNP A5ZY13
B	169	TYR	TRP	engineered mutation	UNP A5ZY13
C	-2	SER	-	expression tag	UNP A5ZY13
C	-1	ASN	-	expression tag	UNP A5ZY13
C	0	ALA	-	expression tag	UNP A5ZY13
C	169	TYR	TRP	engineered mutation	UNP A5ZY13
D	-2	SER	-	expression tag	UNP A5ZY13
D	-1	ASN	-	expression tag	UNP A5ZY13
D	0	ALA	-	expression tag	UNP A5ZY13
D	169	TYR	TRP	engineered mutation	UNP A5ZY13

- Molecule 2 is ALPHA-ACARBOSE (three-letter code: ACR) (formula: $C_{25}H_{43}NO_{18}$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 44	C 25	N 1	O 18	0	0
2	B	1	Total 44	C 25	N 1	O 18	0	0
2	C	1	Total 44	C 25	N 1	O 18	0	0
2	D	1	Total 44	C 25	N 1	O 18	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total 94	O 94	0	0
3	B	120	Total 120	O 120	0	0
3	C	203	Total 203	O 203	0	0
3	D	184	Total 184	O 184	0	0

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 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: alpha-glucosidase
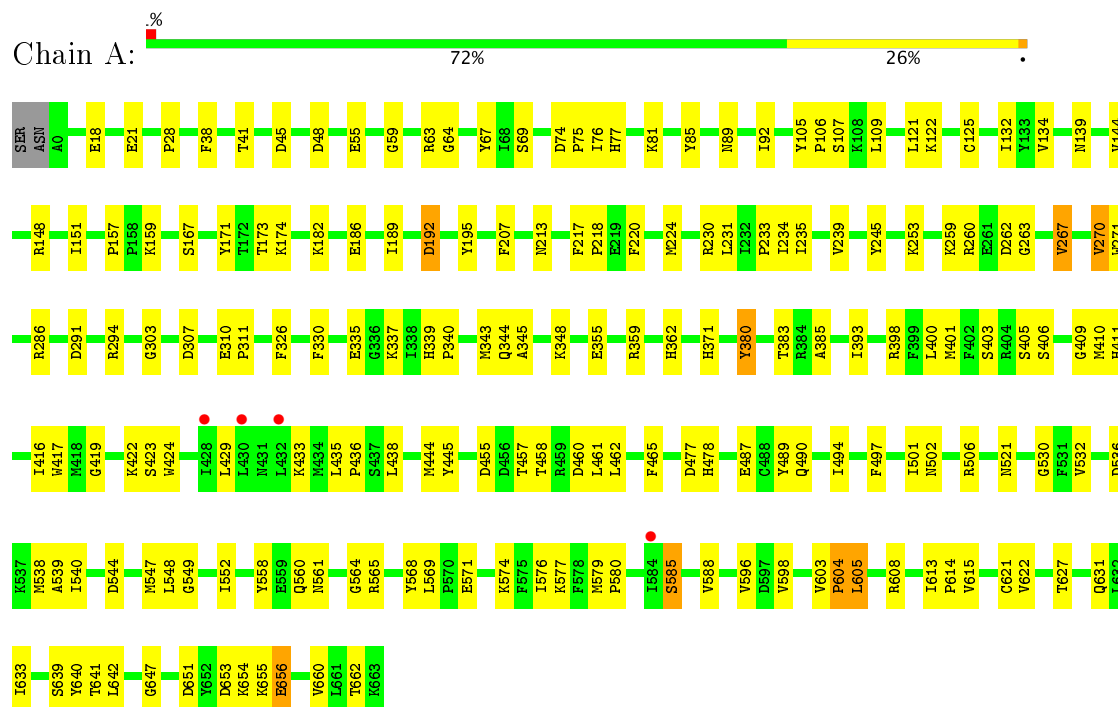
- Molecule 1: alpha-glucosidase

- Molecule 1: alpha-glucosidase

Chain C:

- Molecule 1: alpha-glucosidase

Chain D:
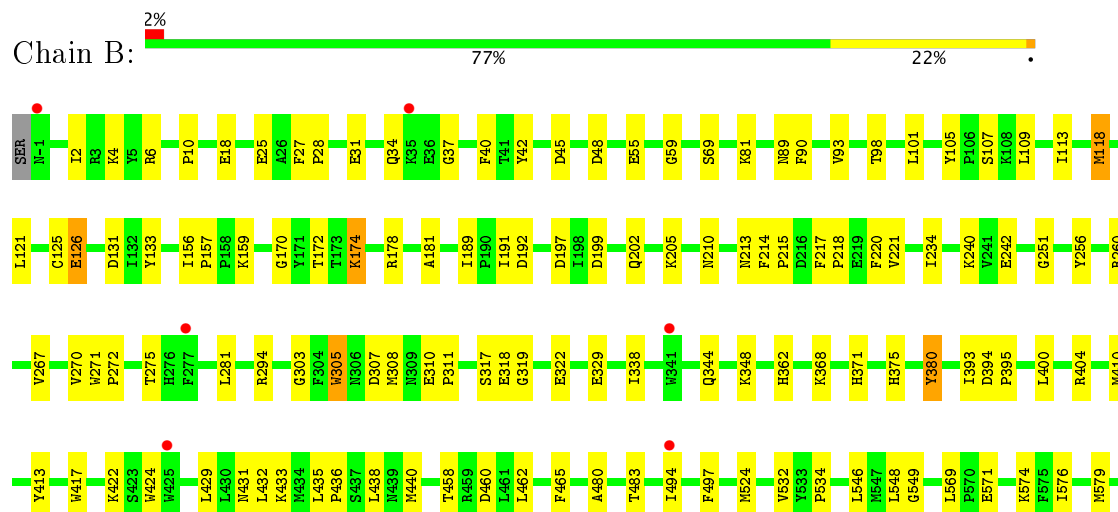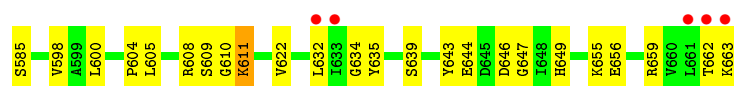
4   Data and refinement statistics (i)

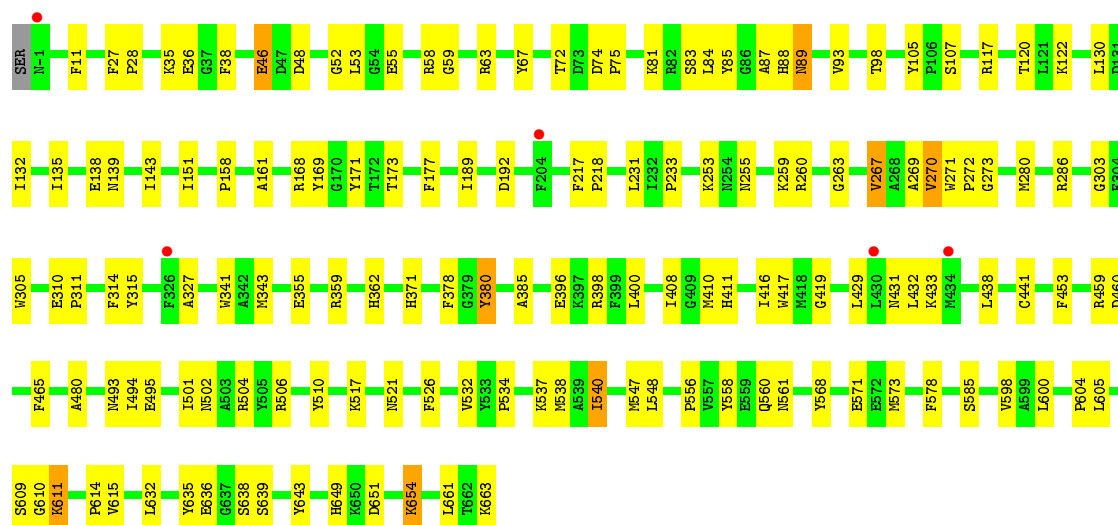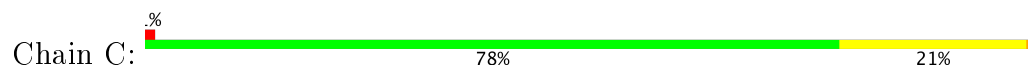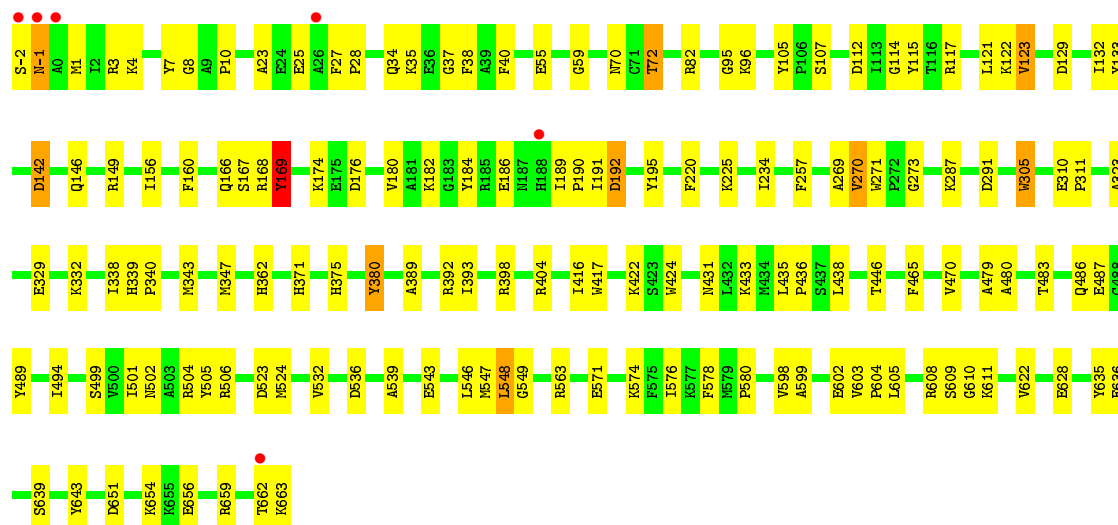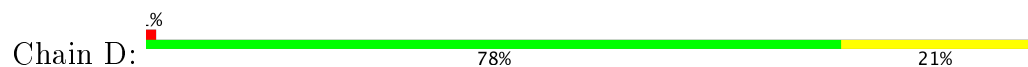| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.03Å 125.95Å 133.58Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	42.41 – 2.17 50.06 – 2.17	Depositor EDS
% Data completeness (in resolution range)	90.4 (42.41-2.17) 97.9 (50.06-2.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.09 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.200 , 0.265 0.197 , 0.262	Depositor DCC
R_{free} test set	7139 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.3	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22569	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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 82.90 % 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 2.4837e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: ACR

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	0.38	0/5585	0.54	0/7531
1	B	0.39	0/5592	0.54	1/7541 (0.0%)
1	C	0.41	0/5593	0.56	0/7542
1	D	0.42	0/5602	0.57	0/7553
All	All	0.40	0/22372	0.55	1/30167 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	432	LEU	CA-CB-CG	5.63	128.25	115.30

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	A	5440	0	5213	135	0
1	B	5447	0	5217	107	0
1	C	5448	0	5219	105	0
1	D	5457	0	5226	100	0
2	A	44	0	43	1	0
2	B	44	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	43	2	0
2	D	44	0	43	3	0
3	A	94	0	0	5	0
3	B	120	0	0	4	0
3	C	203	0	0	11	0
3	D	184	0	0	4	0
All	All	22569	0	21047	450	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 10.

All (450) 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:270:VAL:HG12	1:A:271:TRP:H	1.24	1.00
1:A:330:PHE:HB2	1:A:343:MET:HE3	1.48	0.95
1:C:327:ALA:HA	1:C:343:MET:HE1	1.53	0.88
1:C:429:LEU:HD22	1:C:558:TYR:CE1	2.09	0.87
1:A:59:GLY:HA2	1:A:433:LYS:HD3	1.60	0.82
1:A:330:PHE:CB	1:A:343:MET:HE3	2.12	0.79
1:D:4:LYS:HG3	1:D:133:TYR:CE1	2.18	0.78
1:D:436:PRO:HG3	1:D:546:LEU:HD21	1.66	0.77
1:A:576:ILE:HB	1:A:605:LEU:HD13	1.68	0.75
1:D:270:VAL:HG12	1:D:271:TRP:H	1.52	0.74
1:D:548:LEU:HD12	1:D:549:GLY:N	2.02	0.74
1:A:270:VAL:HG12	1:A:271:TRP:N	2.01	0.74
1:A:310:GLU:N	1:A:311:PRO:HA	2.03	0.73
1:A:21:GLU:HG2	3:A:675:HOH:O	1.88	0.73
1:B:598:VAL:HG11	1:B:604:PRO:HG3	1.71	0.72
1:A:571:GLU:OE2	1:A:608:ARG:HD2	1.90	0.72
1:A:641:THR:HG22	1:A:660:VAL:HG12	1.71	0.71
1:D:651:ASP:OD1	1:D:654:LYS:HE3	1.91	0.71
1:B:210:ASN:HB3	1:B:213:ASN:HB2	1.72	0.70
1:C:432[B]:LEU:HD12	1:C:556:PRO:HG2	1.74	0.70
1:D:532:VAL:HG21	1:D:547:MET:HG3	1.72	0.70
1:B:260:ARG:NH2	1:B:267[B]:VAL:HG12	2.05	0.70
1:B:260:ARG:HH21	1:B:267[B]:VAL:HG12	1.55	0.70
1:D:70:ASN:O	1:D:72:THR:HG22	1.90	0.70
1:B:632:LEU:O	1:B:663:LYS:HE2	1.91	0.70
1:D:362:HIS:NE2	1:D:371:HIS:HD2	1.91	0.69
1:C:310:GLU:N	1:C:311:PRO:HA	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HE3	1:B:215:PRO:HD2	1.76	0.68
1:C:59:GLY:HA2	1:C:433:LYS:HD3	1.75	0.68
1:D:55:GLU:HB2	1:D:438:LEU:HD21	1.77	0.67
1:A:598:VAL:HG11	1:A:604:PRO:HG3	1.77	0.66
1:C:609:SER:HA	1:C:635:TYR:CE2	2.30	0.66
1:B:4:LYS:HG3	1:B:133:TYR:CE1	2.31	0.66
1:C:35:LYS:HG3	1:C:36:GLU:H	1.60	0.66
1:A:639:SER:HB3	1:A:662:THR:HG22	1.77	0.65
1:B:105:TYR:CE2	1:B:107:SER:HB3	2.31	0.65
1:A:362:HIS:NE2	1:A:371:HIS:HD2	1.94	0.65
1:B:267[B]:VAL:HG11	1:B:317:SER:OG	1.95	0.65
1:C:408:ILE:CD1	1:C:441:CYS:HB3	2.27	0.65
1:D:436:PRO:HG3	1:D:546:LEU:CD2	2.26	0.65
1:C:270:VAL:HG12	1:C:271:TRP:H	1.62	0.64
1:B:639:SER:HA	3:B:759:HOH:O	1.96	0.64
1:B:436:PRO:HG3	1:B:546:LEU:HD21	1.80	0.64
2:C:701:ACR:H6C1	2:C:701:ACR:H5B	1.81	0.63
2:D:701:ACR:H3C	3:D:841:HOH:O	1.99	0.63
1:D:310:GLU:N	1:D:311:PRO:HA	2.14	0.62
1:D:59:GLY:HA2	1:D:433:LYS:HD3	1.79	0.62
1:B:234:ILE:HD11	1:B:307:ASP:HB2	1.81	0.62
1:B:59:GLY:HA2	1:B:433:LYS:HD3	1.81	0.62
1:C:327:ALA:HA	1:C:343:MET:CE	2.28	0.62
1:C:560:GLN:O	1:C:561:ASN:HB2	1.99	0.62
1:A:330:PHE:HB2	1:A:343:MET:CE	2.28	0.62
1:A:345:ALA:HA	1:A:348:LYS:HE3	1.82	0.61
1:D:571:GLU:OE2	1:D:608:ARG:HD3	2.01	0.61
1:B:380:TYR:HA	1:B:410:MET:HG3	1.83	0.61
1:C:89:ASN:HD22	1:C:89:ASN:N	1.99	0.61
1:B:294:ARG:HG3	1:B:393:ILE:HD13	1.82	0.61
1:B:436:PRO:HG3	1:B:546:LEU:CD2	2.31	0.61
1:A:55:GLU:HB2	1:A:438:LEU:HD21	1.83	0.60
1:B:2:ILE:O	1:B:2:ILE:HG22	2.02	0.60
1:D:479:ALA:HB1	1:D:483:THR:HG21	1.82	0.60
2:B:701:ACR:H6C1	2:B:701:ACR:H5B	1.83	0.60
1:A:344:GLN:HG2	1:A:348:LYS:HE2	1.84	0.60
1:B:240:LYS:HA	1:B:275:THR:HG22	1.83	0.60
1:B:371:HIS:HE1	1:B:375:HIS:ND1	1.99	0.60
1:D:339:HIS:ND1	1:D:340:PRO:HD2	2.17	0.59
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.84	0.59
1:A:409:GLY:H	1:A:411:HIS:HD2	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:HD3	1:A:455:ASP:OD2	2.02	0.59
1:C:286:ARG:HG3	1:C:385:ALA:HB2	1.84	0.59
1:B:109:LEU:HD12	1:B:125:CYS:HB3	1.85	0.59
1:A:403:SER:O	1:A:416:ILE:HD13	2.03	0.58
1:C:93:VAL:O	1:C:98:THR:HA	2.01	0.58
1:C:651:ASP:OD2	1:C:654:LYS:HD2	2.04	0.58
1:A:231:LEU:O	1:A:233:PRO:HD3	2.03	0.58
1:D:182:LYS:O	1:D:186:GLU:HB2	2.04	0.58
1:A:460:ASP:HB3	1:B:118:MET:CE	2.33	0.58
1:B:234:ILE:HD11	1:B:307:ASP:CB	2.32	0.58
1:C:89:ASN:N	1:C:89:ASN:ND2	2.52	0.58
1:A:260:ARG:NH2	1:A:267:VAL:HG12	2.19	0.58
1:B:172:THR:HG22	1:B:213:ASN:HD21	1.69	0.58
1:B:105:TYR:CZ	1:B:107:SER:HB3	2.39	0.57
1:D:435:LEU:HB2	1:D:436:PRO:HD3	1.85	0.57
1:A:655:LYS:HG3	1:A:656:GLU:OE2	2.04	0.57
1:D:40:PHE:HB3	1:D:123:VAL:HG13	1.85	0.57
1:D:323:ALA:HB1	1:D:347:MET:HE1	1.87	0.57
1:B:404:ARG:HB2	1:B:417:TRP:CH2	2.39	0.57
1:B:303:GLY:HA3	1:B:400:LEU:HB3	1.86	0.56
1:A:171:TYR:HB2	3:A:696:HOH:O	2.05	0.56
1:D:599:ALA:HB3	1:D:602:GLU:HG3	1.86	0.56
1:B:6:ARG:HD3	1:B:131:ASP:OD1	2.05	0.56
1:B:362:HIS:NE2	1:B:371:HIS:HD2	2.03	0.56
1:A:574:LYS:HG2	1:A:588:VAL:HG22	1.86	0.56
1:D:156:ILE:HG22	1:D:398:ARG:HD3	1.86	0.56
1:B:202:GLN:OE1	1:B:210:ASN:HA	2.04	0.56
1:B:310:GLU:N	1:B:311:PRO:HA	2.20	0.56
1:A:538:MET:HG2	1:A:568:TYR:CE1	2.41	0.56
1:B:436:PRO:O	1:B:440:MET:HG3	2.06	0.56
1:C:431:ASN:HB2	3:C:858:HOH:O	2.06	0.56
1:A:286:ARG:HG2	1:A:385:ALA:HB2	1.87	0.55
1:A:560:GLN:O	1:A:561:ASN:HB2	2.05	0.55
1:C:260:ARG:HH22	1:C:267:VAL:HG12	1.70	0.55
1:C:526:PHE:CE1	1:C:548:LEU:HD12	2.41	0.55
1:A:310:GLU:N	1:A:311:PRO:CA	2.69	0.55
1:D:-1:ASN:C	1:D:1:MET:H	2.09	0.55
1:A:654:LYS:HD2	1:A:654:LYS:N	2.21	0.55
1:D:548:LEU:HD12	1:D:548:LEU:C	2.27	0.55
1:C:231:LEU:O	1:C:233:PRO:HD3	2.07	0.54
1:D:329:GLU:HB3	1:D:338:ILE:CD1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HD2	1:B:214:PHE:CD1	2.43	0.54
1:B:609:SER:HA	1:B:635:TYR:CE2	2.42	0.54
1:C:259:LYS:HE3	1:C:263:GLY:O	2.07	0.54
1:B:308:MET:HA	1:B:404:ARG:NH1	2.23	0.54
1:A:45:ASP:HB3	1:A:48:ASP:CG	2.28	0.54
1:B:6:ARG:HD2	1:B:10:PRO:HG2	1.90	0.54
1:C:87:ALA:C	1:C:88:HIS:HD2	2.11	0.54
1:D:329:GLU:HB3	1:D:338:ILE:HD11	1.90	0.54
1:A:157:PRO:HG3	1:A:445:TYR:CD1	2.42	0.54
1:B:644:GLU:OE2	1:B:659:ARG:NH1	2.41	0.54
1:C:362:HIS:NE2	1:C:371:HIS:HD2	2.05	0.53
1:C:460:ASP:HB3	1:C:600:LEU:HD11	1.91	0.53
1:D:480:ALA:O	1:D:483:THR:HG22	2.09	0.53
1:D:639:SER:OG	1:D:662:THR:HG23	2.08	0.53
1:C:48:ASP:O	1:C:63:ARG:HD2	2.09	0.53
1:D:-1:ASN:N	1:D:-1:ASN:HD22	2.06	0.53
1:D:105:TYR:CE2	1:D:107:SER:HB3	2.44	0.53
1:D:121:LEU:HD12	1:D:122:LYS:N	2.24	0.53
1:A:38:PHE:CZ	1:A:132:ILE:HD11	2.43	0.53
1:A:564:GLY:HA3	1:A:596:VAL:O	2.09	0.53
1:A:651:ASP:OD1	1:A:654:LYS:HD3	2.09	0.53
1:B:371:HIS:CE1	1:B:375:HIS:ND1	2.77	0.53
1:C:171:TYR:HB2	3:C:808:HOH:O	2.07	0.53
1:D:416:ILE:HG12	1:D:446:THR:HG22	1.90	0.53
1:D:610:GLY:O	1:D:611:LYS:HD2	2.08	0.53
1:B:435:LEU:HB2	1:B:436:PRO:HD3	1.91	0.53
1:C:610:GLY:C	1:C:611:LYS:HD2	2.29	0.53
1:A:286:ARG:CG	1:A:385:ALA:HB2	2.39	0.52
1:A:383:THR:HG23	1:A:401:MET:HE2	1.91	0.52
1:B:202:GLN:O	1:B:205:LYS:HD3	2.09	0.52
1:A:189:ILE:HD11	1:A:494:ILE:HD11	1.91	0.52
1:B:460:ASP:HB3	1:B:600:LEU:HD11	1.91	0.52
1:D:112:ASP:OD1	1:D:115:TYR:HB3	2.10	0.52
1:B:422:LYS:HD3	1:B:424:TRP:CZ2	2.43	0.52
1:A:230:ARG:HA	3:A:733:HOH:O	2.10	0.52
1:B:646:ASP:OD2	1:B:649:HIS:ND1	2.36	0.52
1:A:303:GLY:HA2	1:A:400:LEU:O	2.10	0.52
1:A:85:TYR:CE2	1:A:419:GLY:HA3	2.44	0.52
1:B:202:GLN:OE1	1:B:202:GLN:HA	2.10	0.52
1:D:167:SER:HB2	1:D:195:TYR:HB2	1.92	0.51
1:C:105:TYR:CE2	1:C:107:SER:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:HD3	3:C:783:HOH:O	2.09	0.51
1:A:532:VAL:HG21	1:A:547:MET:HG3	1.93	0.51
1:C:260:ARG:NH2	1:C:267:VAL:HG12	2.24	0.51
1:D:532:VAL:CG2	1:D:547:MET:HG3	2.40	0.51
1:C:310:GLU:N	1:C:311:PRO:CA	2.73	0.51
1:C:271:TRP:HB2	1:C:272:PRO:HD3	1.93	0.51
1:C:408:ILE:HD11	1:C:441:CYS:HB3	1.91	0.51
1:D:23:ALA:HB1	1:D:25:GLU:OE2	2.09	0.51
1:D:389:ALA:O	1:D:393:ILE:HG13	2.11	0.51
1:C:35:LYS:HG3	1:C:36:GLU:N	2.26	0.51
1:D:-1:ASN:N	1:D:-1:ASN:ND2	2.59	0.51
1:A:76:ILE:HG13	1:A:81:LYS:HE3	1.93	0.51
1:B:126:GLU:CD	1:B:126:GLU:H	2.13	0.51
1:B:318:GLU:O	1:B:322:GLU:HG3	2.11	0.51
1:D:114:GLY:HA2	1:D:117:ARG:O	2.10	0.50
1:D:636:GLU:OE2	1:D:663:LYS:HE3	2.10	0.50
1:A:260:ARG:HH22	1:A:267:VAL:HG12	1.75	0.50
1:B:189:ILE:HD11	1:B:494:ILE:HD11	1.92	0.50
1:C:355:GLU:O	1:C:359:ARG:HG3	2.12	0.50
1:A:291:ASP:HB3	1:A:294:ARG:NH2	2.27	0.50
1:A:38:PHE:CD2	1:A:38:PHE:C	2.85	0.50
1:D:38:PHE:CZ	1:D:132:ILE:HD11	2.46	0.50
1:C:643:TYR:CD2	1:C:643:TYR:C	2.84	0.50
1:C:217:PHE:HB3	1:C:218:PRO:HD3	1.94	0.50
1:B:90:PHE:HD1	1:B:101:LEU:O	1.95	0.50
1:C:168:ARG:HD2	3:C:848:HOH:O	2.11	0.50
1:A:615:VAL:HG21	1:A:633:ILE:HD12	1.94	0.50
1:C:638:SER:HB3	3:C:703:HOH:O	2.12	0.50
1:C:72:THR:HA	3:C:763:HOH:O	2.10	0.50
1:A:502:ASN:O	1:A:506:ARG:HG3	2.12	0.50
1:C:517:LYS:O	1:C:521:ASN:HB2	2.11	0.50
1:A:286:ARG:HG2	1:A:385:ALA:CB	2.42	0.49
2:A:701:ACR:H6C1	2:A:701:ACR:H5B	1.93	0.49
1:A:121:LEU:HD12	1:A:122:LYS:N	2.27	0.49
1:A:435:LEU:HB2	1:A:436:PRO:HD3	1.94	0.49
1:B:69:SER:OG	1:B:89:ASN:ND2	2.46	0.49
1:D:329:GLU:HA	1:D:332:LYS:NZ	2.27	0.49
1:D:55:GLU:O	1:D:55:GLU:HG2	2.12	0.49
1:A:76:ILE:HG13	1:A:76:ILE:O	2.13	0.49
1:A:18:GLU:HB2	3:A:667:HOH:O	2.11	0.49
1:D:536:ASP:HB3	1:D:539:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ASP:O	1:D:146:GLN:HG3	2.13	0.48
1:B:192:ASP:OD2	1:B:622:VAL:HG23	2.13	0.48
1:C:534:PRO:HB2	3:C:758:HOH:O	2.13	0.48
1:D:-1:ASN:C	1:D:1:MET:N	2.66	0.48
1:C:408:ILE:HD13	1:C:441:CYS:HB3	1.93	0.48
1:C:343:MET:CE	1:D:343:MET:HE2	2.42	0.48
1:B:532:VAL:C	1:B:534:PRO:HD3	2.34	0.48
1:C:158:PRO:HG3	1:C:398:ARG:O	2.14	0.48
1:D:598:VAL:HG11	1:D:604:PRO:HG3	1.95	0.48
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.66	0.48
1:A:139:ASN:HB2	3:A:694:HOH:O	2.14	0.48
1:A:182:LYS:HG3	1:A:186:GLU:CD	2.33	0.48
1:A:174:LYS:HG2	1:A:220:PHE:CD1	2.49	0.48
1:B:113:ILE:HG23	1:B:121:LEU:HD13	1.95	0.48
1:D:502:ASN:O	1:D:506:ARG:HG3	2.13	0.48
1:D:654:LYS:HB3	1:D:656:GLU:HG2	1.96	0.48
1:B:574:LYS:HE3	1:B:634:GLY:O	2.14	0.48
1:D:610:GLY:C	1:D:611:LYS:HD2	2.34	0.48
2:C:701:ACR:O5C	2:C:701:ACR:H6D2	2.14	0.48
1:A:548:LEU:HD23	1:A:549:GLY:N	2.29	0.47
1:D:40:PHE:HD2	1:D:123:VAL:CG1	2.26	0.47
1:D:166:GLN:NE2	1:D:184:TYR:OH	2.45	0.47
1:B:251:GLY:HA2	1:B:256:TYR:HB2	1.95	0.47
1:C:122:LYS:HG2	3:C:686:HOH:O	2.12	0.47
1:C:269:ALA:HA	1:C:273:GLY:O	2.14	0.47
1:C:83:SER:O	1:C:84:LEU:HD23	2.14	0.47
1:A:460:ASP:HB3	1:B:118:MET:HE3	1.96	0.47
1:D:192:ASP:OD2	1:D:622:VAL:HG23	2.14	0.47
1:D:174:LYS:HG2	1:D:220:PHE:CD1	2.49	0.47
1:A:497:PHE:O	1:A:501:ILE:HG12	2.14	0.47
1:B:27:PHE:HA	1:B:28:PRO:HD3	1.78	0.47
1:A:457:THR:HG22	1:A:458:THR:H	1.80	0.47
1:B:267[B]:VAL:CG1	1:B:317:SER:OG	2.62	0.47
1:A:224:MET:HA	1:A:224:MET:HE2	1.96	0.47
1:A:28:PRO:HG2	1:A:134:VAL:HG11	1.97	0.47
1:B:655:LYS:HE2	1:B:656:GLU:OE1	2.15	0.47
1:B:93:VAL:O	1:B:98:THR:HA	2.15	0.47
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.74	0.47
1:B:45:ASP:HB3	1:B:48:ASP:OD1	2.14	0.47
1:D:501:ILE:O	1:D:504:ARG:HB3	2.15	0.47
1:A:38:PHE:HZ	1:A:132:ILE:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLU:HB2	1:A:337:LYS:HG3	1.97	0.47
1:B:6:ARG:CD	1:B:10:PRO:HG2	2.44	0.47
1:D:380:TYR:C	1:D:380:TYR:CD1	2.88	0.47
1:D:7:TYR:O	1:D:129:ASP:HA	2.15	0.47
1:C:138:GLU:HG3	1:C:139:ASN:H	1.79	0.46
1:D:523:ASP:OD1	1:D:524:MET:N	2.44	0.46
1:C:161:ALA:CB	1:C:400:LEU:HD13	2.45	0.46
1:C:189:ILE:HD11	1:C:494:ILE:HD11	1.96	0.46
1:C:74:ASP:HA	1:C:75:PRO:HD3	1.74	0.46
1:B:197:ASP:O	1:B:199:ASP:N	2.49	0.46
1:C:639:SER:HB2	1:C:661:LEU:O	2.15	0.46
1:C:151:ILE:HD12	1:C:411:HIS:CE1	2.50	0.46
1:C:87:ALA:C	1:C:88:HIS:CD2	2.89	0.46
1:D:176:ASP:O	1:D:180:VAL:HG23	2.15	0.46
1:A:174:LYS:HG2	1:A:220:PHE:CE1	2.50	0.46
1:A:76:ILE:O	1:A:81:LYS:HE3	2.15	0.46
1:C:537:LYS:HD2	1:C:540:ILE:HD11	1.97	0.46
1:B:40:PHE:CZ	1:B:42:TYR:HB2	2.50	0.46
1:C:253:LYS:HE3	1:C:253:LYS:HB2	1.83	0.46
1:A:253:LYS:HB2	1:A:253:LYS:HE2	1.47	0.46
1:A:521:ASN:N	1:A:521:ASN:HD22	2.14	0.46
1:C:255:ASN:HA	3:C:799:HOH:O	2.15	0.46
1:D:269:ALA:HA	1:D:273:GLY:O	2.16	0.46
1:A:576:ILE:HB	1:A:605:LEU:CD1	2.41	0.46
1:C:85:TYR:CE2	1:C:419:GLY:HA3	2.51	0.46
1:A:48:ASP:O	1:A:63:ARG:HD2	2.16	0.46
1:B:610:GLY:C	1:B:611:LYS:HD2	2.37	0.46
1:B:634:GLY:N	1:B:663:LYS:HE3	2.31	0.45
1:B:271:TRP:HB2	1:B:272:PRO:HD3	1.99	0.45
2:B:701:ACR:H6D1	2:B:701:ACR:H5C	1.99	0.45
1:C:501:ILE:O	1:C:504:ARG:HB3	2.16	0.45
1:C:537:LYS:HA	1:C:540:ILE:CD1	2.46	0.45
1:D:168:ARG:HH22	1:D:483:THR:HG22	1.82	0.45
1:A:294:ARG:HG3	1:A:393:ILE:CD1	2.47	0.45
1:B:329:GLU:HB3	1:B:338:ILE:CD1	2.46	0.45
1:C:432[B]:LEU:HD12	1:C:556:PRO:CG	2.43	0.45
1:D:189:ILE:HD11	1:D:494:ILE:HG12	1.98	0.45
1:B:109:LEU:CD1	1:B:125:CYS:HB3	2.45	0.45
1:C:55:GLU:HB2	1:C:438:LEU:HD21	1.99	0.45
1:D:160:PHE:C	1:D:160:PHE:CD1	2.89	0.45
1:C:105:TYR:CZ	1:C:107:SER:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:NH2	1:C:493:ASN:HB2	2.32	0.45
1:B:191:ILE:HG12	1:B:192:ASP:N	2.31	0.45
1:B:217:PHE:O	1:B:221:VAL:HG23	2.16	0.45
2:D:701:ACR:O5C	2:D:701:ACR:H6D1	2.17	0.45
1:A:217:PHE:HB3	1:A:218:PRO:HD3	1.99	0.45
1:A:45:ASP:HB3	1:A:48:ASP:OD1	2.17	0.45
1:A:564:GLY:CA	1:A:596:VAL:O	2.65	0.45
1:B:240:LYS:HE3	1:B:242:GLU:HB2	1.98	0.45
1:D:146:GLN:O	1:D:149[A]:ARG:HB2	2.17	0.45
1:A:259:LYS:HE3	1:A:263:GLY:O	2.16	0.44
1:B:380:TYR:C	1:B:380:TYR:CD1	2.90	0.44
1:C:270:VAL:HG12	1:C:271:TRP:N	2.30	0.44
1:C:416:ILE:HD12	1:C:416:ILE:C	2.38	0.44
1:C:502:ASN:O	1:C:506:ARG:HG3	2.17	0.44
1:C:67:TYR:CD2	1:C:67:TYR:N	2.85	0.44
1:D:270:VAL:HG12	1:D:271:TRP:N	2.26	0.44
1:A:422:LYS:HD2	1:A:424:TRP:CZ2	2.53	0.44
1:A:653:ASP:C	1:A:654:LYS:HD2	2.38	0.44
1:B:294:ARG:HG3	1:B:393:ILE:CD1	2.46	0.44
1:A:234:ILE:HD11	1:A:307:ASP:CB	2.48	0.44
1:B:574:LYS:O	1:B:576:ILE:HG12	2.18	0.44
1:D:603:VAL:HA	1:D:604:PRO:HD3	1.87	0.44
1:C:259:LYS:CE	1:C:263:GLY:O	2.65	0.44
1:C:654:LYS:CA	1:C:654:LYS:HE3	2.47	0.44
1:B:344:GLN:HG2	1:B:348:LYS:HE3	1.98	0.44
1:B:662:THR:HG23	3:B:759:HOH:O	2.17	0.44
1:A:217:PHE:N	1:A:218:PRO:CD	2.80	0.44
1:B:217:PHE:HB3	1:B:218:PRO:HD3	1.99	0.44
1:D:643:TYR:CD2	1:D:643:TYR:C	2.91	0.44
1:A:380:TYR:CD1	1:A:380:TYR:C	2.91	0.44
1:A:59:GLY:CA	1:A:433:LYS:HD3	2.41	0.44
1:B:305:TRP:CD1	1:B:305:TRP:N	2.86	0.44
1:A:105:TYR:CE2	1:A:107:SER:HB3	2.53	0.44
1:A:67:TYR:CD2	1:A:67:TYR:N	2.86	0.44
1:C:38:PHE:CZ	1:C:132:ILE:HD11	2.53	0.44
1:C:46:GLU:HA	3:C:727:HOH:O	2.17	0.44
1:C:52:GLY:O	1:C:53:LEU:HB2	2.18	0.44
1:A:568:TYR:C	1:A:569:LEU:HD23	2.38	0.43
1:A:69:SER:CB	1:A:89:ASN:HD21	2.31	0.43
1:B:317:SER:HA	3:B:709:HOH:O	2.18	0.43
1:D:479:ALA:HB2	1:D:486:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:C	1:B:605:LEU:HD12	2.38	0.43
1:C:396:GLU:O	1:C:649:HIS:HA	2.17	0.43
1:C:538:MET:HG2	1:C:568:TYR:CE1	2.53	0.43
1:A:536:ASP:HB3	1:A:539:ALA:HB3	1.99	0.43
1:C:135:ILE:CG2	1:C:143:ILE:HG23	2.48	0.43
1:C:314:PHE:O	1:C:315:TYR:HB3	2.18	0.43
1:D:433:LYS:HE2	1:D:543:GLU:HB3	2.01	0.43
1:A:167:SER:HB2	1:A:195:TYR:HB2	1.99	0.43
1:B:34:GLN:HA	1:B:37:GLY:O	2.17	0.43
1:C:578:PHE:HE1	1:C:605:LEU:HD21	1.83	0.43
1:A:270:VAL:CG1	1:A:271:TRP:N	2.72	0.43
1:A:233:PRO:HD2	1:A:303:GLY:O	2.19	0.43
1:A:192:ASP:OD2	1:A:621:CYS:HA	2.18	0.43
1:C:38:PHE:CD2	1:C:38:PHE:C	2.91	0.43
1:D:422:LYS:HD3	1:D:424:TRP:CZ2	2.54	0.43
1:D:487:GLU:HB3	1:D:489:TYR:CE1	2.53	0.43
1:A:487:GLU:HB2	1:A:490:GLN:HG2	1.99	0.43
1:A:603:VAL:HA	1:A:604:PRO:HD3	1.78	0.43
1:B:571:GLU:OE2	1:B:608:ARG:HD2	2.18	0.43
1:B:643:TYR:C	1:B:643:TYR:CD2	2.91	0.43
1:D:578:PHE:HB3	3:D:675:HOH:O	2.18	0.43
1:A:613:ILE:HA	1:A:614:PRO:HD3	1.79	0.43
1:D:225:LYS:HE3	1:D:225:LYS:HB2	1.76	0.43
1:A:339:HIS:CG	1:A:340:PRO:HD2	2.53	0.43
1:A:409:GLY:N	1:A:411:HIS:HD2	2.14	0.43
1:A:536:ASP:OD1	1:A:538:MET:HB3	2.19	0.42
1:B:178:ARG:O	1:B:181:ALA:HB3	2.19	0.42
1:B:462:LEU:HD23	1:B:497:PHE:CE1	2.54	0.42
1:D:329:GLU:HA	1:D:332:LYS:HZ3	1.84	0.42
1:D:416:ILE:O	1:D:446:THR:HA	2.19	0.42
1:A:167:SER:HG	1:A:478:HIS:CE1	2.36	0.42
1:B:25:GLU:CD	1:B:25:GLU:H	2.21	0.42
1:C:453:PHE:CZ	1:C:480:ALA:HB2	2.54	0.42
1:C:571:GLU:O	1:C:573:MET:HG3	2.19	0.42
1:A:462:LEU:O	1:A:462:LEU:HD12	2.19	0.42
2:B:701:ACR:H6D1	2:B:701:ACR:C5C	2.49	0.42
1:C:88:HIS:N	1:C:88:HIS:CD2	2.87	0.42
1:A:577:LYS:HA	1:A:603:VAL:O	2.19	0.42
1:B:174:LYS:O	1:B:178:ARG:HG3	2.19	0.42
1:B:6:ARG:HH11	1:B:10:PRO:HG2	1.84	0.42
1:C:532:VAL:HG21	1:C:547:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:GLU:HB3	1:A:489:TYR:CE1	2.55	0.42
1:A:579:MET:HE2	1:A:585:SER:HB3	2.02	0.42
1:B:429:LEU:HG	1:B:433:LYS:HE2	1.99	0.42
1:C:378:PHE:HB2	3:C:762:HOH:O	2.19	0.42
1:C:611:LYS:HD2	1:C:611:LYS:N	2.34	0.42
1:A:92:ILE:HD11	1:A:144:VAL:HG22	2.01	0.42
1:D:574:LYS:O	1:D:576:ILE:HG12	2.19	0.42
1:D:499:SER:OG	1:D:580:PRO:HA	2.19	0.42
1:A:406:SER:HB3	1:A:416:ILE:HD11	2.02	0.42
1:B:394:ASP:HA	1:B:395:PRO:HD3	1.79	0.42
1:B:462:LEU:HD23	1:B:497:PHE:HE1	1.85	0.42
1:B:159:LYS:HB2	1:B:647:GLY:HA3	2.01	0.42
1:D:4:LYS:HG3	1:D:133:TYR:CZ	2.55	0.42
1:D:605:LEU:C	1:D:605:LEU:HD12	2.40	0.42
1:D:82:ARG:HA	3:D:788:HOH:O	2.18	0.42
1:A:109:LEU:HD12	1:A:125:CYS:HB3	2.01	0.42
1:A:260:ARG:C	1:A:262:ASP:H	2.22	0.42
1:D:95:GLY:O	1:D:96:LYS:C	2.58	0.42
1:A:173:THR:HG22	1:A:213:ASN:ND2	2.34	0.42
1:D:404:ARG:NH2	2:D:701:ACR:H1A	2.34	0.42
1:A:631:GLN:HE21	1:A:633:ILE:HG12	1.85	0.42
1:B:524:MET:HE2	1:B:524:MET:HB3	1.93	0.42
1:C:510:TYR:HB2	1:C:614:PRO:HD2	2.01	0.42
1:A:355:GLU:O	1:A:359:ARG:HG3	2.20	0.41
1:C:168:ARG:HB3	1:C:171:TYR:CZ	2.55	0.41
1:A:380:TYR:HA	1:A:410:MET:HG3	2.02	0.41
1:B:480:ALA:HB3	1:B:483:THR:CG2	2.51	0.41
1:C:380:TYR:HA	1:C:410:MET:HG3	2.01	0.41
1:D:38:PHE:HZ	1:D:132:ILE:HD11	1.85	0.41
1:D:343:MET:HE1	1:D:347:MET:CE	2.49	0.41
1:D:371:HIS:HE1	1:D:375:HIS:ND1	2.18	0.41
1:A:76:ILE:HG13	1:A:81:LYS:CE	2.49	0.41
1:B:579:MET:HE3	1:B:585:SER:HB3	2.02	0.41
1:C:343:MET:HE2	1:D:343:MET:HE2	2.03	0.41
1:C:453:PHE:CE2	1:C:480:ALA:HB2	2.55	0.41
1:B:156:ILE:HA	1:B:157:PRO:HD3	1.91	0.41
1:B:548:LEU:HD23	1:B:549:GLY:N	2.34	0.41
1:C:27:PHE:HA	1:C:28:PRO:HD3	1.82	0.41
1:C:303:GLY:HA2	1:C:400:LEU:O	2.20	0.41
1:D:609:SER:HA	1:D:635:TYR:CE2	2.56	0.41
1:A:239:VAL:HG12	1:A:245:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLY:H	1:A:411:HIS:CD2	2.34	0.41
1:A:398:ARG:NH1	1:A:647:GLY:HA2	2.35	0.41
1:B:174:LYS:HG3	1:B:220:PHE:CE1	2.55	0.41
1:A:64:GLY:O	1:B:458:THR:HG21	2.21	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.87	0.41
1:C:11:PHE:C	1:C:11:PHE:CD2	2.94	0.41
1:C:280:MET:O	1:C:286:ARG:HD3	2.19	0.41
1:C:632:LEU:HD11	1:C:661:LEU:HB3	2.02	0.41
1:A:207:PHE:CE1	1:A:235:ILE:HD12	2.56	0.41
1:A:148:ARG:NH2	1:A:444:MET:SD	2.94	0.41
1:D:169:TYR:C	1:D:169:TYR:CD1	2.92	0.41
1:D:257:PHE:HB2	3:D:758:HOH:O	2.21	0.41
1:A:548:LEU:HB3	1:A:552:ILE:CG1	2.51	0.41
1:A:544:ASP:CG	1:A:565:ARG:HH22	2.23	0.41
1:A:159:LYS:HG2	1:A:622:VAL:HG11	2.03	0.41
1:C:506:ARG:HB3	1:C:615:VAL:HG13	2.03	0.41
1:D:34:GLN:HA	1:D:37:GLY:O	2.19	0.41
1:A:77:HIS:N	1:A:77:HIS:CD2	2.89	0.41
1:A:530:GLY:HA2	1:A:540:ILE:HG22	2.01	0.41
1:A:640:TYR:CE2	1:A:642:LEU:HA	2.56	0.41
1:B:172:THR:CG2	1:B:213:ASN:HD21	2.33	0.41
1:B:368:LYS:HB3	1:B:368:LYS:HE2	1.93	0.41
1:D:105:TYR:CZ	1:D:107:SER:HB3	2.56	0.41
1:D:291:ASP:OD1	1:D:392:ARG:NH2	2.46	0.41
1:A:457:THR:HG22	1:A:458:THR:N	2.34	0.41
1:A:423:SER:C	1:A:461:LEU:HD21	2.40	0.41
1:A:69:SER:OG	1:A:89:ASN:ND2	2.54	0.41
1:C:81:LYS:HA	1:C:81:LYS:HD3	1.81	0.41
1:D:167:SER:CB	1:D:195:TYR:HB2	2.51	0.41
1:A:429:LEU:HD22	1:A:558:TYR:CE1	2.56	0.40
1:C:117:ARG:HB2	1:C:120:THR:HB	2.03	0.40
1:D:27:PHE:HA	1:D:28:PRO:HD3	1.75	0.40
1:D:8:GLY:C	1:D:10:PRO:HD3	2.42	0.40
1:A:239:VAL:HG12	1:A:245:TYR:HE2	1.86	0.40
1:A:326:PHE:CD2	1:A:343:MET:HE2	2.56	0.40
1:B:319:GLY:HA3	3:B:767:HOH:O	2.21	0.40
1:C:260:ARG:NH2	1:C:267:VAL:CG1	2.84	0.40
1:D:190:PRO:HB2	1:D:505:TYR:CE1	2.56	0.40
1:A:151:ILE:HG13	1:A:411:HIS:CE1	2.57	0.40
1:A:579:MET:HA	1:A:580:PRO:HD3	1.90	0.40
1:C:173:THR:O	1:C:177:PHE:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:LYS:HE3	1:C:654:LYS:HA	2.03	0.40
1:D:182:LYS:HG3	1:D:186:GLU:HG3	2.02	0.40
1:D:234:ILE:HB	1:D:305:TRP:CE2	2.57	0.40
1:A:234:ILE:HG12	1:A:235:ILE:N	2.36	0.40
1:A:477:ASP:C	1:A:477:ASP:OD1	2.60	0.40
1:B:413:TYR:N	1:B:413:TYR:CD2	2.90	0.40
1:D:287:LYS:HG3	1:D:392:ARG:NH2	2.35	0.40
1:A:74:ASP:HA	1:A:75:PRO:HD3	1.71	0.40
1:B:532:VAL:O	1:B:534:PRO:HD3	2.21	0.40
1:B:81:LYS:HA	1:B:81:LYS:HD3	1.90	0.40
1:C:632:LEU:O	1:C:663:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/666 (100%)	617 (93%)	44 (7%)	2 (0%)	44	47
1	B	664/666 (100%)	615 (93%)	48 (7%)	1 (0%)	51	56
1	C	664/666 (100%)	622 (94%)	39 (6%)	3 (0%)	32	32
1	D	665/666 (100%)	627 (94%)	34 (5%)	4 (1%)	28	27
All	All	2656/2664 (100%)	2481 (93%)	165 (6%)	10 (0%)	38	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	58	ARG
1	D	169	TYR
1	C	270	VAL
1	B	170	GLY

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Mol	Chain	Res	Type
1	A	270	VAL
1	D	470	VAL
1	A	604	PRO
1	D	270	VAL
1	C	598	VAL
1	D	191	ILE

5.3.2　Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/575 (100%)	563 (98%)	11 (2%)	62	73
1	B	575/575 (100%)	563 (98%)	12 (2%)	59	70
1	C	575/575 (100%)	557 (97%)	18 (3%)	45	54
1	D	576/575 (100%)	558 (97%)	18 (3%)	45	54
All	All	2300/2300 (100%)	2241 (97%)	59 (3%)	51	61

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	192	ASP
1	A	267	VAL
1	A	380	TYR
1	A	405	SER
1	A	417	TRP
1	A	465	PHE
1	A	585	SER
1	A	605	LEU
1	A	627	THR
1	A	656	GLU
1	B	18	GLU
1	B	31	GLU
1	B	118	MET
1	B	126	GLU

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Mol	Chain	Res	Type
1	B	174	LYS
1	B	270	VAL
1	B	305	TRP
1	B	380	TYR
1	B	431	ASN
1	B	465	PHE
1	B	569	LEU
1	B	611	LYS
1	C	46	GLU
1	C	89	ASN
1	C	130	LEU
1	C	169	TYR
1	C	192	ASP
1	C	267	VAL
1	C	305	TRP
1	C	341	TRP
1	C	380	TYR
1	C	417	TRP
1	C	465	PHE
1	C	495	GLU
1	C	540	ILE
1	C	585	SER
1	C	604	PRO
1	C	611	LYS
1	C	636	GLU
1	C	654	LYS
1	D	-2	SER
1	D	-1	ASN
1	D	3	ARG
1	D	35	LYS
1	D	72	THR
1	D	123	VAL
1	D	142	ASP
1	D	169	TYR
1	D	192	ASP
1	D	305	TRP
1	D	380	TYR
1	D	417	TRP
1	D	431	ASN
1	D	465	PHE
1	D	548	LEU
1	D	563	ARG

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Mol	Chain	Res	Type
1	D	628	GLU
1	D	659	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	127	ASN
1	A	166	GLN
1	A	227	GLN
1	A	344	GLN
1	A	371	HIS
1	A	411	HIS
1	A	521	ASN
1	A	631	GLN
1	B	89	ASN
1	B	146	GLN
1	B	166	GLN
1	B	213	ASN
1	B	306	ASN
1	B	344	GLN
1	B	371	HIS
1	C	-1	ASN
1	C	88	HIS
1	C	89	ASN
1	C	202	GLN
1	C	306	ASN
1	C	344	GLN
1	C	371	HIS
1	D	34	GLN
1	D	89	ASN
1	D	166	GLN
1	D	306	ASN
1	D	371	HIS
1	D	431	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	ACR	A	701	-	45,47,47	0.60	0	59,70,70	1.48	10 (16%)
2	ACR	B	701	-	45,47,47	0.70	0	59,70,70	1.76	15 (25%)
2	ACR	C	701	-	45,47,47	0.66	0	59,70,70	1.47	11 (18%)
2	ACR	D	701	-	45,47,47	0.70	0	59,70,70	1.72	14 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACR	A	701	-	-	0/18/98/98	0/4/4/4
2	ACR	B	701	-	-	0/18/98/98	0/4/4/4
2	ACR	C	701	-	-	0/18/98/98	0/4/4/4
2	ACR	D	701	-	-	0/18/98/98	0/4/4/4

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	ACR	C3B-C4B-C5B	-3.75	103.45	110.44
2	B	701	ACR	C3B-C4B-C5B	-3.64	103.66	110.44
2	D	701	ACR	O4C-C1B-O5B	-3.48	102.25	110.70
2	D	701	ACR	O1D-C1D-O5D	-3.21	100.70	110.20
2	D	701	ACR	C2B-C3B-C4B	-3.14	105.67	110.33
2	D	701	ACR	O4D-C1C-O5C	-2.82	103.85	110.70
2	A	701	ACR	O1D-C1D-O5D	-2.82	101.85	110.20
2	B	701	ACR	O4C-C1B-O5B	-2.80	103.90	110.70
2	B	701	ACR	C2B-C3B-C4B	-2.66	106.39	110.33
2	A	701	ACR	C3B-C4B-C5B	-2.65	105.50	110.44
2	B	701	ACR	O1D-C1D-O5D	-2.62	102.45	110.20
2	C	701	ACR	O1D-C1D-O5D	-2.61	102.49	110.20
2	A	701	ACR	O4D-C1C-O5C	-2.60	104.39	110.70
2	C	701	ACR	O4D-C1C-O5C	-2.47	104.70	110.70
2	A	701	ACR	O4C-C1B-O5B	-2.38	104.91	110.70
2	B	701	ACR	O4D-C1C-O5C	-2.36	104.97	110.70
2	C	701	ACR	C2B-C3B-C4B	-2.34	106.86	110.33
2	C	701	ACR	C3B-C4B-C5B	-2.29	106.17	110.44
2	A	701	ACR	C2B-C3B-C4B	-2.23	107.02	110.33
2	D	701	ACR	O4D-C4D-C3D	2.01	112.02	107.19
2	A	701	ACR	C1C-O5C-C5C	2.05	117.57	113.72
2	B	701	ACR	C5B-C4B-N4B	2.07	117.47	111.53
2	C	701	ACR	O4D-C4D-C3D	2.07	112.18	107.19
2	B	701	ACR	C2D-C3D-C4D	2.09	113.95	109.61
2	B	701	ACR	C1C-C2C-C3C	2.12	113.92	109.98
2	B	701	ACR	O3A-C3A-C2A	2.14	115.01	110.36
2	C	701	ACR	C1D-C2D-C3D	2.19	114.61	110.65
2	D	701	ACR	O3A-C3A-C2A	2.26	115.28	110.36
2	A	701	ACR	C1D-O5D-C5D	2.30	117.54	113.39
2	A	701	ACR	C1D-C2D-C3D	2.45	115.08	110.65
2	D	701	ACR	C2C-C3C-C4C	2.45	114.69	109.61
2	B	701	ACR	C1D-O5D-C5D	2.48	117.86	113.39
2	D	701	ACR	C5B-C4B-N4B	2.52	118.75	111.53
2	C	701	ACR	C1C-O5C-C5C	2.58	118.58	113.72
2	D	701	ACR	O4D-C1C-C2C	2.63	114.03	108.11
2	C	701	ACR	O5D-C1D-C2D	2.63	114.40	110.04
2	B	701	ACR	O4D-C1C-C2C	2.69	114.17	108.11
2	A	701	ACR	O5D-C1D-C2D	2.76	114.61	110.04
2	C	701	ACR	O4D-C1C-C2C	2.82	114.47	108.11
2	D	701	ACR	O2A-C2A-C1A	2.83	114.87	109.20
2	D	701	ACR	C1C-O5C-C5C	2.84	119.06	113.72
2	D	701	ACR	C1C-C2C-C3C	3.07	115.69	109.98
2	B	701	ACR	O3B-C3B-C4B	3.14	115.97	109.61

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	ACR	C1D-O5D-C5D	3.38	119.50	113.39
2	B	701	ACR	O5D-C1D-C2D	4.03	116.73	110.04
2	B	701	ACR	C1D-C2D-C3D	4.16	118.16	110.65
2	C	701	ACR	C1B-O5B-C5B	4.26	121.21	113.67
2	B	701	ACR	C1B-O5B-C5B	4.31	121.30	113.67
2	A	701	ACR	C1B-O5B-C5B	4.48	121.60	113.67
2	D	701	ACR	C1B-O5B-C5B	4.60	121.80	113.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ACR	1	0
2	B	701	ACR	3	0
2	C	701	ACR	2	0
2	D	701	ACR	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	664/666 (99%)	0.12	4 (0%)	89	89	32, 50, 78, 116	1 (0%)
1	B	665/666 (99%)	0.09	11 (1%)	70	70	27, 48, 76, 108	1 (0%)
1	C	665/666 (99%)	-0.15	5 (0%)	86	86	23, 38, 64, 103	2 (0%)
1	D	666/666 (100%)	-0.15	6 (0%)	84	84	22, 38, 68, 111	1 (0%)
All	All	2660/2664 (99%)	-0.02	26 (0%)	82	82	22, 44, 74, 116	5 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-2	SER	8.2
1	C	-1	ASN	3.7
1	B	-1	ASN	3.5
1	B	661	LEU	3.4
1	A	584	ILE	3.2
1	C	326	PHE	3.0
1	C	204	PHE	3.0
1	C	434	MET	2.7
1	D	0	ALA	2.6
1	D	662	THR	2.5
1	B	633	ILE	2.4
1	B	662	THR	2.4
1	B	632	LEU	2.4
1	C	430	LEU	2.3
1	B	341	TRP	2.3
1	D	26	ALA	2.3
1	A	428	ILE	2.2
1	B	35	LYS	2.2
1	B	425	TRP	2.2
1	D	-1	ASN	2.1
1	B	494	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	277	PHE	2.1
1	A	430	LEU	2.1
1	A	432	LEU	2.0
1	D	188	HIS	2.0
1	B	663	LYS	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ACR	D	701	44/44	0.93	0.15	1.12	29,58,117,124	0
2	ACR	B	701	44/44	0.93	0.15	0.65	38,61,109,111	0
2	ACR	C	701	44/44	0.93	0.13	0.10	31,55,118,128	0
2	ACR	A	701	44/44	0.95	0.12	-0.19	32,65,116,120	0

6.5　Other polymers (i)

There are no such residues in this entry.