Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2025 – 12:23 PM JST

PDB ID	:	8Y9U
Title	:	Crystal structure of nanobody MY6323 bound to human serum albumin (HSA)
Authors	:	Ding, Y.; Zhong, P.Y.
Deposited on	:	2024-02-07
Resolution	:	3.10 Å(reported)

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

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

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

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

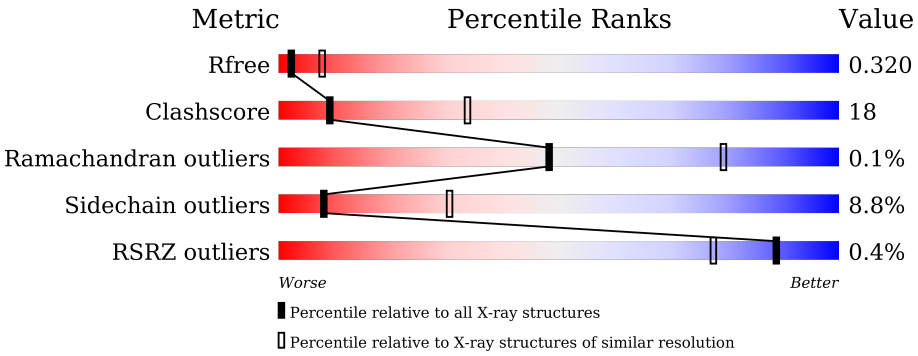
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.10 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))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	591	60% 30% 5% ·
1	C	591	65% 27% 5% ·
2	B	126	64% 31% 5%
2	D	126	2% 71% 26% ··

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11068 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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	1	0
			4499	2833	764	862	40			
1	C	578	Total	C	N	O	S	0	0	0
			4601	2903	778	879	41			

- Molecule 2 is a protein called nanobody MY6323.

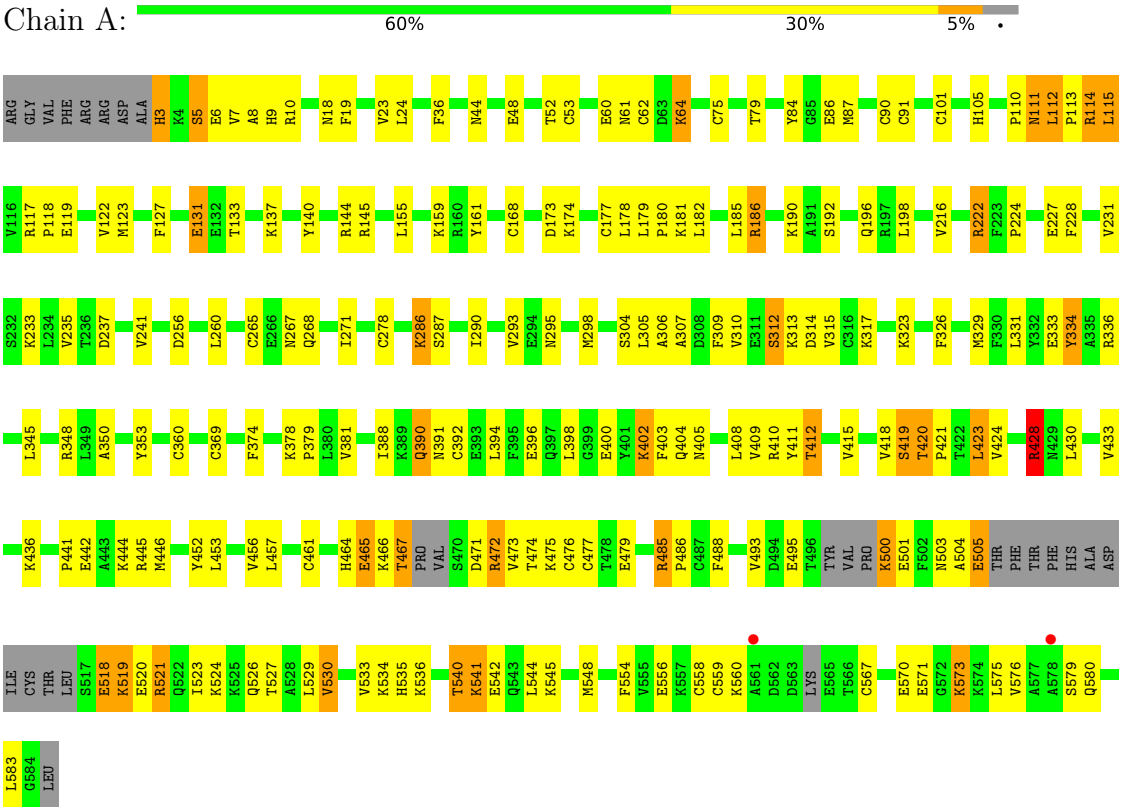
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			984	615	174	191	4			
2	D	126	Total	C	N	O	S	0	0	0
			984	615	174	191	4			

3 Residue-property plots (i)

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

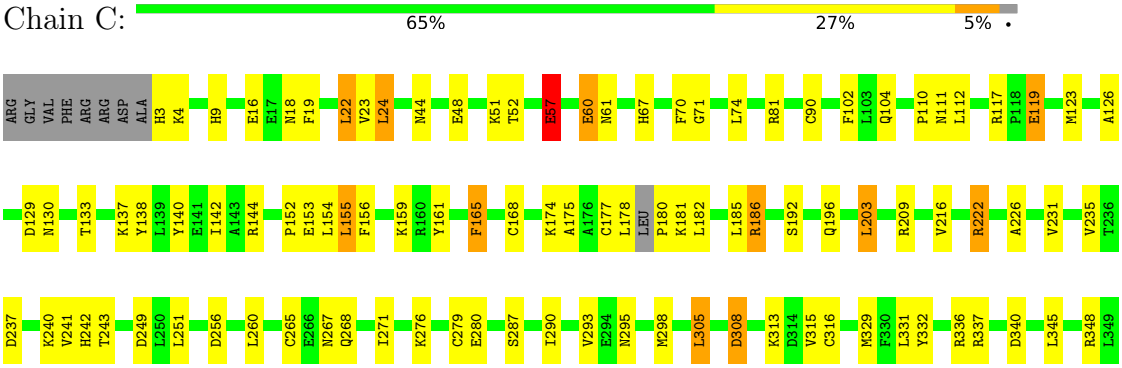
• Molecule 1: Albumin

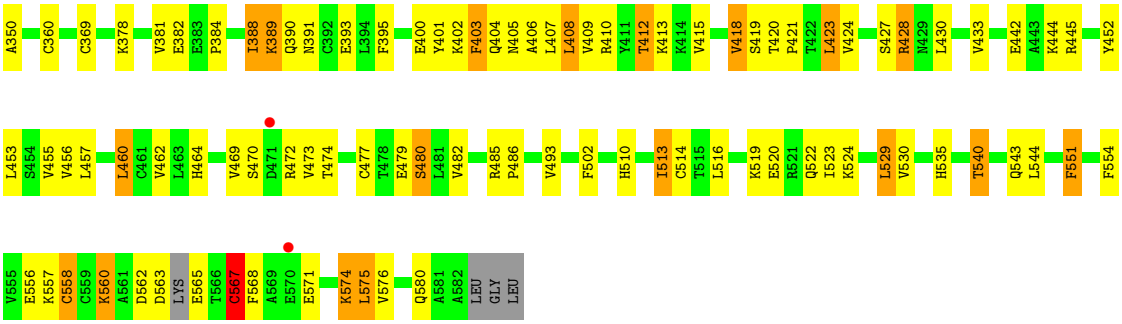
Chain A:



• Molecule 1: Albumin

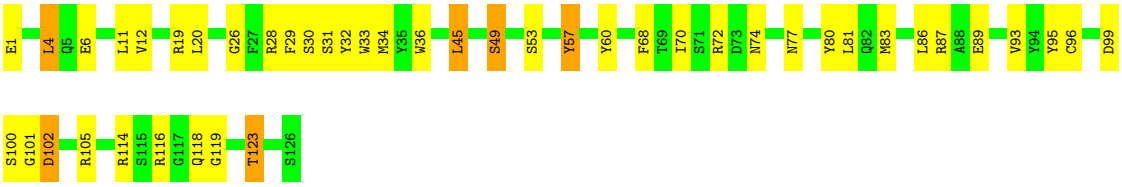
Chain C:





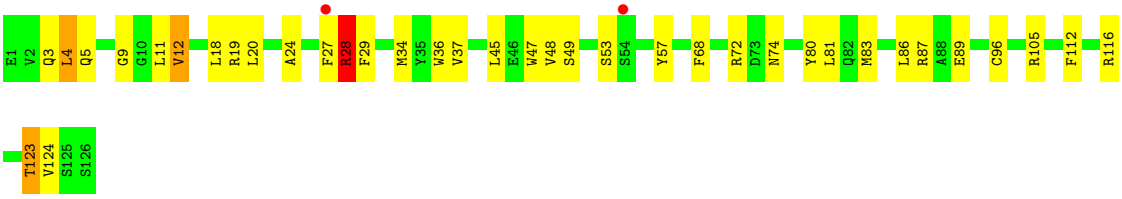
• Molecule 2: nanobody MY6323

Chain B:



• Molecule 2: nanobody MY6323

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.42Å 65.89Å 118.71Å 104.85° 103.41° 91.73°	Depositor
Resolution (Å)	63.40 – 3.10 63.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.9 (63.40-3.10) 96.1 (63.40-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.273 , 0.316 0.275 , 0.320	Depositor DCC
R_{free} test set	1510 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	85.3	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 9.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l 0.009 for -h,k,-k-l 0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11068	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.50	0/4579	0.71	0/6164
1	C	0.48	0/4689	0.73	3/6321 (0.0%)
2	B	0.56	0/1007	0.85	2/1358 (0.1%)
2	D	0.52	0/1007	0.80	1/1358 (0.1%)
All	All	0.50	0/11282	0.74	6/15201 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	C	0	11
2	B	0	1
2	D	0	2
All	All	0	23

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	57	TYR	N-CA-CB	7.71	124.47	110.60
1	C	567	CYS	CB-CA-C	7.69	125.77	110.40
2	D	57	TYR	N-CA-CB	7.09	123.37	110.60
1	C	477	CYS	CB-CA-C	5.93	122.25	110.40
2	B	102	ASP	CA-CB-CG	5.64	125.82	113.40
1	C	57	GLU	CB-CA-C	5.10	120.60	110.40

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	348	ARG	Sidechain
1	A	410	ARG	Sidechain
1	A	428	ARG	Sidechain
1	A	472	ARG	Sidechain
1	A	485	ARG	Sidechain
1	A	521	ARG	Sidechain
2	B	87	ARG	Sidechain
1	C	186	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	222	ARG	Sidechain
1	C	336	ARG	Sidechain
1	C	348	ARG	Sidechain
1	C	428	ARG	Sidechain
1	C	445	ARG	Sidechain
1	C	472	ARG	Sidechain
1	C	479	GLU	Mainchain
1	C	480	SER	Mainchain
1	C	81	ARG	Sidechain
2	D	28	ARG	Sidechain
2	D	87	ARG	Sidechain

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	4499	0	4438	167	0
1	C	4601	0	4533	164	0
2	B	984	0	934	32	0
2	D	984	0	934	22	0
All	All	11068	0	10839	376	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 18.

All (376) 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:402:LYS:HA	1:A:402:LYS:HZ2	1.14	1.11
1:C:418:VAL:HG13	1:C:469:VAL:HG21	1.40	1.04
1:A:168:CYS:HB2	1:A:178:LEU:HD13	1.38	1.02
1:C:510:HIS:O	1:C:513:ILE:HD12	1.63	0.98
1:A:398:LEU:HD21	1:A:402:LYS:HB3	1.46	0.96
1:A:418:VAL:HB	1:A:423:LEU:HD11	1.53	0.91
1:C:4:LYS:HG2	1:C:57:GLU:HB3	1.54	0.89
1:A:402:LYS:HA	1:A:402:LYS:NZ	1.86	0.88
1:C:155:LEU:HD23	1:C:155:LEU:O	1.72	0.88
1:C:298:MET:CE	1:C:337:ARG:HA	2.07	0.85
1:A:90:CYS:HG	1:A:101:CYS:HG	0.90	0.83
1:A:420:THR:HA	1:A:423:LEU:HD22	1.59	0.83
1:C:178:LEU:C	1:C:180:PRO:N	2.33	0.83
1:A:420:THR:HB	1:A:530:VAL:HG21	1.61	0.82
1:C:513:ILE:HD11	1:C:568:PHE:CZ	2.15	0.81
1:A:461:CYS:HG	1:A:477:CYS:HG	1.03	0.81
1:A:267:ASN:O	1:A:271:ILE:HD12	1.81	0.80
1:A:398:LEU:HD21	1:A:402:LYS:CB	2.11	0.79
1:A:392:CYS:O	1:A:396:GLU:HG2	1.81	0.79
2:B:101:GLY:HA2	2:B:114:ARG:HD2	1.65	0.79
1:C:267:ASN:O	1:C:271:ILE:HD12	1.82	0.79
1:A:398:LEU:HD23	1:A:398:LEU:C	2.02	0.78
1:C:430:LEU:CD1	1:C:456:VAL:HG11	2.13	0.78
1:C:3:HIS:CE1	1:C:9:HIS:CE1	2.71	0.78
1:A:405:ASN:HD21	1:A:526:GLN:HG2	1.47	0.78
1:C:567:CYS:O	1:C:571:GLU:HG2	1.85	0.77
1:A:500:LYS:HD2	1:A:534:LYS:HB3	1.65	0.76
1:C:571:GLU:O	1:C:574:LYS:HG3	1.85	0.76
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.68	0.76
2:B:11:LEU:HD12	2:B:123:THR:HB	1.67	0.75
1:C:567:CYS:SG	1:C:571:GLU:OE2	2.44	0.75
2:D:36:TRP:O	2:D:48:VAL:HG12	1.87	0.75
2:B:101:GLY:HA2	2:B:114:ARG:CD	2.16	0.74
1:C:360:CYS:HG	1:C:369:CYS:HG	0.77	0.74
1:A:529:LEU:O	1:A:533:VAL:HG23	1.86	0.74
1:A:114:ARG:H	1:A:114:ARG:HD3	1.53	0.73
1:A:419:SER:O	1:A:423:LEU:HD13	1.88	0.73
1:C:395:PHE:HB2	1:C:403:PHE:CE2	2.24	0.73
1:A:471:ASP:O	1:A:474:THR:HG22	1.89	0.72
1:A:500:LYS:HE3	1:A:535:HIS:H	1.54	0.72
1:C:4:LYS:CG	1:C:57:GLU:HB3	2.20	0.72
1:C:298:MET:HE1	1:C:337:ARG:HA	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:VAL:HG23	1:C:423:LEU:HD11	1.71	0.71
1:C:203:LEU:HD12	1:C:203:LEU:O	1.89	0.71
1:C:576:VAL:O	1:C:580:GLN:HG3	1.91	0.70
1:A:576:VAL:O	1:A:580:GLN:HG3	1.92	0.70
1:A:227:GLU:OE2	2:B:32:TYR:HD1	1.75	0.69
1:C:70:PHE:CE2	1:C:74:LEU:HD21	2.28	0.69
1:A:536:LYS:HG3	1:A:583:LEU:HD13	1.75	0.68
1:C:400:GLU:HG2	1:C:404:GLN:HE21	1.57	0.68
1:A:360:CYS:HG	1:A:369:CYS:HG	0.68	0.68
1:C:420:THR:HG23	1:C:530:VAL:HG11	1.75	0.68
1:A:345:LEU:HD21	1:A:381:VAL:HG22	1.76	0.67
1:A:398:LEU:CD2	1:A:402:LYS:HB3	2.21	0.67
1:C:117:ARG:HG2	1:C:123:MET:HE3	1.74	0.67
1:A:398:LEU:HD21	1:A:402:LYS:CA	2.25	0.67
1:C:418:VAL:CG2	1:C:423:LEU:HD11	2.24	0.66
1:C:329:MET:HE1	2:D:112:PHE:CD1	2.31	0.66
1:C:412:THR:HG23	1:C:423:LEU:HD23	1.77	0.66
1:A:398:LEU:HD21	1:A:402:LYS:C	2.15	0.65
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.77	0.65
1:C:345:LEU:HD21	1:C:381:VAL:HG22	1.77	0.65
1:A:5:SER:O	1:A:8:ALA:HB3	1.95	0.65
1:C:241:VAL:HG22	1:C:256:ASP:HB3	1.78	0.65
1:A:290:ILE:O	1:A:293:VAL:HG12	1.97	0.64
1:A:402:LYS:NZ	1:A:405:ASN:OD1	2.29	0.64
1:C:384:PRO:O	1:C:388:ILE:HD13	1.98	0.64
1:C:419:SER:O	1:C:423:LEU:HD13	1.97	0.63
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.80	0.63
1:A:420:THR:HB	1:A:530:VAL:CG2	2.28	0.63
1:C:117:ARG:HG2	1:C:123:MET:CE	2.28	0.63
1:C:290:ILE:O	1:C:293:VAL:HG12	1.99	0.63
1:A:464:HIS:HA	1:A:467:THR:OG1	1.99	0.62
1:C:110:PRO:HB2	1:C:112:LEU:HG	1.80	0.62
1:A:168:CYS:SG	1:A:181:LYS:HD2	2.39	0.62
1:C:389:LYS:HD3	1:C:393:GLU:OE2	2.00	0.62
1:C:418:VAL:CG1	1:C:469:VAL:HG21	2.24	0.62
1:C:520:GLU:O	1:C:524:LYS:HD3	2.00	0.62
1:A:398:LEU:HD23	1:A:398:LEU:O	2.00	0.61
1:C:4:LYS:HG2	1:C:57:GLU:CB	2.26	0.61
1:A:227:GLU:OE2	2:B:32:TYR:CD1	2.54	0.61
1:A:500:LYS:CE	1:A:535:HIS:H	2.14	0.61
1:C:433:VAL:HG22	1:C:452:TYR:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG22	1:A:452:TYR:HB3	1.83	0.60
1:A:405:ASN:ND2	1:A:526:GLN:HG2	2.16	0.60
1:C:453:LEU:HD12	1:C:457:LEU:HD11	1.83	0.60
1:C:133:THR:O	1:C:137:LYS:HG3	2.01	0.60
2:B:60:TYR:CE1	2:B:70:ILE:HG22	2.36	0.60
1:C:178:LEU:HG	1:C:182:LEU:HD13	1.82	0.60
1:C:130:ASN:HB3	1:C:133:THR:OG1	2.00	0.60
2:D:11:LEU:HD23	2:D:123:THR:HB	1.84	0.60
1:A:112:LEU:HD23	1:A:113:PRO:HD2	1.84	0.59
1:A:119:GLU:O	1:A:122:VAL:HG12	2.02	0.59
1:C:203:LEU:HD12	1:C:203:LEU:C	2.23	0.59
1:C:557:LYS:HA	1:C:560:LYS:HE2	1.83	0.59
1:A:398:LEU:HD22	1:A:403:PHE:N	2.17	0.59
1:A:408:LEU:O	1:A:412:THR:OG1	2.20	0.59
1:A:411:TYR:HE2	1:A:430:LEU:HD22	1.68	0.59
1:C:216:VAL:HG22	1:C:235:VAL:HG21	1.84	0.59
1:C:513:ILE:HD13	1:C:514:CYS:N	2.18	0.59
1:A:305:LEU:HD11	1:A:334:TYR:HA	1.85	0.59
1:C:408:LEU:O	1:C:412:THR:OG1	2.20	0.59
1:A:233:LYS:HD3	2:B:57:TYR:CE2	2.38	0.58
1:C:168:CYS:SG	1:C:177:CYS:O	2.62	0.58
1:C:420:THR:HG23	1:C:530:VAL:CG1	2.31	0.58
1:A:475:LYS:O	1:A:479:GLU:HG2	2.03	0.58
1:A:412:THR:HG21	1:A:530:VAL:HG23	1.85	0.58
1:A:540:THR:O	1:A:544:LEU:HD23	2.03	0.58
1:A:114:ARG:H	1:A:114:ARG:CD	2.17	0.58
1:A:420:THR:HA	1:A:423:LEU:HB2	1.86	0.57
1:C:155:LEU:HD21	1:C:159:LYS:HE3	1.86	0.57
1:A:421:PRO:O	1:A:424:VAL:HG22	2.04	0.57
1:A:520:GLU:HA	1:A:523:ILE:HD12	1.86	0.57
1:C:237:ASP:HB3	1:C:260:LEU:HD13	1.87	0.57
2:B:30:SER:HA	2:B:74:ASN:OD1	2.05	0.57
1:C:556:GLU:O	1:C:560:LYS:HB3	2.05	0.57
1:A:186:ARG:O	1:A:190:LYS:HG3	2.05	0.57
1:A:398:LEU:CD2	1:A:403:PHE:N	2.68	0.57
1:A:541:LYS:HG3	1:A:542:GLU:OE1	2.05	0.56
1:A:61:ASN:OD1	1:A:64:LYS:HE2	2.04	0.56
1:A:161:TYR:CD1	1:A:185:LEU:HD13	2.41	0.56
1:C:90:CYS:HB2	1:C:102:PHE:CE1	2.39	0.56
2:D:12:VAL:HG12	2:D:124:VAL:HG22	1.87	0.56
1:C:408:LEU:HD22	1:C:427:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ARG:O	2:D:29:PHE:HB3	2.05	0.56
1:C:133:THR:HG22	1:C:137:LYS:HD2	1.86	0.56
1:A:5:SER:HA	1:A:62:CYS:O	2.05	0.56
1:C:152:PRO:O	1:C:156:PHE:CD2	2.59	0.55
1:C:558:CYS:HB3	1:C:568:PHE:CZ	2.41	0.55
1:C:192:SER:O	1:C:196:GLN:HG3	2.06	0.55
1:C:513:ILE:HD13	1:C:514:CYS:H	1.71	0.55
1:A:579:SER:O	1:A:583:LEU:HG	2.06	0.55
1:C:412:THR:HG21	1:C:530:VAL:HG13	1.88	0.55
1:A:5:SER:HB3	1:A:8:ALA:CB	2.37	0.54
1:C:19:PHE:O	1:C:23:VAL:HG23	2.07	0.54
1:A:192:SER:O	1:A:196:GLN:HG3	2.07	0.54
2:B:101:GLY:HA2	2:B:114:ARG:NE	2.22	0.54
1:A:329:MET:HE1	2:B:105:ARG:NE	2.22	0.54
1:C:155:LEU:O	1:C:155:LEU:CD2	2.53	0.54
1:A:333:GLU:OE2	2:B:105:ARG:NH2	2.40	0.54
2:B:29:PHE:CD2	2:B:77:ASN:HA	2.43	0.54
1:C:395:PHE:HD2	1:C:403:PHE:CD2	2.26	0.54
1:A:430:LEU:HD12	1:A:456:VAL:HG11	1.89	0.54
1:C:574:LYS:HD2	1:C:574:LYS:C	2.28	0.54
1:C:276:LYS:O	1:C:280:GLU:HG3	2.08	0.53
1:C:177:CYS:O	1:C:178:LEU:HB2	2.09	0.53
1:A:84:TYR:HB3	1:A:87:MET:HE3	1.90	0.53
1:A:312:SER:O	1:A:315:VAL:HG23	2.08	0.53
1:A:400:GLU:O	1:A:404:GLN:HG3	2.09	0.53
1:A:398:LEU:C	1:A:398:LEU:CD2	2.77	0.53
1:C:415:VAL:HG13	1:C:415:VAL:O	2.09	0.53
1:A:19:PHE:O	1:A:23:VAL:HG23	2.09	0.53
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.24	0.53
1:A:390:GLN:HE21	1:A:391:ASN:ND2	2.07	0.53
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.38	0.53
1:C:413:LYS:HB3	1:C:493:VAL:HG13	1.91	0.53
1:C:112:LEU:HD11	1:C:144:ARG:HE	1.74	0.52
1:C:391:ASN:HD21	1:C:410:ARG:HH12	1.58	0.52
1:C:153:GLU:HA	1:C:156:PHE:HD2	1.74	0.52
1:C:329:MET:HE1	2:D:112:PHE:CG	2.44	0.52
1:A:117:ARG:HG3	1:A:123:MET:HE1	1.92	0.52
1:A:424:VAL:O	1:A:428:ARG:HG3	2.10	0.52
1:A:228:PHE:CE2	1:A:329:MET:HG3	2.45	0.51
1:C:452:TYR:O	1:C:455:VAL:HG12	2.10	0.51
1:C:155:LEU:HD23	1:C:155:LEU:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:PHE:HD2	1:C:403:PHE:HD2	1.56	0.51
1:C:513:ILE:HA	1:C:516:LEU:HD23	1.91	0.51
2:B:100:SER:O	2:B:114:ARG:HD2	2.10	0.51
1:C:395:PHE:HB2	1:C:403:PHE:HE2	1.74	0.51
1:C:216:VAL:CG2	1:C:235:VAL:HG21	2.41	0.51
1:C:404:GLN:OE1	1:C:428:ARG:HA	2.11	0.51
1:A:222:ARG:HD3	1:A:295:ASN:OD1	2.11	0.51
1:C:308:ASP:N	1:C:308:ASP:OD1	2.43	0.51
1:A:400:GLU:HG2	1:A:404:GLN:HE21	1.76	0.51
1:C:395:PHE:CD2	1:C:403:PHE:HD2	2.27	0.51
1:C:519:LYS:O	1:C:523:ILE:HG13	2.11	0.51
1:C:540:THR:O	1:C:544:LEU:HD23	2.11	0.50
1:A:453:LEU:O	1:A:457:LEU:HD23	2.10	0.50
1:A:519:LYS:O	1:A:523:ILE:HG13	2.11	0.50
2:D:36:TRP:C	2:D:48:VAL:HG12	2.31	0.50
1:C:554:PHE:CE1	1:C:571:GLU:HG3	2.46	0.50
1:C:558:CYS:SG	1:C:568:PHE:N	2.85	0.50
1:C:104:GLN:OE1	1:C:104:GLN:HA	2.11	0.50
1:C:415:VAL:HG13	1:C:418:VAL:CG2	2.41	0.50
1:A:5:SER:OG	1:A:62:CYS:HB3	2.11	0.49
2:B:1:GLU:O	2:B:26:GLY:HA3	2.12	0.49
1:C:305:LEU:N	1:C:305:LEU:HD23	2.27	0.49
1:A:323:LYS:O	1:A:326:PHE:N	2.45	0.49
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.93	0.49
1:C:155:LEU:CD2	1:C:155:LEU:C	2.81	0.49
1:C:90:CYS:CB	1:C:102:PHE:CE1	2.96	0.49
1:A:179:LEU:N	1:A:180:PRO:HD2	2.27	0.49
1:A:75:CYS:CB	1:A:91:CYS:HG	2.22	0.49
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.95	0.49
1:C:420:THR:O	1:C:424:VAL:HG13	2.13	0.49
2:B:29:PHE:O	2:B:72:ARG:NH2	2.46	0.48
1:C:70:PHE:CD2	1:C:74:LEU:HD21	2.47	0.48
1:C:412:THR:CG2	1:C:530:VAL:HG13	2.43	0.48
1:C:126:ALA:O	1:C:129:ASP:O	2.31	0.48
2:B:4:LEU:HD22	2:B:96:CYS:SG	2.54	0.48
2:B:6:GLU:OE1	2:B:6:GLU:N	2.46	0.48
1:C:405:ASN:HA	1:C:408:LEU:HB2	1.95	0.48
1:C:231:VAL:O	1:C:235:VAL:HG23	2.13	0.48
1:C:402:LYS:HA	1:C:405:ASN:OD1	2.14	0.48
1:C:424:VAL:O	1:C:428:ARG:HG3	2.13	0.48
1:A:527:THR:O	1:A:530:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:CYS:O	1:A:286:LYS:HG3	2.14	0.48
1:A:534:LYS:O	1:A:536:LYS:N	2.43	0.48
1:C:3:HIS:HE1	1:C:9:HIS:CE1	2.31	0.47
1:C:551:PHE:CD1	1:C:551:PHE:C	2.88	0.47
1:A:306:ALA:HB1	1:A:310:VAL:HB	1.95	0.47
1:C:408:LEU:HD11	1:C:530:VAL:CG2	2.44	0.47
1:A:503:ASN:O	1:A:504:ALA:HB3	2.13	0.47
1:A:36:PHE:CE1	1:A:137:LYS:HA	2.50	0.47
1:A:464:HIS:ND1	1:A:467:THR:HG21	2.30	0.47
2:B:99:ASP:OD2	2:B:105:ARG:NH1	2.47	0.47
2:D:45:LEU:HD11	2:D:116:ARG:HH11	1.78	0.47
1:A:442:GLU:C	1:A:442:GLU:OE1	2.53	0.47
1:C:554:PHE:HB2	1:C:575:LEU:CD2	2.45	0.47
2:D:20:LEU:CD1	2:D:83:MET:HE3	2.45	0.47
1:C:16:GLU:OE2	1:C:51:LYS:NZ	2.45	0.47
1:A:173:ASP:O	1:A:174:LYS:C	2.51	0.46
2:B:118:GLN:HG2	2:B:119:GLY:N	2.30	0.46
1:C:265:CYS:SG	1:C:279:CYS:CB	3.03	0.46
1:A:5:SER:OG	1:A:53:CYS:HB3	2.15	0.46
1:C:67:HIS:HE1	1:C:249:ASP:OD2	1.98	0.46
1:C:177:CYS:SG	1:C:181:LYS:NZ	2.84	0.46
1:A:420:THR:CA	1:A:423:LEU:HD22	2.39	0.46
1:A:500:LYS:HE3	1:A:500:LYS:HB2	1.50	0.46
1:C:3:HIS:CE1	1:C:9:HIS:ND1	2.84	0.46
1:C:305:LEU:HD21	1:C:337:ARG:HD2	1.96	0.46
1:A:117:ARG:CG	1:A:123:MET:HE1	2.46	0.46
1:C:473:VAL:O	1:C:474:THR:C	2.53	0.46
2:B:49:SER:HB2	2:B:60:TYR:CD1	2.50	0.46
1:C:408:LEU:CD1	1:C:530:VAL:CG2	2.94	0.46
1:C:24:LEU:HD23	1:C:24:LEU:O	2.16	0.46
1:A:231:VAL:O	1:A:235:VAL:HG23	2.16	0.46
1:C:442:GLU:C	1:C:442:GLU:OE1	2.53	0.46
1:C:502:PHE:HB2	1:C:535:HIS:NE2	2.31	0.46
2:D:29:PHE:HE1	2:D:74:ASN:HA	1.80	0.46
1:A:86:GLU:O	1:A:87:MET:C	2.55	0.45
1:A:113:PRO:O	1:A:145:ARG:NH1	2.50	0.45
1:A:309:PHE:HB3	1:A:353:TYR:OH	2.16	0.45
1:C:329:MET:CE	2:D:112:PHE:CD1	2.98	0.45
2:D:4:LEU:HD22	2:D:96:CYS:SG	2.56	0.45
1:A:18:ASN:HD21	1:A:159:LYS:NZ	2.14	0.45
1:A:545:LYS:HA	1:A:548:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:ARG:NH2	2:B:80:TYR:CD2	2.85	0.45
1:C:469:VAL:HG23	1:C:470:SER:N	2.31	0.45
1:A:476:CYS:HB3	1:A:488:PHE:CD1	2.52	0.45
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.51	0.45
1:A:420:THR:O	1:A:423:LEU:HB2	2.17	0.45
1:C:249:ASP:OD1	1:C:251:LEU:N	2.50	0.45
1:A:60:GLU:HG3	1:A:61:ASN:ND2	2.32	0.45
1:A:420:THR:HA	1:A:423:LEU:CD2	2.38	0.45
1:A:168:CYS:CB	1:A:178:LEU:HD13	2.28	0.45
1:A:309:PHE:O	1:A:315:VAL:HG21	2.17	0.45
1:A:534:LYS:C	1:A:536:LYS:H	2.18	0.45
1:C:226:ALA:O	1:C:332:TYR:OH	2.29	0.45
2:B:33:TRP:O	2:B:34:MET:HE2	2.16	0.45
2:D:29:PHE:O	2:D:72:ARG:NH2	2.49	0.45
1:A:177:CYS:O	1:A:181:LYS:HG3	2.17	0.45
1:A:442:GLU:HA	1:A:445:ARG:CD	2.47	0.45
1:C:71:GLY:HA2	1:C:74:LEU:HD23	1.98	0.45
1:A:18:ASN:HD22	1:A:155:LEU:HD21	1.82	0.44
1:A:464:HIS:CE1	1:A:473:VAL:HG21	2.51	0.44
2:B:20:LEU:HD22	2:B:83:MET:HE2	1.98	0.44
1:A:3:HIS:HE1	1:A:9:HIS:CD2	2.34	0.44
1:A:237:ASP:HB3	1:A:260:LEU:HD13	1.99	0.44
1:A:306:ALA:O	1:A:310:VAL:N	2.50	0.44
2:B:45:LEU:HD21	2:B:116:ARG:NH1	2.32	0.44
1:C:119:GLU:CD	1:C:119:GLU:N	2.71	0.44
1:A:441:PRO:HG2	1:A:444:LYS:HD3	2.00	0.44
1:C:70:PHE:O	1:C:74:LEU:HD22	2.17	0.44
1:A:44:ASN:O	1:A:48:GLU:HG2	2.18	0.44
1:A:198:LEU:C	1:A:198:LEU:HD23	2.37	0.44
1:A:267:ASN:O	1:A:271:ILE:CD1	2.61	0.44
1:A:415:VAL:HG12	1:A:418:VAL:HG23	2.00	0.44
1:C:237:ASP:CB	1:C:260:LEU:HD13	2.47	0.44
1:C:378:LYS:O	1:C:382:GLU:HG3	2.18	0.44
1:A:117:ARG:HG2	1:A:123:MET:CE	2.48	0.44
2:B:28:ARG:HG2	2:B:31:SER:OG	2.18	0.44
1:C:222:ARG:HD3	1:C:295:ASN:OD1	2.18	0.44
1:C:408:LEU:HD22	1:C:427:SER:CB	2.48	0.44
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.99	0.44
1:A:573:LYS:H	1:A:573:LYS:HG2	1.58	0.44
1:C:529:LEU:O	1:C:529:LEU:HD12	2.18	0.44
1:C:60:GLU:HG3	1:C:61:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:MET:SD	1:C:165:PHE:HZ	2.41	0.44
2:D:24:ALA:HB1	2:D:27:PHE:CE1	2.53	0.44
1:A:228:PHE:CE1	1:A:329:MET:HA	2.53	0.43
1:A:286:LYS:HB2	1:A:286:LYS:HE3	1.72	0.43
2:B:68:PHE:HB3	2:B:81:LEU:HD11	2.00	0.43
1:C:406:ALA:O	1:C:409:VAL:HG22	2.18	0.43
1:A:378:LYS:HB3	1:A:379:PRO:HD3	2.00	0.43
1:A:465:GLU:HG2	1:A:466:LYS:N	2.32	0.43
1:C:18:ASN:HD22	1:C:155:LEU:HD11	1.83	0.43
1:C:408:LEU:HD11	1:C:530:VAL:HG23	2.00	0.43
1:C:130:ASN:HB3	1:C:133:THR:CB	2.49	0.43
1:C:331:LEU:HD13	1:C:350:ALA:HB2	2.00	0.43
1:C:395:PHE:HB2	1:C:403:PHE:CD2	2.53	0.43
1:A:101:CYS:O	1:A:105:HIS:HD2	2.02	0.43
1:C:418:VAL:HB	1:C:423:LEU:HD11	2.00	0.43
1:A:265:CYS:O	1:A:268:GLN:HG3	2.18	0.43
1:A:442:GLU:HA	1:A:445:ARG:HD2	2.00	0.43
1:A:457:LEU:O	1:A:461:CYS:SG	2.77	0.43
1:A:222:ARG:HD3	1:A:222:ARG:HA	1.87	0.43
1:C:421:PRO:O	1:C:424:VAL:HG22	2.18	0.43
1:A:133:THR:O	1:A:137:LYS:HB2	2.19	0.43
1:A:420:THR:HG23	1:A:421:PRO:HD3	2.01	0.43
1:C:174:LYS:O	1:C:175:ALA:HB3	2.19	0.42
1:C:401:TYR:CD1	1:C:522:GLN:NE2	2.87	0.42
1:C:418:VAL:CB	1:C:423:LEU:HD11	2.49	0.42
1:C:140:TYR:OH	1:C:144:ARG:NH1	2.51	0.42
1:C:265:CYS:O	1:C:268:GLN:HG3	2.18	0.42
1:C:430:LEU:HD11	1:C:456:VAL:HG11	1.95	0.42
1:C:44:ASN:O	1:C:48:GLU:HG2	2.19	0.42
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.35	0.42
1:A:140:TYR:OH	1:A:144:ARG:NH1	2.52	0.42
1:A:241:VAL:HG22	1:A:256:ASP:CB	2.45	0.42
2:B:72:ARG:HE	2:B:74:ASN:HD21	1.66	0.42
1:A:174:LYS:H	1:A:174:LYS:HG3	1.67	0.42
1:C:460:LEU:O	1:C:460:LEU:HD23	2.19	0.42
1:A:558:CYS:SG	1:A:567:CYS:C	2.98	0.42
2:B:74:ASN:N	2:B:74:ASN:HD22	2.18	0.42
1:C:22:LEU:HD22	1:C:155:LEU:HD12	2.01	0.42
1:C:242:HIS:O	1:C:243:THR:C	2.58	0.42
1:C:464:HIS:NE2	1:C:469:VAL:HG22	2.35	0.42
1:C:415:VAL:HG13	1:C:418:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ARG:N	1:C:486:PRO:HD2	2.35	0.42
2:D:19:ARG:NH2	2:D:80:TYR:CD2	2.88	0.42
1:A:307:ALA:O	1:A:312:SER:HB3	2.20	0.41
1:A:390:GLN:HG3	1:A:391:ASN:N	2.35	0.41
1:A:503:ASN:O	1:A:505:GLU:HG2	2.20	0.41
1:C:516:LEU:HD12	1:C:520:GLU:CB	2.50	0.41
1:A:224:PRO:HB3	1:A:336:ARG:HB2	2.02	0.41
1:A:388:ILE:HD11	1:A:446:MET:HA	2.01	0.41
1:C:110:PRO:O	1:C:111:ASN:HB2	2.21	0.41
1:C:408:LEU:CD1	1:C:530:VAL:HG22	2.49	0.41
1:A:398:LEU:HD21	1:A:403:PHE:N	2.35	0.41
1:C:186:ARG:HE	1:C:186:ARG:HB3	1.74	0.41
1:A:48:GLU:O	1:A:52:THR:HG23	2.20	0.41
1:A:305:LEU:HD11	1:A:334:TYR:CA	2.50	0.41
1:A:519:LYS:HG2	1:A:520:GLU:N	2.36	0.41
1:C:315:VAL:HG12	1:C:316:CYS:N	2.35	0.41
1:C:329:MET:SD	2:D:105:ARG:NH1	2.93	0.41
2:D:27:PHE:HZ	2:D:34:MET:SD	2.43	0.41
2:D:68:PHE:HB3	2:D:81:LEU:HD11	2.02	0.41
1:A:110:PRO:O	1:A:111:ASN:ND2	2.53	0.41
1:A:306:ALA:HB2	1:A:374:PHE:CE2	2.55	0.41
2:B:20:LEU:HD22	2:B:83:MET:CE	2.49	0.41
2:B:93:VAL:HG12	2:B:95:TYR:CE1	2.55	0.41
1:C:48:GLU:O	1:C:52:THR:HG23	2.21	0.41
1:A:518:GLU:HB3	1:A:519:LYS:H	1.72	0.41
1:A:536:LYS:HG3	1:A:583:LEU:CD1	2.47	0.41
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.94	0.41
1:A:118:PRO:O	1:A:123:MET:HE2	2.21	0.41
1:A:178:LEU:O	1:A:182:LEU:HG	2.20	0.41
1:A:534:LYS:O	1:A:535:HIS:HB3	2.20	0.41
2:B:12:VAL:HG21	2:B:86:LEU:HD13	2.03	0.41
1:C:168:CYS:CB	1:C:177:CYS:O	2.69	0.41
1:C:267:ASN:O	1:C:271:ILE:CD1	2.62	0.41
1:C:540:THR:HG22	1:C:543:GLN:HG3	2.02	0.41
2:D:19:ARG:NH2	2:D:80:TYR:CE2	2.88	0.41
1:A:390:GLN:HE21	1:A:391:ASN:HD21	1.68	0.41
1:A:570:GLU:HG3	1:A:571:GLU:HG2	2.03	0.40
1:C:298:MET:HB2	1:C:298:MET:HE2	1.94	0.40
2:D:9:GLY:HA2	2:D:18:LEU:HD13	2.03	0.40
2:D:37:VAL:HG12	2:D:47:TRP:HA	2.03	0.40
1:C:161:TYR:CD1	1:C:185:LEU:HD23	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LYS:HE3	1:C:444:LYS:HB2	1.83	0.40
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.51	0.40
1:A:314:ASP:HB3	1:A:317:LYS:HE2	2.02	0.40
1:A:493:VAL:HG12	1:A:495:GLU:H	1.87	0.40
1:C:24:LEU:CD2	1:C:24:LEU:C	2.90	0.40
1:C:222:ARG:HD3	1:C:222:ARG:HA	1.92	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	556/591 (94%)	537 (97%)	19 (3%)	0	100	100
1	C	572/591 (97%)	547 (96%)	24 (4%)	1 (0%)	44	74
2	B	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
2	D	124/126 (98%)	117 (94%)	7 (6%)	0	100	100
All	All	1376/1434 (96%)	1322 (96%)	53 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	480	SER

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	494/516 (96%)	446 (90%)	48 (10%)	6 25
1	C	506/516 (98%)	465 (92%)	41 (8%)	9 33
2	B	101/101 (100%)	94 (93%)	7 (7%)	13 39
2	D	101/101 (100%)	91 (90%)	10 (10%)	6 24
All	All	1202/1234 (97%)	1096 (91%)	106 (9%)	8 30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	5	SER
1	A	6	GLU
1	A	7	VAL
1	A	24	LEU
1	A	64	LYS
1	A	79	THR
1	A	111	ASN
1	A	112	LEU
1	A	114	ARG
1	A	115	LEU
1	A	131	GLU
1	A	286	LYS
1	A	287	SER
1	A	298	MET
1	A	304	SER
1	A	312	SER
1	A	313	LYS
1	A	334	TYR
1	A	390	GLN
1	A	394	LEU
1	A	402	LYS
1	A	409	VAL
1	A	412	THR
1	A	419	SER
1	A	420	THR
1	A	423	LEU
1	A	428	ARG
1	A	436	LYS
1	A	465	GLU
1	A	467	THR

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Mol	Chain	Res	Type
1	A	472	ARG
1	A	500	LYS
1	A	501	GLU
1	A	505	GLU
1	A	518	GLU
1	A	519	LYS
1	A	521	ARG
1	A	524	LYS
1	A	530	VAL
1	A	540	THR
1	A	541	LYS
1	A	554	PHE
1	A	556	GLU
1	A	559	CYS
1	A	560	LYS
1	A	573	LYS
1	A	575	LEU
2	B	4	LEU
2	B	45	LEU
2	B	49	SER
2	B	53	SER
2	B	89	GLU
2	B	102	ASP
2	B	123	THR
1	C	22	LEU
1	C	24	LEU
1	C	57	GLU
1	C	60	GLU
1	C	119	GLU
1	C	138	TYR
1	C	142	ILE
1	C	154	LEU
1	C	155	LEU
1	C	165	PHE
1	C	203	LEU
1	C	240	LYS
1	C	287	SER
1	C	305	LEU
1	C	308	ASP
1	C	313	LYS
1	C	340	ASP
1	C	388	ILE

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Mol	Chain	Res	Type
1	C	389	LYS
1	C	390	GLN
1	C	403	PHE
1	C	407	LEU
1	C	408	LEU
1	C	412	THR
1	C	418	VAL
1	C	423	LEU
1	C	460	LEU
1	C	462	VAL
1	C	482	VAL
1	C	513	ILE
1	C	529	LEU
1	C	540	THR
1	C	551	PHE
1	C	558	CYS
1	C	560	LYS
1	C	562	ASP
1	C	563	ASP
1	C	565	GLU
1	C	567	CYS
1	C	574	LYS
1	C	575	LEU
2	D	3	GLN
2	D	4	LEU
2	D	5	GLN
2	D	12	VAL
2	D	28	ARG
2	D	49	SER
2	D	53	SER
2	D	86	LEU
2	D	89	GLU
2	D	123	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	9	HIS
1	A	18	ASN
1	A	67	HIS
1	A	105	HIS

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Mol	Chain	Res	Type
1	A	111	ASN
1	A	170	GLN
1	A	390	GLN
1	A	440	HIS
1	A	483	ASN
1	A	580	GLN
1	C	3	HIS
1	C	18	ASN
1	C	61	ASN
1	C	67	HIS
1	C	130	ASN
1	C	391	ASN
1	C	440	HIS
1	C	483	ASN
1	C	522	GLN
1	C	535	HIS
1	C	580	GLN
2	D	5	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	565/591 (95%)	-0.24	2 (0%)	89	77	19, 38, 38, 38	1 (0%)
1	C	578/591 (97%)	-0.27	2 (0%)	90	81	38, 38, 38, 38	0
2	B	126/126 (100%)	0.08	0	100	100	38, 38, 38, 38	0
2	D	126/126 (100%)	0.08	2 (1%)	70	52	33, 38, 38, 38	0
All	All	1395/1434 (97%)	-0.20	6 (0%)	89	77	19, 38, 38, 38	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	27	PHE	2.3
1	C	570	GLU	2.3
2	D	54	SER	2.3
1	C	471	ASP	2.1
1	A	561	ALA	2.1
1	A	578	ALA	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.